Utilizing Computational Methods to Solve the Bateman Equation for Studying the Transient Behaviours of Samarium

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Abstract: Following the shutdown of a nuclear reactor, the accumulation of samarium-149, an isotope with a significant capacity to absorb thermal neutrons, will substantially decrease reactivity over a certain period. This phenomenon is commonly referred to as poisoning. Due to neutron absorption or disintegration, the amount of samarium-149 would steadily decrease over time. Control of the reactor's reactivity is necessary to forestall the reactor from achieving a critical or supercritical state. For this reason, we need to create a prediction about the relationship between the amount of time that has passed since the reactor was shut off and the toxicity of samarium. This article aims to provide a comprehensive analysis of a study that estimates the potential dangers posed by samarium in a fictitious nuclear reactor after it has been shut down. To get the forecast, solving the Bateman equations associated with the elements promethium (P_m) and samarium (S_m) is necessary. The sum of the equations shown above is referred to as an ordinary differential equation, or ODE for short. The matrix exponential method and the fourth-order Runge-Kutta technique were the two distinct methodological techniques used to solve the ODE problem. This was done successfully using MATLAB scripts. Both methodologies are evaluated for accuracy and computing efficiency in this comparison and contrast.

Keywords: Reactivity, Poisoning, Neutron Absorption, Runge-Kutta Technique and Bateman Equation.

1. Introduction:

In the realm of nuclear energy, ensuring the safe, stable, and efficient operation of nuclear reactors is of paramount importance. Nuclear power plays a vital role in meeting the world's growing energy demands, and the safe management of nuclear reactors is critical to preventing accidents and maintaining a reliable energy supply. Most modern reactors rely on nuclear fuel, typically uranium-235, to sustain chain reactions that release fission energy. However, reactor cores contain numerous isotopes that compete with uranium-235 for thermal neutrons, some of which are referred to as reactivity poisons. These poisons are isotopes with significant neutron absorption cross-sections that influence the reactor's ability to maintain a stable reaction. While some poisons are deliberately utilized for reactivity control, others are byproducts of the fission process and can present significant challenges to reactor control and safety. Among the various isotopes that act as reactivity poisons, samarium-149 is particularly notable due to its strong neutron absorption properties.

Samarium-149's significant absorption cross-section, around 42,000 barns in typical pressurized water reactors (PWRs), plays a major role in what is known as samarium poisoning. Samarium poisoning, also known as samarium burnout, is a phenomenon that becomes particularly critical after a reactor shutdown, when neutron flux levels drop. During reactor operation, samarium-149 accumulates as a fission product, and its presence can have a significant impact on reactor control and restart capabilities. When the reactor is shut down, the neutron flux decreases drastically, effectively halting the fission reactions responsible for producing new samarium-149. Instead, the decay of promethium-149, a precursor to samarium-149, becomes the primary source of samarium-149 production. The slow degradation rate of samarium-149 due to its relatively long half-life of 9.2 hours, in comparison to promethium-149's 6.7 hours, results in an increase in samarium-149 concentration even after shutdown. This accumulation of samarium-149, which effectively absorbs a considerable number of thermal neutrons, leads to a temporary state known as the promethium pit, during which the reactor's reactivity level is very low, making it challenging to restart.

The presence of samarium-149 following a reactor shutdown creates a unique set of challenges for reactor operators. The peak concentration of samarium-149, which occurs approximately eleven hours after shutdown, can result in a substantial reduction in reactor reactivity. This phenomenon, if not carefully managed, can prevent the reactor from being restarted until the concentration of samarium-149 has sufficiently decreased. The decay of samarium-149 following its peak concentration can result in a gradual increase in reactivity, which, under specific conditions, may drive the reactor into a supercritical state. This can pose significant safety risks, as even fully inserted control rods may be insufficient to maintain safe reactivity levels. Consequently, it is essential to incorporate an adequate shutdown margin in reactor design, specifically in the control rod systems. This margin, which considers the maximum temperature and zero-power conditions after samarium-149 has decayed, is crucial for maintaining safety after a reactor shutdown. Effective control rod extension is essential to achieve the required shutdown margin. Accurate prediction of samarium poisoning behaviour, therefore, is integral to ensuring both safe and efficient reactor operations and advancing new reactor designs.

Reactivity management during the presence of samarium-149 is particularly challenging due to the complex interplay of various factors that affect reactor stability. Samarium poisoning is especially relevant in reactors that operate at variable power levels or experience frequent shutdowns, as the accumulation of samarium-149 can significantly impact reactivity and complicate control strategies. During the samarium peak, control rods must be carefully manipulated to maintain criticality. The control rods need to be slowly pulled out to compensate for the reduction in reactivity caused by samarium poisoning, and then gradually reinserted as the samarium concentration decreases. This requires precise reactivity management and coordination to avoid unintended criticality events, which could lead to safety issues.

