Validation of reduced nuclide chains by the adjoint formulation of the Bateman equations

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Dedicated to my mom...I wish things were the way they used to be

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PRESENTATION OF WORKING ENVIRONMENT

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The research work has be conducted at SERMA (Service d'Études des Réacteurs et de Mathématiques Appliquées), to which we will give a brief presentation.

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Abstract

In this document, we present the validation of reduced nuclide chains by the use of adjoint Bateman equations. The neutron transport equation and the nuclide evolution equations (Bateman equations) have been analysed in detail over the entire document where we have set and tried to resolve the so called "Trasport-Burnup" problem.

Depletion chain simplification method takes its origin by the generalized perturbation theory (GPT) and the method we are going to discuss, was firstly introduced by Go Chiba and his colleagues of Hokkaido University, Japan, with the intent to select relative important nuclides and to simplify depletion chains. This method defines a fundamental function named Contribution Function (CF) which has been derived and calculated thanks to the definition of the Adjoint Nuclide Number Density function (ANND). Anyway, the definition of Go Chiba applies only in one time step interval and CF 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. So we have generalized the CF definition at any time step in order to achieve full understanding of this method and to validate it. We have developed a Bateman equation solver which includes neutron flux calculation module that has been obtained with the $B1$ leakage model. Without this module, burnup matrix will be constant during calculation, which produces low accuracy result while with this module we could update neutron flux in each iteration so that the calculation result could be more accurate.

However, the CF defined by Go Chiba resolves directly the adjoint transport equation while we have not implemented the resolution of the latter since it would be too difficult to resolve the adjoint transport equation because there will be one more unknown quantity (B^2) and the problem is intrinsically a nonlinear eigenvalue problem. This last modification led to a new procedure for the calculation of CF which will be shown off. For testing the depletion chain simplification method we have chosen two of the most important fission products nuclides in terms of reactor criticality controll, Xe135 and Sm149 and for both of them we started from an equilibrium steady state. In this steady state case, after resolving Bateman equations and adjoint Bateman equations using Bateman solver, we calculated contribution function. In both cases, CF could select correctly important nuclides. In the end we will give some physical interpretations of CF, further tests to conduct in the near future and improvements to the method.

Contents

Chapter one

In the first chapter, we briefly descibe some theoretical references on the neutron transport equation and on Bateman Equations that will be followed by the review of Go Chiba's method.

1 Introduction

In Transport-Burnup problem, two equations are important for its resolution: the neutron transport equation and the Bateman equations. The first one, which historically is known as the Boltzmann equation, descibes the neutron density evolution with time while the second one describes the variation of concentration of each isotope in depletion chains with time.

From their formulation, we notice that the solution of one equation appears in the other as a parameter, therefore in reactor calculation we always need to resolve those two equations at the same time. In addition the Bateman equations are a non-linear differential in time equation system because of the coupled relation between neutron flux and isotopic abundance, so its resolution becomes quite cumbersome. Of course, we are aware that 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. So, we need to find a balance between the number of isotopes in the chains and the needed accuracy. In this sense we highlight that the issue is a case dependent problem since it depends on whether or not we have to simplify complex depletion chains which influence the wanted accuracy.

The aim of this work is to simplify depletion chains according to a specif target quantity by the use of the adjoint Bateman equations. To achieve this goal we will make use of a solver created by us which is capable of resolving both direct and adjoint Bateman equations. Then after proving the validity and reliability of this solver we will make use of a theory developed by Go Chiba and his colleagues of Hokkaido University, Japan to demonstrate our goals. During the exposition of our work we will highlight many modifications that have be done to the original method which is based on the definition of Contribution Function, our selective function for semplification method.

The basic idea of the method is to introduce a perturbation of a nuclide number density (our reference quantity) at the beginning of calculation and observe its influence to the target's nuclide number density. Those nuclides producing important variation of target quantity are regarded as important nuclides. Basically this

procedure can be applied to each nuclide respect to a target nuclide but, because of the great number of nuclides, it will pretty long and not practical. That's why we will make use of Perturbation Theory and connected adjoint functions since it permits to analyze the response of small perturbation to the system more quickly than the direct approach. In this chapter, we will proceed with the key method of this work which is the one of Go Chiba where we will make use of some notations of adjoint formulation used in generalized perturbation theory (GPT). After that, in chapter two and three, we will higlight our own improvements of the method and in chapter four and five we will test it for few case of interest.

2 Transport-Burnup problem

2.1 The Neutron Transport Equation

The transport equation is introduced to describe a population of neutral particles such as neutrons in a close domain, under transient or steady state condition. Its derivation is based on the principle of particle conservation but here we won't present it whereas we will focus on its meaning ad application in many fields of nuclear engineering, notably: reactor physics, safety and criticality, radiation shielding and protection.

This fundamental equation describes all the possible interations that a neutron can encounter during his entire lifetime. In fact, since its birth, neutrons can escape from the reactor or interact with a nucleus (basically they do not interact with electrons since they are globaly neutral). This interaction might be the absorption by this nucleus and it might deduce the emission of other particles resulting in a change of atomic number in the nucleus. Before its end of life, one neutron could also interact with several nucleus along its travel in space and it's called scattering reaction; those kind of interaction result in a change of energy or in a change in its propagation direction. All these possibly route of interaction are accounted by the transport equation and since the great numbers of neutrons present in a rector, the approach for its definition is statistical. We therefore introduce the neutron density $n(\vec{r}, E, \vec{\Omega}, t)$ which represents the average number of neutrons in unit volume at instant t. We must remember that here the unit volume is to be intended as the one in phase space which includes six dimensions: three for space geometry, two for velocity direction and one for energy (velocity module). Anyway, in reactor physics we make use of a derivative quantity of the neutron density which is the neutron flux, where we have taken into account velocity direction in the definition of n:

$$\phi(\vec{r}, E, \vec{\Omega}, t) = v \cdot n(\vec{r}, E, \vec{\Omega}, t) \tag{2.1}$$

The neutron flux is a fundamental quantity and it permits the definition of the reaction rate which is the number of (specific) reactions per unit time and per unit volume:

$$R(\vec{r}, E, \vec{\Omega}, t) = v \cdot n(\vec{r}, E, \vec{\Omega}, t) \cdot \Sigma(\vec{r}, E, \vec{\Omega}, t) \tag{2.2}$$

where $\Sigma(\vec{r}, E, \vec{\Omega}, t)$ is the macroscopic reaction cross section of a particular event, defined as the product of microscopic reaction cross section and target NND. The importance of the reaction rate relies in the fact that this quantity is measurable. If we refer to the fission event, by knowing the average energy released per fission event and by measuring the reactor power we can deduce the reaction rate. Now it follows the definition of transport equation [3]:

$$\frac{1}{v}\frac{d\phi(\vec{r},E,\vec{\Omega},t)}{dt} = -\left(\mathbf{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega},t) + \Sigma_f(\vec{r},E,\vec{\Omega},t)\cdot\phi(\vec{r},E,\vec{\Omega},t)\right)$$

$$+\int_0^\infty dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\vec{r},E\leftarrow E',\mathbf{\Omega}\leftarrow\mathbf{\Omega}')\phi(\vec{r},E',\mathbf{\Omega}') \quad (2.3)$$

$$+\frac{\chi(E)}{4\pi k_{eff}}\int_0^\infty dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E')$$

where we have introduced the macroscopic scattering (fission) cross section Σ_s (Σ_f), the effective multiplication factor k_{eff}, the fission spectrum $\chi(E)$ and the average number of neutron emitted isotropically per fission ν.

If we refer at the right side of the equation, we notice that we can compact it into positive terms that are the source of neutrons and negative terms, that using the language of particle conservation equations, can be regarded as the sink term. The negative terms in parenthesis refer to the leakage of neutrons from the system through the surfaces while the second one refers to all the possible reactions between neutrons and material; the positive terms which represent the source of the system, refers to the neutron's production due to the fission events, the decay production and the scattering that could change its energy in phase space. However it must be said that the source term depends on the situation and in our case we won't need any external source since it is supposed that we are in critical conditions.

This is the general form of Boltzmann equation but we must say that it's not of easy resolution and many simplified models have been implemented in nuclear codes for easier calculations. Furthermore, in many applications, we shall be concerned with time indipendent neutron distribution. In our work we have decided to implement $B1$ leakage model, a neutron leakage model used for lattice calculations. Further derivations and semplifications will be given later on.

2.2 Isotopic depletion: Bateman equations

With the term isotopic depletion we refer to all those phenomena that consist in a nuclide field variation and nucleus modification. During the operation of a nuclear power reactor, neutrons produced by the fission reactions can "react" with all possible materials in the reactor, including a large amount of isotopes (this is the first complexity: large numbers of isotopes included in the calculations). The exposure of those nuclides to neutrons can led to nucleus modification like the change of numbers of protons and neutrons. The new produced isotope may be unstable and this instability could led to radioactive decay which is a way of searching a stable energy configuration (here we should also consider metastable states which are considered as a completely brand new nuclide); the daughter nuclide of course, under the influence of neutron flux, can undergo further modification.

In isotopic depletion we make use of the parameter Burnup which is the integration of power with time per unit initial mass. With fuel Burnup, the nuclide number density (NND) will change and this will affect the macroscopic cross section present in the Boltzmann equation, which ultimately affects neutron flux. Reversely the neutron flux could determine the variation of nuclide field. This is the complex relation that exists between neutron flux and NND. In practise most of the time

we will barely find single linear chains and since one nuclide can come from several different reactions due to the large kinds of reaction types, we will be more likely to have cyclic or multiple branches in chains.

Another point to underline is that the influence of neutron flux to the production or depletion of a general nuclide is different and it depends on the nuclide we are looking up to; for instance, very high absorbing fission products in epithermal regions like Xe135 and Sm119, will be higly dependent on the level of neutron flux while another isotopes that have very low absorbing cross section won't. So again we find that flux and nuclide number density are pretty far to be consider close friends for our calculation purposes. For a generic nuclide k, the variation of its NND with time depends on its generation and disappearance at each instant. The variation of N_k with time can be expressed as follows[9]:

$$
\begin{aligned}
\frac{dN_k}{dt} &= \Delta\dot{N}_{gener} - \Delta\dot{N}_{disapp} \\
&= + \sum_{l=1}^{N_{decay}} \lambda_{l_k} N_l(t) + \sum_{l=1}^{N_{nucleus}} \langle \sigma_{n,l}\phi(t)\rangle N_l(t) \\
&\quad + \sum_{l=1}^{N_{Fission}} Y_{l_k} \langle \sigma_{f,l}\phi(t)\rangle N_l(t) - (\lambda_k + \langle \sigma_{a,k}\phi(t)\rangle)N_k(t)
\end{aligned}
\tag{2.4}
$$

where Y_{l_k} is the fission yield of fissile isotope l to fission product k and the quantities in square brackets are the integration over space and energy of neutron flux and microscopic cross section for isotope k and for all the possible reaction types (absorbtion, fission and radioactive capture). For each isotope k we have the previous form of Bateman equation. If we take into account all the nuclides in exam (in number n), the nuclide evolution can be written also in its vectorial form by using the nuclide number density vector **NND** so defined $\mathbf{N(t)} = [N_1(t), N_2(t), ..., N_n(t)]$ and the burnup matrix **M**. So, we have:

$$
\frac{d\mathbf{N}}{dt} = \mathbf{MN}.
\tag{2.5}
$$

Bateman equations are a set of ordinary non linear differential equations because of the non linearity between flux and nuclide number density that appears in the burnup matrix and it must be solved numerically. Different methods for its resolution are possible and we will discuss it later on when we will test our Bateman solver.

2.3 Depletion chain simplification method

Adjoint formulation

Here we describe the method introduced by Go Chiba and his colleagues of Hokkaido University. However, the analytical derivation makes use of the adjoint formulation for both the transport and Bateman equations; so firstly we have to give some basic concepts and since the complete derivation is out of the purpose of this master thesis, we present just what will be used later.

