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INVESTIGATIONS OF THE ADJOINT BATEMAN EQUATIONS FOR RADIOACTIVE DECAY

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Abstract

In this work, the application of adjoint Bateman equations for radioactive decay is investigated and its application in this work is to simplify depletion chains. In this work, we also develop a Bateman equations solver, which could combine with neutron transport calculation to solve Transport-Burnup problem.

The depletion chains simplification method was proposed by Go Chiba, which originated from the generalized perturbation theory (GPT). In order to select important nuclides and simplify depletion chains, this method defines the contribution function. In Go Chiba's work, there is only the derivation of contribution function in one time step. In this case, contribution function could only calculate the influence of perturbation at initial moment to the system at final moment. Therefore, we will not be able to know the evolution of contribution function in this process. This work gives a complete derivation of calculating contribution function at any time step. Based on the original contribution function definition, we propose a new definition of contribution function. The difference is that the original one conserves the final target variation but the new one conserves the final adjoint condition.

In this work, we develop a Bateman equations solver, which could resolve Bateman equations and adjoint Bateman equations. Besides, this solver contains neutron flux calculation module, which uses B_1 leakage model. Without this module, burnup matrix will be constant during calculation, which produces low accuracy calculation result. Our Bateman equations solver could update neutron flux in each iteration so that the calculation result could be more accurate. But this model couldn't be applied to calculate contribution function, so we also modify the method of calculating contribution function.

For testing this depletion chains simplification method, ^{135}Xe is chosen as target nuclide because of its essential importance to reactor criticality control. We test for two cases: steady state and transient state. In each state, after resolving Bateman equations and adjoint Bateman equations using Bateman solver, we calculate contribution function. In each case, contribution function could select correctly important nuclides. We also give detailed analysis about the performance of two contribution functions, so that we could better understand the physical meaning of contribution function. We also discuss the time-dependence of those two contribution functions to choose adequate definition under different situations

Keywords: Batemann equations, Burnup calculation, Simplified chains, Adjoint formulation

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1. Presentation of working environment

1.1 Presentation of CEA

The French Alternative Energies and Atomic Energy Commission (CEA) is a key player in research, development and innovation in four main areas: defence and security, low carbon energies (nuclear and renewable energies), technological research for industry, fundamental research in the physical sciences and life sciences. Drawing on its widely acknowledged expertise, the CEA actively participates in collaborative projects with a large number of academic and industrial partners.

The CEA is established in nine centers spread throughout France. It works in partnership with many other research bodies, local authorities and universities. Within this context, the CEA is a stakeholder in a series of national alliances set up to coordinate French research in energy (ANCRE), life sciences and health (AVIESAN), digital science and technology (ALLISTENE), environmental sciences (AllEnvi) and human and social sciences (ATHENA).

CEA in figures (2016):

- 9 research centres,
- 16 010 technicians , engineers, researchers and staff
- 51 joint research units (UMR)
- 55 framework agreements with universities and schools
- 743 priority patents filed in 2016
- 27 Equipex (facilities of excellence)
- 33 Labex (Laboratories of excellence)
- 3 Idex (Initiatives of excellence)
- 195 start-ups since 1972 in the innovative technologies sector
- 4,1 billion euros budget
- 422 ongoing European projects in 2016

The CEA is active internationally in a variety of areas. As a multidisciplinary scientific and technological research organisation, it develops European and international collaborative programmes. It also performs sovereign missions entrusted to it by the State. It supports the deployment of French companies internationally. Finally, it works within the framework of the European Community.

The CEA is also one of Europe's largest major research bodies. It is active in the fields of low carbon energies, information and healthcare technologies, defence and security. The Companies area is intended for firms interested in R&D collaboration with the CEA as well as those seeking to offer their services to the CEA.

1.2 Presentation of service SERMA

The SERMA unit (Service d'Études des Réacteurs et de Mathématiques Appliqués) of CEA (Commissariat à l'Énergie Atomique) based in Saclay, France, develops scientific computer codes and mathematical methods for the simulation of nuclear reactors and physical problems under radiation exposure.

The field of neutronics covers nuclear reactor core physics, criticality safety, radiation protection and nuclear instrumentation. These skills are capitalized by producing computer software that is then used to carry out innovative studies. This software deals with all the issues related to the deterministic and stochastic transport of neutrons and photons and to the isotopic evolution of the media in which neutrons propagate.

On this basis, SERMA develops computational schemes (physico-numerical modeling and computational linkings / couplings) adapted to complex physical configurations, for example nuclear reactors or cycle installations. Moreover, it industrialises and maintains in operational condition these numerical simulation tools, for the specific needs of the CEA as for those of its industrial partners, in particular AREVA and EDF. This activity includes the control of the nuclear data processing chain required by the different software.

The design of all these digital tools is based on an active, transdisciplinary and innovative "multi-scale and multi-physics" R&D of international level, as well as on skills in applied mathematics, numerical modeling, nuclear physics, computer science and software engineering. The R&D conducted is revitalized by various national and international scientific collaborations, as well as by the reception of PhD students and trainees. SERMA also transmits up-to-date scientific and technical knowledge through the lessons it leads and / or those it provides, particularly in Universities, Grandes Écoles, and INSTN. SERMA's strong point and originality lies in the existence and proximity of its four business divisions: studies, R&D, production of computing tools and lessons, which enrich the world of industry, that of research and the academic world at the same time.

2. Introduction

In the calculation of nuclear physics, there are two important equations: the transport equation which describes the neutron density evolution with time and is also known as Boltzmann equation and the famous Bateman equations which describe the variation of concentration of each isotope in depletion chains with time. For those two equations, the solution of one equation appears in the other question as a parameter. Therefore, in reactor calculation, we always need to solve those two coupled equations at the same time and this is called Transport-Burnup calculation. In general, the Bateman equations form a set of first-order differential equations in time, the number of which is equal to that of isotopes included in the system. Moreover, because of the coupled relation between neutron flux and isotopic abundance, the Bateman equations are a non-linear equation system, which increases its resolution difficulty. For doing accurate burnup calculation, depletion chains should be accurate enough. However, denser chains will cause longer calculation time because more isotopic concentrations need to be calculated and more variables appear in Bateman equations. Therefore, a balance between the number of isotopes in the chains to calculate and the recommended accuracy is needed. Moreover, it follows that the production of the reduced depletion chains is fully a case-dependent problem. Therefore, the determination of the list of isotopes in depletion chains for a specific calculation is the key step in the numerical resolution of Bateman equations.

The aim of this work is to investigate the application of adjoint Bateman equations for radioactive decay and in this work the application is to simplify depletion chains according to a specific target quantity which is case-dependent. Moreover, in this work, we develop a Bateman equations solver, which combines with neutron transport calculation.

The depletion chains simplification method was proposed by Go Chiba[3] which originated from the generalized perturbation theory. By applying this method, we could find important isotopes to the calculation of target quantity and then reconstruct depletion chains using those important nuclides. With simplified depletion chains, we could get accurate enough result using much less calculation time. In this work, the target quantity is the nuclide number density(NND) of a specific nuclide. The idea is to introduce a perturbation of nuclide number density at the beginning of calculation and observe its influence to the target nuclide's nuclide number density. Those nuclides producing important variation of target quantity are therefore regarded as important nuclides. For simplifying depletion chains and selecting important nuclides, in Go Chiba's theory, the contribution function is defined and it presents the ratio of relative change of final target nuclide's NND to the initial relative perturbation of nuclide number density vector.

In the first chapter of this report, we will firstly present the derivation of Boltzmann and Bateman equations, also some basic quantities and conceptions in the derivation will be highlighted. Next, several numerical methods for resolving Bateman equations will be presented including Runge-Kutta method used

in our Bateman equations solver. Next, we will present the key method in this work: Go Chiba's method for simplifying depletion chains. In this method, we will need to resolve adjoint Boltzmann and adjoint Bateman equations, therefore, we will firstly introduce the adjoint formulation, then we could begin to present Go Chiba's method.

In next chapter, we will present those improvements about our Bateman solver and the depletion chains simplification method. The Bateman equation solver developed in our work could resolve the direct and adjoint Bateman equations for finally calculating contribution function. Besides, this solver contains neutron flux calculation module, which uses B_1 leakage model. Therefore, we will firstly present the B_1 leakage model. For different nuclear data types, we give complete derivation of calculating neutron flux in different cases. We also discuss their difference and how to choose adequate method under different situations.

However, this model is not compatible with the derivation of contribution function in Go Chiba's method, because we couldn't solve adjoint B_1 equations. Therefore, we modify the depletion chains simplification method so that we could obtain final contribution function without resolving for the generalized adjoint neutron flux. Moreover, the derivation of contribution function is presented only in one time step, in which the burnup matrix is regarded as constant. Our work shows the complete derivation for calculating contribution function at any time step. Meanwhile, based on the original definition of contribution function, we propose a new definition of contribution function and make the comparison between those two methods.

After that, for checking the physical state of nuclear data and checking our implementation of Bateman solver, a series of tests are realized to observe the NND evolution of ^{135}Xe and ^{135}I with time under different operation conditions. Then, ^{135}Xe is chosen as the target nuclide. For selecting important nuclides, we do burnup calculation using our Bateman solver and then calculate contribution function. Besides, we also analyze the evolution of contribution function with time.

Finally, we will summarize the calculation result and discuss possible applications of this method in the future. For the last point, future work about this subject will be listed for better understanding and applying this depletion chains simplification method.

3. Literature review

3.1 Transport-Burnup Problem

1-a Neutron transport equation

For the whole life of a neutron created in the reactor, it will end with escape from the reactor or interaction with a nucleus (due to its electric neutrality, neutron doesn't react with electron). This interaction might be the absorption by one nucleus or this neutron might deduce the emission of other particles resulting in a change of atomic number or neutron number in the nucleus. Before this end of life, one neutron could interact with several nucleus along with its travel in space and it's called scattering reaction. The scattering reaction usually doesn't change the atomic number or neutron number of the nucleus but the energy or the propagating direction of neutron. And all those interactions described above result in the change of neutron flux and this is what the neutron transport equation describes.

In the reactor, there are nearly $10^6 n/cm^3$, therefore it's impossible to describe the trajectory and interactions of each neutron. The only solution is to do the statistics treatment and we define therefore the neutron density:

$$n(\vec{r}, \vec{v}, t), \quad (1)$$

which presents the average number of neutrons in unit volume at instant t . But in this definition, the unit volume is not the usual one in our physical world, but the one in the phase space[6] which includes six dimensions: three for physical geometry, two for velocity direction and one for energy or velocity module.

For describing the neutrons moving in the reactor, only the definition of neutron density is not sufficient, we need to define one of the most important notation in neutron physics: neutron flux[6]

$$\Phi(\vec{r}, E, \vec{\Omega}, t) = v \cdot n(\vec{r}, E, \vec{\Omega}, t). \quad (2)$$

In this definition, the velocity is only the module because the definition of neutron density has already considered the velocity direction.

After having the statistical description of neutron, we could then define the reaction rate, the number of reaction with neutron per unit time and per unit volume

$$R(\vec{r}, E, \vec{\Omega}, t) = v \cdot n(\vec{r}, E, \vec{\Omega}, t) \cdot \Sigma(\vec{r}, E, \vec{\Omega}, t) = \Sigma(\vec{r}, E, \vec{\Omega}, t) \cdot \Phi(\vec{r}, E, \vec{\Omega}, t), \quad (3)$$

in which the $\Sigma(\vec{r}, E, \vec{\Omega}, t)$ is the macroscopic reaction cross section and it's equal to the product of microscopic reaction cross section and target NND. This is one of fundamental quantities because it's measurable: for each reaction like the fission, we could measure the energy that this reaction releases. Then we could deduce the reaction rate by measuring the reactor power. In reverse, if we could calculate the reaction rate, we could then predict the reactor power under specific conditions for the operation or

security analysis. Generally, we prefer using the formula including the neutrons flux because then the reaction rate could be divided into two variables: one is known or measurable and another is unknown. What's more, in the transport or isotope equation, the neutron density could also be combined with velocity, which could really reduce the number of unknown variable and is more practical.

After introducing all necessary knowledge, now we could introduce the derivation of neutron transport equation which describes the conservation of neutrons[6]:

$$\frac{dn}{dt} = -(\vec{\Omega} \cdot \vec{\nabla} \Phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(\vec{r}, E, \vec{\Omega}, t) \cdot \Phi(\vec{r}, E, \vec{\Omega}, t)) + Q, \quad (4)$$

where n is the local neutron density, and its temporal variation depends on the rate of disappearance: the flux of neutron through the position(the term $\vec{\Omega} \cdot \vec{\nabla} \Phi(\vec{r}, E, \vec{\Omega}, t)$) and the all possible reactions between neutrons and materials(the term $\Sigma_t(\vec{r}, E, \vec{\Omega}, t) \cdot \Phi(\vec{r}, E, \vec{\Omega}, t)$) and also on the creation of neutron(the source term Q) which could include the fission production, the decay production or just the scattering which could change its energy(in phase space). The expression of source term depends on the situation, for example, in fuel rod, there is U235 or other fissile isotopes which could produce neutron by fission, but in the used fuel storing pool, the main source becomes the decay production. In our calculation, we will need the neutron flux in a reactor without external source, therefore the source term Q has the following expression[6]:

$$Q = \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(r, E \leftarrow E', \Omega \leftarrow \Omega') \Phi(\mathbf{r}, E, \Omega) + \frac{1}{4\pi K_{eff}} \chi(E) \int_0^\infty dE' \nu \Sigma_f(\mathbf{r}, E') \Phi(\mathbf{r}, E'), \quad (5)$$

where Σ_s is the macroscopic scattering cross section, K_{eff} is the effective multiplication factor in the reactor, $\chi(E)$ is the fission spectrum, ν is the number of neutron emitted per fission, Σ_f is the fission cross section. Besides, we could replace the neutron density term bu neutron flux using equation 2:

$$\frac{dn}{dt} = \frac{1}{v} \frac{d\Phi}{dt}. \quad (6)$$

Therefore, we could obtain a general form of neutron transport (Boltzmann) equation[6]:

$$\begin{aligned} \frac{1}{v} \frac{d\Phi}{dt} = & -(\vec{\Omega} \cdot \vec{\nabla} \Phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(\vec{r}, E, \vec{\Omega}, t) \cdot \Phi(\vec{r}, E, \vec{\Omega}, t)) \\ & + \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(r, E \leftarrow E', \Omega \leftarrow \Omega') \Phi(\mathbf{r}, E, \Omega) \\ & + \frac{1}{4\pi K_{eff}} \chi(E) \int_0^\infty dE' \nu \Sigma_f(\mathbf{r}, E') \Phi(\mathbf{r}, E'). \end{aligned} \quad (7)$$

This is the general form of Boltzmann equation for solving the neutron transport in the reactor, but in the real neutron transport calculation, there are also other models which simplify the expression and therefore, the calculation difficulties. In this work, one of those models: B_1 leakage model[6] will be used and implemented in our code. And the details about this model will be presented later in the report.

1-b Isotopic depletion

In this part, some basic knowledge about the isotopic depletion would be presented. Then we could write another important equation in nuclear physics: Bateman depletion equations. During the the operation of nuclear power plant, the neutron produced by fission reaction reacts with all possible materials in the reactor including a large range of isotopes. And the exposure to the neutron flux might deduce the modification of its nucleus like the change of number of protons or number of neutrons or state. After the modification of nucleus, the new produced isotope might be unstable and this instability could cause a radioactive decay. Moreover, the daughter nucleus might undergo another series of modifications under the influence of neutron flux. All those changes are collected and presented in the form of isotope chains and they are called depletion chains[6]. And the phenomenon of those nuclides field variation and nucleus modifications is called isotopic depletion.

In general, we don't use time to describe this evolution of nuclide field because it also depends on the reactor power(or neutron flux). Therefore, the parameter burnup is defined which means the integration of power with time per unit initial mass. With the burnup of fuel rod, the nuclide number density(NND) will change and this will modify the macroscopic reaction cross section which appears in the Boltzmann transport equation and influence the resolution of neutron flux. Reversely, the neutron flux could determine the variation of nuclide field. This is the origin of the coupling relation of neutron flux and NND and the complexity of this coupled relation will be explained in the rest part of isotopic depletion

The first complexity is the huge number of isotopes included in the calculation. As it's said before, all isotopes in the reactor exposed to neutron flux could be one element in depletion chains. Moreover, all of those new isotopes created after the exposure are also in the chains, which increases the difficulty of solving the Bateman equations. In addition, the created new daughter might be in a meta-stable state which is called isomeric state and we will add an m in the notation. Generally, meta-stable nucleus will release energy in the form of gamma ray to reach the ground state. But in this case, this meta-stable state could be maintained for a measurable period and during this period of time, those nucleus characteristics of this isomeric state like the spin or binding energy are different from those for ground state. Therefore, we prefer regarding it as a distinct isotope with its own properties and has a distinct position in depletion chains.

Another complexity is the different kinds of reaction types: radioactive capture (n,r), fission reaction(n,f), (n,xn) reaction, (n,a) transmutation, (n,p) transmutation. What's more, for one isotope, it could come from several different isotopes via different reaction and it could undergo several different reactions to produce several different daughter nucleus. Therefore, the real depletion chains is much more complex than a single linear chains[21], it could be sometimes cyclic or have many different branches or intersections. For calculating the density of one isotope, we need to consider all those relevant isotopes

and reactions.

In addition, the influence of neutron flux to the depletion rate is not linear. The neutron-induced depletion is essentially a neutron absorption reaction and it depends on the neutron flux. Moreover, the influence of neutron flux to different isotopes is obviously different: there are some isotopes whose concentrations are sensible to the neutron flux like Xe135 and there are some isotopes which will only undergo pure radioactive decay like Ac208. Moreover, even the distribution of neutron flux in different time interval will have an important influence to depletion reaction rate. From all the above discussion, we could conclude that the neutron flux has an important, non-linear effect to the NND calculation.

For one nuclide k , the variation of its NND with time depends on its generation and disappearance at each instance. The production and destruction both come from four modes:radioactive decay, nucleus reaction(for example: (n, n) reaction, (n, α) reaction...), neutron absorption and fission reaction. It should be noted that for most isotopes fission reaction is only their generation mode and only for fissile isotopes they could be consumed by fission reaction. Therefore, the variation of N_k could be expressed as[25]

$$\begin{aligned} \frac{dN_k}{dx} &= \Delta \dot{N}_{generation} - \Delta \dot{N}_{disappearance} \\ &= \sum_{l=1}^{N_{decay}} \lambda_{l \rightarrow k} N_l(t) + \sum_{l=1}^{N_{nucleus}} \langle \sigma_{n,l \rightarrow k} \phi(t) \rangle N_l(t) \\ &\quad + \sum_{l=1}^{N_{fission}} Y_{l \rightarrow k} \langle \sigma_{f,l} \phi(t) \rangle N_l(t) - (\lambda_k + \langle \sigma_{a,k} \phi(t) \rangle) N_k(t), \end{aligned} \quad (8)$$

where $N_i(t)$ is the NND of isotope i at time t , $\lambda_{l \rightarrow k}$ is the decay constant of nuclide l , $Y_{l \rightarrow k}$ is the fission yield of fissile isotope l to fission product k and $\langle \sigma_{x,l} \phi(t) \rangle = \int_0^\infty dE \sigma_{x,l,E} \phi(t, E)$ is the integration of neutron flux and microscopic cross section for isotope k and reaction type x (absorption, fission or radioactive capture). In this derivation, we suppose that the microscopic cross section is independent of time and we have $\langle \sigma_{x,y} \phi(t) \rangle = \int_0^\infty dE \sigma_{x,y}(E) \phi(E, t)$ with $x = f, x = a, x = n$ and $y = k, y = l \rightarrow k$. For each isotope, we have one equation with the above form and if we write the NND of all isotopes in one vector $\mathbf{N}(t) = [N_1(t), N_2(t), \dots, N_n(t)]$ [26] which we call nuclide number density vector(NNDV), all of those equations could be written in form of matrix \mathbf{M} and we have[25]

$$\frac{d\mathbf{N}}{dt} = \mathbf{M}\mathbf{N}. \quad (9)$$

This ordinary differential equation system (ODES) describing the variation of NNDs during the burnup process is called Bateman equations and the matrix \mathbf{M} is called burnup matrix.

