Modified Equations for Radioactive Decay
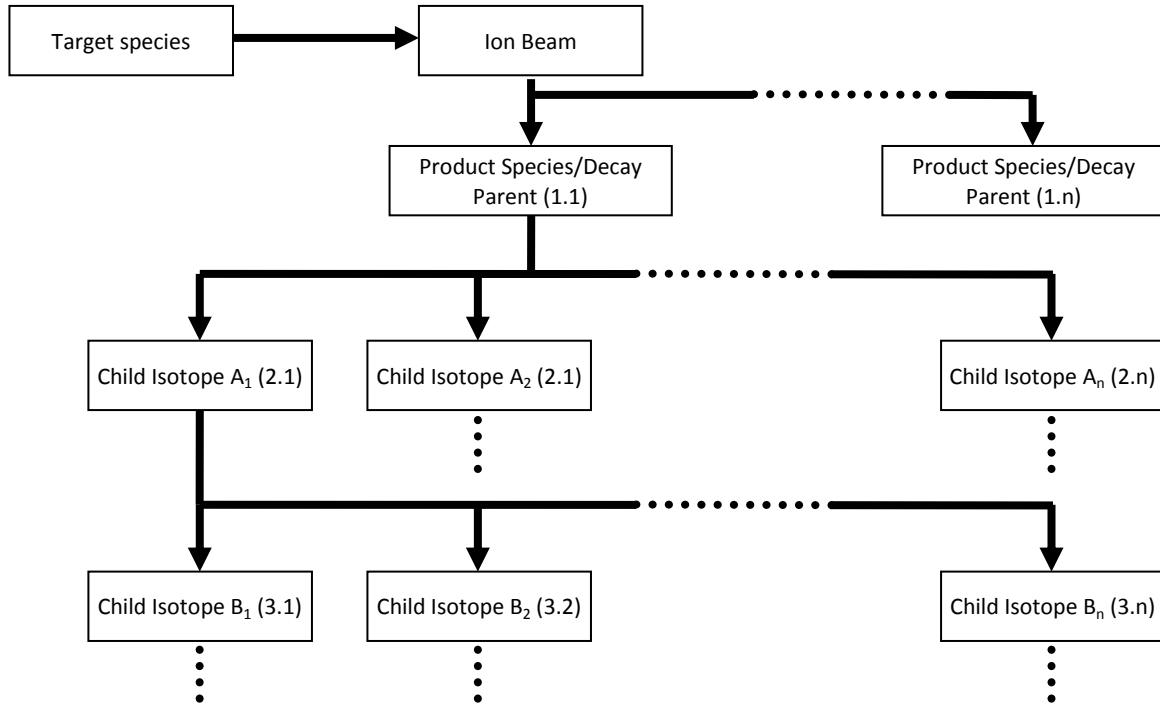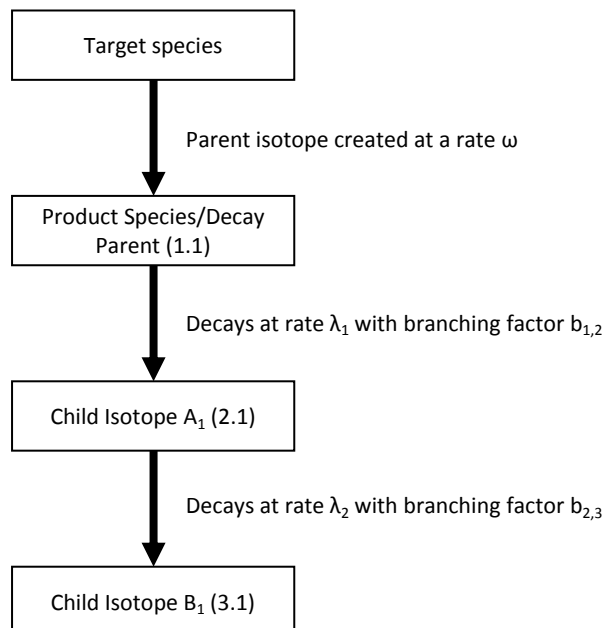
The Bateman equations in their original form do not include variable starting amounts for each child in the decay chain, the various branching factors from one isotope to the next and a variable rate of production of the parent isotope.

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┌─────────────────┐              ┌─────────────────┐
│  Target species │ ──────────►  │    Ion Beam     │
└─────────────────┘              └─────────────────┘
                                          │········································┐
                                          ▼                                      ▼
                              ┌─────────────────────┐              ┌─────────────────────┐
                              │ Product Species/Decay│              │ Product Species/Decay│
                              │    Parent (1.1)     │              │    Parent (1.n)     │
                              └─────────────────────┘              └─────────────────────┘
                        ┌──────────────┼···············································┐
                        ▼              ▼                                           ▼
            ┌────────────────────┐ ┌────────────────────┐            ┌────────────────────┐
            │ Child Isotope A_1 (2.1)│ │ Child Isotope A_2 (2.1)│        │ Child Isotope A_n (2.n)│
            └────────────────────┘ └────────────────────┘            └────────────────────┘
                        │ :              :                                      :
                        ▼              ▼                                        ▼
            ┌────────────────────┐ ┌────────────────────┐            ┌────────────────────┐
            │ Child Isotope B_1 (3.1)│ │ Child Isotope B_2 (3.2)│        │ Child Isotope B_n (3.n)│
            └────────────────────┘ └────────────────────┘            └────────────────────┘
                        :              :                                      :
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The target species is irradiated by an ion beam that creates a number of radioactive (and some stable) parent isotopes. The unstable of these then decay, and at each level there may be a chance that the parent decays into several different child isotopes with varying probabilities (branching factors).