The adjoint operator originates from functional analysis and it's defined on Hilbert space which generalizes the notion of Euclidean space, by extending the methods of vector algebra and calculus from the two-dimensional Euclidean plane and three-dimensional space to spaces with any finite or infinite number of dimensions. We have to introduce at first the inner product over all the independent variables of phase space[8]:

$$\langle f, g \rangle = \int d\vec{r} \int dE \int d\vec{\Omega} f(\vec{r}, E, \vec{\Omega}) g(\vec{r}, E, \vec{\Omega}) \qquad (2.6)$$

where suscript after brakets have been obmitted for a general derivation. Now refering to the definition and meaning of a mathematical operator (for instance it could be the trasport operator defined later), we introduce for an operator C, its adjoint operator, defined as the one which satisfies the following condition[2]:

$$\langle f, Cg \rangle = \langle C^* f, g \rangle \qquad (2.7)$$

Where C^* is the adjoint operator of C and f and g are two generic functions defined in phase space. Moreover, if we suppose that f is the adjoint of g which will be indicated as g^*, the previous relation becomes the following:

$$\langle g^*, Cg \rangle = \langle C^* g^*, g \rangle = \langle g, C^* g^* \rangle. \qquad (2.8)$$

The last identity is possible since the inner product is defined on Euclidean space. As previously said, we won't resolve adjoint transport equation so our only adjoint system equation is the one of Bateman. Actually we have to prove the existance of the adjoint but from a mathematical theorem, linear and real-valued functions have their adjoint operator (8). Let's consider now the generic function f as the NND vector. In our model, this vector does not depend on the position, angle or energy and we will considered each term of the burnup matrix **M** as energy, angle intergrated and spatial averaged so that there is no longer dependence between **MN** and the space variables $(\vec{r}, E, \vec{\Omega})$. So,

$$\langle \mathbf{M}, \mathbf{N} \rangle = \mathbf{MN} \qquad (2.9)$$

and equation (2.9) becomes:

$$\langle \mathbf{N}^* \mathbf{MN} \rangle = \langle \mathbf{NM}^* \mathbf{N}^* \rangle = \langle \mathbf{NM}^T \mathbf{N}^* \rangle \qquad (2.10)$$

which means that the adjoint of Burnup matrix is just its transpose.

Introduction to Go Chiba's Method

In the recent past, identifications of important FPs for a simplified burnup chain have been conducted manually based on experts' knowledge and experiences. Of course, the task is still nowadays quite cumbersome and more accurate numerical simulations of them are required. For instance, the fuel management of a fission reactor can benefit from a more reliable and higher calculation efficiency which at the same time could save calculation time. The present procedure for the indentification of important fission product (FP) nuclides, which are required to construct a simplified burnup chain, makes use of the adjoint nuclide number density (ANND) which was initially proposed in the framework of the generalized perturbation theory[2]. The aim of GPT, which has so many application in reactor theory, is to study the sensitivity of reactor characteristic to reactor parameters. Then, with the introduction of ANND, it has been defined a function named Contribution function (CF) which will be the selector of our important nuclides.

However, up to now, we have talked about important nuclides but we have not yet referred this importance to something; well, the importance of NND of a generic nuclide k is related to a specif target nuclear characteristic, which in our case will be the NND of specif nuclide after burnup. The procedure that we are going to show has the goal of computing those CF and by comparison with a thresold value, it will choose the important ones that will be included in the simplified depletion chains. Moreover, during the construction of those chains, the decay relation should also be redifined because a large number of nuclides in those chians will be eliminated and there might not be direct decay relation between two adiacent selected nuclides. Now we will go over the main steps of Go Chiba's method.

In Transport-Burnup problem, the neutron flux distribution is tipically assumed to be time-invariant and it is calculated by solving the following neutron transport equation [1]

$$B^i \phi^i = \left(A^i - \frac{1}{k_{eff}^i} F^i\right)\phi^i = 0 \tag{2.11}$$

where we have indicated with B^i the trasport operator which has been devided into a neutron destruction operator A^i and a fission generation operator F^i; in the original derivation the k_{eff}^i term is not present but it has been introduced for keeping the equality between the disappearance and production rate. Another explanation of the quasi-static approximation applied to the transport equation relies in the fact that burnup calculations are long term calculations respect to the time scale of the neutronic transport one and this enhance our hypotesy.

The transport equation, obeyed by the neutron distribution in a reactor is homogeneous, thus the solution can be determined only to within an arbitrary multiplicative constant; in principle, the flux distribution can have any amplitude between zero and infinity while in practice, it is limited by heat removal considrations and by temperature feedback effects. The flux is so normalized by a reactor power P^i, which is constant during the burnup period and defined as:

$$P^i = \int_{r \in V_f} \sum_j k_j N_j(t_i) \sum_g \sigma_{f,j,g}^i {\phi_g}^i(r) dr = \sum_j k_j N_j(t_i) \langle \sigma_{f,j}^i \phi_i \rangle \tag{2.12}$$

where brackets denote the integration over all the energy groups and whole volume of the system, V_f is a total volume of a fuel region, $N(t_i)$ and$Nj(ti)$ denote a NND vector and its jth entry (NND of nuclide j) at t $= t_i$ respectively, k_j and $\sigma_{f,g,j}$ are an emitted energy by one fission reaction and a microscopic fission cross section in energy group g of nuclide j, and ϕ_g(r) is a neutron flux of energy group g at a spatial position r. In this study we do not consider spatial dependences of microscopic cross section and neither angular distribution of the flux so that the flux can be considered isotropic.

For simplifing the derivation we write the previous equation as

$$P^i = \mathbf{N}^T(t_i)\mathbf{K}(t_i) \tag{2.13}$$

with obvious meaning of the previous terms. The basic idea of how to quantify importance of NND of nuclide k at t_i, $N_k(t_i)$, to NND of nuclide l at t_{i+1}, is to observe a change in $N_l(t_{i+1})$ due to a change in $N_k(t_i)$ by direct burnup calculation. Whereas importance of every nuclide at t_i to NND of an arbitrary nuclide at t_{i+1} can be calculated with this procedure, it requires a huge number of calculation cases. With the use of GPT we can calculate the importance of NNDs in a more efficient way and next we will show how. We have already written the Bateman equations in his vectorial form as

$$\frac{\partial \mathbf{N}(t)}{\partial t} = \mathbf{M}^i \mathbf{N}(t) \tag{2.14}$$

Considering a time interval $[t_i, t_{i+1}]$ and a initial known condition of $\mathbf{N}(t_i)$, suppose we introduce a perturbation of the initial condition, which we indicate as $\Delta N(t_i)$, the operator B^i of transport equation changes and so the flux ϕ^i and the matrix $\mathbf{M}^i$ too; the system is so perturbed and we have to resolve the new system of differential equation, so defined

$$\frac{\partial \mathbf{N}^{'}(t)}{\partial t} = \mathbf{M}^{i,'}\mathbf{N}^{'}(t) \tag{2.15}$$

where $\mathbf{N}^{'}(t) = \mathbf{N}(t) + \Delta \mathbf{N}(t), \mathbf{M}^{i'} = \mathbf{M}^i + \Delta \mathbf{M}^i$ are respectively the perturbed nuclide number density vector and the perturbed burnup matrix. Substituting those perturbed quantity in the previous equation and neglecting higher order term we have:

$$\frac{\partial \Delta \mathbf{N}(t)}{\partial t} = \Delta \mathbf{M}^i \mathbf{N}(t) + \mathbf{M}^i \Delta \mathbf{N}(t). \tag{2.16}$$

Then we multiply for both side of the above equation a vector $\mathbf{w}^T(t)$ and we integrate over the time intervall in exam $[t_i, t_{i+1}]$, by getting:

$$\int_{t_i}^{t_{i+1}} \mathbf{w}^T(t)\frac{\partial \Delta \mathbf{N}(t)}{\partial t}dt = \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t)\Delta \mathbf{M}^i \mathbf{N}(t)dt + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t)\mathbf{M}^i \Delta \mathbf{N}(t)dt. \tag{2.17}$$

If we resolve the left hand side with intergration per parts and we make some

adjustments, we find

$$
\begin{aligned}
&\mathbf{w}^T(t_{i+1})\Delta\mathbf{N}(t_{i+1}) - \mathbf{w}^T(t_i)\Delta\mathbf{N}(t_i) \\
&= \int_{t_i}^{t_{i+1}} \Delta\mathbf{N}^T(t)\left(\frac{\partial\mathbf{w}(t)}{\partial t} + \mathbf{M}^{i,T}\mathbf{w}(t)\right)dt + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t)\Delta\mathbf{M}^i\mathbf{N}(t)dt.
\end{aligned}
\tag{2.18}
$$

If we define the vector w as a solution to the following equation

$$
\frac{\partial\mathbf{w}(t)}{\partial t} = -\mathbf{M}^{i^T}\mathbf{w}(t)
\tag{2.19}
$$

and the final condition for $\mathbf{w}(t_{i+1})$ is given as $\mathbf{w}(t_{i+1}) = \mathbf{e}_l$ [1], Equation (3.19) can be rearranged as

$$
\Delta N_l(t_{i+1}) = \mathbf{w}^T(t_i)\Delta\mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{w}^T(t)\Delta\mathbf{M}^i\mathbf{N}(t)dt.
\tag{2.20}
$$

First of all, we notice that with $\mathbf{e}_l$ we refer to the unit vector in which the lth entry is unity and the others are zero. The above equation is of great importance since it tells us that for calculating the perturbation on the lth target nuclide density, we need to calculate the $\mathbf{w}$ in advanced and the second term inside the integral, where we should focus on the expression of $\Delta\mathbf{M}^i$. We have seen in paragraph (2.3.1) that the adjoint of $\mathbf{M}^i$ is just its transpose (since our hypotesis of space indipendence) so $\mathbf{w}$ in (2.20) can be written as $\mathbf{N}^*$ which it will be called the adjoint nuclide number density (**ANND**) vector.

Let us consider how ΔM^i, a change in the burnup matrix due to the perturbation in the initial number density vector, can be calculated with the GPT-based procedure. We saw that the perturbation in the initial number density vector gives changes to the neutron flux distribution, however also the multi-group microscopic cross sections during burnup are affected because they are avaraged respect to the flux distribution. The latter change, however, is considered negligible since the resonance self-shielding effect in conventional thermal neutron reactors is dominantly affected by the neutron fuel escape cross section, which is dependent on cross sections in non-fuel regions. Thus, the term ΔM^i can be written as a function on flux only

$$
\Delta M^i = \frac{d\mathbf{M}^i}{d\bar{\phi}^i}\frac{\int_{r\in V_f}\Delta\phi^i(r)dr}{V_f}
\tag{2.21}
$$

where $\bar{\phi}^i$ is an averaged neutron flux in the fuel region. In the previous relation we still not know how to calculate the $\int_{r\in V_f}\Delta\phi^i(r)dr$ expression which is the term that gives us the effect of the introduced perturbation to the averaged neutron flux in the region of interest. So, we have to introduce the adjoint neutron transport equation in order to get this relation:

$$
\mathbf{B}^{i*}\Gamma^{i*} = \mathbf{S}^{i*}
\tag{2.22}
$$

$$
\mathbf{S}^{i,*} = \frac{\int_{t_i}^{t_{i+1}}\mathbf{N}^{*,T}\frac{d\mathbf{M}^i}{d\bar{\phi}^i}\mathbf{N}dt}{V_f} - \left(\int_{t_i}^{t_{i+1}}\mathbf{N}^{*,T}\bar{\mathbf{M}}^i\mathbf{N}dt\right)\sum_j k_j N_j(t_i)\sigma_{f,j}^i p^i
\tag{2.23}
$$

where $\mathbf{B}^{i*}$ is an adjoint operator to $\mathbf{B}^i$, Γ^* is a so-called generalized adjoint neutron flux and $\bar{M}^i$ is a component of a burnup matrix M^i, in which all the entries are dependent on ϕ_i. Note that the source S^i is orthogonal to the neutron flux ϕ_i and this last equation is valid where $r \in V_f$ and it's zero elsewhere. Now we multiply $\Delta \phi^i$ to both side of equations (2.23) and we integrate this equation over all energy group and volume V_f. By introducing the definition of the source term, we obtain:

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

$$(2.24)$$

in which we have put $P^{i*} = \dfrac{\int_{t_i}^{t_{i+1}} \mathbf{N}^{*T} \bar{M}^i \mathbf{N} dt}{P^i}$ as the adjoint power, P^i as the reactor power and we have set the following identity

$$\langle \Gamma^{i*} \mathbf{B}^{i*} \Delta\phi^i \rangle = \langle \Delta\phi^i \Gamma^{i*} \mathbf{B}^{i*} \rangle = \langle \mathbf{B}^{i*} \Gamma^{i*} \Delta\phi^i \rangle \tag{2.25}$$

in which the first equality comes from the symmetry of real inner product and the second one from property of adjoint operator.

The last step is to get the relation between neutron flux and nuclide perturbation $\Delta \mathbf{N}(t_i)$ and since the influence of the latter works indirectly by modifying the transport operator, its deriation is not immediate and needs further steps.