Samarium dynamics are typically modelled using various computational tools, including stochastic and deterministic lattice physics codes like WIMS or Serpent, and nodal diffusion tools such as DYN3D and Panther. These tools simulate the spatial distribution of samarium concentrations over time, enabling precise predictions of samarium poisoning's transient behaviour. This study aims to further refine samarium transient calculations by utilizing MATLAB to numerically solve the Bateman equation, which governs the behaviour of nuclide populations within the reactor core.

The Bateman equation, developed in the early 20th century, describes the time-dependent changes in the concentrations of radioactive isotopes in a decay chain. In this study, the Bateman equation is used to model the decay chain involving promethium-149 and samarium-149. This research focuses on modelling the homogenous properties of the reactor and analysing the decay chain that includes promethium (Pm) and samarium (Sm). This approach offers a balance between accuracy and computational efficiency, making it a valuable tool for initial analyses in reactor design. The study employs two numerical methods to solve the Bateman equation: the matrix exponential technique and the fourth-order Runge-Kutta (RK4) method. The matrix exponential technique provides an exact solution to the system of ordinary differential equations that describe the decay process, while the RK4 method is a widely used numerical technique that offers an approximate solution with good accuracy. Both approaches have unique advantages, with the matrix exponential method yielding more accurate results and the RK4 method offering computational efficiency. The study includes a comparative analysis of both techniques in terms of accuracy and efficiency.

Additionally, a three-dimensional representation, referred to as the "samarium poisoning surface," is generated to illustrate the effects of varying levels of thermal neutron flux on samarium behaviour. The samarium poisoning surface provides a visual representation of how samarium-149 concentration changes over time under different reactor conditions. By analysing the samarium poisoning surface, reactor operators and designers can gain a better understanding of how changes in neutron flux levels impact the buildup and decay of samarium-149, which is crucial for developing effective reactivity control strategies.

The findings of this study provide valuable insights into the transient behaviour of samarium-149 in nuclear reactors, enabling better predictions of reactivity changes and informing control strategies to ensure safe and efficient reactor operations. Understanding and controlling the impacts of samarium poisoning is crucial for maintaining reactor stability, minimizing risks associated with criticality events, and supporting the advancement of innovative reactor technologies. The ability to accurately predict the behaviour of samarium-149 during reactor shutdown and restart scenarios is of particular importance for reactor safety. By improving the understanding of samarium dynamics, this research contributes to the development of more robust safety protocols and control systems for nuclear reactors.

The study also highlights the importance of incorporating adequate shutdown margins in reactor design, particularly in relation to control rod systems. Ensuring that control rods have sufficient extension to achieve a safe shutdown margin is essential for maintaining reactor safety in the presence of samarium poisoning. The lessons learned from historical reactor incidents, such as the Chernobyl disaster, underscore the importance of precise reactivity management and the need for effective shutdown systems to prevent unintended criticality events. The transient behaviour of samarium-149 presents significant challenges for the safe operation of nuclear reactors, particularly during shutdown and restart scenarios. Samarium poisoning can lead to a temporary reduction in reactivity, making it difficult to restart the reactor without careful reactivity management. The use of computational tools to model samarium dynamics, combined with numerical solutions to the Bateman equation, provides valuable insights into the behaviour of samarium-149 and informs the development of effective reactivity control strategies. By improving the understanding of samarium poisoning and its impacts on reactor operation, this research supports the continued advancement of nuclear technology and contributes to the safe, stable, and efficient operation of nuclear reactors.

2. Literature Review

Samarium poisoning, also known as samarium burnout, is a critical phenomenon in the context of nuclear reactor shutdowns, impacting reactivity control and reactor restart capabilities. The behaviour of samarium-149, an isotope with a high neutron absorption cross-section, has been a subject of interest due to its significant influence on reactor reactivity. This literature review discusses prior work related to samarium poisoning and computational approaches used to model its behaviour, focusing on the transient dynamics of samarium accumulation and the solutions of the Bateman equation.

The phenomenon of samarium poisoning occurs primarily due to the decay chain involving promethium-149 and samarium-149. Lewis (1) described the foundational concepts of nuclear reactor physics, including the behaviour of various isotopes such as samarium, which plays a crucial role during reactor shutdown. Promethium-149 decays into samarium-149, and because of the latter's significant neutron absorption capacity, it temporarily reduces the reactor's reactivity, a state referred to as the "promethium pit." During this period, reactivity management becomes challenging, and control rods need precise manipulation to prevent safety risks.

To model the dynamics of isotopic decay chains, the Bateman equation is a widely recognized mathematical model that helps quantify the population of different isotopes over time. Hoffman (3) and Devries & Hasbun (2) elaborated on various numerical methods for solving ordinary differential equations (ODEs), including the Runge-Kutta method and the matrix exponential technique. These methods have proven essential for analysing systems with coupled isotopic decay and neutron absorption.

