## Simulation of Iodine-Xenon Transients After Reactor Shutdown

Comparison of RK4 and Matrix Exponential Methods

Sajib Sakhawat

April 2025

### Introduction

#### Introduction

#### Goal

Simulate behavior of I-135 and Xe-135 after reactor shutdown.

#### Introduction

#### Goal

Simulate behavior of I-135 and Xe-135 after reactor shutdown.

### Why Important?

- Xe-135 is a strong neutron absorber.
- Accurate simulation ensures reactor safety.

## Nuclear Physics Background

#### Isotopes Involved

- lodine-135 (I-135): Decays to Xe-135.
- Xenon-135 (Xe-135): Produced directly and from I-135.
- Xe-135 is termed a neutron poison because of its extremely high microscopic absorption cross-section

## Nuclear Physics Background

#### Isotopes Involved

- lodine-135 (I-135): Decays to Xe-135.
- Xenon-135 (Xe-135): Produced directly and from I-135.
- Xe-135 is termed a neutron poison because of its extremely high microscopic absorption cross-section

### Key Challenge

Xe-135 has a high neutron absorption cross-section.

## Bateman equations and Parameters

### Bateman equations

The equations for the I-135 and Xe-135 populations in a reactor, where  $\lambda_T$  is the decay constant for tellurium-135:

$$\frac{d}{dt}I(t) = \lambda_T T(t) - \lambda_I I(t)$$

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

## Bateman equations and Parameters

#### Bateman equations

The equations for the I-135 and Xe-135 populations in a reactor, where  $\lambda_T$  is the decay constant for tellurium-135:

$$\frac{d}{dt}I(t) = \lambda_T T(t) - \lambda_I I(t)$$

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

#### Fixed Nuclear Constants

Symbol	Description	Value
$\lambda_I$	Decay constant of I-135	$2.874 \times 10^{-5} \text{ s}^{-1}$
$\lambda_X$	Decay constant of Xe-135	$2.027 \times 10^{-5} \text{ s}^{-1}$
$Y_I, Y_X$	Fission yields	0.061, 0.003
$\sigma_{aX}$	Absorption cross-section of Xe-135	$2.75  imes 10^{-18} \;  ext{cm}^2$

## Equilibrium Before Shutdown

The equilibrium concentrations  $I_0$  and  $X_0$  represent the steady-state levels of lodine-135 and Xenon-135 during full-power operation of the reactor.

#### Initial Concentrations

$$I_0 = \frac{Y_I \cdot \Sigma_f \cdot \phi}{\lambda_I}$$
$$X_0 = \frac{Y_X \cdot \Sigma_f \cdot \phi + \lambda_I I_0}{\lambda_X + \sigma_{aX} \cdot \phi}$$

## Equilibrium Before Shutdown

The equilibrium concentrations  $I_0$  and  $X_0$  represent the steady-state levels of lodine-135 and Xenon-135 during full-power operation of the reactor.

#### Initial Concentrations

$$I_0 = \frac{Y_I \cdot \Sigma_f \cdot \phi}{\lambda_I}$$
$$X_0 = \frac{Y_X \cdot \Sigma_f \cdot \phi + \lambda_I I_0}{\lambda_X + \sigma_{aX} \cdot \phi}$$

- φ: Neutron flux
- $\Sigma_f$ : Macroscopic fission cross-section

## Equilibrium Before Shutdown

The equilibrium concentrations  $I_0$  and  $X_0$  represent the steady-state levels of lodine-135 and Xenon-135 during full-power operation of the reactor.

#### Initial Concentrations

$$I_0 = \frac{Y_I \cdot \Sigma_f \cdot \phi}{\lambda_I}$$

$$X_0 = \frac{Y_X \cdot \Sigma_f \cdot \phi + \lambda_I I_0}{\lambda_X + \sigma_{aX} \cdot \phi}$$

- φ: Neutron flux
- $\Sigma_f$ : Macroscopic fission cross-section

#### Significance

- As Initial Conditions
- Incorrection of values leading to inaccurate poisioning forecast

### Simulation Methods

### Simulation Methods

### RK4 (Runge-Kutta 4th Order)

- Step-by-step numerical integration
- It uses combinations of explicit and implicit iterative methods in temporal discretization to approximate solutions of ordinary differential equations.

#### Simulation Methods

### RK4 (Runge-Kutta 4th Order)

- Step-by-step numerical integration
- It uses combinations of explicit and implicit iterative methods in temporal discretization to approximate solutions of ordinary differential equations.

### Matrix Exponential

- The matrix exponential is a matrix function on square matrices analogous to the ordinary exponential function.
- It is used to solve systems of linear differential equations.
- Efficient and compact via exp(At)

## Analytical Reference Solution

7 / 18

Sajib Sakhawat I-X Transient Simulation April 2025

## Analytical Reference Solution

#### Xe-135 Concentration Over Time

$$X(t) = X_0 e^{-\lambda_X t} + \frac{\lambda_I I_0}{\lambda_X - \lambda_I} (e^{-\lambda_I t} - e^{-\lambda_X t})$$

• Used as benchmark for simulation accuracy.