The last point for the isotopic depletion is its contribution for the reactor control. As is known, most neutrons generated in the reactor are prompt neutrons which means that they are emitted as soon as the fission reaction occurs. However, the period of prompt neutrons generation is about microsecond scale. Therefore, if the multiplication factor of prompt neutrons is slowly higher than 1, the reactor power would

be increased dramatically even in 1 second and it would be out of control. In fact, the reactor could be controlled thanks to the delayed neutron which is only a small proportion of total neutrons (only about 0.5%). The delay neutron originates from the isotopic depletion. For some fission products, if the energy released during its decay is high enough, it could emit one or more neutrons with its radioactive decay. So this part of neutrons are generated a little later to sustain the whole generation of neutron and the total neutrons generation time becomes longer. And the reactor could be therefore under control.

3.2 Numerical methods for solving Bateman equations

After presenting the isotopic depletion and introducing the Bateman equations, the next step is to know how to solve it. In the process of simplifying depletion chains, we need to solve Bateman equations to finally calculate contribution function. Because of the coupling of Bateman equations with neutron balance(Boltzmann) equation, it's nearly impossible to get an analytic solution of Bateman equations. The only possible way is to solve it by numerical methods.

Firstly, Bateman equations form an ordinary differential equations system(ODES), therefore all those numerical methods for ODE could in theory be applied for solving Bateman equations. However, in reality it's more difficult because the resolution of Bateman equations is a stiff problem[23] which means that certain numerical methods could be numerically unstable and the time step[20] should be extremely small or even unacceptable for eliminating this instability. Therefore, only several methods could be applied and they will be presented later. Moreover, for better presenting those methods, we will rewrite this equation in a more mathematical way[9]:

$$y'(t) = F(y(t), t)y(t), \quad (10)$$

where $y(t)$ is the NND vector $\mathbf{N}(t)$ and $F(y(t), t)$ is the burnup matrix \mathbf{M} . The neutron flux component in the burnup matrix depend on $y(t)$ because the NND vector appears in the Boltzmann equation, so F is a function of t and $y(t)$.

2-a Matrix exponential methods

Firstly, for simplifying the question, we suppose that during each time step, the reaction rate is constant. Therefore, from the equation (??), we could deduce the solution as[9]

$$\mathbf{N} = \mathbf{N}(0)e^{\mathbf{M}t}, \quad (11)$$

where the exponential of matrix is defined as[18]

$$e^{\mathbf{M}t} = \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{M}t^k. \quad (12)$$

There are several ways for calculating the exponential of matrix[9][12][15]. The first method of evaluating the exponential is cutting and taking first K terms in the decomposition series[15]

$$e^{\mathbf{M}t} = \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{M}t^k \approx \sum_{k=0}^{K-1} \frac{1}{k!} \mathbf{M}t^k. \quad (13)$$

Moreover, for reduce the calculation, we could separate the short-lived isotopes from the burn-up matrix, add their contribution to long-lived isotopes by modifying the initial concentrations of long-lived isotopes and calculate their concentrations by combining the contribution of short-lived and long-lived ones[7].

Another method for estimating the exponential term is the Chebyshev rational approximation method[17], this method is appropriate for solving the burnup equation because the distribution of eigenvalues of matrix \mathbf{M} concentrates around the negative real axis[7]. And an order of (k, k) approximation is[7]

$$e^{\mathbf{M}t} \approx \frac{P_k(z)}{Q_k(z)} = a_0 + \sum_{i=1}^k \frac{a_i}{z + \theta_i} = a_0 + 2Re[\sum_{i=1}^{k/2} \frac{a_i}{z + \theta_i}], \quad (14)$$

where k is at the same time order of the polynomial $P_k(z)$ and $Q_k(z)$ and k is even so that those poles could construct $k/2$ conjugate pairs to eliminate those imaginary parts, a_0 is the infinity limit of this approximation, a_i are the residues and θ_i are poles. The matrix exponential method concentrates on the decomposition and evaluation of the exponential term appearing in the solution.

2-b Predictor-corrector method

The Predictor-corrector method[8] is just like Rung-Kutta method. Firstly, for equation (10), if F is just a constant as we supposed in the previous chapter, the problem would be much easier, because we could resolve this question analytically and get the precise solution[9]

$$y(t) = y(0)e^{Ft}, \quad (15)$$

and the next step is to do the development of matrix exponential. Finally, we could get the precision of the solution as we like and it just depends on the estimation of exponential function. However, it's not so simple in real case, F has a complex expression which even contains the unknown function $y(t)$. Therefore, as in the previous chapter, the first assumption we can make in the numerical resolution is that the function $F(y(t), t)$ is constant in each time interval and we take the value of $F(y(t), t)$ at the beginning of each time step[9]

$$F_n = F(y_n, t_n), \quad \text{for } t_n \leq t \leq t_{n+1}. \quad (16)$$

Therefore the integration above this time interval could be realized simply as[9]

$$y_{n+1} = y_n e^{F_n \Delta t}, \quad (17)$$

where $\Delta t = t_{n+1} - t_n$. Using this method, we could resolve this equation. However, its limitation is the precision is not enough: for this method, it will converge to $O(\Delta t)$. If we want to have a smaller error, then Δt must be small enough. However, this could increase the calculation time, sometimes it could even be unacceptable. Therefore, some higher order methods are developed to overcome this limitation and to make the calculation easier. For example, we could not only use the value at the beginning of time step, but also some intermediate values could be evaluated and all those values could contribute to the calculation of final value at the end of this time step. Its general two-stage structure is as follow[9]:

$$\begin{aligned} x &= y_n e^{c_{11}F(y_n, t_n)\Delta t} \\ y_{n+1} &= y_n e^{(c_{21}F(y_n, t_n) + c_{22}F(x, t_n + c_{11}\Delta t))\Delta t}. \end{aligned} \quad (18)$$

In this structure, the value of y is firstly evaluated at $t = t_n + c_{11}\Delta t$, then the matrix F is updated according to this calculation. Finally, the value of y_{n+1} is evaluated by weighting the combination of matrix F at $t = t_n$ and $t = t_n + c_{11}\Delta t$. And, c_{11} , c_{21} and c_{22} are three coefficients to be determined and it depends on the method of interpolation used. For example, for the linear interpolation we have[9]

$$\begin{aligned} x &= y_n e^{F(y_n, t_n)\Delta t} \\ y_{n+1} &= y_n e^{[0.5F(y_n, t_n) + 0.5F(x, t_n + \Delta t)]\Delta t}. \end{aligned} \quad (19)$$

This time, after using more than one point, the precision could reach $O(\Delta t^2)$. In fact, we could realize that it is similar to the normal low-order Runge-Kutta method. Therefore, just like higher order Runge-Kutta methods, we could think to add more intermediate steps in our integration and also like in Runge-Kutta methods we could arrange those coefficients like c_{ij} into a Butcher's table. Therefore, the final structure of higher order methods would be as follows[9]:

$$\begin{aligned} x_1 &= y_n \\ x_i &= y_n e^{\Delta t \sum_{j=1}^{i-1} a_{ij} F(x_j, t_n + c_j)} \\ y_{n+1} &= y_n e^{\Delta t \sum_{j=1}^s b_j F(x_j, t_n + c_j)}, \end{aligned} \quad (20)$$

where the corresponding Butcher's table is[9]

0					
c_2	a_{21}				
c_3	a_{31}	a_{32}			
\vdots	\vdots		\ddots		
c_s	a_{s1}	a_{s2}	\cdots	$a_{s,s-1}$	
	b_1	b_2	\cdots	b_{s-1}	b_s

and s is the number of

points in the extrapolation used to evaluate the value of y_{n+1} . There is one point should be noted: the precision of this method couldn't increase rapidly like expected. Even we use the Butcher's table which is high order for scalar functions, the result of this vector function could only have an order of 2 which is showed in research of C. Josey[9].

2-c Runge-Kutta method

Runge-Kutta method is a family of numerical algorithms of different precision orders which could solve the general differential equation(s) with a given initial condition. This method firstly estimates several points at different time by iteration and then it could evaluate the final value using all those estimation points to reach a high order convergence.

The general structure of Runge-Kutta method for solving equation (10) is as follow[22]:

$$\begin{aligned}
 x_1 &= y_n \\
 x_i &= y_n + \Delta t \sum_{j=1}^{i-1} a_{ij} F(x_j, t_n + c_j) x_j \\
 y_{n+1} &= y_n + \Delta t \sum_{j=1}^s b_j F(x_j, t_n + c_j) x_j,
 \end{aligned} \tag{21}$$

and those coefficients are also summarized in the Butcher's table[22]

0					
c_2	a_{21}				
c_3	a_{31}	a_{32}			
\vdots	\vdots		\ddots		
c_s	a_{s1}	a_{s2}	\cdots	$a_{s,s-1}$	
	b_1	b_2	\cdots	b_{s-1}	b_s

There are many similarities between the Runge-Kutta method and the predictor-corrector method, but the most important difference is the way doing the integration. For the Runge-Kutta method, the integration is done simply by:

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} y'(t) dt = y_n + \int_{t_n}^{t_{n+1}} F(y(t), t) y(t) dt, \tag{22}$$

but for the predictor-corrector method, it's

$$\begin{aligned}
 \ln(y_{n+1}) &= \ln(y_n) + \int_{t_n}^{t_{n+1}} F(y(t), t) dt \\
 y_{n+1} &= y_n e^{\int_{t_n}^{t_{n+1}} F(y(t), t) dt}.
 \end{aligned} \tag{23}$$

In fact, there are still other ways from different points of view to resolve the Bateman equations, for examples: the Transition Probabilities Method[19], Krylov Subspace Method[1][11], Magnus Method[2], Laplace Transform Method[29], etc. But there we just present the most basic ways for solving the Bateman equations and we won't present all of them.

3.3 Depletion chains simplification method

In this part, we will present the depletion chains simplification method proposed by Go Chiba. But the adjoint Boltzmann equation and adjoint Bateman equations appear in its derivation, so we need to firstly present the adjoint formulation and then we could begin to show how to simplify depletion chains.

The concept of adjoint operator originates from functional analysis and it's defined on Hilbert space. But in our physical case, we won't present the whole mathematical theory about adjoint(or more seriously in mathematics: Hermitian adjoint) operator. In later part, we will just present all essential knowledge about the adjoint operator used in our derivation and implementation.

Firstly, before giving the definition of adjoint operator, we must define an inner product in space. In previous part about the Boltzmann equation, we define the phase space, which has six dimensions: three for geometry position, two for velocity direction and one for particle energy(or module of velocity) and the inner product will also be defined on this space. Now, we could define the inner product: the integration of two input quantities over the phase space:

$$\langle f, g \rangle = \int dr \int dE \int d\Omega f(r, E, \Omega) g(r, E, \Omega) \quad (24)$$

In general, for an integration inner product, we need to add a subscript after the bracket to indicate the integrated variables. But in this report, the only inner product used is defined on the neutron phase space, so we will use simply the bracket in later parts. After defining the inner product, we will present briefly what an operator is. In mathematics, an operator is a mapping which could create a relation between two elements of space, we could also understand it like a combination of operations acting on one element to produce another one. In neutron physics, for example, in previous part, we introduce the Boltzmann equation(7). It has a very complex expression, but we could just regard it as an operator acting on neutron flux to get a zero result:

$$B\Phi = 0 \quad (25)$$

where B is the operator which contains all the interaction ways between neutron flux and material. Or we could divide it into two parts[22]:

$$(D - \frac{1}{K_{eff}}P)\Phi = 0 \quad (26)$$

where D is the operator causing disappearance of neutron and P is the operator containing all the production of neutron.

Now we can introduce the definition of adjoint operator: for an operator H , its adjoint operator is defined as the operator which could satisfy the following condition[22]:

$$\langle f, Hg \rangle = \langle H^\dagger f, g \rangle \quad (27)$$

where H^\dagger is the adjoint operator of H and (f, g) are two functions defined on phase space. However, in neutron physics, we didn't have so many physical quantities defined on phase space and (f, g) are not two arbitrary functions. In fact, in physics, we will also call f as the adjoint of g and note it as g^\dagger . Besides, by changing the position of two parts (we can do this because this inner product is defined on Euclidean space), we have:

$$\langle g^\dagger, Hg \rangle = \langle H^\dagger g^\dagger, g \rangle = \langle g, H^\dagger g^\dagger \rangle \quad (28)$$

In this definition, the function g could be the neutron flux Φ or NND vector. For Φ , it's a function defined on the phase space, but for resolving the Boltzmann equation numerically, we must do the discretization over phase space: for each unit calculation volume, we will define the average neutron flux value in this volume, so that we have only limited number of unknowns which will construct an vector Φ . For the most common case, we will resolve Boltzmann equation in an unit geometry volume and a discretized direction, so the vector Φ will only contain the neutron flux in different energy groups. In this case, the operator and Φ are both in the form of matrix and inner product is just the common inner product of vectors above the phase space.

In this report, there is only one adjoint equation system to resolve: the adjoint Bateman equations. But before looking for its adjoint form, we must prove its existence. This comes from a mathematical theorem[22]: for linear and real-valued function (or we call it operator), it has an adjoint operator. And this operator in Bateman equations evidently satisfy this condition, therefore we could get its adjoint form. Now the derivation of adjoint Bateman operator will be presented. This work comes from the doctor thesis of Hayes Franklin STRIPLING[22]. Because we will use the phase space, but in our model, the NND vector is a list of densities which don't depend on the position, angle or energy, so we just define an operator m as:

$$\langle m\mathbf{N} \rangle = \mathbf{M}\mathbf{N}, \quad (29)$$

where \mathbf{M} is the burnup matrix described in equation (9). As the term $m\mathbf{N}$ is a vector, the i -th term of this component is defined as:

$$\begin{aligned} (m\mathbf{N})_i = \frac{1}{\langle \rangle} & \left(\sum_{l=1}^{N_{decay}} \lambda_{l \rightarrow k} N_l(t) + \sum_{l=1}^{N_{nucleus}} \langle \sigma_{n,l \rightarrow k} \bar{\phi}(t) \rangle_E N_l(t) \right. \\ & \left. + \sum_{l=1}^{N_{fission}} Y_{l \rightarrow k} \langle \sigma_{f,l} \bar{\phi}(t) \rangle_E N_l(t) - (\lambda_k + \langle \sigma_{a,k} \bar{\phi}(t) \rangle_E) N_k(t) \right), \end{aligned} \quad (30)$$

where $\langle \rangle_E$ means the integration only over energy, $\bar{\phi}(t)$ is the average neutron flux over the whole calculation volume using the B_1 leakage model and all those terms come from equation (8) and they have the same meaning. The derivation of adjoint Bateman operator is quite simple, we know that each term of $\mathbf{M}\mathbf{N}$ is already energy and angle integrated and spatial averaged, therefore there is no longer dependence

between \mathbf{MN} and those variables (r, E, Ω) , so we have

$$\langle \mathbf{N}^\dagger \mathbf{MN} \rangle = \langle \mathbf{NM}^T \mathbf{N}^\dagger \rangle = \langle \mathbf{NM}^\dagger \mathbf{N}^\dagger \rangle, \quad (31)$$

which means that the adjoint of Bateman operator is just its transpose.

After showing those notations about adjoint formulation, we could begin to present depletion chains simplification method. The simplification of depletion chains has always been an important problem, not only because it could improve calculation efficiency and save calculation time, but also for its broad application possibilities. Until now, there aren't many methods for treating this process automatically[3][10] or applications[14][13]. This is mainly because the simplification is a case-dependent work and this raises a lot of difficulties. Therefore, it's important to develop new simplification methods and also optimize existing methods.

For doing the simplification of burnup chains, here we present an adjoint method proposed by Go Chiba[3]. It originates from the Generalized Perturbation Theory(GPT)[4][5][27]. The aim of Generalized Perturbation Theory is to study the sensitivity of reactor characteristic to reactor parameters[6] and this theory has many applications[28][16]. The burnup chains simplification method uses the adjoint formulation and finally it selects those important nuclides with the help of two functions: the adjoint nuclide number density(ANND) and the contribution function(CF). For employing this method, the first step is to define the target nuclear characteristic and also the importance of nuclide. Firstly, the importance of one nuclide means the influence of its number density variation to the goal characteristic like the reactivity or other nuclide densities in the chains after burnup calculations. Besides, the goal quantity could be some calculation result 'response' like the final nuclide number density, the integral of "response function" and neutron flux like the total reaction rate or the ratio of these integrals. Or it could be just a transient which will be studied and we just want to use a simplified depletion chains for saving time and keeping accuracy at the same time. Whatever it is, it should be determined at the beginning.

Then, for determining the importance of nuclide elements, a detailed burnup chains would be carried out to calculate the ANNDs and CFs. Those more important nuclides for a specific target quantity are identified by comparing the values of CFs and the threshold one. After the comparison, those identified nuclides are selected to construct the simplified burnup chains. Moreover, during this construction, the decay relation should also be redefined because a number of nuclides in this chains are eliminated and there might be not direct decay relation between two adjacent selected nuclides. Meanwhile, the contribution for fission reactions(or other neutrons reactions) by those eliminated nuclides should also be conserved and this contribution is given to its non eliminated daughter nuclide.