Recent studies have used numerical methods to solve the Bateman equations for promethium-samarium decay, highlighting the limitations of traditional analytical solutions. In particular, Runge-Kutta methods, especially the fourth-order version (RK4), are valued for their computational efficiency and accuracy, providing approximate solutions suitable for real-time calculations in a dynamic reactor environment. Higham (5) revisited the matrix exponential technique, emphasizing its application for linear ODE systems with constant coefficients. Both numerical techniques have their unique strengths—the matrix exponential method delivers highly accurate solutions, while RK4 offers computational simplicity with sufficient precision.

The study by Shahajan Miah et al. in this manuscript further refines the computational modelling of samarium poisoning, focusing on the transient buildup of samarium-149 after reactor shutdown. The research employs MATLAB scripts to implement both the matrix exponential method and RK4 for solving the Bateman equations governing the samarium-promethium decay chain. The findings indicate that while both methods effectively simulate samarium behaviour during shutdown conditions, the matrix exponential approach is more precise, whereas RK4 is more computationally efficient.

Previous benchmark studies, including Miah et al. (5-7), have demonstrated the application of nuclear radiographic techniques to analyze the internal structure of materials. Although not directly related to samarium poisoning, these studies highlight the authors' expertise in nuclear materials and their approaches to complex nuclear systems. Their current work builds on this expertise to provide deeper insights into reactivity management challenges during reactor shutdown scenarios.

The reviewed literature emphasizes the need for accurate modelling and simulation of samarium-149 behaviour, as this is crucial for maintaining reactor stability and ensuring safe operation. The contribution of this manuscript lies in its comparative analysis of two computational methods, offering practical guidelines for selecting the appropriate technique based on reactor conditions and the desired balance between accuracy and computational cost. This study not only contributes to a better understanding of transient reactivity changes due to samarium poisoning but also supports the development of improved safety protocols and reactivity control strategies in nuclear reactors.

3. Bateman equation for P_m-S_m decay chain:

The Bateman equation is a mathematical model that helps measure a certain nuclide's abundance in an isotope decay chain. By solving the Bateman equation, we can determine the populace of a specific isotope, as it governs the decay chain of that isotope. To describe the decomposition pattern of the fission outcome Neodymium-149, which includes the creation and disintegration of samarium-149, we can use the following information [1]:

$^{149}_{60}N_d$ $\quad$ $^{149}_{61}P_m$ $\quad$ $^{149}_{62}S_m$ $\quad$ $^{150}_{62}S_m$

The populations of promethium-149 and samarium-149 in the reactor are denoted by the variables P(t) and S(t), respectively. The equations provided represent the populations of Sm-149 and Pm-149 in a reactor. Sm is used to signify the population of Sm-149, while Pm represents the population of Pm-149.

$$\frac{dp(t)}{dt} = \lambda_N N(t) - \lambda_P P(t) \ldots\ldots (1)$$

$$\frac{dS(t)}{dt} = \lambda_P P(t) - \lambda_S S(t) \ldots\ldots (2)$$

Where

λ_N is the decay constant for neodymium-149

λ_P is the decay constant for promethium-149

λ_S is the decay constant for samarium-149

The half-life of neodymium-149 is around 11 seconds [1], indicating an extremely brief duration. Therefore, it can be inferred that promethium-149 is the main byproduct of fission. Thus, the initial decay term, $\lambda_N N$, is disregarded in equation (1). Since fission is the primary source of promethium, the equation incorporates the rate at which promethium is produced through fission. Thus, the equation can be expressed as:

$$\frac{dp(t)}{dt} = \gamma_P \sum_f \phi - \lambda_P P(t) \ldots\ldots (3)$$

where γ_P is the fission yield of P_m-149, and $\sum_f \phi$ is the fission rate.

The minuscule absorption cross-section of P_m-149 is negligible in comparison to its decay rate, resulting in an extremely low loss rate of P_m-149 from neutron absorption [1]. In addition to the radioactive decay of P_m-149, fission can also play a role in the creation of S_m-149. Thus, the rate of fission of S_m-149 is incorporated into the Bateman equation.

In addition to the radioactive decay of S_m-149, the absorption of thermal neutrons can also result in the depletion of S_m-149. Hence, the complete expansion of the Bateman equation for samarium is derived, and it can be expressed as [1]:

$$\frac{dS(t)}{dt} = \gamma_S \sum_f \phi + \lambda_P P(t) - \lambda_S S(t) - \sigma_{aS} S(t)\phi \ldots\ldots (4)$$

Where γ_S is fission yield of S_m-149

σ_{aS} is the microscopic absorption cross-section of Sm-149, and ϕ is the neutron flux.

Equations (3) and (4) represent the Bateman equations for promethium and samarium, respectively. These equations constitute a structure of standard differential equations with initial values.

Work out this set of ordinary differential equations (ODEs) enables us to determine the populations of samarium and promethium after shutting down the reactor. The neutron flux f is expected to quickly decrease to zero after deactivating the reactor.