The change in the neutron flux $\Delta\phi^i$ preserves the following equation if we neglect second order terms:

$$B^i \Delta\phi^i + \Delta B^i \phi^i = 0 \tag{2.26}$$

but since reactor power is constant during a burnup period, the next identity holds:

$$\sum_j k_j N_j(t_i) \langle \sigma_{f,j}^i \Delta\phi^i \rangle = -\sum_j k_j \Delta N_j(t_i) \langle \sigma_{f,j}^i \phi^i \rangle \tag{2.27}$$

and in comparison with equation (2.14), we can write it as

$$\sum_j k_j N_j(t_i) \langle \sigma_{f,j}^i \Delta\phi^i \rangle = -\Delta \mathbf{N}^T(t_i) \mathbf{K}(t_i). \tag{2.28}$$

Using this last two equations and equation (2.27), equation (2.25) is written as

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

$$(2.29)$$

and with the last substitutions we can write the equation which gives us the variation of nuclide number density for target nuclide (2.21) as

$$\Delta N_l(t_{i+1}) = \left(\mathbf{N}^{*T}(t_i) - \left\langle \Gamma^{i*} \frac{dB^i}{d\mathbf{N}^T} \phi^i \right\rangle - P^{i*} \cdot \mathbf{K}^T(t_i)\right)\Delta\mathbf{N}(t_i). \tag{2.30}$$

To compact the above equation, we introduce the corrected ANND vector defined as

$$\widehat{\mathbf{N}}^* = \mathbf{N}^*(t_i) - \left\langle \mathbf{\Gamma}^{i,*} \frac{dB^i}{d\mathbf{N}^T} \phi^i \right\rangle - P^{i,*} \cdot \mathbf{K}(t_i). \tag{2.31}$$

so that equation(2.31) becomes:

$$\Delta N_l(t_{i+1}) = \widehat{\mathbf{N}}^{*T}(t_i)\Delta\mathbf{N}(t_i). \tag{2.32}$$

The above equation is of a key importance in determine importace of NND of nuclide k respect to the choosen target NND of nuclide l; in fact, $\Delta N_l(t_{i+1})$ can be regarded as the amplification of the initial perturbation and this is considered as the absolute amplification[8]. However, the perturbed concentrations of different isotopes could lead to different values of the absolute concentration of the key nuclide l, so for better identifing the importance no matter how much bigger or not is the amplitude of the amplification, we would refer to the relative perturbation for Contribution function definition

$$CF_{k,l}(t_i) = \frac{\frac{\Delta N_{k,l}(t_{i+1})}{N_l(t_{i+1})}}{\frac{\Delta N_k(t_i)}{N_k(t_i)}} = \frac{\frac{\widehat{\mathbf{N}}_k^{*T}(t_i)\Delta\mathbf{N}_k(t_i)}{N_l(t_{i+1})}}{\frac{\Delta N_k(t_i)}{N_k(t_i)}} = \frac{\widehat{\mathbf{N}}_k^{*T}(t_i)N_k(t_i)}{N_l(t_{i+1})} \tag{2.33}$$

where we have used the term $\Delta N_{k,l}$ to indicate the variation of target nuclide concentration cause by the perturbation of nuclide *k* number density. Finally we got the definition of CF by which we can quantify the NND importance of all the nuclides during burnup for the NND of the specific nuclide after burnup. However our derivation is different from the one of Go Chiba and it the next chapters we will show our own modifications, by posing the framework for the final results.

Chapter Two

In this chapter we focus entirely on the exposition of B_n leakage model. Firstly we present the set of B_1 equations and we highlight the benefit of using this model, which brings us to obtain more accurate results; in fact, with this module the solver could calculate neutron flux and then update burnup matrix at each time step. After that, we show a new numerical method of solving B_1 equations, method that it's discussed in detail since its use is not only restricted to the Transport Burnup problem.

3   The B_n leakage model

In lattice calculations, we are suppose to calculate neutron flux, leakage and reaction rates of a unit cell or assemby without the knowledge of the exact operating conditions and materials sourronding it. For the applicability of the method, some hypotesis must be posed and those are the following:[3]

1) The flux calculation inside the unit cell or assemhly will be performed under closed conditions. An infinite domain or a finite domain closed with periodic bowndary conditions will be used.

2) We will assume that the real neutron flux of the unit cell or assembly is under steady-state conditions and a leakage model will be introduced to enforce the hypotesis of $K_{eff} = 1$ in the unit cell or assembly. This is done by the introduction of a *fundamental* mode approximation. The principle is to considered the neutron flux as the product of a macroscopic distribution in space $\psi(\mathbf{r})$ with a homogeneous or periodic fundamental flux $\varphi(\mathbf{r}, E, \mathbf{\Omega})$. So the factorization is written as

$$\phi(\mathbf{r}, E, \mathbf{\Omega}) = \psi(\mathbf{r})\varphi(\mathbf{r}, E, \mathbf{\Omega}) \tag{3.1}$$

3)The macroscopic distribution is assumed to be a property of the complete reactor and to be the solution of a Laplace equation:

$$\Delta^2\psi(\mathbf{r}) + B^2\psi(\mathbf{r}) = 0, \tag{3.2}$$

where $\Delta^2 = \nabla \cdot \nabla$ is the Laplacian operator and B^2 is the geometrical buckling representing the curvature of the flux. The buckling B^2 is modified until matching a unitary multiplication factor, which means also adjusting the leakage rates in case of insufficient or excessive production of neutrons by fission, i.e. positive or negative B^2, respectively. There exist homogeneous and heterogeneous variants of the fundamental mode theory, depending on whether the fundamental flux $\varphi(\mathbf{r}, E, \mathbf{\Omega})$ is assumed to be homogeneous or periodic according to the lattice pitch. A general

solution of Eq. (3.2) is $\psi = C \exp{(i\mathbf{B} \cdot \mathbf{r})}$ where C is constant and the magnitude of the vector $\mathbf{B}$ is $|\mathbf{B}| = \sqrt{\mathbf{B} \cdot \mathbf{B}} = B$. The neutron flux will therefore be factorized as

$$\phi(\mathbf{r}, E, \mathbf{\Omega}) = \varphi(\mathbf{r}, E, \mathbf{\Omega}) \exp{(i\mathbf{B} \cdot \mathbf{r})}, \tag{3.3}$$

where $\varphi(\mathbf{r}, E, \mathbf{\Omega})$ is a complex quantity. For our purposes, we will make use of the homogeneous $B1$ model which is the standard choice in lattice calculations; the equations of the model are obtained after substituting the factorization of equation (3.3) into the transport equation defined in (3.4) with the semplification of steady state reactor and for the case of a finite and homogeneous geometry (the mathematical derivation can be find in "Applied Reactor Physics" by Alain Hébert)[3], we obtain:

$$[\Sigma(E) + d(B, E)B^2]\phi(E) = \int_0^\infty dE' \Sigma_{s,0}(E \leftarrow E')\phi(E') + \frac{\chi(E)}{k_{eff}} \int_0^\infty dE' \nu \Sigma_f(E')\phi(E') \tag{3.4}$$

and with d defined as:

$$d(B, E) = \frac{1}{3\gamma[B, \Sigma(E)\Sigma(E)]} \left\{ 1 + 3 \int_0^\infty dE' \Sigma_{s,0}(E \leftarrow E')d(B, E') \frac{\phi(E')}{\phi(E)} \right\} \tag{3.5}$$

where Σ is the total cross section, Σ_f is the fission cross section, d is the leakage coefficient, ϕ is the neutron flux, $\Sigma_{s,0}$ and $\Sigma_{s,1}$ 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 neutrons emitted per fission, and the quantity $\gamma[B, \Sigma(E)]$ is a term that appearts during the derivation of these equations and so approximated

$$\gamma[B, \Sigma(E)\Sigma(E)] \approx 1 + \frac{4}{15}\left(\frac{B}{\Sigma}\right)^2 - \frac{12}{175}\left(\frac{B}{\Sigma}\right)^4 + \frac{92}{2625}\left(\frac{B}{\Sigma}\right)^6 + O\left(\frac{B}{\Sigma}\right)^8. \tag{3.6}$$

we will see in the next paragraph that the previous function will be the key function for the brand new proposed solution of B_1 system equation. Looking up to those equations, we note that neutron flux depends only on neutron energy E because this is already an angular and volume integrated quantity. The final goal is to get the total neutron flux in the calculation zone but those equations are also used to find the critical *buckling*, i.e., the value of B^2 that will led lead to an *effective* multiplication factor k_{eff} equal to one.

After this brief introduction on B_1 equations, we could do the condensation over different energy groups. We define G energy groups, where we indicate with E_G the minimum thermal neutron energy (order of 0.025 eV) and with E_0 the maximum fast neutron energy (order of 20 MeV). If we condensate each quantity present in those previous equations we have the following definitions:

$$\phi_g = \int_{E_{g+1}}^{E_g} dE\phi(E), \tag{3.7}$$

$$\chi_g = \int_{E_{g+1}}^{E_g} dE\chi(E), \tag{3.8}$$

$$D_g = \frac{1}{\phi_g} \int_{E_{g+1}}^{E_g} dEd(B,E)\phi(E), \tag{3.9}$$

$$\Sigma_g = \frac{1}{\phi_g} \int_{E_{g+1}}^{E_g} dE\Sigma(E)\phi(E), \tag{3.10}$$

$$\Sigma_{f,g} = \frac{1}{\nu\phi_g} \int_{E_{g+1}}^{E_g} dE\Sigma_f(E)\phi(E)\nu, \tag{3.11}$$

$$\Sigma_{s0,g\leftarrow h} = \frac{1}{\phi_g} \int_{E_{g+1}}^{E_g} dE \int_{E_{h+1}}^{E_h} dE'\Sigma_{s,0}(E \leftarrow E')\phi(E'), \tag{3.12}$$

$$\Sigma_{s1,g\leftarrow h} = \frac{1}{D_g\phi_g} \int_{E_{g+1}}^{E_g} dE \int_{E_{h+1}}^{E_h} dE'\Sigma_{s,1}(E \leftarrow E')d(B,E)\phi(E'), \tag{3.13}$$

$$\langle\gamma(B,\Sigma)\rangle_g = \frac{1}{D_g(B)\Sigma_g\phi_g} \int_{E_{g+1}}^{E_g} dE\gamma(B,\Sigma(E))d(B,\Sigma)\Sigma(E)\phi(E) \tag{3.14}$$

which can be used in the integration of B_1 equation over the generic energy integral $[E_g, E_{g+1}]$. After the integration and further semplification, the condensed form of B_1 equations is:

$$[\Sigma_g + B^2 D_g]\phi_g = \sum_{h=1}^{G} \Sigma_{s0,g\leftarrow h}\phi_h + \frac{\chi_g}{K_{eff}} \sum_{h=1}^{G} \nu\phi_h\Sigma_{f,h} \tag{3.15}$$

and

$$3D_g(B)\gamma(B,\Sigma_g)\Sigma_g\phi_g = \phi_g + 3\sum_{h=1}^{G} \Sigma_{s1,g\leftarrow h}D_h(B)\phi_h. \tag{3.16}$$

A further semplification can be done by rewriting the last one as it follows:

$$D_g(B)\phi_g = \frac{1}{w(B,\Sigma_g)} \left\{ \phi_g + 3\sum_{h=1}^{G} \Sigma_{s1,g\leftarrow h}D_h(B)\phi_h \right\} \tag{3.17}$$

with $w(B,\Sigma_g) = 3\gamma(B,\Sigma_g)\Sigma_g$. Since we have considered G energy groups in our energy condensation, we will have G equations for each of the B_1 equations. The resolving system is easier to visualize if we refer to its vectorial formulation:

$$\Sigma\Phi + B^2\mathbf{D}\Phi = \Sigma_{s0}\Phi + \frac{1}{k_{eff}}\chi \otimes (\mathbf{F}\Phi) \tag{3.18}$$

and

$$\mathbf{W}\mathbf{D}\Phi = \Phi + 3\Sigma_{s1}\mathbf{D}\Phi \tag{3.19}$$

where we have defined the vectorial quantities as

$$\Sigma = \begin{bmatrix} \Sigma_1 & 0 & ... & 0 \\ 0 & \Sigma_2 & ... & 0 \\ ... & ... & ... & 0 \\ 0 & ... & 0 & \Sigma_G \end{bmatrix} \tag{3.20}$$

$$\Phi = \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ ... \\ \Phi_G \end{bmatrix} \tag{3.21}$$

$$\mathbf{D}\Phi = \begin{bmatrix} D_1\Phi_1 \\ D_2\Phi_2 \\ ... \\ D_G\Phi_G \end{bmatrix} \tag{3.22}$$

$$\chi = \begin{bmatrix} \chi_1 \\ \chi_2 \\ ... \\ \chi_G \end{bmatrix} \tag{3.23}$$

$$\mathbf{F} = [\nu\Sigma_{f,1}, ..., \nu\Sigma_{f,G}] \tag{3.24}$$

$$\mathbf{W} = \begin{bmatrix} w(B,\Sigma_1) & 0 & ... & 0 \\ 0 & w(B,\Sigma_2) & ... & 0 \\ ... & ... & ... & 0 \\ 0 & ... & 0 & w(B,\Sigma_G). \end{bmatrix} \tag{3.25}$$

The ultimate aim of the vectorial equations presented above is to calculate the value of neutron flux and if we refer to equation (3.18), firstly we have to set this equation in order to have Φ as the only unknown variable, so from equation (3.19) we find the value of the product $\mathbf{D}\Phi$

$$[\mathbf{W} - 3\Sigma_{S1}]\mathbf{D}\Phi = \Phi \tag{3.26}$$

and by the inversion of the term $[\mathbf{W} - 3\Sigma_{S1}]$, that we suppose invertible most of the time, we have

$$\mathbf{D}\Phi = [\mathbf{W} - 3\Sigma_{S1}]^{-1}\Phi \tag{3.27}$$

which substitute in(3.18) gives

$$\Sigma\Phi + B^2[\mathbf{W} - 3\Sigma_{S1}]^{-1}\Phi = \Sigma_{s0}\Phi + \frac{1}{k_{eff}}\chi \otimes (\mathbf{F}\Phi) \tag{3.28}$$

We see that now we have the unknown Φ comparing in each term of the previous equation and since the trivial solution of the flux does not make any phisical sense, we have to apply a constraint which is often called *normalization* constrain, as

$$k_{eff} = \mathbf{F}\Phi \tag{3.29}$$

and so our resolving equation becomes

$$[\Sigma + B^2[\mathbf{W} - 3\Sigma_{S1}]^{-1} - \Sigma_{s0}]\Phi = \chi \tag{3.30}$$

from where we obtain the flux

$$\Phi = [\Sigma + B^2[\mathbf{W} - 3\Sigma_{S1}]^{-1} - \Sigma_{s0}]^{-1}\chi \tag{3.31}$$

So, to recap we firstly suppose a value of B^2 since the matrix $\mathbf{W}$ depends both on the total cross section and the buckling; then we calculate the inverse of $[\mathbf{W} - 3\Sigma_{S1}]$ and we subsitute it in equation (3.31) from which we calcualte the neutron flux and therefore the moltiplication factor thanks to the normalization factor. However, one of the hypotesis of the leakage model was that the value of k_{eff} was equal to one, since we added the leakage term to enfore this hypotesis. After that, we must say that the value of B^2 should not be guessed but it should be calculate in order to satisfy the unitary value of the multiplicative factor and this is actually a non linear eigenvalue problem which is generally solved iteratively by root-finding algorithm. In the next paragraph we will briefly introduce a new method developed by Dr. Daniele Tomatis (CEA Saclay), which has been implemented in our code and which leads to an easier resolution of the problem.