For doing burnup calculation, the neutron flux in the calculated region is needed therefore we firstly consider the neutron transport equation. Moreover, we will consider the steady-state situation, which is

quite normal in the reactor.

$$B\phi = (M - \frac{1}{k_{eff}}F)\phi = 0 \quad (32)$$

where M and F represent respectively the disappearance and fission generation operator, and k_{eff} is the effective neutron multiplication factor. But it should be noted that this factor isn't present in the original derivation of transport equation but an additional term for keeping the equality of the disappearance and production of neutrons. If not, the steady-state couldn't be maintained. The burnup calculation is a long-term calculation and its time scale is much larger than that for the neutron transport calculation. Therefore, we could suppose that during the resolution of Bateman equations the reactor is always at steady-state which is the quasi-static approximation applied to the above equation (32). From the form of the static neutron transport equation, we know that it's a homogeneous equation and for normalizing the neutron flux, a constraint condition of constant fission power is added and it's generally called power normalization[3]

$$\begin{aligned} P &= \int_{r \in V_f} \left(\sum_j \kappa_{f,j} N_j \sum_g \sigma_{f,j,g} \phi_g(r) + \sum_l \kappa_{c,l} N_l \sum_g \sigma_{c,l,g} \phi_g(r) \right) dr \\ &= \sum_j \kappa_{f,j} N_j \langle \sigma_{f,j} \phi \rangle + \sum_l \kappa_{c,l} N_l \langle \sigma_{c,l} \phi \rangle \end{aligned} \quad (33)$$

where P is the reactor power, V_f is the calculated region, $\kappa_{m,j}(m = f, c)$ are respectively the average energy emitted per fission reaction or per gamma capture reaction for isotope j , N_j is the nuclide number density of which could absorb neutron and trigger fission reaction or just emit gamma ray, $\sigma_{m,j,g}(m = f, c)$ are respectively the multi-group microscopic fission or gamma capture reaction cross section and $\phi_g(r)$ is neutron flux for energy group g . And for simplification, we use the brackets to present the integration of all energy groups over the whole calculated region. For obtaining this formula, several hypothesis are made: the first one is that the nuclide density is independent with space position r and the second is that the neutron flux is isotropic so there is not the angle distribution $\vec{\Omega}$. For the aim of simplifying later derivation, we could still simplify this equation[3]

$$P = \mathbf{N}^T \mathbf{K}, \quad (34)$$

where \mathbf{N}^T denotes the transpose of the nuclide number density vector containing all nuclides in our calculation and the j th term in the \mathbf{K} vector is defined as

$$K_j = \delta_{f,j} \kappa_j \langle \sigma_{f,j} \phi \rangle + \delta_{c,j} \kappa_j \langle \sigma_{c,j} \phi \rangle, \quad (35)$$

where $\delta_{m,j}(m = f, c)$ is equal to 1 if isotope j could undergo reaction m and equal to 0 if not.

The simplest method of observing the importance of one nuclide k to the target nuclide l is that we could change the initial NND of nuclide k and observe the final NND of nuclide l after the burnup

calculation, this is what we call the sensitivity calculation. In this type of calculation, we define the sensitivity as the ratio of relative change of target nuclide's NND to the relative perturbation of nuclide k :

$$S_k = \frac{\frac{\Delta N_l(t_f)}{N_l(t_f)}}{\frac{\Delta N_k(t_i)}{N_k(t_i)}} \quad (36)$$

where t_i and t_f are respectively the begin and the end of burnup calculation, N_l and N_k are respectively the NND of target nuclide l and another nuclide k . However, this method requires a large number of calculations because not only we need to change the initial NND variation of nuclide k , but also should we change the nuclide k to test the importance of different nuclides. We must solve a large number of times the Bateman equations and it really takes a lot of time. Moreover, if we would like to be more rigorous, we should also change the initial NND of all nuclides to observe the coherence of those results. This is because the influence of other isotopes to a specific target nuclide is not linear: for a nuclide k , we give it a perturbation $\Delta N_k(t_{initial})$ we could get a final variation of target nuclide l 's NND $\Delta N_l(t_{final})$; for another nuclide j , after the same process, we could get another $\Delta N_l(t_{final})$; but if we give the variation $\Delta N_k(t_{initial})$ and $\Delta N_j(t_{initial})$ at the same time, the result $\Delta N_l(t_{final})$ is not the sum of those two variations $\Delta N_l^k(t_{final})$ and $\Delta N_l^j(t_{final})$. Therefore, the sensitivity could just give us some references but not the accurate result prediction because the real situation is much more complex.

After all those considerations, the simple method is no longer practical for computational calculation. Another way is to calculate the importance of nuclide by the GPT theory and it will be shown as follow. The key point in this method is to do the linearization of the burnup equation. This point is also mentioned in the last paragraph. In fact, due to the coupling relation between neutron flux and nuclide number densities, the response of a NND perturbation is non-linear, specially when the calculation time interval $[t_{initial}, t_{final}]$ is long. Therefore, the first thing in this derivation is to set a small duration of time $[t_i, t_{i+1}]$ in which the burnup matrix \mathbf{M} could be regarded as a constant[3]:

$$\mathbf{M}(t) = \mathbf{M}(t_i) \quad \text{for } t \in [t_i, t_{i+1}]. \quad (37)$$

This hypothesis is not true in analytical resolution. But in computational calculation this hypothesis is acceptable because discretization of a quantity and supposing it to be a constant during a calculation step is the basic operation in computational science. After introducing this key point, now we write the burnup equation

$$\frac{\partial \mathbf{N}}{\partial t} = \mathbf{M}^i \mathbf{N}(t), \quad t_i \leq t \leq t_{i+1} \quad (38)$$

where \mathbf{M}^i is the burnup matrix at $t = t_i$, and we also have the initial condition $\mathbf{N}(t_i)$. Generally, the process of burnup calculation is to firstly resolve the neutrons transport equation and then several methods could be applied to resolve the Bateman equations. Moreover, depending on the different cases, the Bateman equations has two possible forms: linear form which is the pure decay case and non-linear form

that the matrix \mathbf{M}^i depends on the neutron flux. And there we apply the GPT theory and focus more on its variation. Therefore a variation of initial NND vector $\Delta\mathbf{N}(t_i)$ is given at $t = t_i$. This variation would also cause a change of neutron transport equation because this variation would deduce the variation of macroscopic reaction cross section in operator M and F and also in the constraint constant power condition. And the general procedure of doing neutronic simulation is to firstly resolve the neutron transport equation and then resolve the burnup equation using the resolved neutron flux. And the new neutron flux also appears in the operator \mathbf{M} , therefore the new perturbed burnup equation is written as[3]

$$\frac{\partial \mathbf{N}'}{\partial t} = \mathbf{M}' \mathbf{N}'(t), \quad t_i \leq t \leq t_{i+1} \quad (39)$$

where $\mathbf{N}'(t)$ and \mathbf{M}' are NND vector and burnup matrix after the variation and we have $\mathbf{N}'(t) = \mathbf{N}(t) + \Delta\mathbf{N}(t)$ and $\mathbf{M}' = \mathbf{M}^i + \Delta\mathbf{M}^i$. After combining the equation with and without variation, we could deduce the equation about $\Delta\mathbf{N}(t)$ as follow[3]

$$\frac{\partial \Delta\mathbf{N}}{\partial t} = \Delta\mathbf{M}^i \mathbf{N}(t) + \mathbf{M}^i \Delta\mathbf{N}(t), \quad t_i \leq t \leq t_{i+1} \quad (40)$$

It should also be noted that in the derivation of above equation, the high order term $\Delta\mathbf{N}(t)\Delta\mathbf{M}^i$ are neglected. Then we multiply for both side of the above equation a vector $\mathbf{w}^T(t)$ and do the integration over $[t_i, t_{i+1}]$

$$\int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \frac{\partial \Delta\mathbf{N}}{\partial t} dt = \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \Delta\mathbf{M}^i \mathbf{N}(t) dt + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \mathbf{M}^i \Delta\mathbf{N}(t) dt. \quad (41)$$

We also have

$$\begin{aligned} \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \frac{\partial \Delta\mathbf{N}}{\partial t} dt &= [\mathbf{w}^T(t) \Delta\mathbf{N}]_{t_i}^{t_{i+1}} - \int_{t_i}^{t_{i+1}} \frac{\partial \mathbf{w}^T(t)}{\partial t} \Delta\mathbf{N} dt \\ &= \mathbf{w}^T(t_{i+1}) \Delta\mathbf{N}(t_{i+1}) - \mathbf{w}^T(t_i) \Delta\mathbf{N}(t_i) - \int_{t_i}^{t_{i+1}} \frac{\partial \mathbf{w}^T(t)}{\partial t} \Delta\mathbf{N} dt, \end{aligned} \quad (42)$$

therefore[3]

$$\begin{aligned} &\mathbf{w}^T(t_{i+1}) \Delta\mathbf{N}(t_{i+1}) - \mathbf{w}^T(t_i) \Delta\mathbf{N}(t_i) \\ &= \int_{t_i}^{t_{i+1}} \Delta\mathbf{N}^T(t) \left(\frac{\partial \mathbf{w}}{\partial t} + \mathbf{M}^{iT} \mathbf{w}(t) \right) dt + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \Delta\mathbf{M}^i \mathbf{N}(t) dt \end{aligned} \quad (43)$$

For further simplifying this formula, if the vector \mathbf{w} is a solution of the follow equation[3]

$$\frac{\partial \mathbf{w}}{\partial t} = -\mathbf{M}^{iT} \mathbf{w}(t), \quad t_i \leq t \leq t_{i+1} \quad (44)$$

with condition $\mathbf{w}(t_{i+1}) = \mathbf{e}_l$ where \mathbf{e}_l is the l -th component of the orthonormal basis vector. Then we could obtain a simpler form of equation (43)[3]:

$$\Delta N_l(t_{i+1}) = \mathbf{w}^T(t_i) \Delta\mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t) \Delta\mathbf{M}^i \mathbf{N}(t) dt \quad (45)$$

From the previous part, we already know that the above functions are the adjoint Bateman equations. In previous part, we prove that the adjoint of Bateman operator is its transpose. Now we have the complete form of this adjoint equation and the minus comes from the integration by parts. In our derivation, we just use the property of space independence to prove that the adjoint is the transpose, but if we doing the integration according the to definition of adjoint operator (27), we could then get the above equation (44). Therefore, we will rewrite the term \mathbf{w} as $\Delta \mathbf{N}^*$ according to the notation showed in the definition (28) and it's called the adjoint nuclide number density(ANND). Another point is that there we introduce the vector \mathbf{w} as a selection: after introducing equation (44), we could get a simplified scalar function which only calculate $\Delta N_l(t_{i+1})$. Conversely, we need to resolve the adjoint Bateman equations for \mathbf{w} . From above equation, we could know that the variation of target nuclide l at $t = t_{i+1}$ is deduced by the variation of $\Delta \mathbf{N}(t_i)$ at $t = t_i$ and $\Delta N_l(t_{i+1})$ could be calculated using the above formula (45). In the right-hand side of formula (45), the vector $\mathbf{w}(t)$ could be obtained by solving the equation (44) with the final condition, $\Delta \mathbf{N}(t_i)$ is the given initial variation and is known, the integration could therefore be calculated as soon as we know the expression of $\Delta \mathbf{M}^i$.

In our work, the variation of \mathbf{M}^i originates from the variation of initial NND vector, the presence of $\Delta \mathbf{N}$ will cause the modification of B^i in neutron transport equation (equation 32) and therefore modify the resolved neutron flux which is included in \mathbf{M}^i . So for calculating the variation of \mathbf{M}^i , the first step is to write its relation with the modified neutron flux[3]:

$$\Delta \mathbf{M}^i = \frac{d\mathbf{M}^i}{d\phi^i} \Delta \bar{\phi}^i = \frac{d\mathbf{M}^i}{d\phi^i} \frac{\int_{r \in V_f} \Delta \phi^i(r) dr}{V_f}, \quad (46)$$

where $\Delta \bar{\phi}^i = \frac{\int_{r \in V_f} \Delta \phi^i(r) dr}{V_f}$ represents the average of variation of neutron flux over the calculated region and this variation deduced by initial perturbation $\Delta \mathbf{N}(t_i)$ is calculated at $t = t_i$. In previous part, it's mentioned that in the burnup equation, the microscopic cross section and the NND vector are both independent of space variation for simplification. Therefore, the \mathbf{M}^i and $\Delta \mathbf{M}^i$ should also be independent to variable r and in the expression of \mathbf{M}^i (or $\Delta \mathbf{M}^i$), the term of $\phi(r)^i$ (or $\Delta \phi^i$) could be averaged and regarded as a homogeneous region result. For the aim of calculating the term $\int_{r \in V_f} \Delta \phi^i(r) dr$ which is caused by the perturbation of $\Delta \mathbf{N}(t_i)$, we need to introduce the adjoint neutron transport equation to reveal the relation between $\Delta \phi^i$ and $\Delta \mathbf{N}(t_i)$ [3].

$$\mathbf{B}^{i*} \mathbf{I}^{i*} = \mathbf{S}^{i*} \quad (47)$$

$$\mathbf{S}^{i*} = \begin{cases} \left(\frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{d\mathbf{M}^i}{d\phi^i} \mathbf{N} dt}{V_f} \right) - \left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \right) \frac{\sum_j \kappa_j N_j(t_i) \sigma_{f,j}^i}{p^i}, & \text{if } r \in V_f \\ 0, & \text{if } r \notin V_f \end{cases} \quad (48)$$

where \mathbf{B}^{i*} and \mathbf{I}^{i*} are respectively the adjoint form of B^i and ϕ^i , \mathbf{S}^{i*} is the adjoint source term, $\bar{\mathbf{M}}^i$ is a

component of \mathbf{M}^i and all elements in $\bar{\mathbf{M}}^i$ depend on ϕ^i . And in later derivation, we will see that we could construct a relation between $\Delta\phi^i$ and $\Delta\mathbf{N}(t_i)$ to finally obtain the contribution function only because we construct an adequate source term. What's more, for the adjoint source term, we must have $\langle S^{i*}\phi^i \rangle = 0$ [3], so

$$\begin{aligned}
\langle S^{i*}\phi^i \rangle &= \int_{r \in V_f} \sum_g \left(\frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} \mathbf{N} dt}{V_f} \right) \phi_g^i(r) dr - \int_{r \in V_f} \sum_g \left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \right) \frac{\sum_j \kappa_j N_j(t_i) \sigma_{f,j,g}^i \phi_g^i(r)}{p^i} dr \\
&= \sum_g \left(\frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} \mathbf{N} dt}{V_f} \right) \int_{r \in V_f} \phi_g^i(r) dr - \sum_g \left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \right) \frac{\int_{r \in V_f} \sum_j \kappa_j N_j(t_i) \sigma_{f,j,g}^i \phi_g^i(r) dr}{p^i} \\
&= \sum_g \left(\frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} \mathbf{N} dt}{V_f} \right) \bar{\phi}_g^i V_f - \left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \right) \frac{\sum_j \kappa_j N_j(t_i) \langle \sigma_{f,j}^i \phi \rangle}{p^i} \\
&= \sum_g \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} \mathbf{N} dt \cdot \bar{\phi}_g^i - \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \\
&= \left(\frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} \mathbf{N} dt}{V_f} \right) \phi^i - \left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt \right) \frac{p^i}{p^i V_f} \\
&= \phi^i \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \left(\frac{\partial \mathbf{M}^i}{\partial \bar{\phi}_g^i} - \frac{\bar{\mathbf{M}}^i}{\phi^i} \right) \mathbf{N} dt \\
&= 0
\end{aligned} \tag{49}$$

In this derivation, we could see that the hypothesis of constant burnup matrix \mathbf{M}^i in time interval $[t_i, t_{i+1}]$ is very important. Without this assumption, we could not obtain the above demonstration of orthogonality between the adjoint source term and neutron flux. After proving the equality, now we multiply $\Delta\phi^i$ to both sides of equation (47) and integrate this equation over all energy group and the volume V_f . By introducing equation (48) in it, finally we obtain[3]

$$\left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{d\mathbf{M}^i}{d\bar{\phi}^i} \mathbf{N} dt \right) \frac{\int_{r \in V_f} \Delta\phi^i(r) dr}{V_f} = \langle \mathbf{\Gamma}^{i*} \mathbf{B}^{i*} \Delta\phi^i \rangle + P^{i*} \cdot \sum_j \kappa_j N_j(t_i) \langle \sigma_{f,j}^i \Delta\phi^i \rangle \tag{50}$$

where $P^{i*} = \frac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{\mathbf{M}}^i \mathbf{N} dt}{p^i}$ is the adjoint power, P^i is the reactor power and we have $\langle \mathbf{B}^{i*} \mathbf{\Gamma}^{i*} \Delta\phi^i \rangle = \langle \Delta\phi^i \mathbf{B}^{i*} \mathbf{\Gamma}^{i*} \rangle = \langle \mathbf{\Gamma}^{i*} \mathbf{B}^i \Delta\phi^i \rangle$ in which the first equality comes from the symmetry of real inner product and the second equality comes from property of adjoint operator.

Until now we haven't got the relation between the variation of neutron flux and nuclide perturbation $\Delta\mathbf{N}(t_i)$, this is because the influence of perturbation $\Delta\mathbf{N}(t_i)$ works indirectly by modifying the transport operator \mathbf{B}^i . Therefore we need one more step to deduce the expression of $\Delta\phi^i$ from the neutron transport equation[3]

$$B^i \Delta \phi^i + \Delta B^i \phi^i = 0 \quad (51)$$

And for the conservation of reactor power during the burnup calculation, we could deduce[3]

$$\begin{aligned} \Delta P^i &= \sum_j \kappa_j N_j(t_i) \left\langle \sigma_{f,j}^i \Delta \phi^i \right\rangle + \sum_j \kappa_j \Delta N_j(t_i) \left\langle \sigma_{f,j}^i \phi^i \right\rangle \\ &= \sum_j \kappa_j N_j(t_i) \left\langle \sigma_{f,j}^i \Delta \phi^i \right\rangle + \Delta \mathbf{N}^T(t_i) \mathbf{K}(t_i) = 0 \end{aligned} \quad (52)$$

Using equation (51) and (52), we could rewrite the equation (50) as[3]

$$\left(\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \frac{d\mathbf{M}^i}{d\phi^i} \mathbf{N} dt \right) \frac{\int_{r \in V_f} \Delta \phi^i(r) dr}{V_f} = - \left\langle \mathbf{\Gamma}^{i*} \Delta \mathbf{B}^i \phi^i \right\rangle - P^{i*} \cdot \Delta \mathbf{N}^T(t_i) \mathbf{K}(t_i). \quad (53)$$

then rewrite equation (45) as[3]

$$\begin{aligned} \Delta N_l(t_{i+1}) &= \left(\mathbf{N}^{*T}(t_i) - \left\langle \mathbf{\Gamma}^{i*} \frac{dB^i}{d\mathbf{N}^T} \phi^i \right\rangle - P^{i*} \cdot \mathbf{K}^T(t_i) \right) \Delta \mathbf{N}(t_i) \\ &= \widehat{\mathbf{N}}^{*T}(t_i) \Delta \mathbf{N}(t_i) = \sum_k \widehat{N}_k^*(t_i) \Delta N_k(t_i) \end{aligned} \quad (54)$$

where we have the corrected ANND vector $\widehat{\mathbf{N}}^* = \mathbf{N}^*(t_i) - \left\langle \mathbf{\Gamma}^{i*} \frac{dB^i}{d\mathbf{N}} \phi^i \right\rangle - P^{i*} \cdot \mathbf{K}(t_i)$. In the above equations, we could see that the term $\widehat{\mathbf{N}}^{*T}(t_i)$ could be regard as the amplification of the initial perturbation of nuclide k to the target nuclide l and this is the absolute amplification. But in the reactor, the concentration of different isotopes could have high difference or even be in different order. Therefore, the absolute value could not show the real importance of different isotopes with different concentrations. And we use the relative perturbation just like the definition of sensitivity to define the contribution function as follow:

$$CF_k(t_i) = \frac{\frac{\Delta N_{k \rightarrow l}(t_{i+1})}{N_l(t_{i+1})}}{\frac{\Delta N_k(t_i)}{N_k(t_i)}} = \frac{\frac{\widehat{N}_k^*(t_i) \Delta N_k(t_i)}{N_l(t_{i+1})}}{\frac{\Delta N_k(t_i)}{N_k(t_i)}} = \frac{\widehat{N}_k^*(t_i) N_k(t_i)}{N_l(t_{i+1})}, \quad (55)$$

where $\Delta N_{k \rightarrow l}$ is the variation of target nuclide caused by nuclide k which is equal to $\widehat{N}_k^*((t_i) N_k((t_i))$.

