

Date: 21 September 2018

To: Prof. Scott Palmtag, NE301 Instructor

From: Charles Goodman

Re: Numerical Decay Chains

Project 1: Numerical Solutions to Decay Chains

Introduction:

The goal of the project is to create software to generate numerical solutions to a decay chain of arbitrary length. This program may be useful for modelling how the activity of a laboratory sample may change over some time period.

Background:

The Matlab program that I wrote accepts user inputs for the number of isotopes, the half-lives of each, the initial concentrations of each, and the source strength and source duration for the first isotope, as well as the time interval. The program outputs a comma-separated-values file that contains the time and nuclide densities for each isotope. All values are stored with double precision to minimize rounding error.

Results

Part 1: Solution Verification

Test Conditions:

- 2 Nuclides: A and B
- Half-lives: 1 minute and 2 minutes for A and B respectively
- Initial concentrations: Both are 0
- Source of A has strength 1 atom/min
- Time: 0 to 20 minutes

Questions:

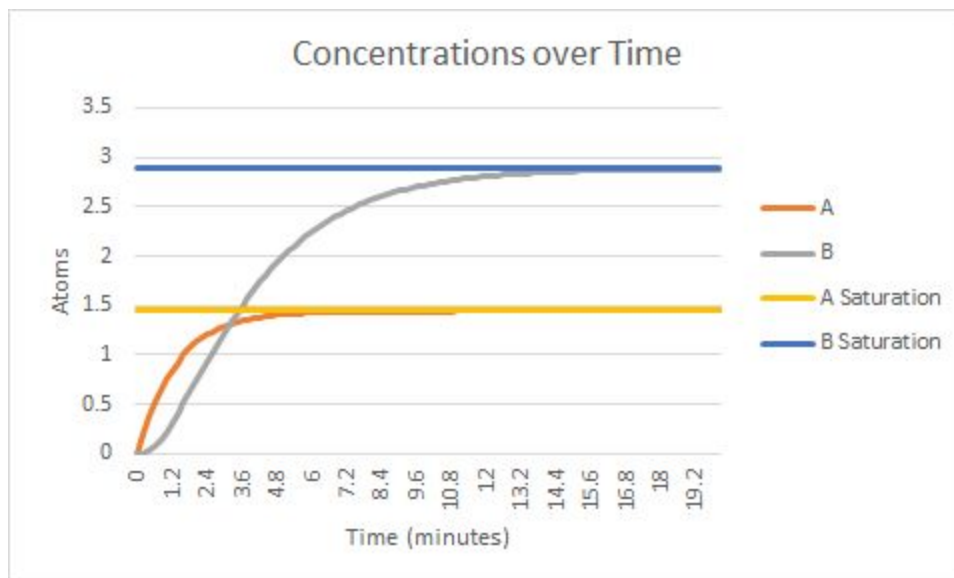
A. Calculate the saturated number densities of A and B.

Saturated Value = Source Strength * Half Life / $\ln(2)$

$A = (1 \text{ atom / min}) * (1 \text{ min}) / \ln(2) = 1.44269504 \text{ atoms}$

$B = (1 \text{ atom / min}) * (2 \text{ min}) / \ln(2) = 2.88539008 \text{ atoms}$

- B. Plot the nuclides A and B as a function of time as calculated by your program. Include lines with the saturated values.



Plot 1: Shows the concentration of A and B over time as well as their saturation lines

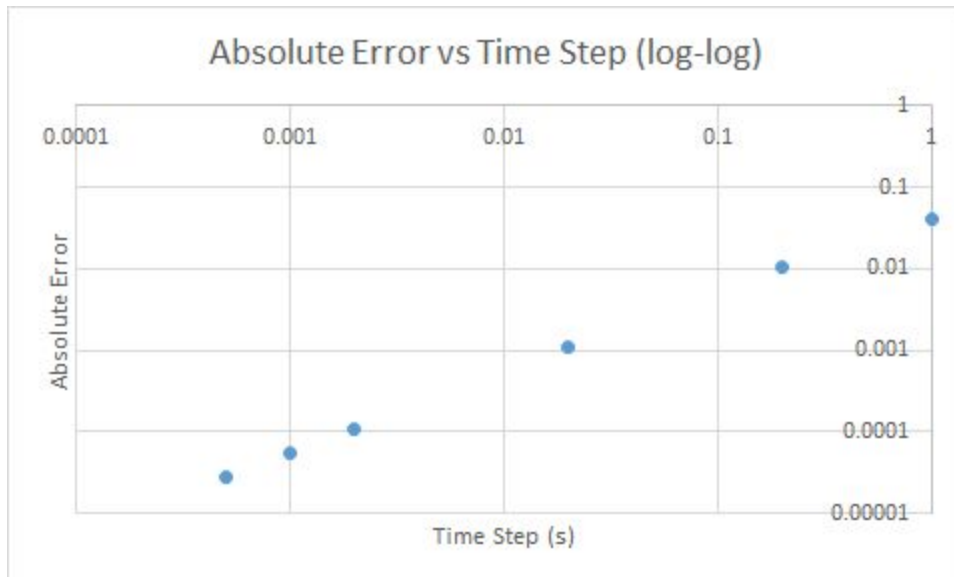
- C. What is the analytic solution for this problem? (refer to HW 2). What is the nuclide concentrations from the analytic solution at 5 minutes?