4 The Homogeneous B_1 model as polynomial eigenvalue problem

We have seen that the B_1 approximation of neutron transport yields mathematically to a non linear eigenvalue problem whose solution is sought iteratively in combination with the eigenvalue problem of the multiplication factor. A root-finding algorith is employed to converge on a given eigenvalue B, representing the curvature of the flux on a microscopic scale while the power method resolves the eigenvalue problem for a fixed value of B to find the unitary multiplication factor. Here we show theoretically, how to achieve the solution using a single linear eigenvalue problem instead of the non linear interative method.

Going back to the quantities introduced in the previous paragraphs, if we first substitute the factorization defined in (3.3) in the neutron transport equation (steady state version) defined in equation (2.4) and then we use the expansion of the differential scattering term using zero and first order Legendre polynomial[10], we obtain the following

$$\left[\Sigma(E) + i\mathbf{B} \cdot \mathbf{\Omega}\right]\varphi(E, \mathbf{\Omega}) = \frac{1}{4\pi}\int_0^\infty dE'$$
$$\cdot\left\{\left[\Sigma_{s,0}(E \leftarrow E') + \frac{\chi(E)}{k}\nu\Sigma_f(E')\right]\Phi(E') + 3\Sigma_{s,1}(E \leftarrow E')\mathbf{\Omega} \cdot \mathbf{J}(E')\right\}, \tag{4.1}$$

with the scalar flux $\Phi = \int d\mathbf{\Omega}\varphi$, the current $\mathbf{J} = \int d\mathbf{\Omega}\mathbf{\Omega}\varphi$ and k, which is here a simple parameter normalizing the fission production, set to one. Now, if we multiply both members of equation (5.1) by the factor

$$\frac{1}{\Sigma(E) + i\mathbf{B} \cdot \mathbf{\Omega}} = \frac{\Sigma(E) - i\mathbf{B} \cdot \mathbf{\Omega}}{\Sigma^2(E) + (\mathbf{B} \cdot \mathbf{\Omega})^2},$$

and integration in angle. Two complex integrals over the unitary sphere arise [11]:

$$\frac{1}{4\pi} \int_{4\pi} d\mathbf{\Omega} \frac{\Sigma^2}{\Sigma^2 + (\mathbf{B} \cdot \mathbf{\Omega})^2} = \alpha(B, \Sigma)\Sigma, \quad \text{with} \tag{4.2a}$$

$$\alpha(B, \Sigma) = \frac{1}{B} \cdot \begin{cases} \arctan \dfrac{B}{\Sigma}, & \text{if } B^2 > 0; \\[2mm] \displaystyle\sum_{n=0}^{\infty} \dfrac{(-1)^{(n)}}{2n+1} \left(\dfrac{B}{\Sigma}\right)^{(2n+1)}, & \text{if } B/\Sigma \approx 0; \\[4mm] \dfrac{1}{2} \ln \left|\dfrac{\Sigma + B}{\Sigma - B}\right|, & \text{if } B^2 < 0. \end{cases} \tag{4.2b}$$

$$\frac{1}{4\pi} \int_{4\pi} d\mathbf{\Omega} \frac{(\mathbf{\Omega} \otimes \mathbf{\Omega}) \cdot \mathbf{B}}{\Sigma^2 + (\mathbf{B} \cdot \mathbf{\Omega})^2} = \beta(B, \Sigma)\mathbf{B}, \quad \text{with} \tag{4.2c}$$

$$\beta(B, \Sigma) = \frac{1 - \alpha(B, \Sigma)\Sigma}{B^2}. \tag{4.2d}$$

By Eqs. 4.2, the weighted integration of Eq. 4.1 yields

$$\Phi(E) = \alpha(B, \Sigma(E)) \int_0^{\infty} dE' \left[\Sigma_{s,0}(E \leftarrow E') + \chi(E)\nu\Sigma_f(E')\right] \Phi(E')$$
$$- 3i\beta(B, \Sigma(E)) \int_0^{\infty} dE' \Sigma_{s,1}(E \leftarrow E')\mathbf{B} \cdot \mathbf{J}(E'). \tag{4.3}$$

The result of the previous derivation is combined with the conservation equation obtained by simple integration in angle of Eq. 4.1:

$$\Sigma(E)\Phi(E) + i\mathbf{B} \cdot \mathbf{J}(E) = \int_0^{\infty} dE' \left[\Sigma_{s,0}(E \leftarrow E') + \chi(E)\nu\Sigma_f(E')\right] \Phi(E'). \tag{4.4}$$

For parity reasons, we must note that the integral in angle of $(\mathbf{\Omega} \cdot \mathbf{J})$ vanishes. The scalar product between the vectors $\mathbf{B}$ and $\mathbf{J}$ can be replaced in all equations by the term (BJ), that is considering only their magnitudes. The substitution of Eq. 4.3 into Eq. 4.4 provides after reordering the new equation:

$$\frac{iJ(E)}{B} = \frac{1}{\Sigma\gamma(B, \Sigma)} \left[\frac{1}{3}\Phi(E) + \int_0^{\infty} dE' \Sigma_{s,1}(E \leftarrow E')\frac{iJ(E')}{B}\right] \tag{4.5}$$

$$\text{with} \quad \gamma(B, \Sigma) = \frac{1}{3\Sigma}\frac{\alpha(B, \Sigma)}{\beta(B, \Sigma)} = \sum_{n=0}^{\infty} c_n \left(\frac{B}{\Sigma}\right)^{2n}. \tag{4.6}$$

The coefficients c_n are determined by Maclaurin expansions for $B/\Sigma \to 0$:

$$c_1 = \frac{4}{15}, \ c_2 = -\frac{12}{175}, \ c_3 = \frac{92}{2625}, \ c_4 = -\frac{7516}{336875}, \ \cdots$$

The last definition introduces the leakage coefficient, which is basically a diffusion coefficient[3]:

$$D(B, E) = \frac{iJ(E)}{B\Phi(E)}. \tag{4.7}$$

If we introduce the energy multigroup formalism like we did in paragraph (3), we obtain the same as equations (3.18) and (3.19) and after some analitical steps we arrive at the following

$$- B^2 \vec{\Phi} = 3 \left(\mathrm{diag}(\vec{\gamma}(B^2)) \cdot \mathbf{T} - \mathbf{S}_1 \right) \mathbf{R} \vec{\Phi}, \tag{4.8}$$

with the removal matrix $\mathbf{R} = \mathbf{T} - \mathbf{S}_0 - \chi \mathbf{F}$ ($\mathbf{T} = \mathrm{diag}(\vec{\Sigma})$). We also introduce the transport matrix $\mathbf{\Gamma} = \mathbf{T} - \mathbf{S}_1$ to simplify the notation hereafter.

Eq. 4.8 shows a non-linear eigenvalue problem to solve. Now, the key for its resolution may be found by a proper change of variable in order to get a simpler problem, thanks to the Maclaurin series expansion of the function γ in a sum of monomial terms as defined in Eq. 4.6. The substitution of the series expansion of γ in Eq. 4.8 yields:

$$
\begin{aligned}
-\frac{B^2}{3} \vec{\Phi} &= \left[\left(\sum_{n=0}^{\infty} c_n B^{2n} \mathbf{T}^{-2n} \right) \cdot \mathbf{T} - \mathbf{S}_1 \right] \mathbf{R} \vec{\Phi} \\
&= \left[\mathbf{\Gamma} + \sum_{n=1}^{\infty} c_n B^{2n} \mathbf{T}^{-(2n-1)} \right] \mathbf{R} \vec{\Phi},
\end{aligned}
\tag{4.9}
$$

which is a polynomial eigenvalue problem of infinite order. After truncation of the sum to the first $(N+1)$ terms, the introduction of the following change of variable:

$$\vec{f}_{n+1} = B^2 \vec{f}_n, \text{ for } n = 0, \dots, N-1, \text{ with } \vec{f}_0 = \vec{\Phi}, \tag{4.10}$$

allows to obtain an ordinary linear generalized eigenvalue problem, where the eigenvalue is always B^2 (cm^{-2}). This kind of problem, it's of easier resolution if we put it in his vectorial form by introducing the vector of the new variables and the related matrices. Of course the better we want to approximize the gamma function and the more eigenvalues we will obtain, leading to a not simple eigenvalue distribution (spectrum). In the next page we show some graphs about gamma function and its polynomial approximation for different orders with connected percentage errors.
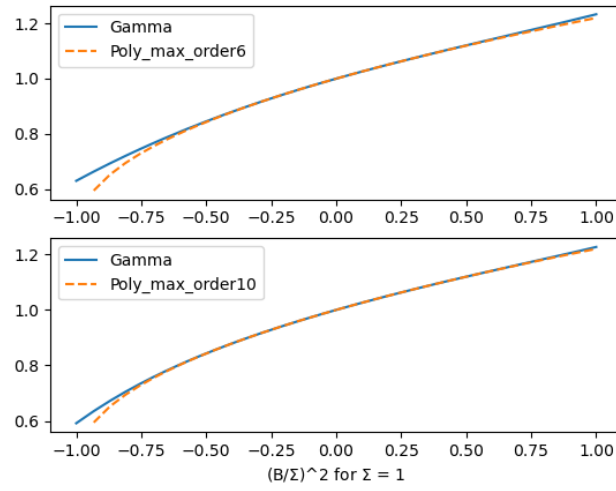
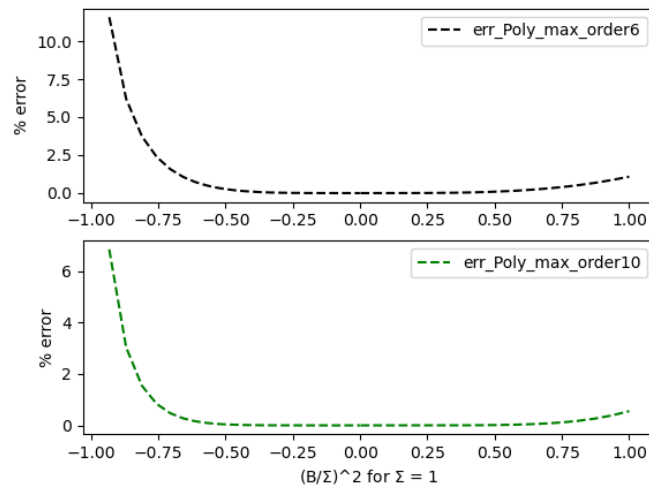**Figure 0.1.** Polynomial approximation for different orders.

Figure 0.2. Percentage error in different polynomial approximation.

Chapter Three

5   Modified depletion chain simplification method

Up to now we have presented the method adopted by Go Chiba who actually calculates neutron flux and the generalized adjoint neutron flux, which are required to obtain ANNDs and CFs with the collision probability method which is based on the spatial discretization of the integral transport equation in moultigroup form, assuming isotropic particle sources. In our derivation we use the B_1 leakage model for flux calculation since it would be very complex to calculate the adjoint neutron flux because we have the leakage constant B^2 as an additional unknown quantity. A modification in the method must be found and it's here presented.