In this section, we present the adjoint formulation and depletion chains simplification method. Finally we get the expression of contribution function in time interval $[t_i, t_{i+1}]$. By calculating each term in the expression, we could get the contribution function of each nuclide and therefore selecting important ones. But in the process of applying this method, we found some defects of this method and so we did some modifications to improve its applicability and we will present those improvements in next chapter.

4. Improvements about Bateman equations solver and depletion chains simplification method

4.1 Improvements about Bateman equations solver: B_n leakage model

For resolving direct and adjoint Bateman equations appearing in depletion chains simplification method, we develop a Bateman equations solver in this work. And this solver contains the neutron flux calculation module. With this module, the solver could calculate neutron flux and then update burnup matrix at each iteration, therefore the result will be more accurate. In this section, we will present the neutron flux calculation model used in the neutron flux module and show the detailed derivation of calculating neutron flux for different nuclear data types.

In our work, we use the B_1 leakage model to calculate neutron flux. Leakage model is generally applied in lattice calculation with reflection or translation boundary condition. The aim of this model is to determine the neutron flux and other quantities without detailed information about the lattice. The only assumption made in this model is $K_{eff} = 1$ and this is always true for the steady-state reactor. The reflection or translation boundary condition assumes that the near cells have the same working situation and the condition $K_{eff} = 1$ is satisfied by controlling the leakage rate. Moreover, by assuming the reflection or translation boundary condition, we could get a homogeneous or periodic flux distribution $\varphi(r, E, \Omega)$ in each calculated lattice, this is the fundamental mode approximation and this flux is called fundamental flux. Under all those assumptions, the leakage rate of each cell is controlled by macroscopic neutron flux distribution in all calculation lattices which only depends on the lattice position $\psi(r)$, moreover, the neutron leakage could be regarded as neutron diffusion in the reactor, therefore $\psi(r)$ satisfies the following Laplace equation[6]:

$$\nabla^2 \psi(r) + B^2 \psi(r) = 0 \quad (56)$$

where B^2 is a real number to determine the form of $\psi(r)$ so that we could get $K_{eff} = 1$. After getting the local neutron flux distribution in one lattice and the macroscopic neutron flux distribution, the neutron flux is defined as the product of those two terms[6]:

$$\phi(r, E, \Omega) = \psi(r) \varphi(r, E, \Omega) \quad (57)$$

From equation(56), we could get a general solution $\psi(r) = \psi_0 e^{i\mathbf{B}r}$ and in this expression \mathbf{B} is a vector satisfying $\mathbf{B} \cdot \mathbf{B} = B^2$. And in the homogeneous fundamental mode of B_1 leakage model, we could further do the homogenization of neutron flux in the calculation lattice and therefore, we have[6]:

$$\phi(r, E, \Omega) = \varphi(E, \Omega) e^{i\mathbf{B}r} \quad (58)$$

By putting this form of neutron flux in the neutron transport equation (7) and after a series of mathematical operations shown in the book of Alain Hébert: <Applied Reactor Physics>[6], we obtain the B_1 equations[6]:

$$[\Sigma(E) + D(B, E)B^2]\phi(E) = \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E')\phi(E') + \frac{\chi(E)}{K_{eff}} \int_0^\infty dE' \nu \Sigma_f(E')\phi(E') \quad (59)$$

and[6]

$$D(B, E) = \frac{1}{3\gamma[B, \Sigma(E)]\Sigma(E)} \left\{ 1 + 3 \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') D(B, E') \frac{\phi(E')}{\phi(E)} \right\}, \quad (60)$$

where Σ is the total cross section, D is the leakage coefficient, ϕ is the neutron flux, Σ_{s0} and Σ_{s1} are respectively the zero and first order Legendre polynomial differential scattering cross section terms, $\chi(E)$ is the fission spectrum, K_{eff} is the effective multiplication factor, ν is the number of neutron emitted per fission, Σ_f is the fission cross section and $\gamma[B, \Sigma(E)]$ is a quantity appearing during the derivation of equations and we have[6]

$$\gamma[B, \Sigma(E)] \approx 1 + \frac{4}{15} \left(\frac{B}{\Sigma} \right)^2 - \frac{12}{175} \left(\frac{B}{\Sigma} \right)^4 + \frac{92}{2625} \left(\frac{B}{\Sigma} \right)^6 + O \left(\frac{B}{\Sigma} \right)^8. \quad (61)$$

In the B_1 equations, we could note that the neutron flux depends only on neutron energy E , because this is already an angular and volume integrated neutron flux. Therefore, the solution of those two equations is the total neutron flux in the calculation zone. Besides, in those above equations, we should note that what we will resolve is the neutron flux ϕ and the real number B^2 , but not the value B .

After introducing the B_1 equations, we could do the condensation over different energy groups. We first define G energy groups: $[E_G, E_{G-1}][E_{G-1}, E_{G-2}] \dots [E_1, E_0]$. Generally, E_G is the minimum thermal neutron energy which is considered in the calculation and E_0 is the maximum fast neutron energy which is 20MeV for most cases. In this definition, the high energy is always with lower subscript, this is because the neutron is produced with the highest energy E_0 (0 means the initial energy) and then its energy decreases with its march in the space. Therefore, with a bigger subscript, the neutron energy becomes in fact smaller. And for $g = 1, 2 \dots G$, we could define those notations as follows[6]:

$$\phi_g = \int_{E_g}^{E_{g-1}} dE \phi(E), \quad (62)$$

$$D_g(B) = \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE d(B, E) \phi(E), \quad (63)$$

$$\Sigma_g = \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma(E) \phi(E), \quad (64)$$

$$\Sigma_{s0, g \leftarrow h} = \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \int_{E_h}^{E_{h-1}} dE' \Sigma_{s0}(E \leftarrow E') \phi(E'), \quad (65)$$

$$\Sigma_{s1, g \leftarrow h} = \frac{1}{D_g \phi_g} \int_{E_g}^{E_{g-1}} dE \int_{E_h}^{E_{h-1}} dE' \Sigma_{s1}(E \leftarrow E') D(B, E) \phi(E'), \quad (66)$$

$$\chi_g = \int_{E_g}^{E_{g-1}} dE \chi(E), \quad (67)$$

$$\Sigma_{f,g} = \frac{1}{v\phi_g} \int_{E_g}^{E_{g-1}} dE v \Sigma_f(E) \phi(E) \quad (68)$$

and

$$\langle \gamma(B, \Sigma) \rangle_g = \frac{1}{D_g(B) \Sigma_g \phi_g} \int_{E_g}^{E_{g-1}} dE \gamma(B, \Sigma(E)) D(B, E) \Sigma(E) \phi(E). \quad (69)$$

If we use a large number of energy groups, we could make sure that[6]

$$\langle \gamma(B, \Sigma) \rangle_g = \gamma(B, \Sigma_g) \quad (70)$$

and finally

$$\gamma(B, \Sigma_g) = \frac{1}{D_g(B) \Sigma_g \phi_g} \int_{E_g}^{E_{g-1}} dE \gamma(B, \Sigma(E)) D(B, E) \Sigma(E) \phi(E). \quad (71)$$

After introducing all of those necessary definitions, we could integrating those B_1 equations over energy interval $[E_{g-1}, E_g]$ and obtain the condensed form:

$$\begin{aligned} [\Sigma_g + B^2 D_g] \phi_g &= \int_{E_g}^{E_{g-1}} dE \Sigma(E) \phi(E) + \int_{E_g}^{E_{g-1}} dE B^2 D(B, E) \phi(E) \\ &= \int_{E_g}^{E_{g-1}} dE [\Sigma(E) + D(B, E) B^2] \phi(E) \\ &= \int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E') \phi(E') \\ &\quad + \int_{E_g}^{E_{g-1}} dE \frac{\chi(E)}{K_{eff}} \int_0^\infty dE' v \Sigma_f(E') \phi(E') \\ &= \sum_{h=1}^G \int_{E_g}^{E_{g-1}} dE \int_{E_h}^{E_{h-1}} dE' \Sigma_{s0}(E \leftarrow E') \phi(E') \\ &\quad + \sum_{h=1}^G \int_{E_g}^{E_{g-1}} dE \frac{\chi(E)}{K_{eff}} \int_{E_h}^{E_{h-1}} dE' v \Sigma_f(E') \phi(E') \\ &= \sum_{h=1}^G \Sigma_{s0,g \leftarrow h} \phi_h + \frac{\chi_g}{K_{eff}} \sum_{h=1}^G v \phi_h \Sigma_{f,h} \end{aligned} \quad (72)$$

and now when we do the integration of equation (60), we could use directly those integrated values, so we have

$$\begin{aligned} 3D_g(B) \gamma(B, \Sigma_g) \Sigma_g \phi_g &= \int_{E_g}^{E_{g-1}} dE \gamma(B, \Sigma(E)) D(B, E) \Sigma(E) \phi(E) \\ &= \int_{E_g}^{E_{g-1}} dE \left\{ \phi(E) + 3 \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') D(B, E') \phi(E') \right\} \\ &= \int_{E_g}^{E_{g-1}} dE \phi(E) \\ &\quad + 3 \int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') D(B, E') \phi(E') \\ &= \phi_g + 3 \sum_{h=1}^G \Sigma_{s1,g \leftarrow h} D_h(B) \phi_h. \end{aligned} \quad (73)$$

For simplifying the expression and calculating $D_g(B)$, we could rewrite the second equation in the following form:

$$D_g(B)\phi_g = \frac{1}{\omega(B, \Sigma_g)} \left\{ \phi_g + 3 \sum_{h=1}^G \Sigma_{s1, g \leftarrow h} D_h \phi_h \right\}, \quad (74)$$

where $\omega(B, \Sigma_g) = 3\gamma(B, \Sigma_g)\Sigma_g$. Then all those equations for different energy groups construct two equation systems (each of which has G equations) as follows:

$$\Sigma \Phi + B^2 \mathbf{D} \Phi = \Sigma_{s0} \Phi + \frac{1}{K_{eff}} \chi \otimes (\mathbf{F} \Phi), \quad (75)$$

where

$$\Sigma = \begin{bmatrix} \Sigma_1 & 0 & \cdots & 0 \\ 0 & \Sigma_2 & \cdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & \Sigma_G \end{bmatrix}, \quad (76)$$

$$\mathbf{D} \Phi = \begin{bmatrix} D_1 \phi_1 \\ D_2 \phi_2 \\ \vdots \\ D_G \phi_G \end{bmatrix}, \quad (77)$$

$$\Sigma_{s\ell} = [\Sigma_{s\ell, g \leftarrow h}]_{1 \leq g, h \leq G} \quad \ell = 0, 1, \quad (78)$$

$$\Phi = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_G \end{bmatrix}, \quad (79)$$

$$\chi = \begin{bmatrix} \chi_1 \\ \vdots \\ \chi_G \end{bmatrix} \quad (80)$$

and

$$\mathbf{F} = [\nu \Sigma_{f,1} \cdots \nu \Sigma_{f,G}]. \quad (81)$$

and

$$\mathbf{W} \mathbf{D} \Phi = \Phi + 3 \Sigma_{s1} \mathbf{D} \Phi, \quad (82)$$

where

$$\mathbf{W} = \begin{bmatrix} \omega(B, \Sigma_1) & 0 & \cdots & 0 \\ 0 & \omega(B, \Sigma_2) & \cdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & \omega(B, \Sigma_G) \end{bmatrix}. \quad (83)$$

After obtaining those two equations, we should recall that the aim of all those operations is to calculate the neutron flux then to calculate the final contribution function. Therefore, next step is to calculate neutron flux, but before doing it, the unknown matrix $\mathbf{D}\Phi$ need to be determined firstly. From equation (82), we have

$$\begin{aligned} [\mathbf{W} - 3\Sigma_{s1}]\mathbf{D}\Phi &= \Phi \\ \mathbf{D}\Phi &= [\mathbf{W} - 3\Sigma_{s1}]^{-1}\Phi \end{aligned} \quad (84)$$

This equation holds as long as $[\mathbf{W} - 3\Sigma_{s1}]$ is invertible. For this condition, it yields for most cases because the singular matrix must satisfy $\det(\mathbf{W} - 3\Sigma_{s1}) = 0$ and this is rare in real numerical calculation.

Now, we could begin to calculate the neutron flux, from equation (84), we have the expression of $\mathbf{D}\Phi$ and we could substitute it in equation (75):

$$\Sigma\Phi + B^2[\mathbf{W} - 3\Sigma_{s1}]^{-1}\Phi = \Sigma_{s0}\Phi + \frac{1}{K_{eff}}\chi \otimes (\mathbf{F}\Phi) \quad (85)$$

In this equation, we have Φ appearing in each term which means that we need to add one constraint above the neutron flux to determine the unique and non trivial(zero) solution. This is also called normalization. This time we do the normalization as:

$$K_{eff} = \mathbf{F}\Phi. \quad (86)$$

Then we have

$$\begin{aligned} [\Sigma + B^2[\mathbf{W} - 3\Sigma_{s1}]^{-1} - \Sigma_{s0}]\Phi &= \chi, \\ \Phi &= [\Sigma + B^2[\mathbf{W} - 3\Sigma_{s1}]^{-1} - \Sigma_{s0}]^{-1}\chi. \end{aligned} \quad (87)$$

For a given B^2 , we could calculate the inverse of matrix $[\mathbf{W} - 3\Sigma_{s1}]$ and substitute it in equation (87), then we could calculate neutron flux Φ and therefore the effective multiplication factor K_{eff} with the normalization $K_{eff} = \mathbf{F}\Phi$. In effect, we have constructed a function $K_{eff} = f(B^2)$. However, it should be noted that the factor K_{eff} should be equal to 1 because in the B_1 leakage model, we add the leakage term to enforce that $K_{eff} = 1$. It isn't true for any B^2 value. Therefore, the last mission is to calculate the right leakage factor B^2 satisfying $K_{eff} = 1$. This is a root finding problem and we could use several existing algorithms to realize it. Finally, we could use the right B^2 to get the right neutron flux vector Φ .

In the above part, we have the complete derivation of B_1 leakage model. However, there is one point that should be noted: in the B_1 equations, the fission source term is expressed as $\frac{\chi(E)}{K_{eff}} \int_0^\infty dE' \nu \Sigma_f(E') \phi(E')$ which means that there is only one $\nu \Sigma_f(E')$ and one fission spectrum $\chi(E)$. This depends on the nuclear data in the calculation. Sometimes in the data base, there is only one total fission macroscopic cross section and one average fission spectrum for all fissile nuclides. Therefore, we could apply the previous method in this case. But sometimes in the data base, there is one fission spectrum for each fissile isotope

so we can't apply the previous method. And we will modify the derivation to realize the neutron flux calculation. Sometimes there are both two kinds of data in the data base, the method will be chosen according to its resolution complexity. This will be discussed after the derivation.

Firstly, we consider the multiple fissile isotopes with different fission spectrum and we could therefore write the following B_1 equations[6]:

$$\begin{aligned} [\Sigma(E) + D(B, E)B^2]\phi(E) &= \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E')\phi(E') \\ &+ \frac{1}{K_{eff}} \sum_{i=1}^{N_{fissile}} \chi_i(E) \int_0^\infty dE' \nu \Sigma_{f,i}(E')\phi(E') \end{aligned} \quad (88)$$

where $N_{fissile}$ is the number of fissile isotopes, χ_i is the fission spectrum for the fissile isotope i and $\Sigma_{f,i}$ is the macroscopic fission cross section for isotope i . For another equation, the multiple fission spectrum won't change it, so we don't need to list it there. Now we could write down the multi-group energy form of the above equation:

$$[\Sigma_g + B^2 D_g]\phi_g = \sum_{h=1}^G \Sigma_{s0,g \leftarrow h} \phi_h + \frac{1}{K_{eff}} \sum_{i=1}^{N_{fissile}} \chi_{i,g} \sum_{h=1}^G \nu \phi_h \Sigma_{f,i,h} \quad (89)$$

with new definition

$$\chi_{i,g} = \int_{E_g}^{E_{g-1}} dE \chi_i(E), \quad (90)$$

and

$$\Sigma_{f,i,g} = \frac{1}{\nu \phi_g} \int_{E_g}^{E_{g-1}} dE \nu \Sigma_{f,i}(E) \phi(E). \quad (91)$$

The next step is to write the matrix form of this equation. This time the term of fission reaction source won't use the outer product and the new form is

$$\Sigma \Phi + B^2 \mathbf{D} \Phi = \Sigma_{s0} \Phi + \frac{1}{K_{eff}} \chi \mathbf{F} \Phi, \quad (92)$$

where the new definitions about those fission relevant quantities are

$$\chi = \begin{bmatrix} \chi_{1,1} & \chi_{2,1} & \cdots & \chi_{N_{fissile},1} \\ \chi_{1,2} & \chi_{2,2} & \cdots & \chi_{N_{fissile},2} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_{1,G} & \chi_{2,G} & \cdots & \chi_{N_{fissile},G} \end{bmatrix}, \quad (93)$$

and

$$\mathbf{F} = \begin{bmatrix} \nu \Sigma_{f,1,1} & \nu \Sigma_{f,1,2} & \cdots & \nu \Sigma_{f,1,G} \\ \nu \Sigma_{f,2,1} & \nu \Sigma_{f,2,2} & \cdots & \nu \Sigma_{f,2,G} \\ \vdots & \vdots & \ddots & \vdots \\ \nu \Sigma_{f,N_{fissile},1} & \nu \Sigma_{f,N_{fissile},2} & \cdots & \nu \Sigma_{f,N_{fissile},G} \end{bmatrix}. \quad (94)$$

This time, after doing the same operation in equation (82) to get the expression of $\mathbf{D}\Phi$ and substitute it into equation (92), we have

$$[\Sigma + B^2[\mathbf{W} - 3\Sigma_{s1}]^{-1} - \Sigma_{s0}]\Phi = \frac{1}{K_{eff}}\chi\mathbf{F}\Phi \quad (95)$$

This time we could no longer eliminate the $\mathbf{F}\Phi$ term by simply doing the normalization of neutron flux because the product of \mathbf{F} and Φ is not a scalar number but a matrix. Therefore, we will present new method for solving this equation.