Taking the example of one decay chain:

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                ┌─────────────────────┐
                │    Target species   │
                └─────────────────────┘
                          │  Parent isotope created at a rate ω
                          ▼
                ┌─────────────────────┐
                │ Product Species/Decay│
                │    Parent (1.1)     │
                └─────────────────────┘
                          │  Decays at rate λ_1 with branching factor b_{1,2}
                          ▼
                ┌─────────────────────┐
                │ Child Isotope A_1 (2.1)│
                └─────────────────────┘
                          │  Decays at rate λ_2 with branching factor b_{2,3}
                          ▼
                ┌─────────────────────┐
                │ Child Isotope B_1 (3.1)│
                └─────────────────────┘
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Bateman took advantage of Laplace Transforms and, after exploring the complexities of solving the differential equations in the time domain, I decided to use the Laplace Transform 's' domain instead. By using Laplace Transforms the differential equation can be solved by algebraic manipulation.

The transform is defined as follows:

$$F(s) \equiv \int_0^\infty f(t)e^{-st}dt$$

[Mathematical Methods for Physics and Engineering Riley, Hobson, Bence]

First, the equation must be constructed in the time domain. The rate of change of the parent isotope is determined by the rate of production due to the ion beam and the rate of loss due to radioactive decay.

$$N_1'(t) = \omega - \lambda_1 N_1(t)$$

This can be transformed into the 's' domain using a table of standard transforms.

$$\mathcal{L}\{N_1'(t)\} = sN_1(s) - N_1(0)$$

$$\mathcal{L}\{\omega - \lambda_1 N_1(t)\} = \frac{\omega}{s} - \lambda_1 N_1(s)$$

The terms are manipulated algebraically in the 's' domain to make $N_1(s)$ the subject.

$$sN_1(s) - N_1(0) = \frac{\omega}{s} - \lambda_1 N_1(s)$$

$$N_1(s) = \frac{1}{(s + \lambda_1)}\left(\frac{\omega}{s} + N_1(0)\right)$$

A table of standard transforms may then be used to transform the function into the time domain.

$$N_1(s) = \omega \frac{1}{s(s + \lambda_1)} + N_1(0)\frac{1}{(s + \lambda_1)}$$

$$N_1(t) = \omega \left(\frac{1}{\lambda_1} - \frac{e^{-\lambda_1 t}}{\lambda_1}\right) + N_1(t)e^{-\lambda_1 t}$$

This process may be applied further down the decay chain, and the branching factors from a parent isotope to a possible child isotope are added. For example, the rate of change of the first child isotope is determined by the decay of the parent, the branching factor of the parent to the child and the rate of decay of the child (if it is unstable).

$$N_2'(t) = b_{1,2}\lambda_1 N_1(t) - \lambda_2 N_2(t)$$

This leads to the solution in the 's' and time domain as follows:

$$N_2(s) = \frac{1}{(s + \lambda_2)}\left(\frac{b_{1,2}\lambda_1}{(s + \lambda_1)}\left(\frac{\omega}{s} + N_1(0)\right) + N_2(0)\right)$$

$$N_2(t) = b_{1,2}\lambda_1\omega\left[\frac{1}{\lambda_1\lambda_2} + \frac{e^{-\lambda_1 t}}{\lambda_1(\lambda_1 - \lambda_2)} - \frac{e^{-\lambda_2 t}}{\lambda_2(\lambda_1 - \lambda_2)}\right] + b_{1,2}\lambda_1 N_1(0)\left[\frac{e^{-\lambda_1 t}}{\lambda_2 - \lambda_1} + \frac{e^{-\lambda_2 t}}{\lambda_1 - \lambda_2}\right] + N_1(0)e^{-\lambda_2 t}$$

The solution in the Laplace Transform 's' domain remains neat and manageable, but the solution in the time domain becomes cumbersome with many terms. The time domain solution also "breaks" if there are two isotopes with the same decay constant, as this causes a singularity. There are two options to avoid this issue:

1. Vary decay constants that are the same value by a small amount
2. Solve in the 's' domain and transform numerically into the time domain

Numerical Inversion of the Laplace Transform

The solution in the 's' Laplace Transform domain can be represented with a recursive function.

$$N_1(s) = \frac{1}{(s + \lambda_1)}\left(\frac{\omega}{s} + N_1(0)\right)$$

$$N_n(s) = \frac{1}{(s + \lambda_n)}[b_n L_{n-1} F_{n-1}(s) + N_n(0)]$$

The Gaver-Stehfest algorithm was developed in the 1960s and 1970s and is a method of calculating the inverse of a Laplace Transform in the real number domain. It is an easy to implement and reasonably accurate method, although it is an approximation to the real value.

$$f(t) \approx f_n(t) = \frac{\ln(2)}{t}\sum_{k=1}^{2n} a_k(n)F(s) \qquad where \ \ n \geq 1, t > 0$$

$$s = \frac{k\ln(2)}{t}$$

$$a_k(n) = \frac{(-1)^{n+k}}{n!}\sum_{j=Floor(\frac{k+1}{2})}^{Min(k,n)} j^{n+1}\binom{n}{j}\binom{2j}{j}\binom{j}{k-j}$$