   Throughout all the exposition we have stressed how the perturbation $\Delta N(t_i)$ affects the system of equations in study and now we want to give a better understanding of this influence; this perturbation affects the burnup matrix which changes directly because of flux, which itself changes indirectly because of the NND perturbed vector which acts on the transport operator B in the neutron transport equation. So, we want to find a relation between $\Delta N(t_i)$ and the variation of burnup matrix ΔM^i and replace this correlation in equation (2.21). Because of what we said before, it is logical to write firstly the relation between the burnup matrix $\mathbf{M}$ and the neutron flux vector Φ. Since in the B_1 leakage model we calculate the volume integrated multigroup neutron flux and we divide it by the whole calculation volume to get the averaged neutron flux, we could express relation (2.22) as

$$\Delta \mathbf{M}^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi^i{}_g} \Delta \phi_g^i \tag{5.1}$$

where ϕ_g^i is the g-th energy group neutron flux and where the total energy groups has been set to N_G. The partial derivative term can be calculated analytically, however we still don't know how to evaluate the variation of neutron flux $\Delta \phi_g^i$ due to $\Delta N(t_i)$; so we write the following

$$\Delta \mathbf{M}^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi_g^i} \Delta \phi_g^i = \sum_{g=1}^{N_G} \frac{\partial \mathbf{M}^i}{\partial \phi^i{}_g} \frac{d\phi^i}{d\mathbf{N}^{iT}} \Delta \mathbf{N}^i. \tag{5.2}$$

The derivative of the multi-group neutron flux to the NND vector has been estimated by us by means of the incremental ratio

$$\frac{d\phi^i}{d\mathbf{N}^{iT}} = \left[\frac{\partial \phi^i}{\partial N_1^T}, \frac{\partial \phi^i}{\partial N_2^T}, \cdots, \frac{\partial \phi^i}{\partial N_n^T} \right] \tag{5.3}$$

where for a generic nuclide k, the incremental ratio is equal to

$$\frac{\partial \phi^i}{\partial N_k{}^T} = \lim_{\epsilon \to 0} \frac{\phi_g^i \left(N_k(t_i) + \epsilon N_k(t_i) \right) - \phi_g^i(N_k(t_i))}{\epsilon N_k(t_i)} \tag{5.4}$$

and the definition is extended for $k \in [1,n]$ with n the number of isoptes taken into account. Now that we have a relation to express the variation of the burnup matrix, let's substitute it in equation (2.21), by getting in few steps the following

$$
\begin{aligned}
\Delta N_l(t_{i+1}) &= \mathbf{N}^{*T}(t_i)\Delta \mathbf{N}(t_{i+1}) + \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\Delta \mathbf{M}^i \mathbf{N}(t)dt \\
&= \mathbf{N}^{*T}(t_i)\Delta \mathbf{N}(t_{i+1}) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\frac{\partial \mathbf{M}^i}{\partial \phi^i{}_g}\frac{d\phi^i}{d\mathbf{N}^{iT}}\Delta \mathbf{N}^i \mathbf{N}(t)dt \\
&= \left(\mathbf{N}^{*T}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\frac{\partial \mathbf{M}^i}{\partial \phi^i{}_g}\frac{d\phi^i}{d\mathbf{N}^{iT}}\mathbf{N}(t)dt \right)\Delta \mathbf{N}^i \\
&= \widehat{\mathbf{N}}^{*T}(t_i)\Delta \mathbf{N}(t_i)
\end{aligned}
\tag{5.5}
$$

where $\widehat{\mathbf{N}}^{*T}(t_i) = \mathbf{N}^{*T}(t_i) + \sum_{g=1}^{N_G} \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\frac{\partial \mathbf{M}^i}{\partial \phi^i{}_g}\frac{d\phi^i}{d\mathbf{N}^{iT}}\mathbf{N}(t)dt$ has been defined and named as the corrected adjoint nuclide number density. Up to now both Go Chiba's method and our method have been applied in a generic time interval $[t_i, t_{i+1}]$, which means that if this time interval is small enough, the burnup matrix can be regarded as constant. If we want to extend the calculations to a longer period and so to valuate its influence, the burnup matrix must be updated for each generic timestep and it will affect both the adjoint nuclide number density (ANND) and contribution function (CF). Now we will discuss how it is possible to make this time step extension of the method.

The first proposed calculation method is basically an extension of the one of Go Chiba's; in each of the generic timestep $[t_i, t_{i+1}] \in [t_{initial}, t_{final}]$, we conserve the final adjoint condition of the adjoint bateman equations which is $\mathbf{N}^*(t_{i+1}) = \mathbf{e}_l$ and so we keep the same definition of the corrected adjoint nuclide number density (and CF definition too). This timestep extension enable us to calculate the value of CF in each time interval, showing the local (in terms of time) importance of other nuclides to the target one.

The second proposed calculation conserves the final target nuclide perturbation; for the last time step, $[t_{final-1}, t_{final}]$, we calculate

$$\Delta N_l(t_{final}) = \widehat{\mathbf{N}}^{*T}(t_{final-1})\Delta \mathbf{N}(t_{final-1}) \tag{5.6}$$

and we keep it apart while for the other timesteps we will use the corrected adjoint nuclide number density as the final adjoint condition so $\mathbf{N}^*(t_{i+1}) = \widehat{\mathbf{N}}^*(t_{i+1})$. If we go back to equation (2.21) without the new final condition, we have

$$\mathbf{N}^*(t_{i+1})\Delta \mathbf{N}(t_{i+1}) = \mathbf{N}^*(t_i)\Delta \mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\Delta \mathbf{M}^i \mathbf{N}(t)dt \tag{5.7}$$

and after it

$$\widehat{\mathbf{N}}^*(t_{i+1})\Delta \mathbf{N}(t_{i+1}) = \mathbf{N}^*(t_i)\Delta \mathbf{N}(t_i) + \int_{t_i}^{t_{i+1}} \mathbf{N}^{*T}(t)\Delta \mathbf{M}^i \mathbf{N}(t)dt \tag{5.8}$$

where we recognise that the right hand side can be written as $\widehat{\mathbf{N}}^*(t_i)\Delta\mathbf{N}(t_i)$, leading to the following

$$\widehat{\mathbf{N}}^*(t_{i+1})\Delta\mathbf{N}(t_{i+1}) = \widehat{\mathbf{N}}^*(t_i)\Delta\mathbf{N}(t_i). \qquad (5.9)$$

We notice that if the perturbation $\Delta\mathbf{N}(t_{i+1})$ is induced by the variation from last time step, we have:

$$\Delta N_l(t_{final}) = \widehat{\mathbf{N}}^*(t_i)\Delta\mathbf{N}(t_i), \forall t \in [t_i, t_{final-1}]. \qquad (5.10)$$

With this new condition, the contribution function keeps the same meaning of identifing the importance of nuclides respect to a targe nuclide characteristic but this time it's giving us a global importance over the entire time interval and no more the local one. For keeping the definition of CF congruent with it's formulation, we have to change its formulation such as that

$$CF_{k,l}(t_i) = \frac{\widehat{\mathbf{N}_k}^{*T}(t_i)N_k(t_i)}{N_l(t_{final})}. \qquad (5.11)$$

Both those proposed calculation methods will be tested in the last chapter where we will comment the results and give it a physical meaning.

Chapter Four

6   Application of Bateman solver

In this chapter we will test our Bateman solver in order to understand if it gives reliable results and to check if it has been implemented correctly. The cases of interests, has previously said, will be the Xe^{135} and Sm^{149}, two of the most important fission product nuclides in reactor control; we will reserve firstly a section in which we describe the behaviour of this two particular nuclides, then we introduce the numerical method for Bateman equation resolution and in the end we set some tests to make sure that we obtain congruent results with the theory of fission product nuclide evolution.

6.1   Analyze Data

Before we start, we have to determine the physical state of nuclear data that will be used for the tests. This data file, named MPO, has been produced by the use of APOLLO3 which is the new multi-purpose deterministic nuclear code developed in the frame of the neutronics simulation project of the nuclear division energy (DES) of the CEA and with financial support from AREVA and EDF. The starting point of APOLLO3 is in fact the upload of isotopic physical data that are provided by four external libraries for the storage of the nucleus cross sectons, shelf shielding data, depletion data and for the kinetics parameters [12]. Anyway we won't present how this data has been obtained (for connected reserved reason) but we will briefly describe its structure. We will refer to our data has obtained by condensation in 2 energy groups and homogenized in a UO2 fuel pin cell, typical of the 17×17 AFA 3G fuel assembly used in PWR. However our treatment, for a simplified discuss, will be applied to a infinite homogeneous reactor and not to a heterogenous reactor. The dataset structure is summarized in the following, and in Table 0.1:

- 105 state points, since for 21 Burnup points considered, we have 5 linear power values;

- 158 nuclides in exam of which 122 of them are fission products, 19 are fissile nuclides and the rest are some very low atomic number nuclides;

- the number of energy groups for energy discretization is equal to two (an extention to 281 groups will be developed in the near future);

- the order of scattering anisotropy is equal to one.

Table 0.1. Data specifications of the parameters.

Burnup values (MWd/ tHM) :	0, 10, 20, 40, 70, 100, 200, 300, 400, 500, 750, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000, 9000, 10000
Linear power values (W/cm) :	0.0 , 44.5, 89.0 , 133.5, 178.0
Moderator Temperature (K) :	542.48

We said that we have 105 state points instead of 21 because those burnup points are referring to a definite power level which actually defines the different operation conditions on which the reactor is working. In fact if the reactor power changes, also the cross section of some isotopes will change for temperatures effects like the Doppler effect or by other means.

For checking further our nuclear data, we will get the nuclide concentration evolution with burnup under at full power level of some of the isotopes that we will use later on for the validation of the depletion chains simplified method. The ones that will be checked are ^{135}Xe and Sm^{149} respectively with their close progenitors I^{135} and Pm^{149}; since those nuclides are very important for Reactor Control, we should firstly give some basic notions about the poisoning fission products.

6.2 Cases of study

Xenon Poisoning

The isotope Xe^{135} is of extreme importance in thermal reactors because it has a resonance in the thermal range ($\approx$0.08 eV) whose average thermal cross section in about $8 \cdot 10^6$ barn [1]; some xenon is found directly as a fission product, but more is produced as the result of a radioactive decay chain which begins with Te^{135} (half-life, 2 min) and proceeds through I^{135} (half-life, 6.7)to Xe^{135}. The Xenon itself is radioactive and it decays in 9.2 h. As the Beginning Of Cycle (BOG) starts, there is initially no iodine or xenon and just after a certain lenght of time, equilibrium concentrations of these quantities are reached; for instance, the production of xenon by direct formation plus decay of iodine is just balanced by its removal by radioactive decay plus burnup. Bateman equation for I^{135} and Xe^{135} formalize in a first order differential equation exactly what we said in words[7]:

$$\frac{dI(t)}{dt} = \gamma_I \bar{\Sigma}_f \phi - \lambda_I I(t) \tag{6.1}$$

and

$$\frac{dX_e(t)}{dt} = \lambda_I I(t) + \gamma_{Xe} \bar{\Sigma}_f \phi - \lambda_{Xe} Xe(t) - \bar{\sigma}_{a,Xe} \phi X_e(t) \tag{6.2}$$

where we have used λ_I, λ_{Xe} respectively as decay constant $(s^{-}1)$ of iodine and xenon and γ_I, γ_{Xe} for the effective yield of each isotope and $\bar{\sigma}_{a,Xe}$ as the average thermal absorbtion cross section. It's interesting to notice that the macroscopic fission cross section $\bar{\Sigma}_f$ and ϕ might be functions of time and the solutions to these equations depend upon the nature of these functions.

---

[1]1 barn is equal to 10^{-24} cm^2.

Because the half lives of iodine and xenon are so short and the absorbtion cross section of xenon is large, the concentrations of these isotopes, in all the reactors except those operating at low flux, quickly rise to their saturation or equilibrium values that can be found by setting the time derivatives equal to zero; those equilibrium values are[7]:

$$I_{eq} = \frac{\gamma_I \bar{\Sigma}_f \phi}{\lambda_I} \tag{6.3}$$

and

$$Xe_{(eq)} = \frac{(\gamma_I + \gamma_{Xe})\Sigma_f \phi \bar{\sigma}_{a,Xe}}{\lambda_{Xe} + \bar{\sigma}_{a,Xe}\phi} \tag{6.4}$$

Samarium Poisoning

Sm^{149} has a termal cross section of 40000 barns and it also must be included separately in reactor calculations; it's not formed directly in fission but apperars as the result of decay of Nd^{149} that decays comparatively rapidly to Pm^{149} (the intermidiate one in the chain), and so the Pm^{149} may be assumed to be produced directly in fission. The concentration of promethium is given by the equation[7]

$$\frac{dP(t)}{dt} = \gamma_P \bar{\Sigma}_f \phi - \lambda_P P(t) \tag{6.5}$$

and since samarium is stable, it disappears only as the result of neutron capture. The relevant equation is [7]:

$$\frac{dS_m(t)}{dt} = \lambda_P P(t) - \bar{\sigma}_{a,Sm}\phi S_m(t) \tag{6.6}$$

with the same quatity described before but now refered to prometio and Samarium. Since the absorbtion cross section of samarium is much less that the one of xenon and the half-life of promethium is longer than those of iodine and xenon, it follows that it takes somewhat longer for the promethium and samarium concentrations to reach their equilibrium values than it does for xenon. Placing the the time derivates equal to zero in both the previous two equations, we find the equilibrium concentrations as:[7]

$$P_{eq} = \frac{\gamma_P \bar{\Sigma}_f \phi}{\lambda_P} \tag{6.7}$$

and

$$Sm_{(eq)} = \frac{\gamma_P \Sigma_f}{\bar{\sigma}_{a,Sm}} \tag{6.8}$$

We have already noticed that in the derivation of equlibrium concentration of xenon and samarium, we assumed that $\bar{\Sigma}_f$ and ϕ were both constant, whereas in reality they are functions of time. So, as the macroscopic fission cross section decreases due to the burnup of the fuel, the flux should inscrease if the reactor has to operate at constant power[5].

