NPRE 247

3 Component Decay Chain Computation

Author

Ally Kepford

May 6, 2024

Introduction

The purpose of this project is to understand the advantages and disadvantages of two methods of solving decay chains and the mathematical theory behind both. The first of the two methods in question is solving the differential equations for each decay chain component such that any point in time can be calculated independently of every prior point (this is the analytical solution). The second method is using the half-life equation to compute the decayed fraction of material each 'timestep' of set length until the desired final time is reached, where each step after the first uses the previously calculated fractions for its initial values, and as such have to be calculated in sequence (this is the numerical solution).

Practical applications for calculating decay chain values over time can include delayed neutrons in a fission reactor, determining xenon decay in a shutdown reactor, and radioactive sample analysis.

Theory

In order to analytically solve for the mass percentages of the decay chain at any point in time, we must solve these three differential equations (1.01-1.03):

$$\frac{dN_A}{dt} = \lambda_A * N_A(t) \tag{1.01}$$

$$\frac{dN_B}{dt} = \lambda_A * N_A(t) - \lambda_B * N_B(t) \tag{1.02}$$

$$\frac{dN_C}{dt} = \lambda_A * N_B(t) \tag{1.03}$$

All of them are straightforward to solve but get progressively more computationally intensive as every equation nests in the one succeeding it (2.01 in 2.02, 2.02 in 2.03, and so on if this was a longer decay chain).

$$N_A(t) = N_A(0)e^{-\lambda_A t} \tag{2.01}$$

$$N_B(t) = N_B(0)e^{-\lambda_A t} + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\left(e^{-\lambda_A t} - e^{-\lambda_B t}\right) \tag{2.02}$$

$$N_C(t) = N_C(0) + N_B(0)\left(1 - e^{-\lambda_B t}\right) + \frac{N_A(0)}{\lambda_B - \lambda_A}\left(\lambda_B\left(1 - e^{-\lambda_A t}\right) - \lambda_A\left(1 - e^{-\lambda_B t}\right)\right) \tag{2.03}$$

As such, is an efficient method of accurately calculating small lengths of decay chains but quickly expands to unreasonable lengths when computing complex decay chains.

Analytical solution mathematical derivation sourced from citation [1]

For longer decay chains, in can be useful to use a mathematically simpler approach for *approximating* the values instead of computing them absolutely. The Numerical solution employed in this project uses a forward-difference approximation and a small "iteration length" between each calculation to achieve very similar (but not identical) results compared to the analytical solution.

Starting with the generic limit definition (3.01):

$$f' = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \tag{3.01}$$

We can substitute in Equation 1.01 and drop the limit to obtain a more applicable equation for our calculation which will test multiple iteration lengths (Δt) to observe their accuracies relative to the Analytical Solution (equation sets 1 and 2).

$$-\lambda_A N_A = \frac{N_A(t + \Delta t) - N_A(t)}{\Delta t} \tag{3.02}$$

Rearranging Equation 3.02 to find $N_A(t + \Delta t)$:

$$N_A(t + \Delta t) = -\lambda_A N_A \Delta t + N_A(t) \tag{3.03}$$

Repeating the steps taken in Equations 3.02 and 3.03 for isotopes N_B and N_C respectively:

$$N_B(t + \Delta t) = -\lambda_B N_B \Delta t + N_B(t) \tag{3.04}$$

$$N_C(t + \Delta t) = -\lambda_C N_C \Delta t + N_C(t) \tag{3.05}$$

And then substituting known values into Equations 3.04 and 3.05 to obtain their final forms (as their quantities are based on what decayed in the prior isotope):

$$N_B(t + \Delta t) = \left(\lambda_A N_A(t) - \lambda_B N_B(t)\right) + N_B(t) \tag{3.06}$$

$$N_C(t + \Delta t) = \left(\lambda_B N_B(t) - \lambda_C N_C(t)\right) + N_C(t) \tag{3.07}$$

To find the maximum value for N_B from the analytical solution, we can take the derivative of Equation 2.02 and set it equal to 0 as due to the nature of the three component decay chain, the maximum will be the only critical point on the graph of N_B.

