Bateman equations

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Theoretical introduction on the Physics

Introduction

Bateman's equations are part of a mathematical model firstly idealized by the physicist Ernest Rutherford and solved analytically by the mathematician Harry Bateman.
The model deal with the abundances and activity of a decay chain as function of time, based on the decay rates and the initial abundances of the species.
Many chemical species are employed in reactors today, for example producing nuclear fuel like Uranium-235 to maintain chain reaction to provide fission energy.
However, there are many other isotopes present in the core that compete with Uranium-235 for thermal neutrons absorption, of which the isotopes with notably large cross-sections are referred to as reactivity poisons.
Poisons can affect the reactivity management in many ways. Some poison materials are used in reactors for reactivity control or fuel management, whereas some fission products poisons, for example, can cause trouble to reactivity control and inherent safety of reactors.

Xenon-135 has a most substantial effect on the reactivity due to its large absorption cross-section (2.75 Mbarns). This phenomenon is called "poisoning". After the shutdown of the reactor, the flux of thermal neutron will drop to almost zero. Consequently, the Xe-135 stops being produced from fission. Therefore, it is only produced through the decay of another nuclide: Iodine-135.
This presentation starts by introducing the Bateman's equations for different isotopes as a system of ODE. Then, it shows two methods to solve the equations numerically: the fourth-order Runge-Kutta method and the matrix exponential method. The first one is much more speed in the calculation, but the last one results with much higher accuracy.

Bateman's equations

Bateman's equations

Bateman's equations for Iodine-135 and Xenon-135 are introduced as follows:

$$\frac{dI(t)}{dt} = \gamma_I \Sigma_f \phi - \lambda_I I(t)$$

$$\frac{dX(t)}{dt} = \lambda_I I(t) - \lambda_X X(t)$$

That system can be solved analytically using Lagrange method. The solutions are:

$$I(t) = \frac{1}{\lambda_I}(\gamma_I \Sigma_f \phi - A e^{-\lambda_I t})$$

$$X(t) = \Sigma_f \phi [\frac{\gamma_I + \gamma_X}{\gamma_X + \sigma_{aX}\phi} e^{-\lambda_X t} + \frac{\lambda_I}{\lambda_I - \lambda_X}(e^{-\lambda_X t} - e^{-\lambda_I t})]$$

where

$$A = \lambda_I \gamma_I - \lambda_I I(0).$$

Runge-Kutta method and algorithm

Runge-Kutta method and algorithm

Runge-Kutta method is an iterative method which approximates a solution of a differential equation. It's based on the Taylor expansion of a function involving the derivatives of it to represent the correct behaviour. Here there are the formula of fourth-ordere Runge-Kutta method adapted to the current problem.

$$I_{n+1} = I_n + \frac{1}{6}(\Delta I_1 + 2\Delta I_2 + 2\Delta I_3 + \Delta I_4)$$

$$X_{n+1} = X_n + \frac{1}{6}(\Delta X_1 + 2\Delta X_2 + 2\Delta X_3 + \Delta X_4)$$

In which

$$\Delta I_1 = \Delta t[\gamma_I \Sigma_f \phi - \lambda_I I_0]$$

$$\Delta X_1 = \Delta t[\gamma_X \Sigma_f \phi + \lambda_I I_0 - (\lambda_X + \sigma_{aX}\phi) X_0]$$

$$\Delta I_2 = \Delta t[\gamma_I \Sigma_f \phi - \lambda_I (I_0 + \frac{1}{2}\Delta I_1)]$$

$$\Delta X_2 = \Delta t[\gamma_X \Sigma_f \phi + \lambda_I (I_0 + \frac{1}{2}\Delta I_1) - (\lambda_X + \sigma_{aX}\phi)(X_0 + \frac{1}{2}\Delta X_1)]$$

$$\Delta I_3 = \Delta t[\gamma_I \Sigma_f \phi - \lambda_I (I_0 + \frac{1}{2}\Delta I_2)]$$

$$\Delta X_3 = \Delta t[\gamma_X \Sigma_f \phi + \lambda_I (I_0 + \frac{1}{2}\Delta I_2) - (\lambda_X + \sigma_{aX}\phi)(X_0 + \frac{1}{2}\Delta X_2)]$$

$$\Delta I_4 = \Delta t[\gamma_I \Sigma_f \phi - \lambda_I (I_0 + \Delta I_3)]$$

$$\Delta X_4 = \Delta t[\gamma_X \Sigma_f \phi + \lambda_I (I_0 + \Delta I_3) - (\lambda_X + \sigma_{aX}\phi)(X_0 + \Delta X_3)]$$

Matrix exponential method and algorithm

Matrix exponential method and algorithm

The matrix exponential method is a matrix function on square matrices analogous to the ordinary exponential function. It's used to solve systems of linear ODE. The solution of Bateman's equations can be collected into a vector and the system transforms as:

$$\begin{bmatrix} I_{n+1} \\ X_{n+1} \end{bmatrix} = \mathsf{e}^{\Delta t} \begin{bmatrix} -\lambda_I & 0 \\ \lambda_I & -\lambda_X - \sigma_{aX}\phi \end{bmatrix} \begin{bmatrix} I_0 \\ X_0 \end{bmatrix}$$

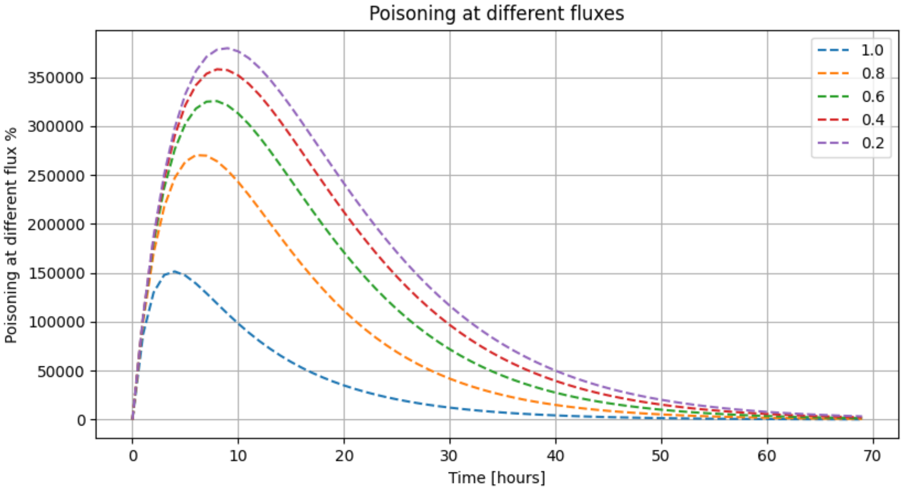

Figure: Curves that represent Xenon poisoning at different fluxes

Conclusion

Conclusion

As we can notice, as many Iodine-135 nuclides decay, many Xenon-135 nuclides grow until reaching a maximum that takes different values as different fluxes are used.
Here there's a table of parameters I used:

γ_I	Fission yield of I-135	0.061
γ_X	Fission yield of Xe-135	0.003
λ_I	Decay constant of I-135 (s^{-1})	2.874×10^{-5}
λ_X	Decay constant of Xe-135 (s^{-1})	2.027×10^{-5}
σ_{aX}	Microscopic absorption cross-section of Xe-135 (cm^2)	2.75×10^{-18}
ν	# of neutrons released per fission	2.3
ϕ	Thermal neutron flux ($cm^{-2}s^{-1}$)	4.42×10^{20}
Σ_f	Macroscopic absorption cross-section (cm^2)	0.008

Figure: Parameters.

Thank you!