6.3   Numerical method for solving Bateman equations

In the process of simplifying depletion chains, we need to solve both Bateman equations and its adjoint formulation in order to calculate contribution functions. We have seen that because of the coupling with the transport equation it's almost impossible to get analytic solutions of Bateman equations. The only way is to solve it by the use of numerical methods; the nuclide evolution equation is an ordinary differential equation (ODE) and must be solved with numerical methods that approximate the real solution in a discrete number of points. Those methods evaluate the unknown function by means of one step iterative algorithm, so defined since for the evaluation of the function at one step, it needs the value of the same function at the prievious or futher step (here we refer to time steps since the nature of the problem is on time demain). Let's now go into details for a better understanding.

Runge-Kutta algorithm

In our differential equation system the nuclide number density is the unknown function while time is our indipendent variable whom the NND is dependent on; the system can be generalized as

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) \tag{6.9}$$

with $\mathbf{y}(0) = \mathbf{y}0$ and $t \in [0, t_{end}]$; the goal of a numerical simulation to solve Equation (6.9) is to compute a sequence of time instants $0 = t_0 < t_1 <, ..., < t_N = t_{end}$ (not necessarily equidistant) and a sequence of states $\mathbf{y}_0, ..., \mathbf{y}_N$ such that $\forall\ l \in [0,N]$, $\mathbf{y}_l \approx \mathbf{y}(t_l, \mathbf{y}_{l-1})$, obtained by the help of an integration scheme.
A Runge-Kutta method, starting from an initial value $\mathbf{y}_l$ at time t_l and a finite time horizon h, the step-size, produces an approximation $\mathbf{y}_{l+1}$ at time t_{l+1}, with $t_{l+1} - t_l$ = h, of the solution $\mathbf{y}(t_{l+1}; \mathbf{y}_l)$. Furthermore, to compute $\mathbf{y}_{l+1}$, a Runge-Kutta method computes s evaluations of f at predetermined time instants. The number s is known as the number of stages. More precisely, a Runge-Kutta method is defined by[6]:

$$\mathbf{y}_{l+1} = \mathbf{y}_l + h \sum_{i=1}^{s} b_i \mathbf{k}_i \tag{6.10}$$

with

$$\mathbf{k}_i = \mathbf{f}\left(t_l + c_i h, y_l + h \sum_{i=1}^{s} a_{ij} \mathbf{k}_j\right). \tag{6.11}$$

The coefficient c_i, a_{ij} and b_i, for $i, j = 1, 2, ..., s$ fully characterize the Runge-Kutta methods and their are usually synthesized in a Butcher tableau [6] that has different shape depending on the kind of R-K method we are applying; in fact we could have explicit and implicit R-K methods that differ from each other wheter or not the function $\mathbf{k}_i$ (which assume the meaning of the spatial slope valuated at each interval) is computed just on previous steps or on intermediate steps involving $\mathbf{k}_i$ itself. The one that has been used in our solver is the explicit Runge-Kutta method of order 5(4) and the implicit Runge-Kutta method of the Radau IIA family of order

5[4]. Those methods have been choosed since they have strong stability properties (the present ODE system is a stiff problem[6]) which are not present for other numerical integration methods such as multi-step methods and the specified order of the algorithms was choosen to ensure good approxition with the exact solution (actually impossible to obtain analitically).

6.4 Numerical Tests

The first test is actually a check of nuclear data as we plot nuclide concentration of few nuclides (Xe^{135}, I^{135}, Sm^{149}, Pm^{149}) with Burnup under full power level.
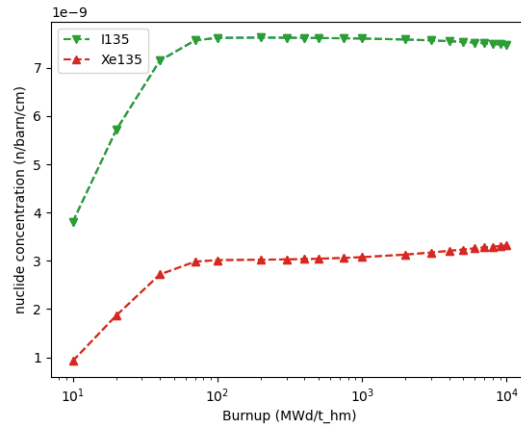
Figure 0.3. I135 and Xe135 concentration with Burnup
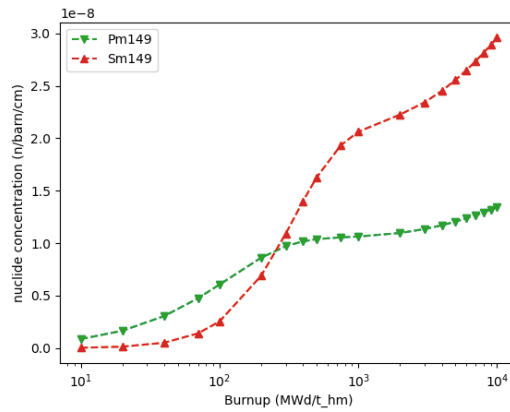
Figure 0.4. Pm149 and Sm149 concentration with Burnup

From the above figures we can see that for Xe^{135} and I^{135} we get the asymptotic concentrations for low values of Burnup (almost the same value for the two of them) while for Pm^{149} and Sm^{149} we need higher values of Burnup and this behavior was expected as highlighted in paragraph 6.2; of course different values will be obtained if we get the concentrations for different power level. If the operating conditions are

the one of full power level, we already have the equilibrium state (as the previous concentrations) while for other power level the initial concentrations are not the equilibrium ones. Let's check how the system evolves in time if we have, for a fixed Burnup value [here assumed as 2000 MWd $/t_H M$], different power levels. For iodine in Figure 0.5, we can see that the equilibrium state for full power level corresponds to a horizontal line since the system does not change in time (or better it changes very little) while for the other power levels the system evolves to its equilibrium concentration that of course are of lower value because of the minor neutron flux associated to linear power. Because of the decrease of iodine concentration with time we can say also confirm that initial concentrations were obtained in the condition of full power level and this justifies the decrement of the concentration since we have lowered the power level. For completeness, we show also the time evolution of the other nuclides for different power levels. For Xenon (Figure 0.6), we have a
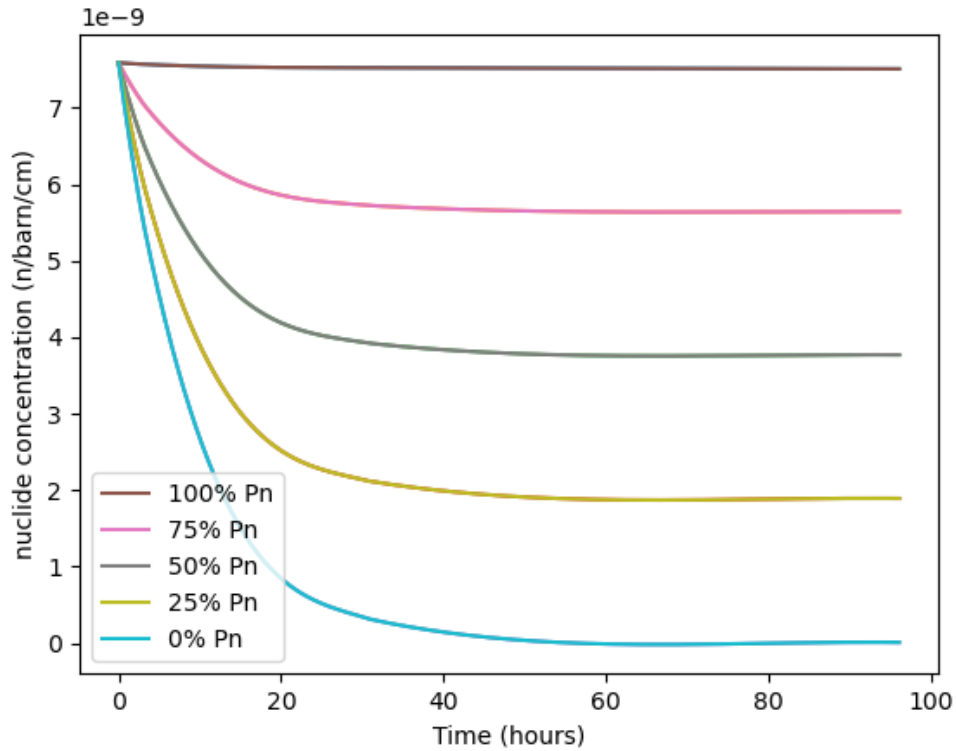
Figure 0.5. Time evolution of I^{135} for different power level (fixed BU)

particular behavior, firstly it increase since the buildup of Xe (due to the lowering of flux) is bigger than its depletion (always for the decrement of flux), it reaches a peak when rates of formation and depletion equalize and then it decreases to its equilibrium concentration.

Then for Pm^{149} (Figure 0.7) we have a similar behavior of the one of iodine (depletion equations have the same form), with the difference that the decrement
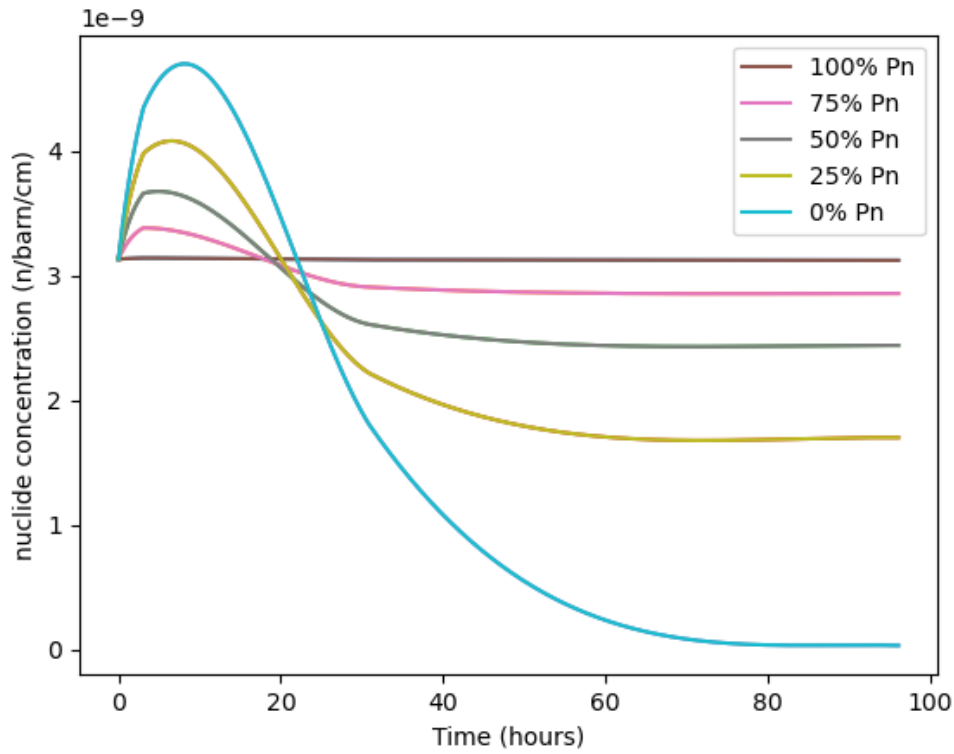
Figure 0.6. Time evolution of Xe^{135} for different power level (fixed BU)

is less rapid because of the longer half-life of promethium; Sm^{149} (Figure 0.8) is instead pretty different from the other nuclides since its equilibrium concentration increases with the decrease of power level and this is due to the fact that in its depletion equation the term with the flux is negative and power level will give less important to this term when lowered.