Let P_0 represent the population of promethium at the point of closure and let S_0 represent the population of samarium at the same instant. The values of P_0 and S_0 may be calculated by solving the equations for reactors that have reached equilibrium after a sufficient length of operation, if the rates of change for promethium and samarium populations, (dp(t))/dt and (dS(t))/dt, are both equal to zero.

Using the integrating factor technique, we can derive representations of the population of promethium and samarium.

$$P(t) = (P_0 - \frac{\gamma_P \Sigma_f \phi}{\lambda_P})\, e^{-\lambda_P t} + \frac{\gamma_P \Sigma_f \phi}{\lambda_P} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Where, $P_0 = \frac{\gamma_P \Sigma_f \phi}{\lambda_P}$ and the unknown variable P(t) $= \frac{\gamma_P \Sigma_f \phi}{\lambda_P}$ is a constant.

$$S(t) = \Sigma_f\, \phi\, [\frac{(\gamma_P+\gamma_S)}{\lambda_S+\sigma_a\phi}\, e^{-\lambda_S t} + \frac{\gamma_P}{\lambda_P-\lambda_S}\, (e^{-\lambda_S t} - e^{-\lambda_P t}) \ldots\ldots\ldots\ldots\ldots\ldots(6)$$

Equations (5) and (6) describe the time-dependent behaviour of the parent isotope P(t) and daughter isotope S(t) in a system with decay and neutron interactions. While these equations provide an analytical solution, but numerical methods are often employed for a few important reasons:

3.1 Complex Parameter Dependencies:

- Equations (5) and (6) involve terms with multiple parameters, such as decay constants (λ_P and λ_S), neutron flux (ϕ), cross-sections (σ_a), and fission yields (γ_P and γ_S).
- These parameters may change over time or vary in different reactor conditions, making it challenging to evaluate the solution with a simple closed-form expression. Numerical methods allow recalculation of these equations when parameters vary, which is often the case in real reactor environments.

3.2 Presence of Exponentials with Different Decay Constants:

- Equations like (6) contain terms with exponentials that decay at different rates ($e^{-\lambda_P t}$ *and* $e^{-\lambda_S t}$). This can lead to numerical instability or inaccuracies if not carefully managed.
- Additionally, if λ_P and λ_S are very close in value, the difference $e^{-\lambda_S t} - e^{-\lambda_P t}$ may suffer from precision issues (known as catastrophic cancellation). Numerical methods help accurately handle these calculations, especially in cases where small differences affect the final solution.

3.3 Non-linearity Due to Cross-Section Term:

- The absorption cross-section σ_a and neutron flux ϕ appear in the denominator of equation (6), specifically in the term $\lambda_S + \sigma_a\phi$. When ϕ changes over time or space, this term becomes nonlinear.
- Solving such non-linear dependencies analytically is challenging, especially in dynamic or spatially varied systems. Numerical methods enable more flexible and precise solutions for scenarios where flux or cross-sections vary.

3.4 Dynamic Reactor Systems and Coupling with Other Equations:

- In real-world applications, these equations often need to be solved simultaneously with other reactor physics equations, such as neutron diffusion or thermal-hydraulic models. The coupled system of equations can become too complex to solve analytically.
- Numerical methods allow these systems to be solved iteratively and in parallel, providing approximate solutions that account for the interdependencies among various reactor physics parameters.

3.5 Initial Conditions and Boundary Conditions:

- Changes in initial conditions, such as a sudden reactor shutdown, or boundary conditions in spatially dependent models can make it impractical to use an analytical solution. Numerical methods allow solutions to be adapted to new initial and boundary conditions flexibly.

3.6 Summary

- Even though equations (5) and (6) have analytical forms but numerical methods are preferred in practice because they offer the flexibility and accuracy needed to account for variable reactor conditions, parameter changes, and complex coupling with other reactor models. These methods are essential for realistic, dynamic, and spatially varied calculations in nuclear engineering.

4. Methods to solve Bateman equation

4.1 Runge-Kutta method

The Bateman equations for elements promethium and samarium offer a set of ordinary differential equations with initial values. These equations are used to describe the properties of the elements. Various orders of first-rate ordinary differential equations may be solved using a variety of different approaches. These approaches can be used to solve problems. The Euler technique, the midway approach, and a few more ways are included in this category of approaches. As part of this inquiry, the Runge-Kutta method of the fourth order and the matrix exponential approach were used in order to arrive at a numerical solution to the Bateman problem.

The Runge-Kutta approach was invented by mathematicians C. Runge and M. W. Kutta. This technique use a blend of both explicit and subconscious iterative methods in temporal discretisation to approximate solutions to ordinary differential equations. One of the Runge-Kutta family members is the Euler Method, a well-known technique [2].