Firstly, we suppose $\mathbf{R}(B^2) = \Sigma + B^2[\mathbf{W} - 3\Sigma_{s1}]^{-1} - \Sigma_{s0}$ so that we could simplify the equation like

$$\mathbf{R}\Phi = \frac{1}{K_{eff}}\chi\mathbf{F}\Phi. \quad (96)$$

Then we have

$$K_{eff}\Phi = \mathbf{R}^{-1}\chi\mathbf{F}\Phi. \quad (97)$$

For changing the form and also the dimension of this equation system, we multiply \mathbf{F} for each side and suppose $\xi = \mathbf{F}\Phi$ so we have

$$K_{eff}\xi = \mathbf{M}\xi, \quad (98)$$

where $\mathbf{M} = \mathbf{F}\mathbf{R}^{-1}\chi$. This time we will have an eigenvalue equation system with N_{fisile} equations. Solving for the eigenvalues and eigenvectors of matrix \mathbf{M} , we could obtain those eigenvalues of equation (97) but not the eigenvectors Φ . Because now we actually resolve for $\mathbf{F}\Phi$. Moreover, the matrix \mathbf{F} is not square which means that there is no inverse of \mathbf{F} to calculate. So we construct a new equation which is very similar to equation (98) as follow:

$$\mathbf{M}\zeta = \zeta\mathbf{K}, \quad (99)$$

where

$$\mathbf{K} = \begin{bmatrix} k_1 & 0 & \cdots & 0 \\ 0 & k_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & k_{N_{fisile}} \end{bmatrix}, \quad (100)$$

$$\zeta = [\xi_1 \cdots \xi_{N_{fisile}}], \quad (101)$$

and $(k_i)_{i=1,2,\dots,N_{fisile}}, (\xi_i)_{i=1,2,\dots,N_{fisile}}$ are respectively the eigenvalues and eigenvectors of matrix \mathbf{M} .

Finally we have

$$\mathbf{F}\Phi = \zeta = \mathbf{M}\zeta\mathbf{K}^{-1} = \mathbf{F}\mathbf{R}^{-1}\chi\zeta\mathbf{K}^{-1}, \quad (102)$$

For any given matrix \mathbf{F} , the above equation is always valid, which means that we have the result below:

$$\Phi = \mathbf{R}^{-1}\chi\zeta\mathbf{K}^{-1}, \quad (103)$$

Now we have a list of eigenvalues K_{eff} and corresponding eigenvectors Φ and the real unique solution pair is the one with the biggest eigenvalues K_{eff} and only this solution pair will have all positive neutron flux components because this is the fundamental solution.

In this part, we propose two methods for solving the B1 leakage model. The choice of method depends not only the reaction data, but also the number of energy groups used. In the first method, the number of equations to be solved is the number of energy groups; but for the second method, after doing several operations, the number of equations in the final system is the number of fissile isotopes. For example, if we have two energy groups and 19 fissile isotopes in our calculation, we will prefer using the first method, but if we have 281 energy groups and only 19 fissile isotopes, the second method could then save much more time in the calculation. Therefore, we should consider both factors to make a good choice for the calculation.

4.2 Improvements about depletion chains simplification method

In previous chapter, we present the depletion chains simplification method proposed by Go Chiba. However, in our work, we can't apply exactly this method. This is because for calculating the neutron flux, we use the B_1 leakage model. But if we use this model, it will be very complex to calculate the adjoint neutron flux because there will be one more unknown quantity: the leakage constant B^2 and this problem will become an eigenvalue problem with source term. Therefore, we must find a solution which could get the final expression of contribution function without solving adjoint neutron transport equation.

As we mentioned several times in previous derivation, the key idea in this method is the linearization of burnup matrix, so that we could find a relation between the variation of burnup matrix $\Delta \mathbf{M}^i$ and the initial perturbation $\Delta \mathbf{N}(t_i)$ and replace $\Delta \mathbf{M}^i$ by an expression containing explicitly the term $\Delta \mathbf{N}(t_i)$ in equation (45). But before finding this, we must recall that the initial perturbation $\Delta \mathbf{N}(t_i)$ will directly influence the transport operator B in the neutron transport equation, so that the neutron flux will be changed, then the changed neutron flux will modify directly the burnup matrix. Therefore, the first step is to write explicitly the relation between the variation of burnup matrix \mathbf{M} and that for the neutron flux vector Φ . In the B_1 leakage model, only the volume-integrated multi-group neutron flux is calculated and we divide it by the whole calculation volume to get the average neutron flux, therefore, we could get a simplified expression of equation (46):

$$\Delta \mathbf{M}^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \Delta \phi_g^i, \quad (104)$$

where ϕ_g^i is the neutron flux of the g - th energy group and there are in total N_G energy groups in the neutron flux calculation. Because of the linearization, from equation (8) we could write the expression of $\frac{\partial \mathbf{M}^i}{\partial \phi_g^i}$ easily: we just pick out all the flux independent terms from $\frac{dN_k}{dt}$ and then the partial derivation to ϕ_g^i is to only take the g - th energy group contribution without neutron flux. Now, as we said before, the variation of neutron flux comes directly from the perturbation of $\mathbf{N}(t_i)$, therefore, we have:

$$\Delta \mathbf{M}^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \Delta \phi_g^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \frac{d\phi_g^i}{d\mathbf{N}^iT} \Delta \mathbf{N}^i \quad (105)$$

Finally, we could rewrite equation(45) as

$$\begin{aligned}
\Delta N_l(t_{i+1}) &= \mathbf{N}^{*T}(t_i) \Delta \mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t) \Delta \mathbf{M}^i \mathbf{N}(t) dt \\
&= \mathbf{N}^{*T}(t_i) \Delta \mathbf{N}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t) \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \mathbf{N}(t) dt \cdot \Delta \phi_g^i \\
&= \mathbf{N}^{*T}(t_i) \Delta \mathbf{N}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t) \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \mathbf{N}(t) dt \cdot \frac{d\phi_g^i}{d\mathbf{N}^{iT}} \Delta \mathbf{N}^i \\
&= \left(\mathbf{N}^{*T}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t) \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \mathbf{N}(t) dt \cdot \frac{d\phi_g^i}{d\mathbf{N}^{iT}} \right) \Delta \mathbf{N}^i \\
&= \widehat{\mathbf{N}}^{*T}(t_i) \Delta \mathbf{N}(t_i) = \sum_k \widehat{N}_k^*(t_i) \Delta N_k(t_i),
\end{aligned} \tag{106}$$

where $\widehat{\mathbf{N}}^{*T}(t_i) = \mathbf{N}^{*T}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t) \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \mathbf{N}(t) dt \cdot \frac{d\phi_g^i}{d\mathbf{N}^{iT}}$. Now, we use another method to get the same final expression and the expression of contribution function is the same. This is the modification in our work to avoid solving adjoint neutron flux equation and now the only rested thing is to calculate the derivation of multi-group neutron flux to the NND vector. In fact, there are two choice. Firstly, we could do the analytical derivation and calculation according to the B_1 leakage equation which will be presented later. However, in our work, we didn't have enough time to do this part of implementation. Therefore, we applied another method: estimating it by the incremental ratio

$$\begin{aligned}
\frac{d\phi_g^i}{d\mathbf{N}^{iT}} &= \left[\frac{\partial \phi_g^i}{\partial N_1^i}, \frac{\partial \phi_g^i}{\partial N_2^i}, \dots, \frac{\partial \phi_g^i}{\partial N_n^i} \right], \\
\frac{\partial \phi_g^i}{\partial N_k^i} &= \lim_{\epsilon \rightarrow 0} \frac{\phi_g^i(N_k(t_i) + \epsilon N_k(t_i)) - \phi_g^i(N_k(t_i))}{\epsilon N_k(t_i)} \quad \text{for } k \in [1, n],
\end{aligned} \tag{107}$$

where n is the number of isotopes in the calculation. As long as we set a small enough ϵ , we could get the approximated value of $\frac{\partial \phi_g^i}{\partial N_k^i}$ and then we could construct the contribution function.

Until now, all the derivation is done in time interval $[t_i, t_{i+1}]$ and we have the linearization assumption if the time interval is small enough. However, if we want to calculate a long-term influence of perturbation, in the whole calculation the burnup matrix \mathbf{M} could no longer be regarded as a constant matrix. Therefore, we need to extend this derivation to any time step case and redefine the contribution function for each time point.

For this case, we have two calculation methods and the difference is the choice of final adjoint condition for resolving adjoint Bateman equations in each time step. For the first one, in each time step $[t_i, t_{i+1}] \in [t_{\text{initial}}, t_{\text{initial}+1}, \dots, t_{\text{final}}]$, we could do the same calculation with the initial perturbation $\Delta \mathbf{N}(t_i)$ and we conserve the same final condition which is $\mathbf{N}(t_{i+1}) = \mathbf{e}_l$. Like this, in each time step $[t_i, t_{i+1}]$, we have $\Delta N_l(t_{i+1}) = \widehat{\mathbf{N}}^{*T}(t_i) \Delta \mathbf{N}(t_i)$, and we keep the same definition of contribution function just like the sensitivity calculation. So we could get a contribution function at each time point and this contribution

show the importance of other nuclides to the target nuclide in each time interval $[t_i, t_{i+1}]$. This is a local value and it's just like the derivation of function which only concentrates on the local variation of values.

For the second method, we conserve the final target nuclide perturbation. For the last time step $[t_{final-1}, t_{final}]$, we apply the above derivation and we have $\Delta N_l(t_{final}) = \widehat{\mathbf{N}}^{*T}(final - 1)\Delta\mathbf{N}(final - 1)$. For all other time steps, we will change the final adjoint condition of adjoint Bateman equations to $N^\dagger(t_{[i+1]}) = \widehat{\mathbf{N}}^*(t_{i+1})$ which is the corrected adjoint nuclide number density (ANND) calculated at time interval $[t_{i+1}, t_{i+2}]$. After resetting the final equation, from equation (43) we could have

$$\begin{aligned}\widehat{\mathbf{N}}^*(t_{i+1})\Delta\mathbf{N}(t_{i+1}) &= \mathbf{N}^{*T}(t_i)\Delta\mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\Delta\mathbf{M}^i\mathbf{N}(t)dt \\ &= \widehat{\mathbf{N}}^{*T}(t_i)\Delta\mathbf{N}(t_i).\end{aligned}\tag{108}$$

The above equation means that for the perturbation $\Delta\mathbf{N}(t_{i+1})$, if this variation is induced by the variation from last time step, then we could get a conservation relation by resetting the final adjoint condition. Combining the expression for last time step, we have

$$N_l(t_{final}) = \widehat{\mathbf{N}}^{*T}(t_i)\Delta\mathbf{N}(t_i), \quad \text{for } t_i \in [t_{initial}, t_{final-1}].\tag{109}$$

From the above method, we could also calculate a contribution function. but this time the contribution function just describe the relation between the perturbation introduced at time t_i and the resulted variation of target nuclide at t_{final} . Therefore, we need to change the definition of contribution function to maintain the principal of relative variation ratio:

$$CF_k(t_i) = \frac{\widehat{N}_k^*(t_i)N_k(t_i)}{N_l(t_{final})}\tag{110}$$

This method could is like the integration: we just care about the global influence between t_i and t_{final} and this method will not show the local importance variation with time. For those two multiple time steps methods, each of them has its own advantages and disadvantages and we will do the detailed analysis in the result analysis chapter.

5. Result Analysis

In previous chapters, we present the depletion chains simplification method and its improvements and in this chapter we will present its application and the result. We apply it to a simple but important case: the depletion of ^{135}Xe . The main reason for choosing this isotope is its importance to the reactor reactivity control: ^{135}Xe is nearly the strongest thermo-neutron absorbant isotope and its neutron absorption cross section could reach the order of 10^6 b in thermal region (for example, one resonance at $E \approx 0.08\text{eV}$)[30]. Therefore, its concentration in reactor is of importance to reactor control and it's important to study the depletion chain of ^{135}Xe . Besides, the depletion chain of ^{135}Xe is already well-known in theoretical study: the depletion chain of ^{135}Xe is very simple which only contains 2 isotopes before ^{135}Xe : ^{135}Te and ^{135}I , moreover, the half-life of ^{135}Te (2 min) is too short compared to that of ^{135}I (6.7h) and ^{135}Xe (9.2h), we could neglect it in the analysis and add its contribution directly to the production of ^{135}I . Therefore, it's really a good beginning to validate the depletion chains simplification method on this case.

After determining the target nuclide, we calculate respectively the contribution function under steady and transient states. According to the values of those contribution functions, we could finally select important isotopes and verify if they are those elements appearing in the depletion chain of ^{135}Xe . In this chapter, we will present the calculation result of test and give detailed analysis about the evolution of contribution function with time.

5.1 System Evolution Analysis

Before showing the calculation result, the first thing in our work is to determine the physical state of the nuclear data. All the nuclear data in our work comes from the MPO file. The MPO file is the standard output file of APOLLO, which is the famous reactor calculation program. In the MPO file, there are 105 state points corresponding 5 parameters: Time(s), Burnup(MWd/t_{HM}), Effective temperature of fuel(K), Moderator temperature(K) and Linear power(W/cm). The simulation is realized under full power level which is a constant. Therefore, there is a linear relationship between time and burnup. Besides, there is also a relation between effective temperature of fuel and linear power which is not linear[24]. Now we list the possible values for those parameters(for time and burnup, we only need to show one, there we choose to list the values of burnup): From the table, we know that there are 21 burnup points and the simulation is realized under full power level. But there are in total 105 state points. This is because for each burnup point, we have 5 linear power values. For each burnup point, when the system arrives at this burnup state under full power level, the linear power decreased to other values, then the data is saved in the MPO file. The reason of doing like this is to output the correct multi-group cross section data. As we know, there are many factors influencing the nuclear reaction cross section, for example: the Doppler

Parameter Name	Values
Burnup(MWd/t_{HM})	0.0, 10, 20, 40, 70, 100, 200, 300, 400, 500, 750, 10^3 , $2 \cdot 10^3$, $3 \cdot 10^3$, $4 \cdot 10^3$, $5 \cdot 10^3$, $6 \cdot 10^3$, $7 \cdot 10^3$, $8 \cdot 10^3$, $9 \cdot 10^3$, 10^4
Effective temperature of fuel(K)	582, 677, 777, 887, 1009
Moderator temperature(K)	582
Linear power(W/cm)	0.0 , 44.5, 89 , 133.5, 178

Table 1: The list of values for different parameters

effect which is a temperature factor. If the reactor power changes, the cross section of some isotopes will have obvious variation like the absorption cross section of U238. Therefore, for realizing our calculation under different operation conditions, the cross section data should be evaluated under each different power level. Therefore, we have 105 state points but not 21. From the correspondence between time and burnup values, we could know the conversion factor between those two parameters which is the quantity called 'power density'. And this is what we could calculate using the data in MPO for different power levels. The result of calculation shows that the correct power density value is that for full power level which checks our previous statement.

For further checking the correct physical state of data, we realize a series of tests. Firstly, we plot the nuclides concentration evolution with burnup under full power level. However, it should be noted that there are about 200 nuclides in the MPO files so we can't plot the concentrations of all of them. Therefore, we choose those important nuclides to our work, in the following work, we will study the depletion chain of ^{135}Xe , therefore, we could choose ^{135}Xe , ^{135}I , also we can choose U235 or U238, but the concentration of U235 or U238 won't change much during the whole burnup process, therefore we just choose to plot the evolution for ^{135}Xe and ^{135}I .

As shown in figure 1, at initial burnup, the concentration of ^{135}Xe (9.2h) and ^{135}I (6.7h) increases from 0, which indicates that this is the burnup of a new fuel rod. Then it reaches an equilibrium rapidly and this corresponds well to our theory, the half life of ^{135}Xe and ^{135}I are not very long. Therefore, after the burnup of $70MWd/t_{HM}$, it nearly reaches the equilibrium and this just corresponds a period less than two days. After this transient, the concentration for ^{135}Xe and ^{135}I are in a relative stable state and their concentrations change slowly with the burnup. In fact, we also check that for each nuclide, its concentrations are the same under different power levels at each burnup point. Therefore, if we plot the burnup evolution of ^{135}Xe and ^{135}I under different power levels, we will see only one line for each nuclide because they are covered. Besides, we have the theoretical equilibrium concentration of ^{135}Xe and ^{135}I as

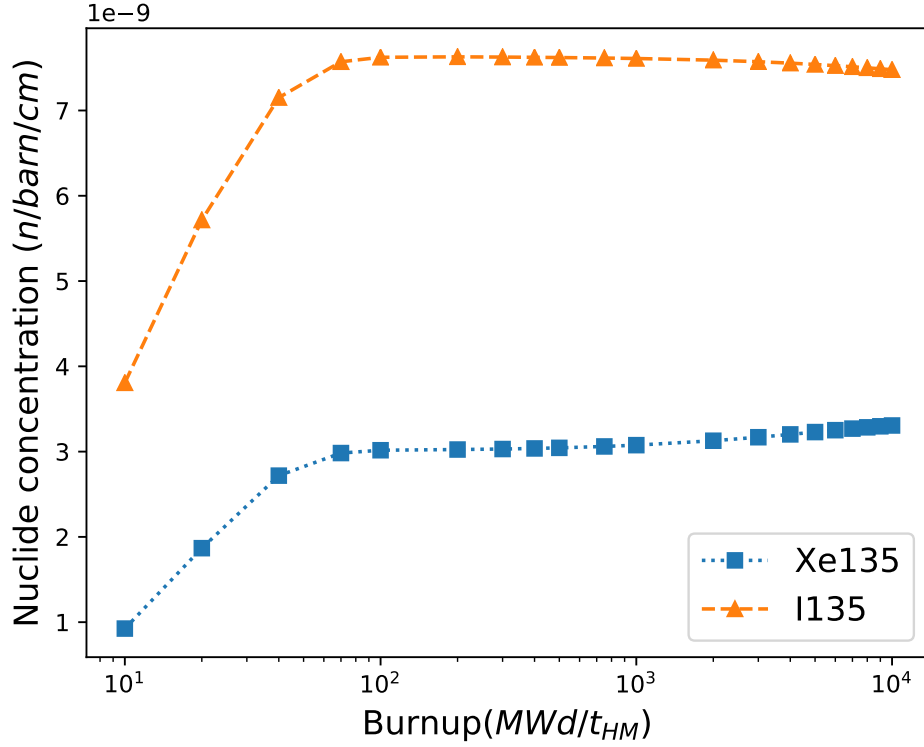


Figure 1: Burnup evolution of ¹³⁵Xe and ¹³⁵I

follow[30]:

$$I_{eq} = \frac{\gamma_I \Sigma_f \Phi}{\lambda_I} \quad (111)$$

$$Xe_{eq} = \frac{\lambda_I I_{eq} + \gamma_{Xe} \Sigma_f \Phi}{\lambda_{Xe} + \Sigma_{Xe,a} \Phi} = \frac{(\gamma_I + \gamma_{Xe}) \Sigma_f \Phi}{\lambda_{Xe} + \Sigma_{Xe,a} \Phi}, \quad (112)$$

where γ_I and γ_{Xe} are the fission yields for ¹³⁵I and ¹³⁵Xe, Σ_f are the total fission reaction, Φ is the neutron flux at equilibrium state, λ_I and λ_{Xe} are decay constants of ¹³⁵I and ¹³⁵Xe and $\Sigma_{Xe,a}$ is the microscopic absorption cross section for ¹³⁵Xe. Besides, there isn't the microscopic absorption cross section of ¹³⁵I because it's just in the order of 10 barn and it's neglected in the calculation. From the above equation, we could see that the equilibrium concentrations of ¹³⁵Xe and ¹³⁵I depend on the neutron flux, if the power is higher, the neutron flux will also be higher causing the increase of ¹³⁵Xe and ¹³⁵I concentrations. Therefore, in the figure, what we obtain is only the equilibrium state for full power level. For other power level, the initial concentrations are not the equilibrium ones. For checking this, we choose a burnup value arbitrarily and plot the ¹³⁵I and ¹³⁵Xe concentration evolution during 48 hours under five power levels and we get figure 2 and figure 3. In figure 2 and figure 3, we could see that there is a horizontal line which means it is the equilibrium state, we could read from the figure that the stable state corresponds to the full power level: $P_{lin} = 178W/cm$. For other linear power values, the ¹³⁵Xe and ¹³⁵I concentrations decrease