$$N_B(t)' = \frac{d}{dt}\left[N_B(0)e^{-\lambda_A t} + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\left(e^{-\lambda_A t} - e^{-\lambda_B t}\right)\right] \tag{4.01}$$

$$0 = -\lambda_A\left(N_B(0) + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\right)e^{-\lambda_A t} + \lambda_B \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A} e^{-\lambda_B t} \tag{4.02}$$

Solving for t:

$$\left(N_B(0) + \frac{\lambda_A N_A(0)}{\lambda_B - \lambda_A}\right)e^{-\lambda_A t} = \lambda_B \frac{N_A(0)}{\lambda_B - \lambda_A} e^{-\lambda_B t} \tag{4.03}$$

$$N_B(0) = \lambda_B \frac{N_A(0)}{\lambda_B - \lambda_A} e^{(\lambda_A - \lambda_B)t} - \lambda_A \frac{N_A(0)}{\lambda_B - \lambda_A} \tag{4.04}$$

$$(\lambda_B - \lambda_A)\frac{N_B(0)}{N_A(0)} = \lambda_B e^{(\lambda_A - \lambda_B)t} - \lambda_A \tag{4.05}$$

$$\frac{(\lambda_B - \lambda_A)}{\lambda_B}\frac{N_B(0)}{N_A(0)} + \frac{\lambda_A}{\lambda_B} = e^{(\lambda_A - \lambda_B)t} \tag{4.06}$$

$$\ln\left(\frac{(\lambda_B - \lambda_A)}{\lambda_B}\frac{N_B(0)}{N_A(0)} + \frac{\lambda_A}{\lambda_B}\right) = (\lambda_A - \lambda_B)t \tag{4.07}$$

$$t = \frac{\ln\left(\frac{(\lambda_B - \lambda_A)}{\lambda_B}\frac{N_B(0)}{N_A(0)} + \frac{\lambda_A}{\lambda_B}\right)}{(\lambda_A - \lambda_B)} \tag{4.08}$$

Necessary simplification as $N_B/N_A = 0$:

$$t = \frac{\ln\left(\frac{\lambda_A}{\lambda_B}\right)}{(\lambda_A - \lambda_B)} \tag{4.09}$$

Finding the maximum value for the numerical solution is as simple as running `[array].argmax()` to find the maximum value index in an array and then multiplying that by the iteration length to find the maximum time.