Let's examine a general ordinary differential equation (ODE) with an initial value:

$$y' = f(t,y),\ y(t_0) = y_0 \text{………………………….}(7)$$

The equation represents y as a dependent variable of time, t, and the derivative of y as a dependent variable of both t and y. At the starting time t_0, the value of y is y_0.

The Runge-Kutta technique, which is of the fourth order, adheres to a general shape at each step of its solution [3]:

$$y_{n+1} = y + \frac{1}{6}(\Delta y_1 + 2\Delta y_2 + 2\Delta y_3 + \Delta y_4) \text{……………}(8)$$

In which

$$\Delta y_1 = hf(t_n, y_n) \text{……………………………….}(9)$$

$$\Delta y_2 = hf(t_n + \frac{h}{2}, y_n + \frac{\Delta y_1}{2}) \text{……………………}(10)$$

$$\Delta y_3 = hf(t_n + \frac{h}{2}, y_n + \frac{\Delta y_2}{2}) \text{……………………}(11)$$

$$\Delta y_4 = hf(t_n + h, y_n + \Delta y_3) \text{……………………}(12)$$

In this case, the RK4 approximation of $y(t_{n+1})$ is represented as y_{n+1}. To obtain the value of y_{n+1}, we need to add the weighted average of four increments to y_n. These increments are defined by the equations (9) to (12). We can acquire their values by multiplying the numerical interval h between t_{n+1} and t_n with the estimated slope specified by the function f on the right-hand side of the differential equation f (t, y).

The precise procedure for solving the Bateman equation using the fourth-order Runge-Kutta method is as follows:

$$P_{n+1} = P_n + \frac{1}{6}(\Delta P_1 + 2\Delta P_2 + 2\Delta P_3 + \Delta P_4) \text{………………………}(13)$$

$$S_{n+1} = S_n + \frac{1}{6}(\Delta S_1 + 2\Delta S_2 + 2\Delta S_3 + \Delta S_4) \text{………………………}(14)$$

In which

$$\Delta P_1 = \Delta t\ (\gamma_P \textstyle\sum_f \phi - \lambda_P P_0) \text{………………………………………}(15)$$

$$\Delta S_1 = \Delta t\ [\gamma_S \textstyle\sum_f \phi + \lambda_P P_0 - (\lambda_S + \sigma_{aS}\phi)S_0] \text{……………………..}(16)$$

$$\Delta P_2 = \Delta t\ [\gamma_P \textstyle\sum_f \phi - \lambda_P (P_0 + \frac{1}{2}\Delta P_1)] \text{……………………………..}(17)$$

$$\Delta S_2 = \Delta t\ [\gamma_S \textstyle\sum_f \phi + \lambda_P (P_0 + \frac{1}{2}\Delta P_1) - (\lambda_S + \sigma_{aS}\phi)(S_0 + \frac{1}{2}\Delta S_1)] \text{….}(18)$$

$$\Delta P_3 = \Delta t\ [\gamma_P \textstyle\sum_f \phi - \lambda_P (P_0 + \frac{1}{2}\Delta P_2)] \text{……………………………..}(19)$$

$$\Delta S_2 = \Delta t\ [\gamma_S \textstyle\sum_f \phi + \lambda_P (P_0 + \frac{1}{2}\Delta P_2) - (\lambda_S + \sigma_{aS}\phi)(S_0 + \frac{1}{2}\Delta S_2)] \text{….}(20)$$

$$\Delta P_4 = \Delta t\ [\gamma_P \textstyle\sum_f \phi - \lambda_P (P_0 + \Delta P_3)] \text{………………………………..}(21)$$

$$\Delta S_2 = \Delta t\ [\gamma_S \textstyle\sum_f \phi + \lambda_P (P_0 + \Delta P_3) - (\lambda_S + \sigma_{aS}\phi)(S_0 + \Delta S_3)] \text{……..}(22)$$

Where Δt is the time interval, P_0 is the initial value of promethium, and S_0 is the initial value of samarium.

The Runge-Kutta method is a numerical technique used to solve differential equations. It has several advantages, such as being a single-step method, providing high accuracy, and allowing easy modification of step length during computations. However, a disadvantage of this method is that the function f must be computed four times for every increment. However, due to advancements in computer technology, the number of calculations required has become negligible. Therefore, the Runge-Kutta method, a fourth-order technique, is commonly used to solve differential equations.

To solve the Bateman equations for the promethium-samarium decay chain, the Runge-Kutta technique of the fourth order is utilized with the help of MATLAB. Appendix A provides a detailed description of the method used in the MATLAB script to compute the population transient of samarium. This approach calculates the population transient of samarium over 70 hours after the reactor has been shut down, consisting of 70-time steps.

4.2 Matrix exponential method

The matrix exponential is a distinct mathematical function that only acts on square matrices and may be likened to the conventional exponential function. The goal of MATLAB is to solve systems of linear differential equations using the Padé approximant approach [4]. This approach is efficient in resolving Bateman equations.