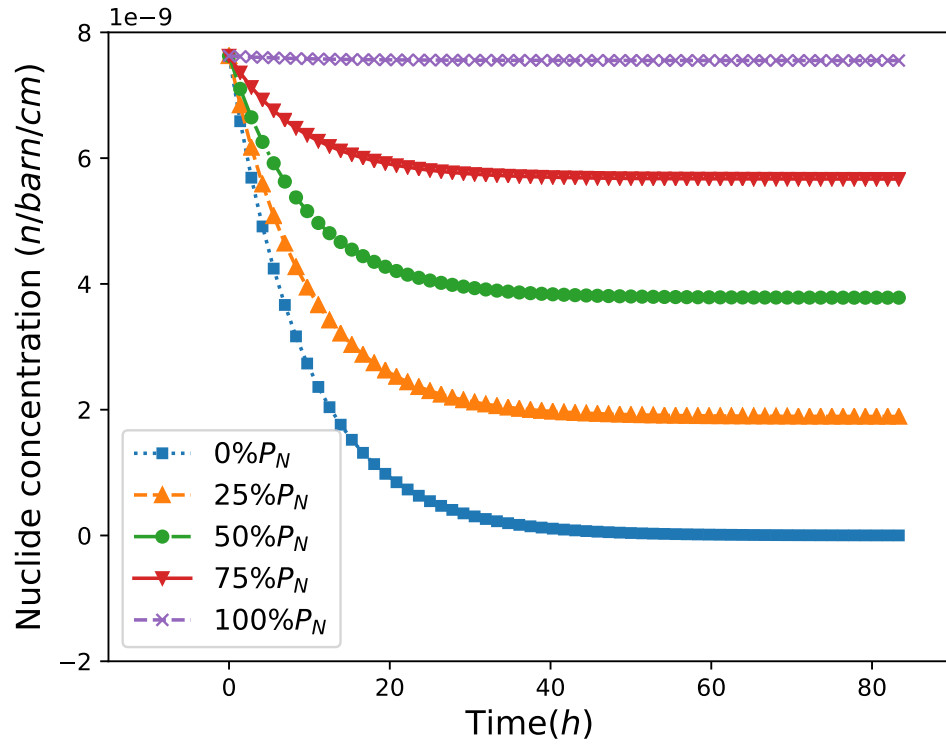


Figure 2: Time evolution of ^{135}I for Burnup= 300.0MWd/ t_{HM}

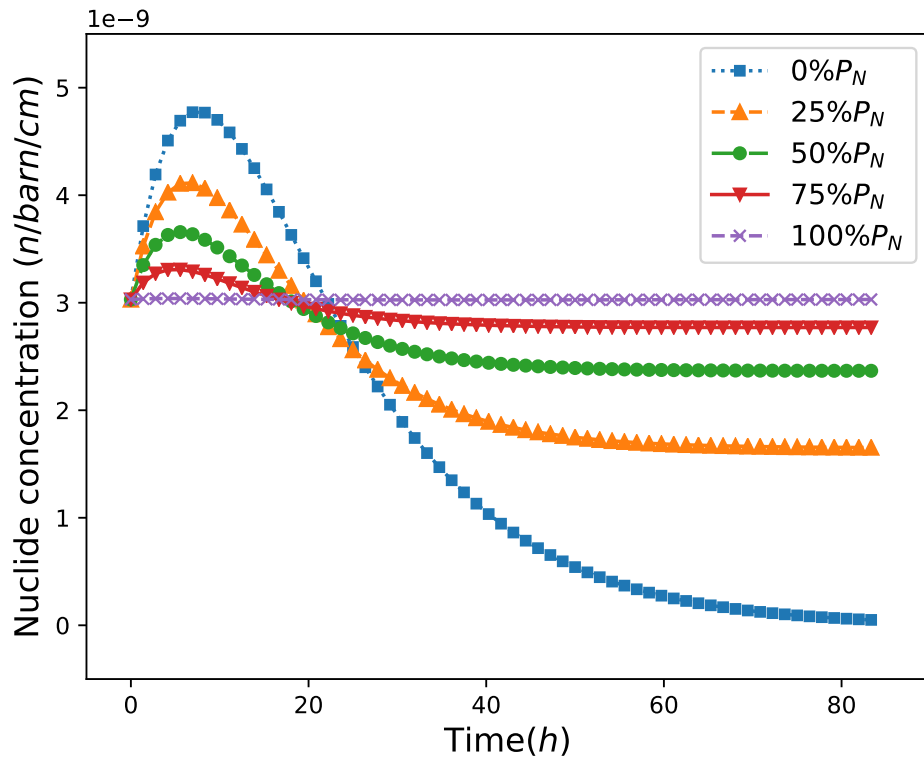


Figure 3: Time evolution of ^{135}Xe for Burnup= 300.0MWd/ t_{HM}

and they correspond to the decrease of neutron flux. Therefore, we check with success the conclusion: the simulation is done under full power level with the burnup evolution. And 21 burnup points are selected on which the power level is changed and then the result is written in the MPO file.

There is another point which should be declared. In previous part, we present the B_1 leakage model which is used to calculate the neutron flux and we implement this part of code and add it to the whole program for solving Bateman equations. However, there is a hypothesis for yielding equation(70): there should be a large number of energy groups in the simulation. However, in our simulation, because of the limitation of nuclear data (the MPO) file, we only have two energy groups and this causes an abnormally high fast neutron flux. For resolving this problem, we set $B^2 = 0$ and therefore we could no longer grantee $K_{eff} = 1$ but $K_{eff} = kinf = constant$ (There is no leakage, so the two multiplication factors are equal).

After determining the operation condition of those state points, for checking further more the physical situation of those state points and also for validating our code if it could resolve correctly the Bateman equations, we realized a series of tests: by changing the power level abruptly, we observe the evolution of ^{135}Xe and ^{135}I concentrations and check if the variation of concentrations is the same as we expect.

Firstly, we realize an abrupt power change from full power (generally we note it P_N and $P_N = 178. W/cm$ for the linear power) to a lower level, and we will see the change of ^{135}Xe and ^{135}I concentrations. From

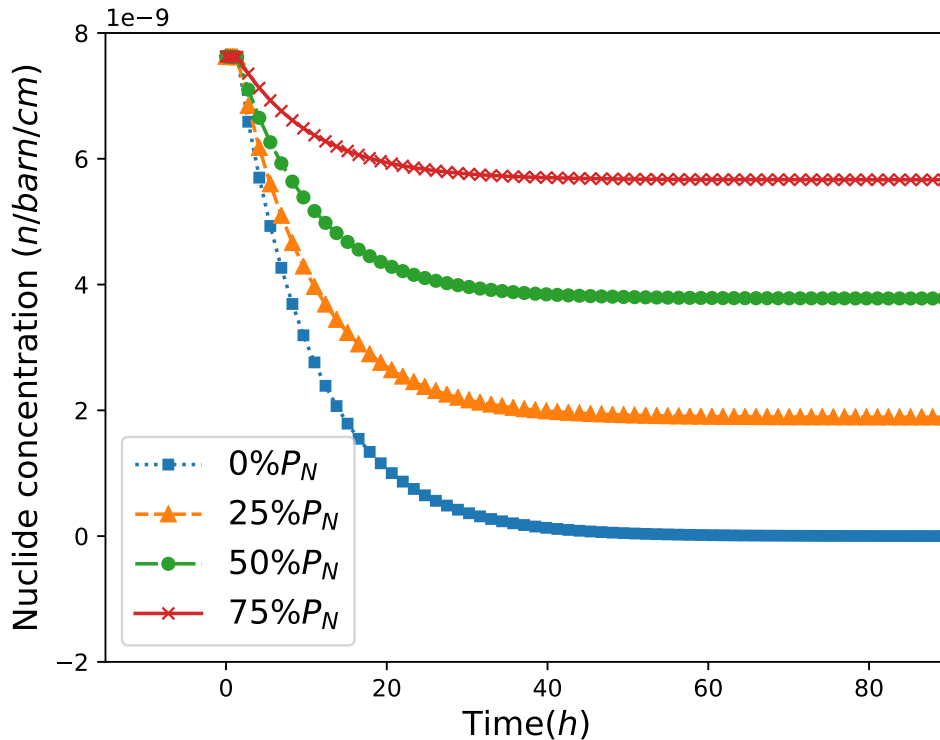


Figure 4: Time evolution of ^{135}I from full power level to a lower power level for Burnup= $300.0 MWd/t_{HM}$

those figures, we could see that the concentrations of ^{135}Xe and ^{135}I both decrease with the decrease

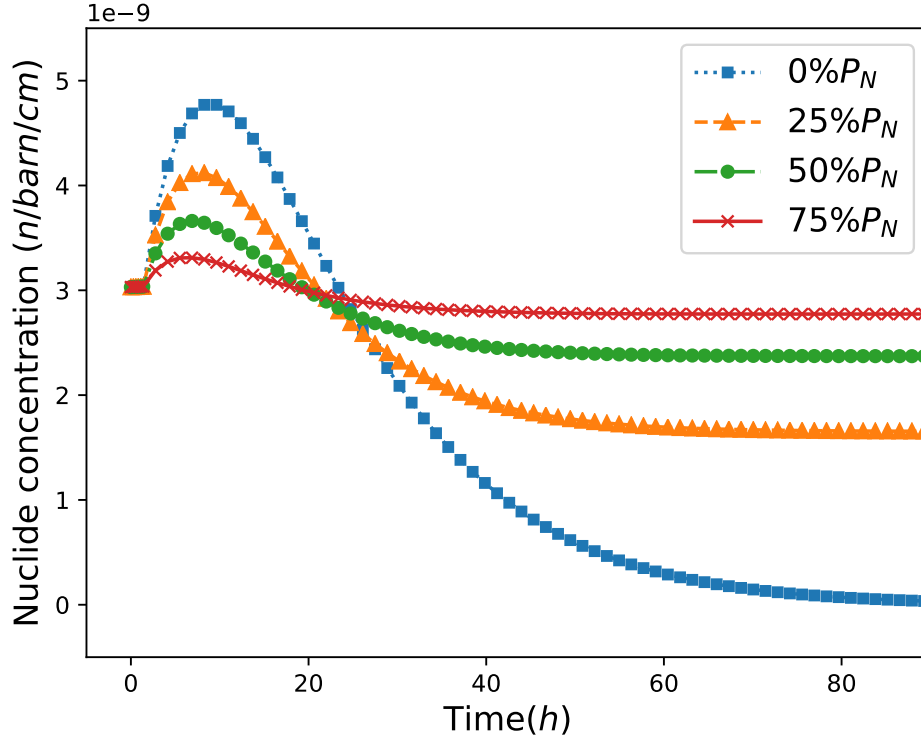


Figure 5: Time evolution of ^{135}Xe from full power level to a lower power level for Burnup= $300.0\text{MWd}/t_{HM}$

of power. For ^{135}I , the decrease of its concentration is proportional to the power level change which is consistent with the formula in equation (111). For ^{135}Xe , its variation is also correct, when the power decrease, the production of ^{135}Xe from decay will not change instantaneously. But the production and consumption of ^{135}Xe from nuclear reaction will be much influenced, specially for the absorption of ^{135}Xe because the absorption cross section of ^{135}Xe is really huge. Therefore, in the transient period, we could observe the temporary increase of ^{135}Xe concentration until it reaches the Xe peak, at which point the variation of nuclear reaction rates is balanced by the decay rates. Then Xe concentration will decrease to its equilibrium concentration. We could also notice that the change of equilibrium ^{135}Xe concentration is not proportional to that of linear power and we could get it from equation (112): there are neutron flux terms in both the numerator and denominator, when the power decreases, the variation of numerator is linear to the power change, but the denominator just decreased, therefore, the change of ^{135}Xe concentration is less violent, but finally it will reach 0 with zero power level. Therefore, we could observe such variation in figure 5. Besides, we could compare figure 4 and 5 with figure 2 and figure 3 and we find that the variation is the same. In fact, for the 0 – th value in the list of linear power, it's a relative small value (order of 10^7 compared to 10^{14}) but in our test the power is set to 0. Therefore there is a little difference in the figure but we can't see it from the figures. Nevertheless, we could still further conform our conclusion about the operation conditions for different state points: it is the burnup under full power level and then the result is

written just after the change of power level which is exactly we test in figure 4 and 5.

Next, we test a power level change from $100\%P_N$ to $0\%P_N$ for different burnup states and we get figure 6. From this figure, we could see that the evolutions for different burnup points don't have much difference. For each chosen point, it's already in steady state and the initial concentrations of ^{135}Xe and ^{135}I don't have much difference. With the increase of burnup, the ^{135}Xe concentration will increase a little, so when the power changes, the Xe concentration for higher burnup is also just a little higher than that of smaller burnup. But the evolution tendency is always the same. For ^{135}I concentration, it is nearly the same thing and the only difference is that the concentration of ^{135}I will decrease a little with the increase of burnup.

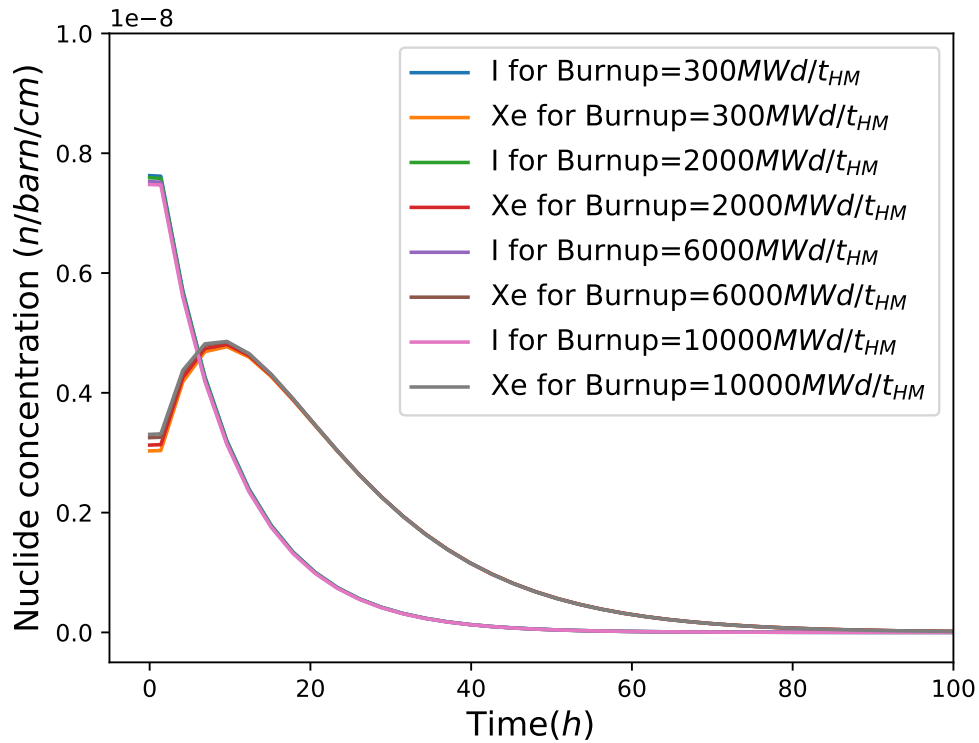


Figure 6: Time evolution of ^{135}I and ^{135}Xe from $100\%P_N$ to $0\%P_N$ for different burnup points

Then, we test the instantaneous power increase from different initial power level to full power and we get figure 7 and figure 8. As we know, the burnup evolution is realized under full power level, the system is not in steady-state for other power levels. Therefore, we need to let the system evolve until it reaches its steady-state. After that, we could give the system a power change and observe the concentration evolution of ^{135}I and ^{135}Xe . From figure 7, we could see that the equilibrium ^{135}I concentration is proportional to power level and when power raises, the ^{135}I concentration will increase in an exponential form. Finally, for all initial states, they all reach the same concentration level. And for ^{135}Xe , the equilibrium concentration is not evenly distributed which is consistent with figure 3. When power increase, the ^{135}Xe concentration

will firstly decreases because of the perturbed balance between disappearance and production. After reaching the Xe (negative) peak, the ^{135}Xe concentration will increase until reaching its final stable level.

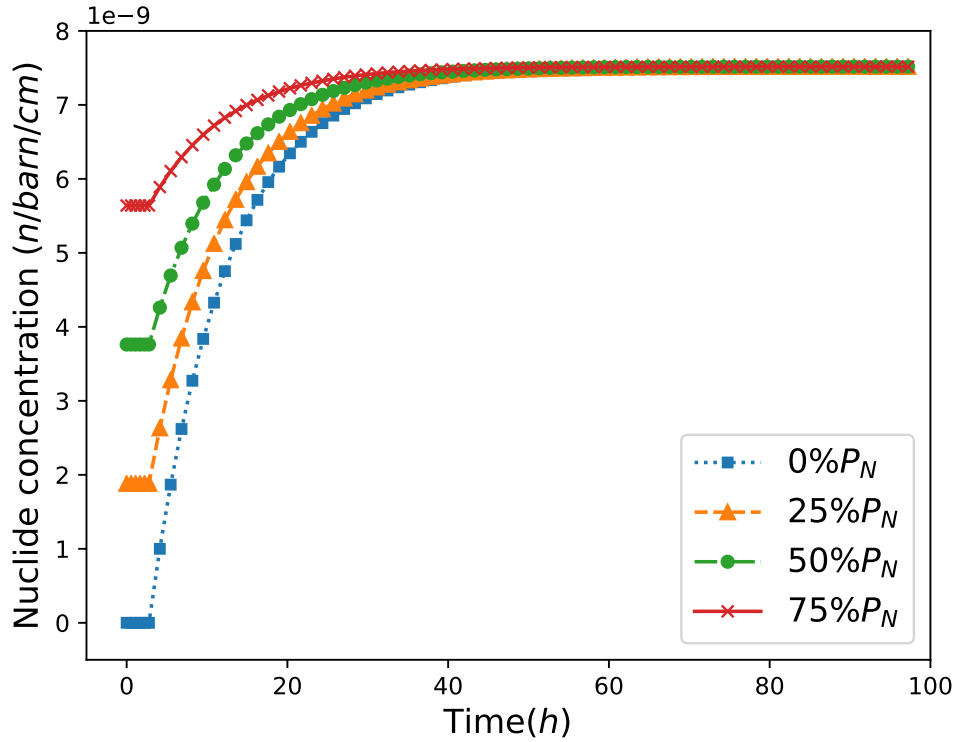


Figure 7: Time evolution of ^{135}I from lower power level to full power level for Burnup= $2000\text{MWd}/t_{HM}$

The last test for the time revolution is to decrease the linear power from different power levels to zero power and observe the time revolution of ^{135}Xe and ^{135}I 's concentrations. After the simulation, we get figure 9 and figure 10. And their variation is also as what we expect: for ^{135}I , its concentration decreases in a exponential form to get close to zero and for ^{135}Xe , it will firstly reach the Xe peak and then decrease to zero.