$$A = A_{\text{sat}} * (1 - (.5)^{\text{time} / \text{Halflife A}}) = (1 - (.5)^t) / \ln(2)$$

$$B = \text{Source} * (\text{Halflife B} - \text{Halflife A}) / \ln(2) * ((.5)^{\text{time}/\text{Halflife B}} - (.5)^{\text{time}/\text{Halflife A}}) + B_{\text{sat}} * (1 - (.5)^{\text{time} / \text{Halflife B}})$$

$$A(5 \text{ min}) = 31 / 32 / \ln(2) = 1.39761082 \text{ atoms} \quad B(5 \text{ min}) = 2.585271 \text{ atoms}$$

- D. Run the problem with at least six time step sizes and plot the absolute error between the calculated solution and analytic solution at time 5 minutes. The plot should show the absolute error vs. the time step size. Choose at least one time step size so the absolute error is less than 0.0001. What relationship between the error and time step size is observed? (e.g. generate a curve fit for error vs. time step size.)



Plot 2: Shows the relationship between error and time step.

There is a proportional relationship between time step and absolute error.

$$\text{Error (atoms)} = (.041113 \text{ atoms / second}) * \text{time step (seconds)}$$

E. What time step is necessary to obtain a maximum absolute error less than 0.0001?

A time step of less than .002432 seconds would have an error less than 0.0001.

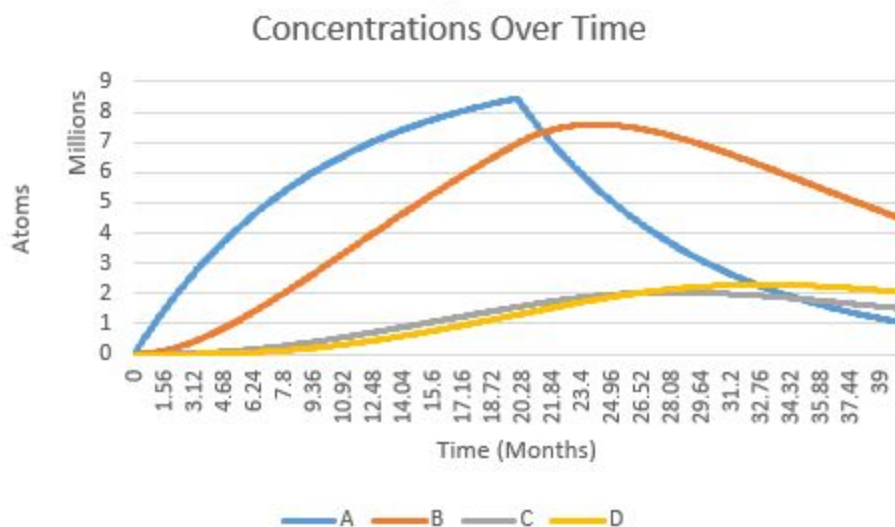
Part 2: Analytical Solution Unknown

Test Conditions:

- 4 Nuclides: A, B, C, and D
- Halflives: 6.7, 9.2, 2.6, and 3.1 months respectively
- Initial concentrations: All are 0
- Source of A has strength 1e6 atoms/month for first 20 months then 0
- Time: 0 to 40 months

Questions:

F. Plot the nuclide concentrations as a function of time.



Plot 3: Shows the concentration of A, B, C, and D over 40 months in millions of atoms. G. What are the values of all the nuclides at 30 months? All of the values should have an absolute error less than 100.

Using a linear fit of concentration of each nuclide against the time step, we can extrapolate the concentration with a time step of 0.

A(30 months) = 3001326.723 atoms

B(30 months) = 6852998.592 atoms

C(30 months) = 2014730.686 atoms

D(30 months) = 2240239.831 atoms

H. What time step size was necessary to obtain this error level? How did you arrive at this conclusion? (Hint: you need to do an error analysis)

The time step such that each nuclide has a absolute error of less than 100 atoms is .000495293 seconds. This was determined by taking the slope of the linear regression to and dividing the maximum allowed error by these slope to find the necessary time step for each nuclide. The minimum time step is chosen.

Summary:

The program creates valid numerical solutions to solve any decay chain fitting the constraint of the project. The error of each model can be quantified simply, which can be used to find the true concentration for any given time.