Sajib Sakhawat I-X Transient Simulation April 2025 7 / 18

## Simulation Setup

### Simulation Setup

The simulation makes several simplifying assumptions for tractability and clarity:

- All neutrons are treated as if they belong to a single energy group.
- This neglects the energy dependence of cross-sections and reactions.
- The reactor core is assumed homogeneous spatial variations in flux and nuclide concentrations are ignored.
- Only I-135 and Xe-135 are modeled.
- Other isotopes or reaction channels are ignored.

### Simulation Setup

The simulation makes several simplifying assumptions for tractability and clarity:

- All neutrons are treated as if they belong to a single energy group.
- This neglects the energy dependence of cross-sections and reactions.
- The reactor core is assumed homogeneous spatial variations in flux and nuclide concentrations are ignored.
- Only I-135 and Xe-135 are modeled.
- Other isotopes or reaction channels are ignored.

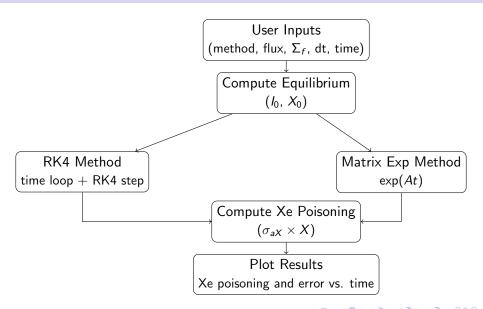
#### **Parameters**

- Time range: up to 70 hours
- Flux levels: 20% to 100% of base flux
- Step size: 3600 seconds (1 hour)



### Simulation Workflow

#### Simulation Workflow



#### Average Runtime Over 300 Runs

Method	Avg. Runtime
RK4	0.001493 s
Matrix Exponential	0.031730 s

#### Average Runtime Over 300 Runs

Method	Avg. Runtime
RK4	0.001493 s
Matrix Exponential	0.031730 s

• RK4 is faster and suitable for linear systems.

### Average Runtime Over 300 Runs

Method	Avg. Runtime
RK4	0.001493 s
Matrix Exponential	0.031730 s

- RK4 is faster and suitable for linear systems.
- The matrix exponential method requires longer calculation time, but it is much more accurate than the Fourth-order Runge-Kutta method.

### Average Runtime Over 300 Runs

Method	Avg. Runtime
RK4	0.001493 s
Matrix Exponential	0.031730 s

- RK4 is faster and suitable for linear systems.
- The matrix exponential method requires longer calculation time, but it is much more accurate than the Fourth-order Runge-Kutta method.

Sajib Sakhawat I-X Transient Simulation April 2025 11 / 18

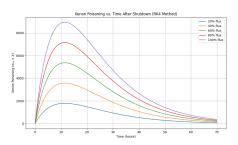


Fig: RK4 Method

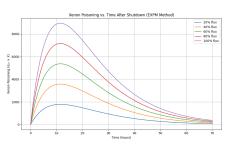


Fig: EXPM Method

Sajib Sakhawat I-X Transient Simulation April 2025 12 / 18

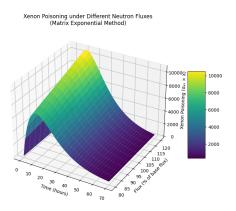


Figure: 3D plot of expm Method

#### Behavior After Shutdown

• Xe-135 builds up then decays.

Sajib Sakhawat I-X Transient Simulation April 2025 13 / 18

#### Behavior After Shutdown

- Xe-135 builds up then decays.
- Poisoning level changes with flux.

Sajib Sakhawat I-X Transient Simulation April 2025 13 / 18

#### Behavior After Shutdown

- Xe-135 builds up then decays.
- Poisoning level changes with flux.
- Xenon poisoning peaks around 11 hrs after reactor shutdown and then decays with a relatively slower rate.

#### Behavior After Shutdown

- Xe-135 builds up then decays.
- Poisoning level changes with flux.
- Xenon poisoning peaks around 11 hrs after reactor shutdown and then decays with a relatively slower rate.
- The greater the flux is, the higher the poisoning peak is.

13 / 18

Sajib Sakhawat I-X Transient Simulation April 2025

#### Behavior After Shutdown

- Xe-135 builds up then decays.
- Poisoning level changes with flux.
- Xenon poisoning peaks around 11 hrs after reactor shutdown and then decays with a relatively slower rate.
- The greater the flux is, the higher the poisoning peak is.