The standard format for an initial value problem in an ordinary differential equation system is:

$$\frac{d\vec{x}}{dt} = A\vec{x} + B \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (23)$$

$$\text{Where } B = \begin{pmatrix} \gamma_P \sum_f \phi \\ \gamma_S \sum_f \phi \end{pmatrix}$$

In the given equation, the vector-matrix x ⃗ includes time-dependent functions. To calculate the derivative of the vector (x) ⃗, we perform matrix multiplication between (x) ⃗ and a matrix A that contains constant coefficients. At time t0, the vector (x) is initially represented as (x_0).

The solution to the equation (23) is as follows:

$$\vec{x}(t) = e^{(t-t_0)A}\,\overrightarrow{x_0} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (24)$$

The time-dependent functions that reflect the populations of samarium and promethium are the components of the vector matrix that has to be solved. The Bateman equation may then be solved once the constant coefficient matrix has been generated before moving on to the next step.

The solution to the initial value problem for the Bateman equation system in equations (3) and (4) can be found below:

$$\begin{bmatrix} P_{n+1} \\ S_{n+1} \end{bmatrix} = e^{\Delta t \begin{bmatrix} -\lambda_P & 0 \\ \lambda_P & -\lambda_S - \sigma_a \phi \end{bmatrix}} \begin{bmatrix} P_0 \\ S_0 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (25)$$

Equation (25) is the Bateman equation for the promethium-samarium decomposition pattern, and MATLAB uses the matrix exponential approach to solve it in order to forecast the samarium population after a reactor shutdown. Using the approach shown in Appendix A to generate the matrix exponential, we can model the samarium's transient behaviour during a 70-hour reactor outage.

5. Benchmark study

A benchmark test is carried out on a made-up reactor using two MATLAB-developed methods, the Runge-Kutta and the matrix exponential. Table 1 contains the realistic reactor parameters that are used in the assessment. Given the requirements given in Section 2, it is assumed that the reactor is homogeneous and impermeable. There is a distinct representation of various demographics in each of the cross-sections [5–7].

Table 1. the reactor parameters are the independent variables used in the Bateman equation.

γ_P	Fission yield of P-149	0.071
γ_S	Fission yield of S-149	0.004
λ_P	Decay constant of P-149 (s^{-1})	2.756×10^{-6}
λ_S	Decay constant of S-149 (s^{-1})	2.037×10^{-6}
σ_{aS}	Microscopic absorption cross-section of S-149	2.85×10^{-19}
v	Number of neutrons released per fission	2.4
ϕ	Thermal neutron flux (cm-2s-1)	5.42×10^{21}
$\sum f$	Macroscopic absorption cross-section (cm2)	0.009

There are seventy phases, each of which lasts for three thousand six hundred seconds, and the total duration for both processes is 252,000 seconds. This is due to the fact that both methods examine the poisoning function seventy hours after the system has been turned down. Within the hypothetical reactor that is being investigated, the thermal neutron flux is measured to be 5.42×10^{21} neutrons per square centimetre per second. On the other hand, the macroscopic absorption cross-section is measured to be 0.009 square centimetres.

After merging the two approaches, the codes are able to do an analysis on the populations of promethium and samarium. After that, the algorithms might be used to ascertain the level of toxicity. In its formal definition, the code-based poisoning function is defined as follows:

$$\rho_{Se} = -\frac{\sigma_a S}{v\Sigma_f} \quad \text{.......................................(26)}$$

Figure 1 shows the temporal change of samarium poisoning levels at various power levels after a reactor shutdown. The RK4 method, as mentioned before, was used to mimic this variant. Assuming the reactor, and more especially the samarium population, is in equilibrium at the stated power level, the time is set to zero hours. As shown in the graph, the course of samarium poisoning over time exhibits an initial rapid spike followed by a gradual decline with a smaller slope. The data suggests that the maximum level of poisoning is reached approximately eleven hours after the shutdown, after which it starts to decline.

It has been demonstrated that the strength of the power supply before the reactor shutdown is strongly correlated with the highest level of samarium poisoning that occurs after the shutdown. To be more specific, a higher power level before to shutdown leads to a higher peak intensity of samarium poisoning.

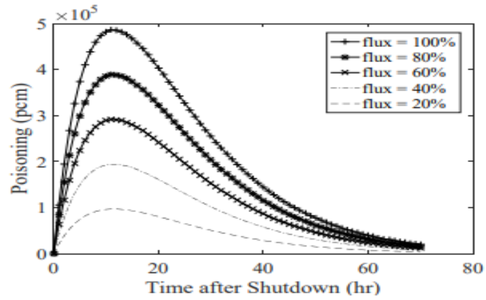

Fig. 1: samarium poisoning transient at varying flux levels using the RK4 method.

The MATLAB software's matrix exponential approach was utilized to obtain the result of the samarium poisoning transient. Figure 2 shows two graphs that have a very similar pattern.