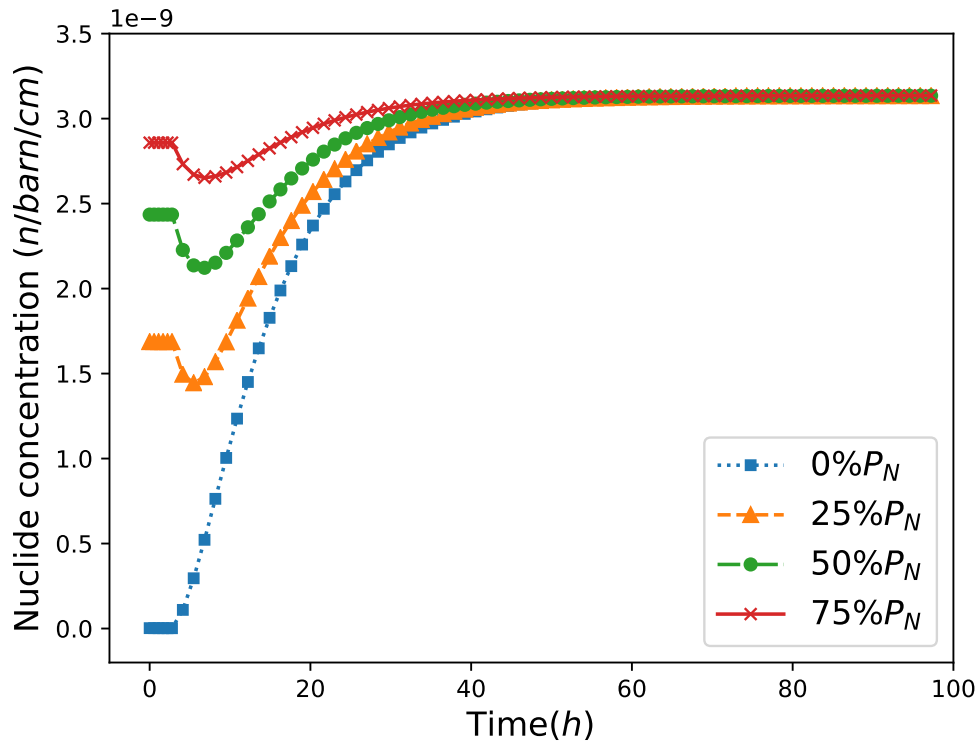


Figure 8: Time evolution of ^{135}Xe from lower power level to full power level for Burnup= $2000\text{MWd}/t_{HM}$

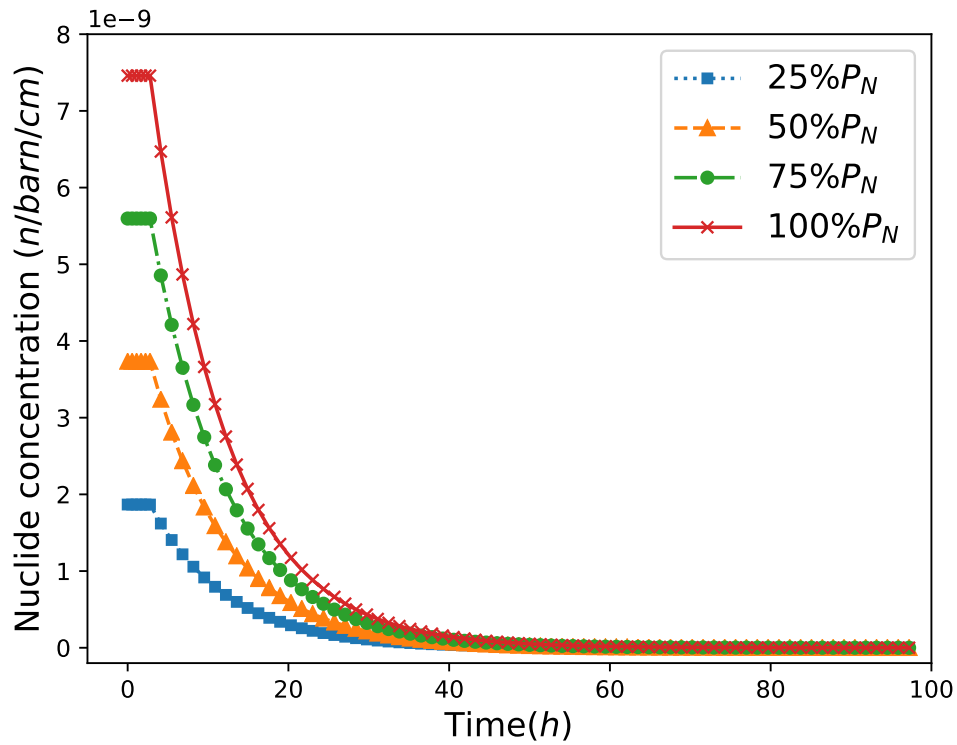


Figure 9: Time evolution of ^{135}I from different power levels to zero power level for Burnup= $6000\text{MWd}/t_{HM}$

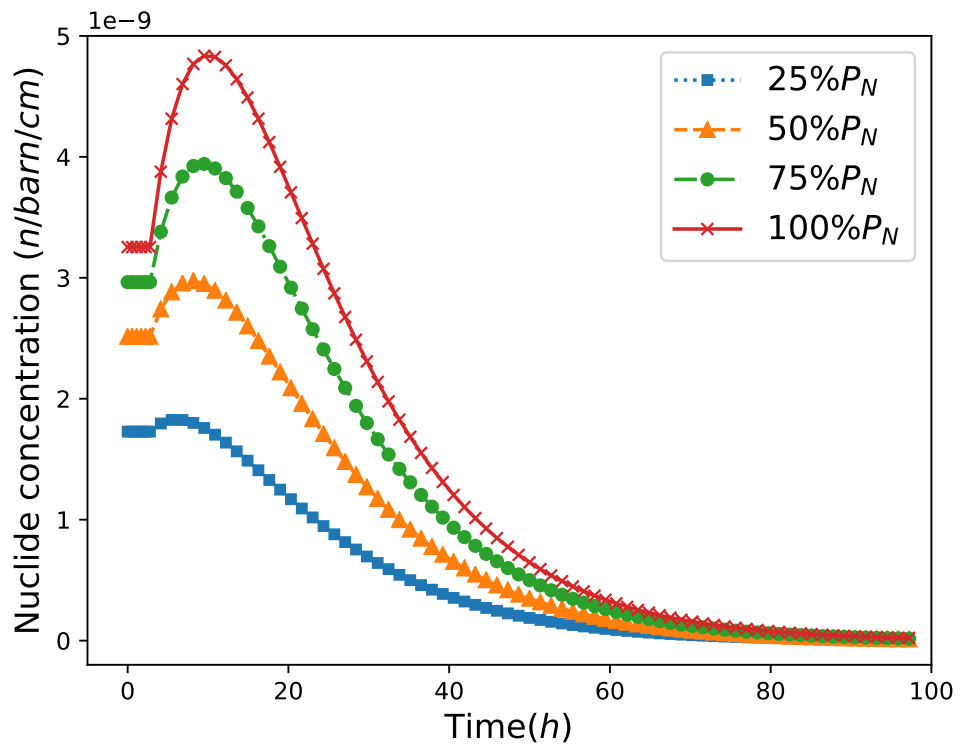


Figure 10: Time evolution of ^{135}Xe from different power levels to zero power level for Burnup= $6000\text{MWd}/t_{HM}$

5.2 Contribution Function Analysis

In this part, we will present the result of calculating the contribution functions. As we present before, two methods will be applied to calculate the contribution functions in a given time interval: the first one conserves the final ^{135}Xe perturbation and the second one conserves the final adjoint condition in each calculation time interval. Now we will analysis the differences between those two methods.

2-a Steady state simulation

Firstly, we choose arbitrarily a state point for which those state parameters are: $\text{Burnup} = 500 \text{ MWd}/t_{HM}$, $T_{eff} = 1009 \text{ K}$, $T_{mod} = 582 \text{ K}$ and $P_{lin} = 178 \text{ W/cm}$. The linear power is at full power level, so the initial state is already steady state. The first test is realized under steady state. Therefore, we resolve the direct and adjoint Bateman equations in the time interval $[0 \text{ s}, 2.5 \cdot 10^5 \text{ s}]$ which is nearly 69.5 hours. We know that in both two contribution functions method, the complete time interval needs to be divided into several parts and we will calculate the contribution function in each time interval. Therefore, we need to choose several intermediate time points. For the first test, those points are given by the Bateman solver: in our code, after constructing the burnup matrix, we will resolve this ordinary differential equation system with implicit Runge-Kutta method. After solving the equations, the solver will output several time points and the corresponding NND vector at each time point. And those values are $[0, 1.6, 18, 1.8 \cdot 10^2, 1.8 \cdot 10^3, 1.8 \cdot 10^4, 1.8 \cdot 10^5, 2.5 \cdot 10^5] (\text{Unit: s})$

Moreover, we do a test: we calculate the time revolution of ^{135}Xe concentration for a given unstable initial state ($P_{lin} = 0 \text{ W/cm}$) so that the ^{135}Xe concentration will change. For calculating this evolution, we used two methods: for a fixed burnup matrix \mathbf{M} at each divided time interval or for a updated burnup matrix \mathbf{M} at each iteration. Then we plot two lines of ^{135}Xe concentration variation in figure 11. From the figure, we could see that there is nearly no difference for two lines. Therefore, we could use the list of time points outputted by resolving Bateman equations with updated \mathbf{M} , because we could get a really accurate result with it.

Now we come back to the calculation of contribution functions. We have two methods: the conservation of final ^{135}Xe perturbation method and the conservation of final adjoint condition method. For each method, we could get a contribution function evolving with time. And we set the threshold value for selecting the important nuclides to ^{135}Xe as : $c_{fmin} = 0.0025$. Then we get the list of important nuclides and as expected, those two methods give the same list of important nuclides: ^{135}I , ^{239}Pu , ^{239}U , ^{238}U and ^{135}Xe . It is logical that we see ^{135}Xe in this list, but we won't study this behavior because the aim of this work is to select important nuclides and construct simplified chains and we will always put the target nuclide itself in the simplified chains. Now, we plot the values of contribution functions for those isotopes at different time points. Figure 12 shows the time revolution of contribution function conserving

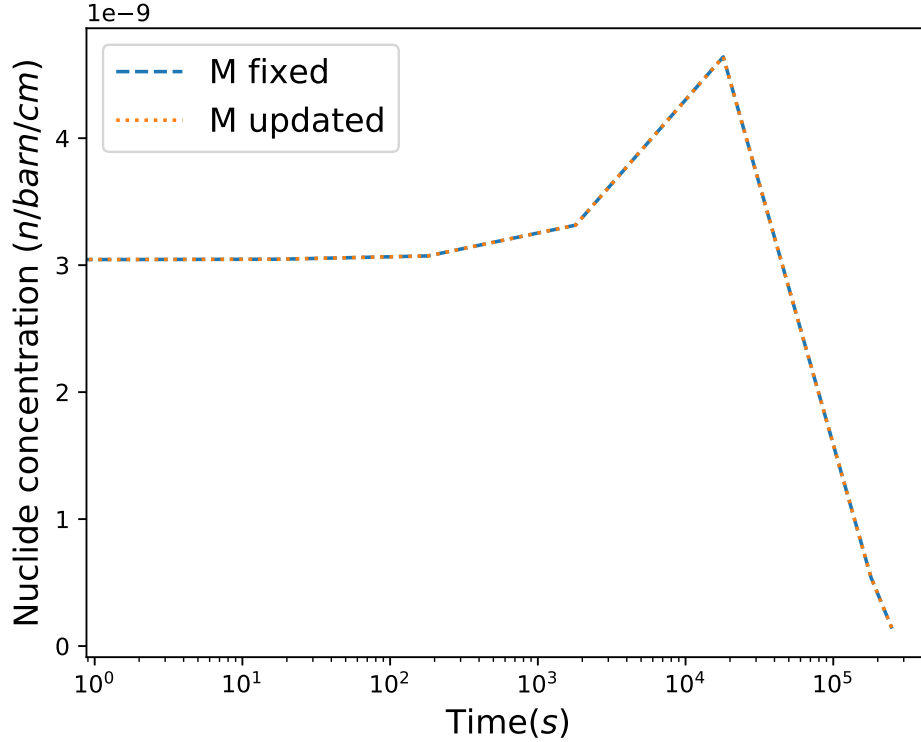


Figure 11: Time evolution of ^{135}Xe

final target nuclide perturbation, in this method, we fix the moment after burnup calculation as t_{final} and calculate the influence to t_{final} from any time point in this burnup calculation $t_i (t_i \in [t_{initial}, t_{final}])$. Besides, in this time division, the time points are in different order, therefore we present time axis in logarithm scale.

From figure 12, we could see that the contribution function values for one isotope are the same except the last one. This is because the time duration of the perturbation burnup calculation $[t_i, t_{final}]$ is long enough so that the system already comes back to its steady state. Therefore, no matter we give the same perturbation at which time point, finally the system is at equilibrium and the response of perturbation is the same. For the last time point, in this case, the perturbation calculation time $[t_i, t_{final}]$ is not long enough, so that the influence of the perturbation hasn't arrived completely at t_{final} , so that for those fissile isotopes, the value of contribution function decreases at the last point because their contributions to the increase of ^{135}Xe 's NND haven't been finished. For ^{135}I , it's in contrary: for long time duration, the perturbation of ΔN_{I135} couldn't change the equilibrium of ^{135}Xe , but if the time duration is not long enough, the system couldn't eliminate completely the influence of ^{135}I to ^{135}Xe therefore its contribution function value increases for the last point. From the above analysis, we could see that the contribution function method is time sensitive. For different perturbation time duration, the result for the same nuclide could be different and the importance is therefore case dependent.

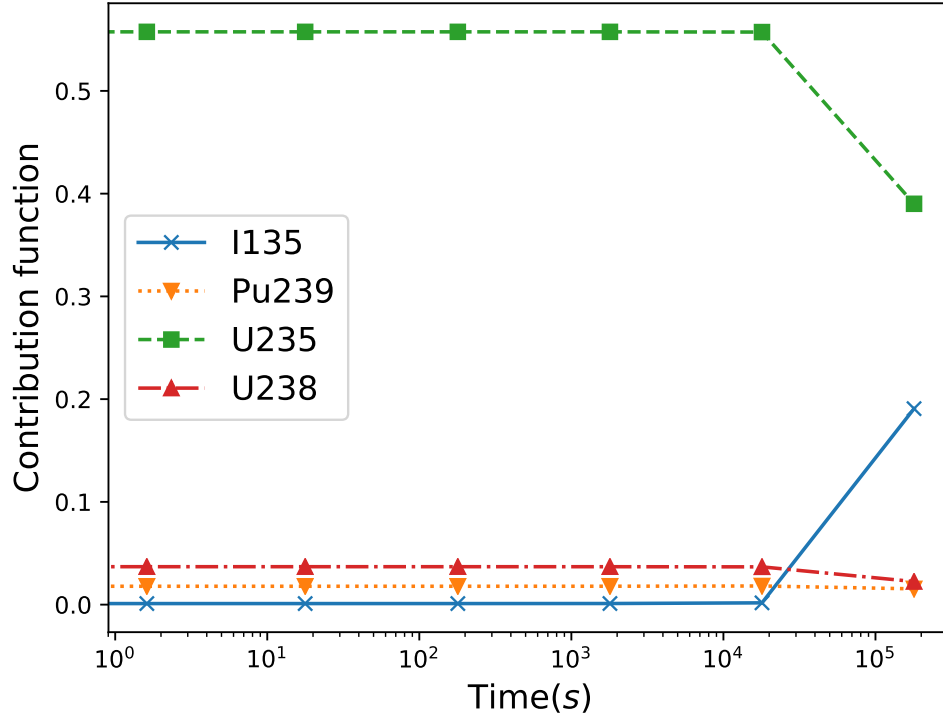


Figure 12: Time evolution of contribution function for selected important isotopes conserving final ^{135}Xe perturbation

For further explaining this phenomenon, we realize another test: we take the same t_{initial} state point, therefore the system is already at equilibrium. We run three simulations: the first one is to keep this state during 72h, and we plot the equilibrium concentrations of ^{135}Xe and ^{135}I as reference; we give the system a perturbation $\Delta N_{I135} = N_{I135}(t_{\text{initial}})$ at t_{initial} , then we plot the time evolution for concentrations of ^{135}Xe and ^{135}I ; we give the system a perturbation $\Delta N_{U235} = N_{U235}(t_{\text{initial}})$ at t_{initial} , then we plot the time evolution for concentrations of ^{135}Xe and ^{135}I . After this test, we get figure 13. From this figure, we know that for the ^{135}I perturbation, the ^{135}Xe concentration will firstly increase because the increase of decay rate, then decrease to equilibrium form a Xe peak. If the perturbation calculation time is long enough, this Xe peak will be cover completely and therefore, the perturbation of ^{135}I nearly has no contribution to the variation of ^{135}Xe concentration. But for ^{235}U , if we increase ^{235}U concentration, the macroscopic fission cross section will increase, but in the simulation, we keep the same reactor power, therefore, neutron flux will decrease but the fission reaction rate won't change. From equation (111) and equation (112), we know that the ^{135}I concentration will keep the same value because fission reaction rate is the same but ^{135}Xe concentration will increase because the neutron absorption rate of ^{135}Xe decreases. Therefore, ^{235}U always has positive contribution and when calculation time is longer, the contribution function value will be higher until the equilibrium state value. This evolution is the same for other fissile isotopes and the

only difference is their different concentrations in the reactor which cause different contribution values.