13 / 18

Sajib Sakhawat I-X Transient Simulation April 2025

Sajib Sakhawat I-X Transient Simulation April 2025 14 / 18

### Comparison of Results

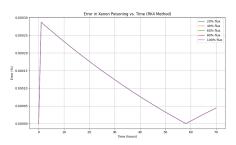


Fig: RK4 Method

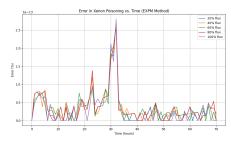


Fig: EXPM Method

## Error Analysis

### **Error Analysis**

#### Comparison with Analytical Solution

- Matrix method shows minimal error.
- RK4 introduces slight numerical error.

### **Error Analysis**

#### Comparison with Analytical Solution

- Matrix method shows minimal error.
- RK4 introduces slight numerical error.
- In expm, there's a small spike in error around 30–35 hours, which might be due to: floating-point precision issues or slight rounding artifacts in matrix operations.
- The RK4 error behavior is largely independent of the flux.
- The smoothness of the curve shows RK4 is stable and doesn't exhibit erratic behavior.

#### Key Takeaways

 With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.

Sajib Sakhawat I-X Transient Simulation April 2025 16 / 18

#### Key Takeaways

- With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.
- The xenon build-up could render the reactor core impossible for restart during some time frame after a shutdown.

Sajib Sakhawat I-X Transient Simulation April 2025 16 / 18

#### Key Takeaways

- With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.
- The xenon build-up could render the reactor core impossible for restart during some time frame after a shutdown.
- Both methods simulate I-X transients effectively. So at this point Matrix exponential method is preferred.

Sajib Sakhawat I-X Transient Simulation April 2025 16 / 18

#### Key Takeaways

- With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.
- The xenon build-up could render the reactor core impossible for restart during some time frame after a shutdown.
- Both methods simulate I-X transients effectively. So at this point Matrix exponential method is preferred.
- When the problem becomes more complicated, computational efficiency might become a much greater concern, the less computationally expensive method RK4 could become the appropriate.

#### Key Takeaways

- With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.
- The xenon build-up could render the reactor core impossible for restart during some time frame after a shutdown.
- Both methods simulate I-X transients effectively. So at this point Matrix exponential method is preferred.
- When the problem becomes more complicated, computational efficiency might become a much greater concern, the less computationally expensive method RK4 could become the appropriate.
- The matrix method matches the analytical solution almost perfectly, making it excellent for benchmarking or high-precision offline simulations.

#### Key Takeaways

- With higher flux, a higher xenon poisoning peak is observed, longer time required to decay.
- The xenon build-up could render the reactor core impossible for restart during some time frame after a shutdown.
- Both methods simulate I-X transients effectively. So at this point Matrix exponential method is preferred.
- When the problem becomes more complicated, computational efficiency might become a much greater concern, the less computationally expensive method RK4 could become the appropriate.
- The matrix method matches the analytical solution almost perfectly, making it excellent for benchmarking or high-precision offline simulations.

#### Limitations of Current Work

 Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.

#### Limitations of Current Work

- Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.
- There are many factors that have not been included in the models that could affect the calculation results, such as spatial variation of nuclide distribution and cross-sections and energy level dependence of the parameters.

#### Limitations of Current Work

- Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.
- There are many factors that have not been included in the models that could affect the calculation results, such as spatial variation of nuclide distribution and cross-sections and energy level dependence of the parameters.

#### Next Steps

 Implementing these factors would require more sophisticated methods such as nodal diffusion methods, Method of Characteristics or Monte-Carlo neutron transport methods

#### Limitations of Current Work

- Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.
- There are many factors that have not been included in the models that could affect the calculation results, such as spatial variation of nuclide distribution and cross-sections and energy level dependence of the parameters.

- Implementing these factors would require more sophisticated methods such as nodal diffusion methods. Method of Characteristics or Monte-Carlo neutron transport methods
- Incorporate real reactor data.

#### Limitations of Current Work

- Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.
- There are many factors that have not been included in the models that could affect the calculation results, such as spatial variation of nuclide distribution and cross-sections and energy level dependence of the parameters.

#### Next Steps

- Implementing these factors would require more sophisticated methods such as nodal diffusion methods, Method of Characteristics or Monte-Carlo neutron transport methods
- Incorporate real reactor data.
- Couple with neutron kinetics and feedback models.

#### Limitations of Current Work

- Can only provide rough estimations of xenon transient as they currently only solve one-group Bateman equations in homogeneous reactor environment.
- There are many factors that have not been included in the models that could affect the calculation results, such as spatial variation of nuclide distribution and cross-sections and energy level dependence of the parameters.

#### Next Steps

- Implementing these factors would require more sophisticated methods such as nodal diffusion methods, Method of Characteristics or Monte-Carlo neutron transport methods
- Incorporate real reactor data.
- Couple with neutron kinetics and feedback models.

### Thank you

# THANK YOU