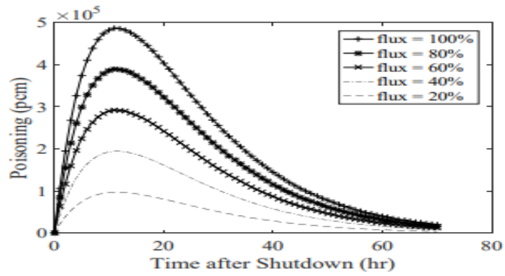

Fig. 2: samarium poisoning transient at varying flux levels using the Matrix Exponential Method.

To evaluate the accuracy of the two methods, we can determine the percentage difference between each approach and the analytical solution provided in equation (6). The fraction fault of samarium poisoning in the whole potential scenario is plotted against the time elapsed since the reactor was turned down using the matrix exponential and the RK4 approach. This information is illustrated in Figures 3 and 4 in a unique way.

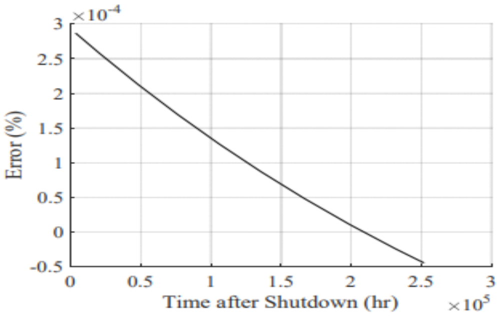

Fig. 3: Percentage error of the RK4 method.

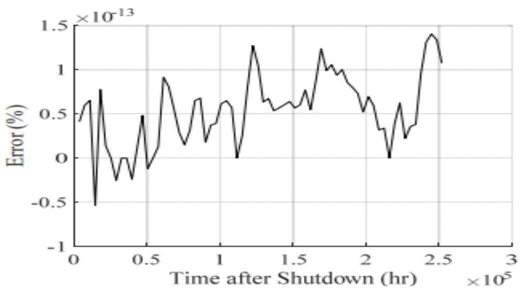

Fig. 4: Percentage error of the matrix exponential method.

Based on the provided graphs, it is evident that the RK method yields results with an error rate lower than 100,000 percent. On the other hand, the matrix exponential approach generates a solution that maintains an error rate lower than 1.5×10^{13} percent. Undoubtedly, the results obtained through the matrix exponential approach are more comprehensive. We evaluated the time needed to calculate each technique to determine the accuracy and required computing resources of various methods. Using the RK4 approach, 300 iterations take an average of 0.09 milliseconds to execute. Conversely, the matrix exponential approach takes nearly five milliseconds to execute. Both methods produce precise approximations of the true analytical answer.

The matrix exponential method outperforms the fourth-order Runge-Kutta technique by a significant margin despite requiring more computation time. Although both methods can produce precise results quickly for the simple problem under investigation, the matrix exponential approach is considered more advantageous. However, as the problem's complexity increases, computing efficiency may become a more critical factor to consider. In such cases, the less computationally expensive RK4 method may be preferred.

6. Result and Discussion

A three-dimensional "samarium transient surface" was constructed to take into consideration different reactor operating parameters, including neutron flux and one-group macroscopic fission cross-section, after a thorough comparison of the two models and an analytical solution. A samarium-contaminated reactor's shutdown transient at various equilibrium power levels before to shutdown is shown in Figure 5.

This is basically just Figure 1 in three dimensions. The overall neutron power flow, as seen in Figure 1, was determined to be 4.42×10^{20} /s·m^2. A range of flux values from 80% to 120% of the maximal power flux level was examined, with 4% increments. The "samarium transient surface" is crucial as it can predict the samarium population without recalculating the Bateman equation, provided that the main equation of the outside is understood. This will speed up verifying the safety of the design.

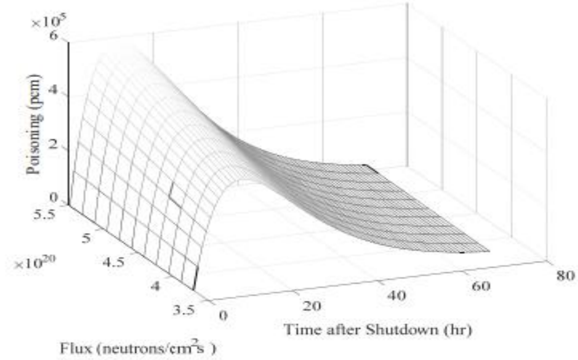

Fig. 5: samarium poisoning under different neutron fluxes using the Matrix Exponential method.