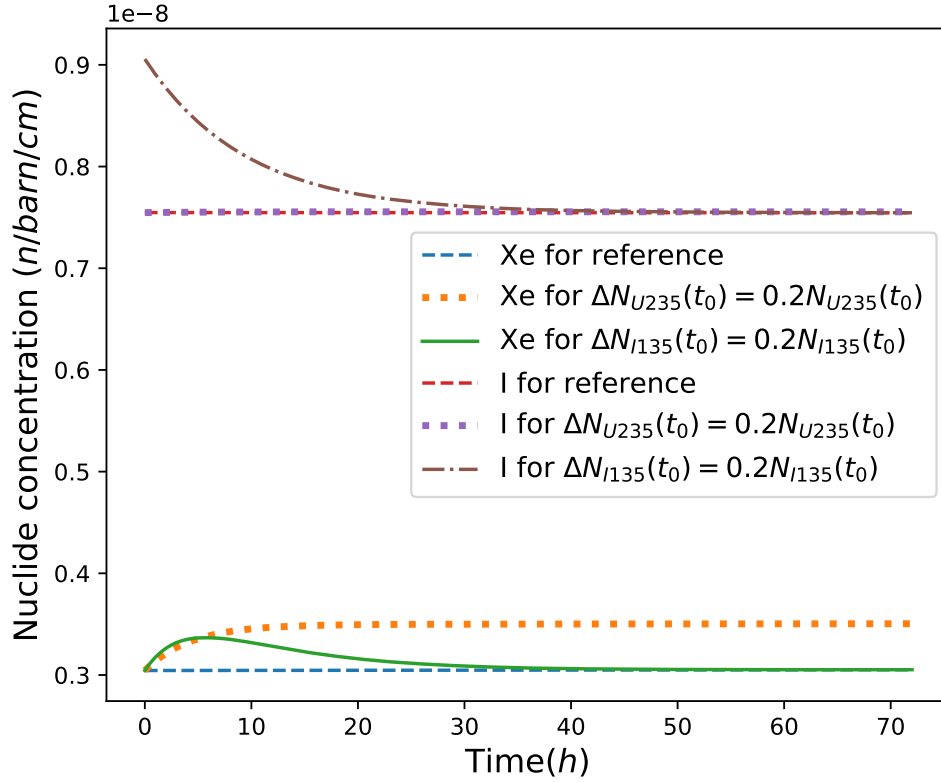


Figure 13: Time evolution of ^{135}Xe and ^{135}I for different perturbation

For another method conserving the final adjoint condition, figure 12 shows the time evolution of this contribution functions for different isotopes. This time for contribution function at t_i , the perturbation calculation duration is $[t_i, t_{i+1}]$ and as we said before, this method is just like calculating the differential derivation. The first thing about this figure is that we should check the values of contribution function at the last time point and they should be the same as those for conserving final perturbation method. Because at this time point, the final adjoint condition is the same for two methods. And this equality proves the correct implementation of those two methods. Next, for all those important isotopes, their contribution values are small at the beginning, this is because for the first several time points t_i , their calculation duration $[t_i, t_{i+1}]$ is small. Therefore, the influence from other nuclides' perturbations haven't arrived yet and the contribution function is small. Then, when the calculation duration increases, the contribution function values for fissile isotopes increase because they contribute to the continuous increase of ^{135}Xe concentration. For the last point, the value decreases is just because the calculation duration decreases. For ^{135}I , the value of contribution function depends on the calculation duration, if the time is near to that for producing the Xe peak, the contribution value will be rather high, for other cases, the values will be smaller. From this figure, we could know that this differential derivation method is very sensitive to

calculation duration, if the time points are not well chosen, it couldn't show the real importance of other nuclides to the target nuclide.

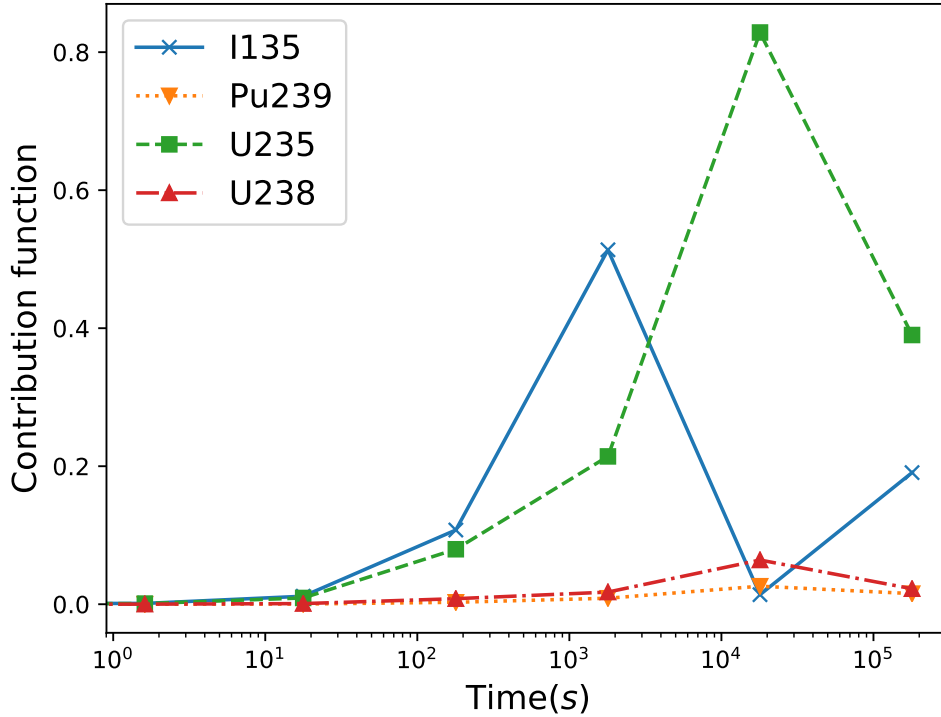


Figure 14: Time evolution of contribution function for selected important isotopes conserving final adjoint condition

2-b Transient state simulation

Now we set another simulation. The first simulation is realized under steady state, It could give us the importance of different isotopes to ^{135}Xe during a long term burnup evolution. However, we haven't know if this function could also do its job during the transient process. As we said, the simplification of depletion chains is a case-dependent problem which should also contain the transient case. So now we will simulate a transient state of about 72 hours and try to get important nuclide to ^{135}Xe .

The initial condition is as follows: $Burnup = 500\text{MWd}/t_{HM}$, $T_{eff} = 582\text{K}$, $T_{mod} = 582\text{K}$, $P_{lin} = 0\text{W}/cm$. As we know, the initial state for zero power level is not stable, therefore we set a evolution time of $83.3h (\approx 3 \cdot 10^5)$ to make sure that the system arrives at the equilibrium state. Then we give increase the linear power to full power level, therefore we could calculate contribution functions during this transient process. In this simulation, we will simulate for $72h$ and we cut the total time interval into 144 parts so that after each 30 min we could get a contribution function vector. Before calculating the contribution function, we firstly test if this time division could present correctly concentration evolution of ^{135}Xe . Therefore, we resolve the Bateman equations using two types of burnup matrix \mathbf{M} : \mathbf{M} is update st each

iteration and \mathbf{M} is fixed during each 30min and plot the evolution ^{135}Xe concentration. Figure 15 shows this evolution and we could observe that for this time division, we could recover the correct concentration evolution of ^{135}Xe with a time step size equal to 30min.

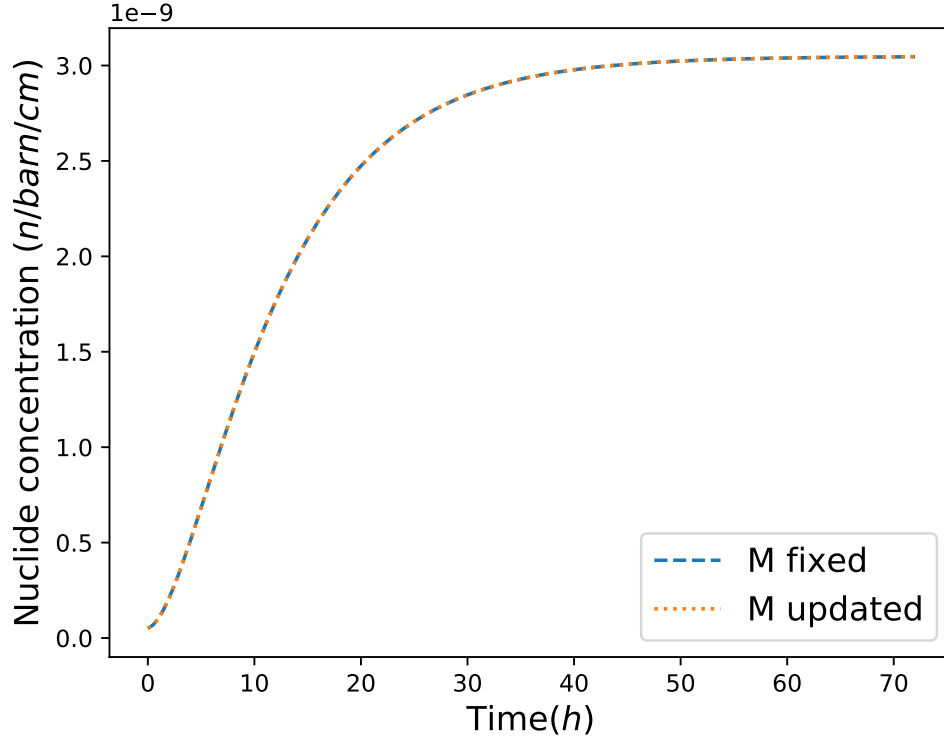


Figure 15: Time evolution of ^{135}Xe for M fixed at each calculation step and updated at each iteration

Now we could begin to calculate contribution functions, we use the method conserving final target perturbation. After calculation, we obtain contribution functions and we set the threshold value $c_{fmin} = 0.0025$ to select important nuclide to the depletion of ^{135}Xe . As expected, we get the same list of nuclides as in the steady state: ^{135}I , ^{239}Pu , ^{239}U , ^{238}U and ^{135}Xe . Figure 16 show the contribution function values of those important isotopes at different time steps.

For the method conserving final target nuclide perturbation, from figure 16, we could see that the contribution function values are constant at the beginning of calculation, this is because the final state is already in steady state, therefore no matter we introduce the perturbation at which time point, finally it will reach the equilibrium and therefore the final variation of target nuclide concentration will always be the same. At the region near end of calculation, for ^{135}I , when the calculation perturbation duration is near the duration producing Xe peak, the value of contribution function will be higher and higher, until the duration is exact for producing Xe peak, then it will decrease as the time goes on. For fissile isotopes, the contribution function will decrease because calculation duration is not enough to completely transfer the influence of perturbation, therefore it will decrease at the end of calculation. We could notice that this

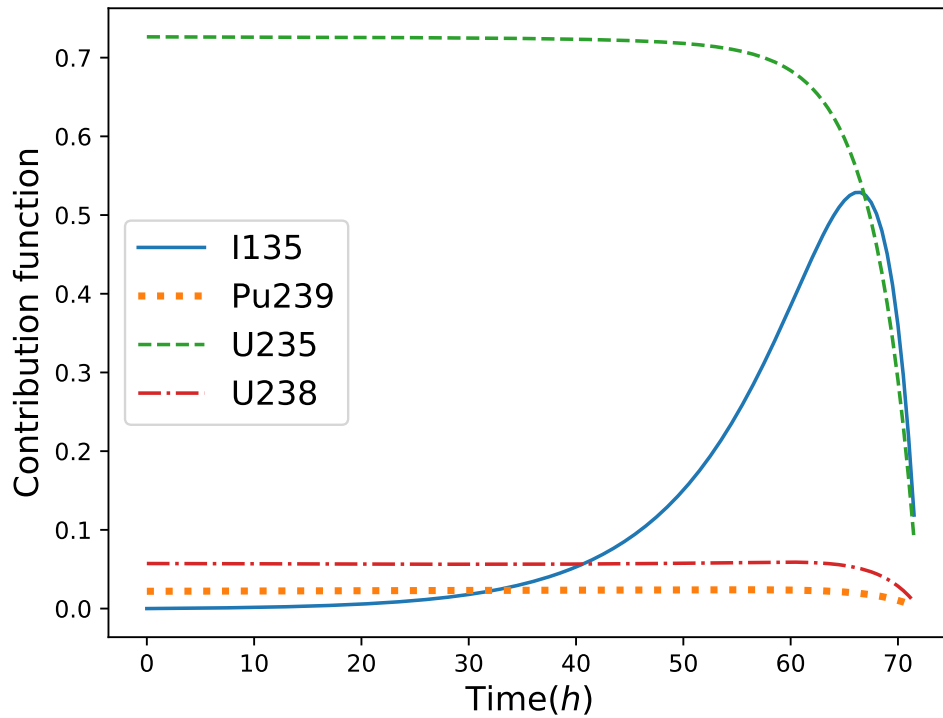


Figure 16: Time evolution of contribution function for selected important isotopes conserving final ^{135}Xe perturbation

part is exactly like figure 12 except that in this test time step is smaller and the variation is clearer. In this method, we could see the variation of importance and select important nuclides.

Figure 17 shows the contribution function conserving final adjoint condition. The important nuclides obtained in this calculation are always the same as previous calculations. From this figure, we could see that the ^{239}Pu and ^{238}U are not important for the transient state. For ^{239}Pu , this is because its small nuclide number density. And for ^{238}U , this is because its small contribution to the fission reaction. We could also see the importance of ^{135}I decreases but the importance of ^{235}U increase, this is because the transient system will finally come back to steady-state and when it is close to reach equilibrium, the behavior of those isotopes are also more similar to those under steady-state. Therefore, we could see this kind of revolution. Besides, in this figure, the contribution function of ^{135}I is higher than that for ^{235}U , this is because the choice of time interval length which shows more the importance of ^{135}I . From this figure, we could see the local importance of nuclides and theirs evolution in the transient state. And this is its advantage compared to last method. Besides, when we combine the calculation of those two contribution functions, we could know more about the nuclide importance evolution with time.

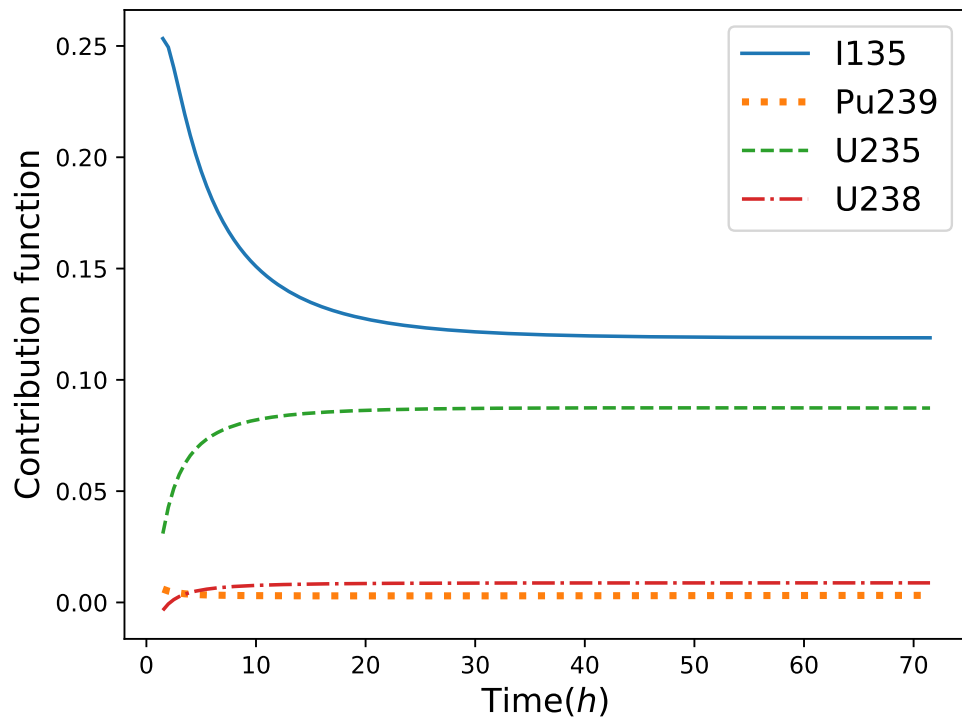


Figure 17: Time evolution of contribution function for selected important isotopes conserving final ^{135}Xe perturbation

6. Conclusion

This work investigates the application of adjoint Bateman equations for radioactive decay and in this work the application is to simplify depletion chains according to a specific target nuclide number density. For doing this, we need to calculate the contribution function of other nuclides to the target one. However, the derivation of Go Chiba's method is presented only in one time step. Faced with this problem, we give the complete derivation for calculating contribution function at any time step so that we could get the evolution of nuclide importance during the whole burnup process. Meanwhile, we propose a new definition of contribution function which is the complement of the original one. With those two definitions, we could know more comprehensively the nuclide importance at different moments.

For solving direct and adjoint Bateman equations, this work develops a Bateman equations solver. Besides, this solver could output other quantities for calculating contribution function. Moreover, this solver contains the neutron flux calculation module. With this module, the solver could update neutron flux at each iteration so that the result could be more accurate. This module uses B_1 leakage model to calculate neutron flux, the derivation of this model uses single fission spectrum. For extending its applicabilities, we give the complete derivation for calculation neutron flux with multiple fission spectrum. And we also compare those two resolution methods and give some instructions for better applying them. In the depletion chains simplification method, we need to resolve adjoint neutron transport equation. But in our work, we use the B_1 leakage equation and we couldn't resolve its adjoint equation. According to this problem, we modify this depletion chains simplification method. After modifications, we won't need to resolving adjoint neutron transport equation, what we need for calculating contribution function are the derivation of burnup matrix to neutron flux(output of Bateman equations solver) and derivation of neutron flux to nuclide number density vector(obtained by applying the incremental ratio method).

Before testing the method, several burnup tests are made to check the correct physical state of data base and the result corresponds well to our theoretical analysis. In this work, ^{135}Xe is chosen as the target nuclide and we calculate contribution functions under steady state and transient state. In each state, two contribution functions are used in the calculation. In both states, the contribution function could select correctly the important nuclides and its response is also case-dependent which satisfies well the requirement of simplifying depletion chains according to different cases. For calculating contribution function, the method conserving final adjoint condition could be regarded as a kind of derivation which could show the local importance of nuclides in a small time duration. This type of contribution function is very sensitive to time step length. In steady state, if the length of time step is not near to that for reproducing the Xe peak, the contribution function value of ^{135}I might be small and there is the possibility of missing important nuclides. But the method conserving final target variation doesn't have this problem:

in steady state it could detect the variation of importance with time and select all important nuclides. But in transient state, the method conserving final target variation could not show the importance during transient state because the contribution depends on final time step, if the final time point is already in equilibrium state, the result will always show the importance of nuclides in steady state. If we fix the final time point in middle of transient, the information after this time point is lost. If we reset the final calculation point, the calculation time will become much longer. In contrary, this problem could be resolved by the method conserving final adjoint condition: in transient, it could present the importance of nuclides at each time point in the evolution.

In this test, only ^{135}Xe is tested. In the future, more work could be done on this topic for testing other nuclides. ^{135}Xe is a little special because it has equilibrium state and the equilibrium concentration only depends on neutron flux. For other isotopes, the situation might be more complex and there are more tests to do using those two contribution functions to see if they could select important nuclides and reproduce rather accurate calculation results using simplified depletion chains.

In fact, the simplification of depletion chains could be done according to a specific target quantity, not only the NND of specific isotope (for example, the effective multiplication factor). If we could know the relation between the target quantity and neutron flux, NND vector and other nuclear data, we could also try to find those important isotopes to this target quantity and then simplify depletion chains. Simplification of depletion chains is a case-dependent work, different requirements could lead to different results. Therefore, this case-dependent calculation method has a good future for the application in several domains like fuel rod storing, pollution control, fuel designing, etc.

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