

Bateman Equations Derivation*

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The purpose of this paper is to derive the Bateman equations, which govern the isotopic composition of a material exposed to a neutron flux.

All quantities discussed can be position-dependent; this dependence is omitted from notation. Consider a point in space which has n isotopes. Let $N_i(t)$ denote the number density (units of atoms/cm³) of isotope i , λ_{ji} denote the decay constant for isotope i to isotope j (typically through β -decay, units of s⁻¹), and $\sigma_{ji}(E)$ denote the microscopic transmutation cross-section for isotope i to isotope j . Normally this is a radiative capture cross-section, often denoted σ_c or σ_γ ; in this case, isotope j is of the same element as i , but with one more neutron. Microscopic cross-sections have the units of b, or “barns”, equal to 10⁻²⁴ cm². Lastly, let $\phi(t, E)$ be the energy-dependent scalar neutron flux density, units of n/cm²s.

Note, that in all cases, two indices of a quantity are always ordered as (to, from). This is an often-used convention in neutron transport.

To derive the rate of change in N_i , we find expressions for all of the loss and the gain mechanisms of isotope i , and balance them.

There are two gain mechanisms for isotope i :

1. Decay from another isotope j to isotope i .
2. Transmutation, due to exposure to neutron flux, of another isotope j to isotope i .

Similarly, there are two loss mechanisms for isotope i :

1. Decay of isotope i to another isotope j .
2. Transmutation, due to exposure to neutron flux, of isotope i to another isotope j .

All four mechanisms above can be characterized through their rate densities: the density in geometric space of the rate of each transmutation/decay occurring. This quantity has the units of events/cm³s, or simply 1/cm³s. The rate of change of the number density of an isotope, dN_i/dt , has the same units.

Decay rate densities from another isotope j to isotope i is governed by:

$$\lambda_{ij} N_j(t). \quad (1)$$

$\phi(t, E)$ is a density in energy, as well as in space.¹ The density in space and energy of some reaction type R rate is given by:

$$\Sigma_R(t, E) \phi(t, E), \quad (2)$$

*Adapted from <http://neutron.kth.se/courses/transmutation/Bateman/Bateman.html>

¹See *Fundamental Definitions* document for details.

in which $\Sigma_R(t, E)$ is the macroscopic cross-section of the corresponding reaction type. Integrating Eq. (2) over all energies yields the reaction rate density in space:

$$\int_0^\infty dE \Sigma_R(E) \phi(t, E). \quad (3)$$

Let the reaction type R above be the transmutation reaction from isotope j to isotope i . The corresponding cross-macroscopic cross-section $\Sigma_{ij}(E)$ can then be given by:

$$\Sigma_{ij}(t, E) = N_j(t) \sigma_{ij}(E). \quad (4)$$

Substituting Eq. (4) into (3) yields the transmutation rate density from isotope j to isotope i :

$$\int_0^\infty dE N_j(t) \sigma_{ij}(E) \phi(t, E) = \left[\int_0^\infty dE \sigma_{ij}(E) \phi(t, E) \right] N_j(t). \quad (5)$$

Summing Eqs. (1) and (5) over all isotopes j other than isotope i , and factoring the common $N_j(t)$ multiplier out of the individual gain terms yields the total gain rate density of isotope i :

$$\sum_{\text{all } j \neq i} \left[\left(\lambda_{ij} + \int_0^\infty dE \sigma_{ij}(E) \phi(t, E) \right) N_j(t) \right]. \quad (6)$$

Loss mechanisms are quantified similarly. The decay rate density of isotope i to isotope j is, similarly to Eq. (1), given by:

$$\lambda_{ji} N_i(t). \quad (7)$$

The transmutation rate density of isotope i to isotope j is, similarly to Eq. (5), given by:

$$\left[\int_0^\infty dE \sigma_{ji}(E) \phi(t, E) \right] N_i(t). \quad (8)$$

Summing Eqs. (7) and (8) over all isotopes j other than isotope i , and factoring the common $N_i(t)$ multiplier out of the sum entirely, yields the total loss rate density of isotope i :

$$\left[\sum_{\text{all } j \neq i} \left(\lambda_{ji} + \int_0^\infty dE \sigma_{ji}(E) \phi(t, E) \right) \right] N_i(t). \quad (9)$$

Subtracting Eq. (9) from Eq. (6) yields the net rate of change in isotope i density:

$$\begin{aligned} \frac{d}{dt} N_i(t) = & \sum_{\text{all } j \neq i} \left[\left(\lambda_{ij} + \int_0^\infty dE \sigma_{ij}(E) \phi(t, E) \right) N_j(t) \right] - \\ & - \left[\sum_{\text{all } j \neq i} \left(\lambda_{ji} + \int_0^\infty dE \sigma_{ji}(E) \phi(t, E) \right) \right] N_i(t). \end{aligned} \quad (10)$$

Equation (10) is the full Bateman equation; when constructed for all n isotopes i in the system, it forms a system of n ordinary differential equations. These equations are linear,

but not constant coefficient, and so must be integrated numerically. MATLAB's `ode15s` command is one of the easier ways to integrate this ODE system.

In many practical cases, the time-dependence of $\phi(t, E)$ is very weak, because for a reactor operating at a steady power level, the flux must be steady as well. Assuming a time-invariant flux $\phi(t, E) = \phi(E)$ allows us to integrate the energy integrals in Eq. (10):

$$\int_0^\infty dE \sigma_{ij}(E) \phi(E) = \sigma_{ij} \phi, \quad (11a)$$

$$\int_0^\infty dE \sigma_{ji}(E) \phi(E) = \sigma_{ji} \phi, \quad (11b)$$

in which σ_{ij} , σ_{ji} and ϕ are all constants. Note, that to construct these constants, $\phi(E)$ must still be known, or assumed. They are known as one-group cross-sections/fluxes, and are usually known prior to integrating the Bateman equations.

Let $\vec{\mathbf{N}}(t)$ be the $n \times 1$ vector of isotopic number densities, and \mathbf{M} be the $n \times n$ constant coefficient matrix. M_{ij} is the row i , column j element of \mathbf{M} , given by:

$$M_{ij} = \lambda_{ij} + \sigma_{ij} \phi. \quad (12)$$

Lastly, let $\vec{\mathbf{N}}^0$ be the vector of initial isotopic number densities. With the above simplifications, we can rewrite the Bateman equations as follows:

$$\frac{d}{dt} \vec{\mathbf{N}}(t) = \mathbf{M} \vec{\mathbf{N}}, \quad (13)$$

which has the following analytical solution:

$$\vec{\mathbf{N}}(t) = \expm(\mathbf{M}t) \vec{\mathbf{N}}^0, \quad (14)$$

in which the \expm function is the matrix exponential. Note, that Eq. (14) can only be used to solve Eq. (13) if \mathbf{M} is constant; the more general Eq. (10) requires numeric integration.