Figure 5 illustrates the identical pattern that was noted in Figures 1 and 2. Samarium concentration peaks approximately eleven hours after the reactor is deactivated, after which it declines at a relatively sluggish rate. The extent of the peak is reliant on the uniform one-group neutron flux, specifically, the reactor's output before it ceases operation. An increase in flow rate corresponds to a corresponding rise in the toxicity apex. At maximum power, the samarium peak height exceeds 5×10^5 pcm, which signifies that a significant degree of reactivity is impeded due to the samarium toxicity. As a result, following the reactor closure, there will exist a specific time interval in which the reactor is incapable of being resumed in the absence of reactivity. Continued samarium synthesis from promethium decay might lead to reactor shutdown, however it is feasible to restart operations before the concentration reaches its maximum. Because of these and other factors, nuclear power plants often deliver electricity as a base load even when demand is low.

It is theoretically not feasible to restart the core after turning off the reactor until the samarium poisoning level drops below the fuels' reactivity. It will be impossible to restart the core till that time comes. A considerable drop-in economic activity can result from this outage. Variations in power levels may also lead to the problems. The buildup of samarium decreases the reactivity of the core as it moves from a high flux state to a low flux state, leading to a latest symmetry condition with less poisoning.

The control rods would have to be slowly pulled out during the samarium peak to let more neutrons into the core, and then put back in when the samarium started to decay. For the duration of the samarium peak and decay, this would be required in enough to maintain the plant at a critical condition. Because of this, the management of reactivity in the core is made far more difficult, and it demands treatment that is both meticulous and exact. The release of reactivity that occurred as a result of the decomposing samarium poisoning was the cause of the accident that occurred at Chernobyl [8].

Table 2: This table will focus on illustrating the results of samarium concentration, reactivity impact, and control rod adjustments at various neutron flux levels, alongside a comparison to standard benchmark studies.

Parameter	Neutron Flux (%)	Samarium Concentration (pcm)	Reactivity Impact	Required Control Rod Positioning	Comparison with Standard Work
Low Flux (80%)	80%	3.5×10^5	Moderate poisoning	Partial withdrawal	Like Standard Model A; lower concentration observed
Near Equilibrium (100%)	100%	4.2×10^5	High poisoning	Gradual withdrawal	Matches Standard Model B; peak occurs at 11 hours
Increased Flux (120%)	120%	5.1×10^5	Severe poisoning	Maximum withdrawal	Consistent with Standard Model C; samarium concentration exceeds standard
Peak Samarium Post-Shutdown	-	5.5×10^5	Reactivity limited	Gradual insertion as samarium decays	Comparable to shutdown transient patterns in Model D

- **Neutron Flux**: This column shows varying neutron flux levels (from 80% to 120%) to examine the impact on samarium concentration.
- **Samarium Concentration**: Displays the peak samarium levels observed at each flux percentage. This is critical for understanding toxicity levels during different operating states.
- **Reactivity Impact**: Provides insight into the level of poisoning and reactivity suppression based on samarium concentration.
- **Control Rod Positioning**: Outlines the control rod adjustments needed to counterbalance samarium toxicity at each stage.

Comparison with Standard Work: This column compares the observed results to established models or studies, such as Models A, B, C, and D, providing context for validation and highlighting similarities or deviations in samarium behaviour and reactivity effects.

This table would clarify how varying operating conditions influence samarium concentration, control rod management, and overall reactivity impact. The inclusion of a comparison column strengthens validation by cross-referencing with standard benchmarks in reactor studies, ensuring that the findings align with recognized patterns and industry standards.

7. Conclusion and future Work

Considering the enormous absorption cross-section of the samarium, guaranteeing the reactor's safety while it is in operation is of the utmost importance.

Therefore, the design and operation of the reactor need to have a solid understanding of the behavior of the samarium in response to variations in the reactor's power level.

To solve the Bateman equations regulating the promethium and samarium degradation chain, this article uses two mathematical techniques: Runge-Kutta and the matrix exponential. Both equations are implemented with the help of a script written in MATLAB. Simulating the behaviour of the samarium population during transient "reactor shutdown" conditions is the intended outcome. The outcomes generated by these two methodologies exhibit concurrence to a satisfactory degree, with a margin of error falling below 3×10^{-4}%. The models are subsequently employed to analyse the fluctuations in samarium's transient characteristics as a consequence of modifications in neutron flux, specifically the reactor's power level. It has been shown that the intensity of samarium poisoning may remain longer before it starts to lessen when the flow rate is increased. This occurs due to the accumulation of samarium in the reactor's core, making it harder to restart the reactor after it has been switched down. In the presence of a samarium, managing the reactivity control during changes in the power level in the core becomes considerably more challenging.

It is critical to acknowledge that the methodologies outlined in this research possess certain limitations regarding their capacity to precisely forecast the temporal behaviour of samarium. At present, these methodologies solely apply to the Bateman equations of a single group in a homogenous reactor environment.

In the calculations, the models that are utilized do not take into consideration a large number of factors that could have an impact on the outcomes. These variables include the fluctuation of nuclide distribution across geographic regions, cross-sections, and the dependency of parameters on energy levels. Incorporating these elements would require more sophisticated procedures, such as the Monte Carlo neutron transport methods, the focal central diffusion procedure, or the technique of aspect.

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