We also noticed throughout these tests that the evolution for different burnup points does not influence the general trend of nuclide evolution and that's why we can even not refer to a particular burnup value; this last observation is verified for the case of xenon and iodine (for instance in the case of full power level to zero power level for different burnup points, Figure 0.8 and Figure 0.9, and for promethium and samarium too but in this last case even if the trend is always the same, the initial and final values vary significantly and this is due to the fact that the concentration of these latter nuclide vary more than the other, for different burnup values (Figure 0.4).
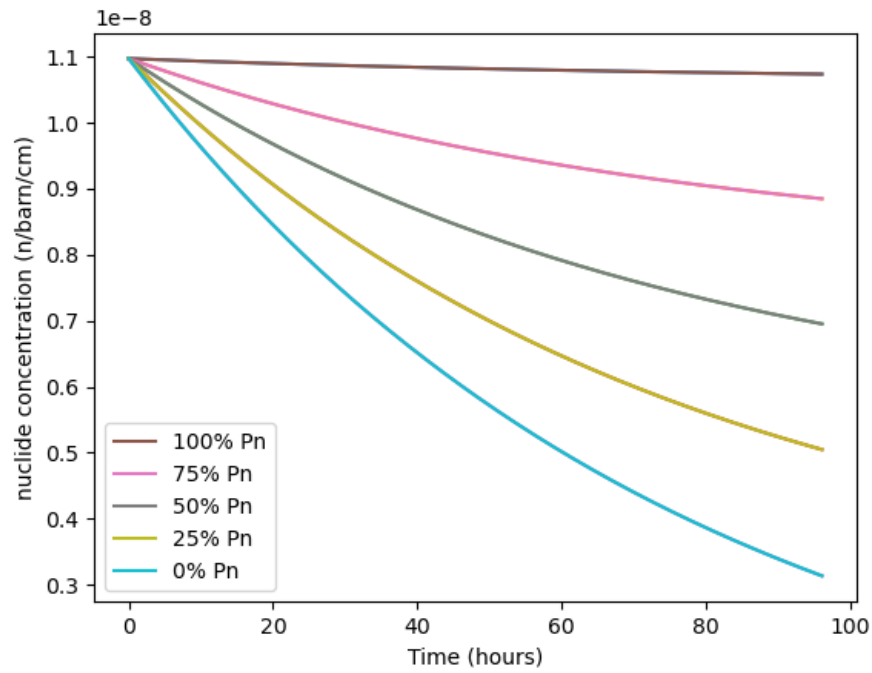
Figure 0.7. Time evolution of Pm^{149} for different power level (fixed BU)
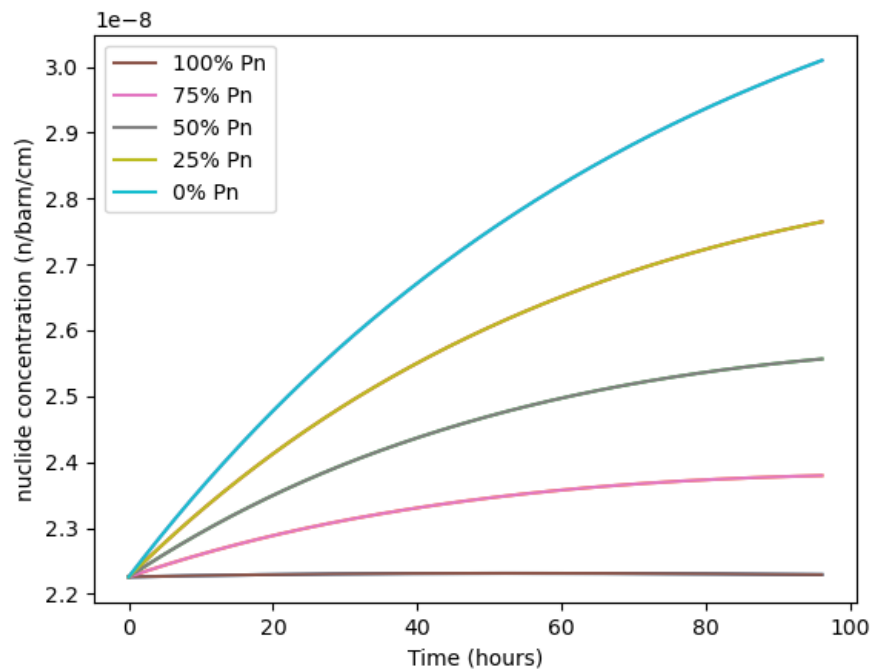

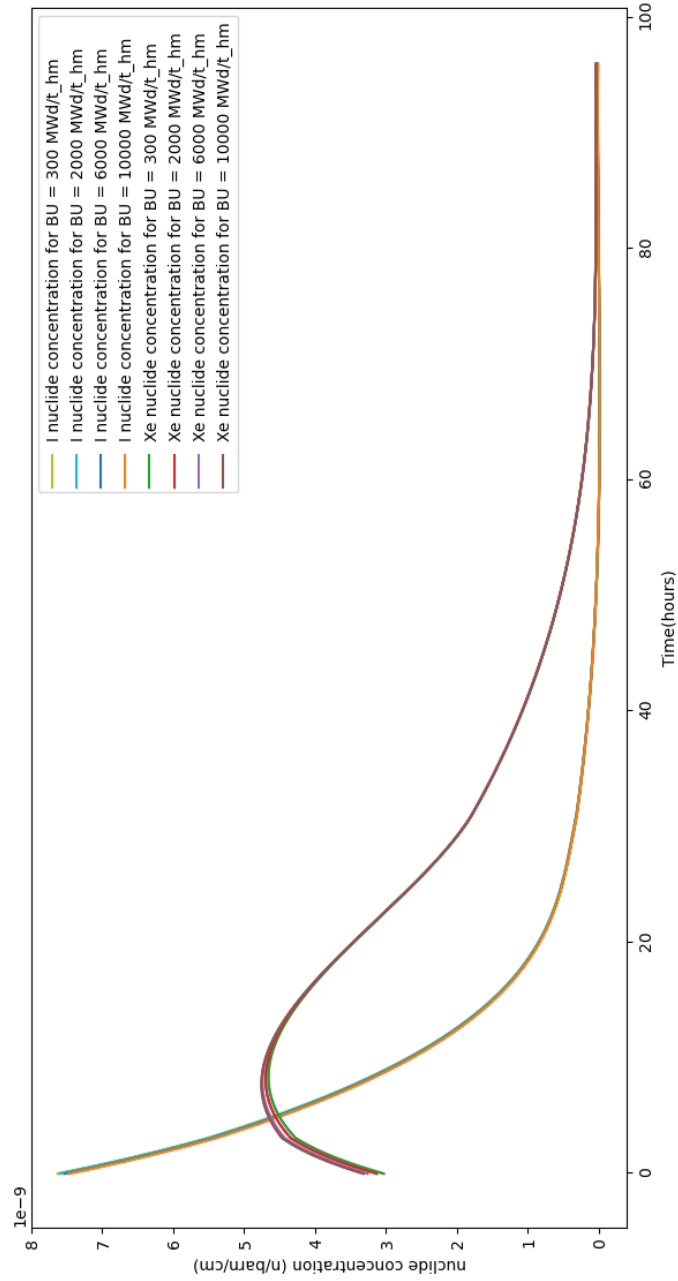**Figure 0.8.** Time evolution of Sm^{149} for different power level (fixed BU)

Figure 0.9. Evolution of I^{135} and Xe^{135} from 100%Pn to 0%Pn for different burnup points
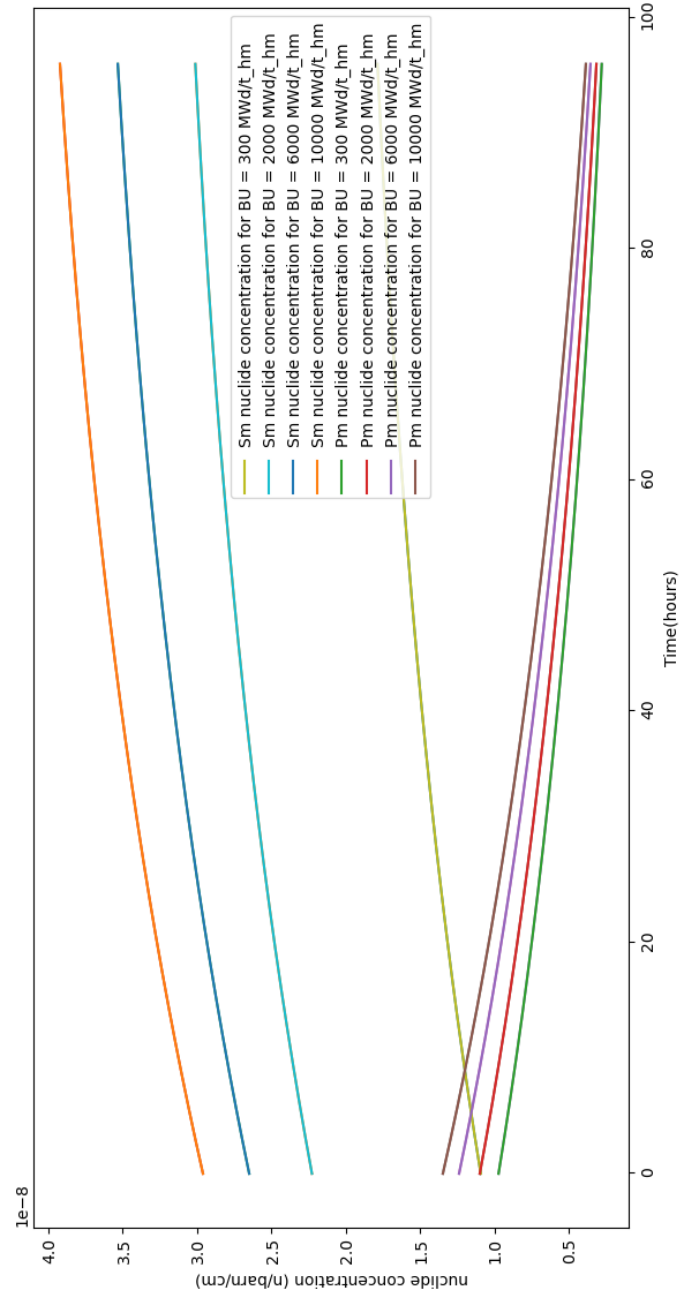
Figure 0.10. Evolution of Sm^{149} and Pm^{149} from 100%Pn to 0%Pn for different burnup points

The last test is about to deal with nuclide evolution from lower power level to full power level in order to understand if Bateman solver can give the right results even during the increasing of power (up to now we have analyzed just decreasing power cases). This time we will show results just for I^{135} and Xe^{135} since the behavior of all the fission products in exam is the same. First of all, since for other power level we said that the system is not in steady state (so in equilibrium), we let the system to evolve to its equilibrium concentration and then we apply a suddenly increase of power level. For both iodine and xenon we expect the reverse situation of Figure 0.5 and 0.6. In fact, iodine increases exponentially from different equilibrium concentrations of different power levels to a common asymptotic value, which is the one of full power level; xenon instead, firstly decrease and then after a minimum increases till it reaches the asymptotic value of full power level. We can say that the behavior is exactly reversed from the one of full power to different power levels and this is in accordance with theory.
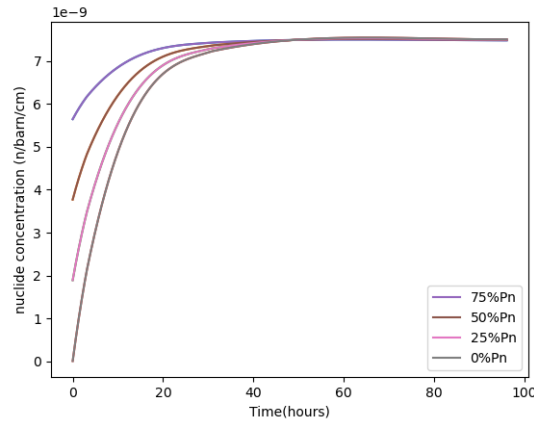

Figure 0.11. Time evolution of I^{135} for low power level to full power level (fixed BU)
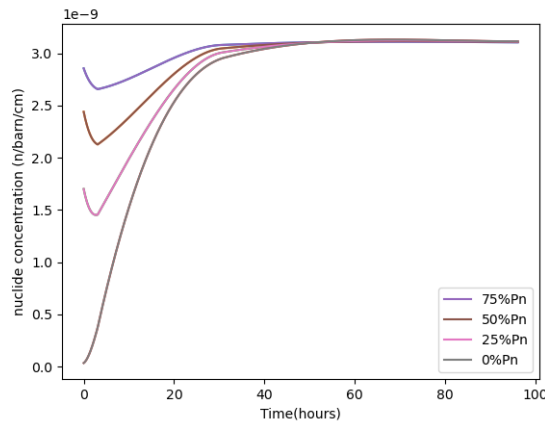

Figure 0.12. Time evolution of Xe^{135} for low power level to full power level (fixed BU)

Chapter Five

In this chapter we present the results of Contribution Functions calculation. We computed this function with the two method described in chapter 3; these methods apply different final adjoint condition for resolving adjoint Bateman equations in each time step and they differ theoretically from each other because one focuses on the local importance in each time interval while the other one focuses on the global importance in the whole time step. Before going into CF analysis we introduce some expected results based on intuition on how the system evolves when we introduce some perturbations on NND vector; those intuitions will be confirmed by CF analysis.

7 Expected results

Let's suppose we want to perform the following test: since we know already the depletion chain of our four target fission product nuclides, we want to prove that with a simple sensitivity analysis we can guess, by solving Bateman equations, which isotopes will be important and how important they could be during the time evolution.