Results

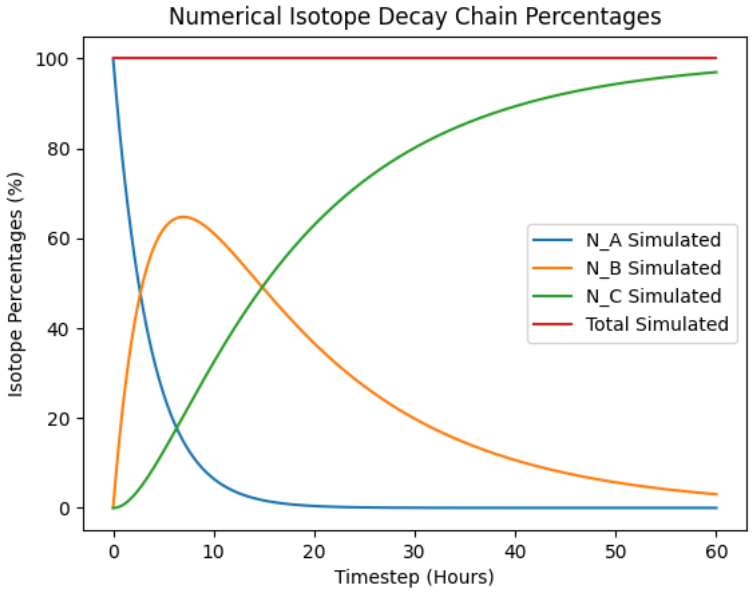

Figure 1: Numerical results using an iteration length of 0.1 hours

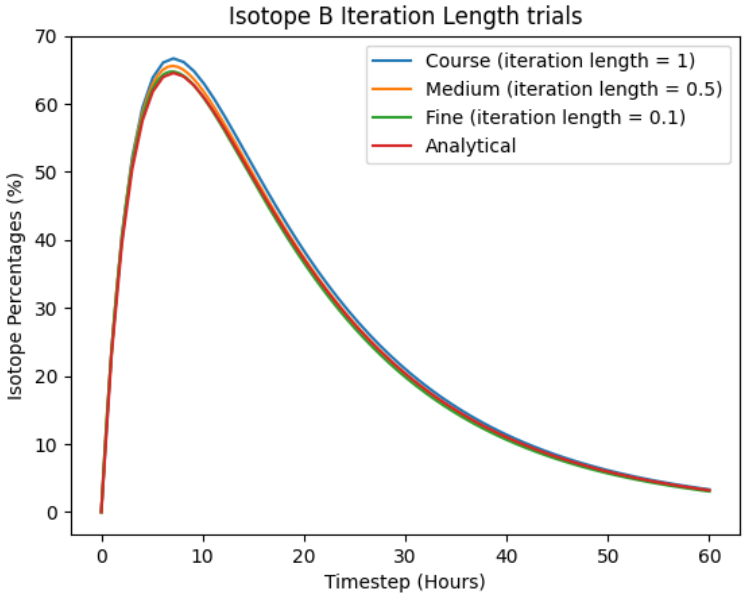

Figure 2: Comparisons between values of N_B with different iteration lengths

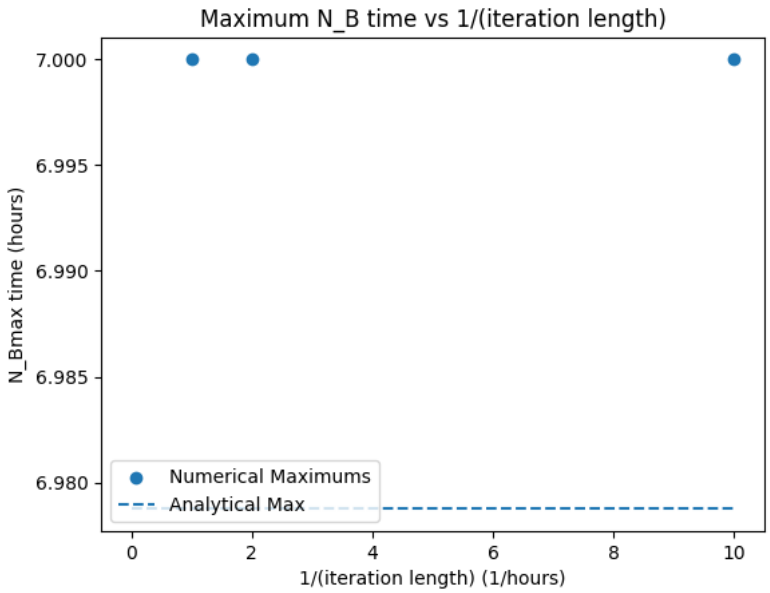

Figure 3: Maximum N_B values as a function of 1/(iteration length)

Conclusion

From Figure 1, a clear relationship between the three isotopes and their half-lives can be observed, with isotope N_C approaching 100% concentration over time from the relatively slow decay of isotope N_B and the initial fast decay of isotope N_A.

From Figure 2, it can be observed that as you decrease the iteration length, the numerical solution's values approach the analytical solution's values but never reaches them.

Figure 3 is an odd graph: from comparing it to Figure 2, we can observe that all of the numerical solutions do indeed have a maximum at 7 hours, and it is reasonable to assume the analytical solution's max is ever so slightly off from 7 hours though imperceivable due to the extreme resolution requirement to see it. The graph itself does not display the expected behavior of rough values approaching the analytically 'correct' value, rather all iteration lengths settle at the same value.

Works Cited

[1] Meisel Z., “Lecture 6: Radioactive Decay,” 2021, Ohio University.

https://inpp.ohio.edu/~meisel/PHYS7501/file/Lecture6_RadioactiveDecay_PHYS7501_F2021_ZM.pdf