We choose a steady state case in order to have the system already in equilibrium and we plot the equilibrium concentrations of Xe^{135}, I^{135}, Sm^{149}, Pm^{149}; then we give separately to the evolving system of xenon a perturbation ΔN_{I-135}, ΔN_{U-235}, ΔN_{U-238}, while to the evolving system of samarium separately we give ΔN_{U-235}, ΔN_{U-238} and ΔN_{Pm-95}.
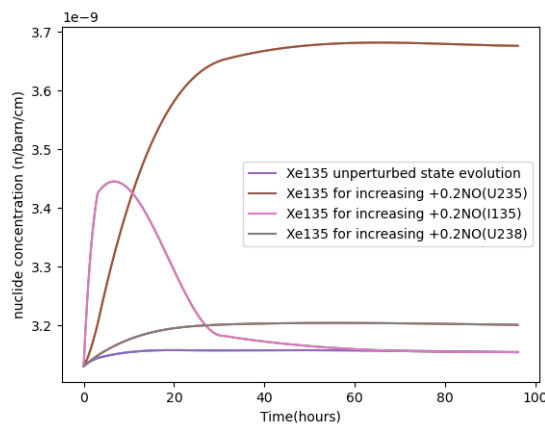

Figure 0.13. Time evolution of Xe^{135} for different nuclide perturbation

The entity of each perturbation is the 20% of the initial concentration at time t_i. After that, we plot the time evolution of this two nuclides and we obtain the results in Figure 0.11 and 0.12.
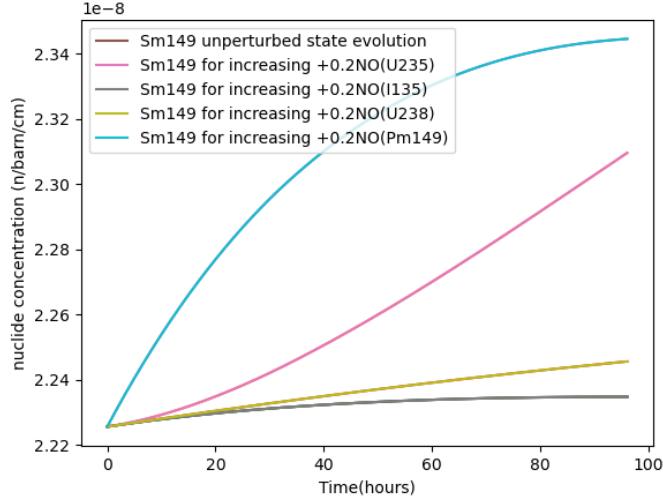

Figure 0.14. Time evolution of Sm^{119} for different nuclide perturbation

For xenon evolution with iodine perturbation, we have a rapid increase because of the increase of positive decay rate of iodine, then the peak and the decrease to the equilibrium value, which approaches the equilibrium concentration; for xenon evolution with uranium perturbation we see that, since an increase in uranium concentration will led to a higher macroscopic fission cross section, the concentration increases very rapidly and then it approaches a new equilibrium value. Even though we keep the same reactor power (which means a decrease of flux if the macroscopic fission cross gets higher), xenon concentration will always increase since the neutron absorbtion rate decreases. The entity of the increase of course is higher for the case of U_{235} that the one of U_{238} because of the higher contribution to fission cross section of the former.

For samarium evolution, we notice that both uranium perturbations led to higher concentrations and so it does promethium (it's so high that it changes concavity); we plotted also the concentration of samarium due to iodine perturbation and since iodine does not appear in the depletion chain of samarium, the evolving concentration is the same as the equilibrium one, as expected. From the above discussion we can say that in terms of importance, iodine and both uranium are the one that will be selected by CF as well as promethium and both uranium for samarium, but the importance will change for different time steps since at different time intervals the influence of the perturbation led to different concentration of the target nuclide. For instance, we can say that U_{235} will incease its importance to Xe_{135} with increasing time and so it will U_{238}; same thing for Sm_{119}. Moreover we say that the same procedure has been done with other initial nuclide perturbations for different nuclides, but since xenon and samarium have well known and short depletion chain, the exposition was limited to it.

8   CF analysis

In this section, we present the result of contribution function calculation. Up to now we have computed the steady state simulation which has shown some important results for a better understanding of contribution function meaning and some properties of the funtion itself, which is our discriminant for the construction of simplified depletion chains. First of all, we start by saying that we choose arbitrarily a state point which state parameters are: $BU = 2000MWd/t_HM$, $Tmod = 582.4K$, $Plin = 178W/cm$; we are at full power level so we do not need to wait for the equilibrium concentration to be reached, since we are already in steady state.

We perform the calculation in a time period of almost 100 hours (in accordance to the timescale buildup of xenon and samarium)for a value of perturbation equal to $\epsilon \cdot N$ with $\epsilon = 10^{-3}$; in both methods (Chapter 3) applied to this calculation, we compute the contribution function in a number of time step equal to the the one of Bateman and Adjoint Bateman equation (the solver could have picked a random number of points but we decided to make an accurate time discretization).

Both methods, for the selection of important nuclide number density of tested nuclide (158 nuclides in our case) respect to the nuclide number density of our targets (Xe^{135} and Sm^{149}), use a threshold value in order to compare it to the value of computed CFs. Only those nuclides that have a higher value than the threshold will be included in the simplified chain. The selected threshold value, here named $CF_{threshold}$, is equal to 10^{-6}; we have to say now that the chosen value of the threshold modifies in part how much do we want to be accurate in depletion chain reconstruction, in fact the more it is lower and the denser will be the chain. In this sense we note that computed CFS of non important nuclides are very small respect to the threshold so there's no risk in picking up wrong nuclides. After those clarification, we show our results for both the methods.
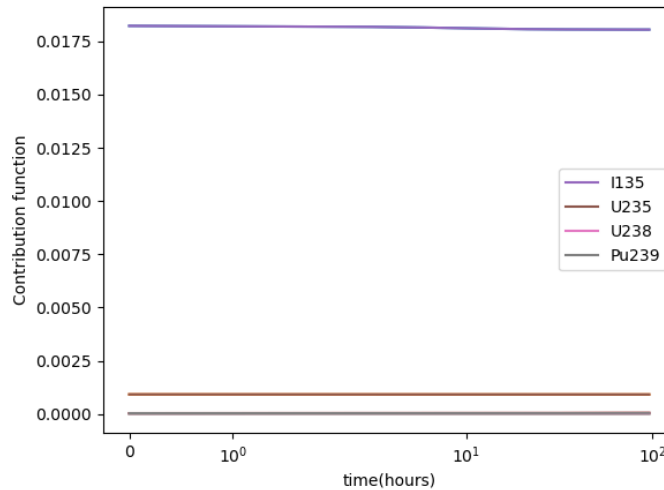

Figure 0.15. Time evolution of contribution function for selected important isotopes conserving initial perturbation respect to Xe^{135}
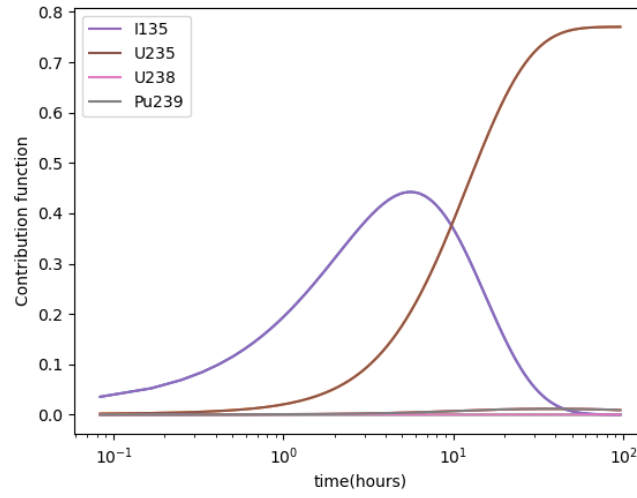
Figure 0.16. Time evolution of contribution function for selected important isotopes conserving final target perturbation for Xe^{135}
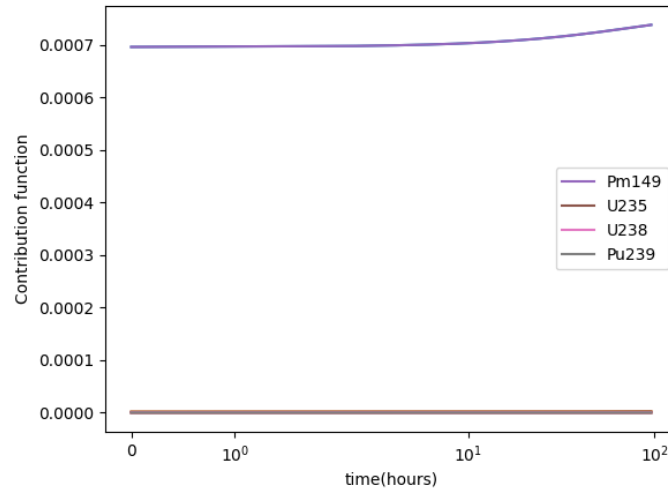

Figure 0.17. Time evolution of contribution function for selected important isotopes conserving initial perturbation respect to Sm^{149}
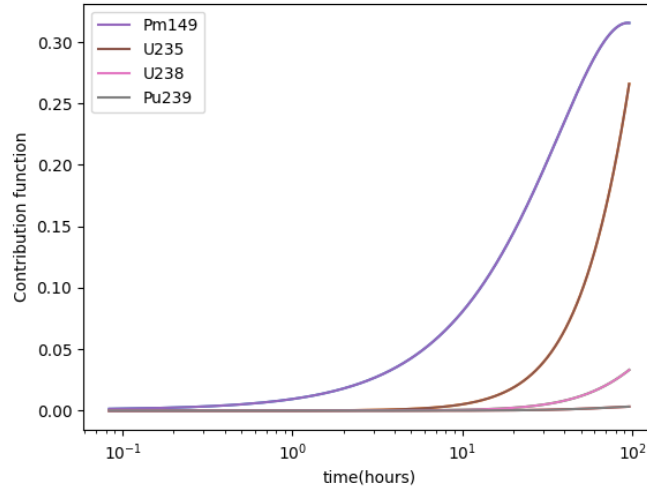
Figure 0.18. Time evolution of contribution function for selected important isotopes conserving final target perturbation for Sm^{149}

From Figure 0.15 and 0.16 we notice that contribution functions, for the first method, is almost constant during the whole time interval with values above the threshold just for the displayed nuclides which are the eexpected ones compared to the depletion chain obtainable in literature. For Xe^{135} the important nuclides are iodine, uranium (fissile and fissionable) and plutonium while for Sm^{119} we find the same nuclide, with promethium instead of iodine.

From the figure above we cannot distinguish the numerical values but from the codes we outplayed it and we saw that plutonium in both cases is very close to the limit value and it can be neglected for a first chain construction. The explanation of the flat behaviour has been indentified in the fact that we have chosen a case in which concentrations were already at the equilibrium value and even though we give the same perturbation at different time point, finally the system is still at equilibrium and the response of perturbation is the same. This behavior probably will not be verified for a transient state (since it takes a bit for reaching equilibrium concentrations and the contribution of different nuclide perturbation might be different).

For the second method, which is the conservation of final target nuclide perturbation, we found a competely different behavior. In this case, if we focus on Figure 0.13 we can see a huge similarity between CF and the nuclide evolution. Focusing on xenon, the trend of CF reflects the one of nuclide concentration evolution for all the nuclides. Respect to the previous method, the moment we give this perturbation is important since CF keeps memory of the previous value of CF and in this case we can say it behaves like a cumulative function since from its definition we are watching the influence on whole time period. Same discussion for Samarium.

The fact that this two methods give different results is because of the meaning that we attribute to CF. In the first case it gives us a local value (which in steady state we do not expect to vary noticeably) while for the second one it gives us global information in the whole period of study. Anyway, CF is able to identify those

important nuclides in both methods with the warning that the selected nuclides used for simplified chain construction, depend on the threshold value imposed to CF; this last choice depends on how much we want to be accurate in simplifying those depletion chains.

9   Conclusion

This work has shown that the procedure of contribution function gives expected results in terms of nuclide importance selection. The modifications to the original method have been done in order to obtain easier calculation (especially on the adjoint transport equation) and to validate a new procedure for the contruction of simplified depletion chains. However, more tests must be done in order to understand if our first intuition was correct. Especially the transient state must be analyzed to understand if the two methods still conserve the same behavior shown in steady state. However, we can say from now that CF is dependent on the time duration of the perturbation and on the instant this perturbation is given. Moreover, even if secondary for the moment, the number of tested nuclides should be incresed in order to understand if the method is able to identify important nuclides also for isotopes that have more complex depletion chains.

From the procedural point of view, in the near future we will extend the energy discretization to 281 groups in order to have more reliable results by increasing also the number of nuclides in our dataset from 158 to almost 1000. Once we have done those improvements we can have enough accurate results to make some comparisons between this method and the one of Hokkaido University, Japan whom we have shown in details procedures and differences.

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