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Validation of ALEPH2 depletion code on the spent fuel isotopic content of samples irradiated in Gösgen PWR core

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Lucien Massinon

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Introduction

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1.1. Context

ALEPH is a Monte-Carlo burn-up code which is being developed in SCK-CEN (Studie Centrum voor de Kernenergie - Centre d'Etude de l'énergie Nucléaire, Belgium) since 2004. It belongs to the category of codes where a Monte-Carlo transport of particles is coupled with the resolution of a depletion system - in order to determine the evolution of material compositions in time.

The first part of the code, the Monte-Carlo calculation, is achieved in this document with MCNP5[1] (a code from the widely used family of codes, MCNP) and gives an estimation of the steady-state Boltzmann neutron transport solution at the beginning of every time step - thanks to neutron interaction data (microscopic reaction cross sections, energy spectra of outgoing neutrons scattered by atoms of the problem, energy spectra of newborn neutrons from fissions of U-235, U-238, Pu-239, etc.) available in files attached to the problem. Regarding the ALEPH-specific part, it first calculates physical reaction rates thanks to the above estimation and the thermal power of the problem at the given time, and finally computes the concentration of every nuclide of the materials at the end of the time step by solving first-order ordinary differential equations which state that the evolution of a nuclide's concentration is equal to the sum of the nuclide's creation rates from the fissions and decays of other nuclides, reduced by its loss rates due to fissions, neutron captures and decays as well.

From the release of ALEPH version 1, several principal modifications have been made to the code. For instance, the nuclear data set has been expanded, the former depletion solver ORIGEN-2.2 [1] has been replaced by a built-in advanced algorithm in order to gain accuracy (at the expense of calculation time, though), the heatings due to α, β and γ radiations are now taken into account in the thermal power produced by a material, the number of required code lines necessary to launch a simulation has been reduced, etc.
All these changes have led to the creation of the second version of the code, entitled ALEPH v2, or ALEPH2 in this document.

In order to extend the bank of its validation cases, the purpose of this document consists thus in testing the ALEPH2 code on a new benchmark case and in seeing whether the results fit the expected values or not.

[1] The Monte-Carlo code can be any version starting from MCNP4C, though: MCNP4C, MCNP5, MCNP6, MCNPX, etc.

1.2. Study case

GU3 and GU3' are two adjacent fuel samples which have been cut in 1997, after a three-cycle neutron irradiation in a fuel rod of Gösgen, a PWR plant located in Däniken, Switzerland. After a two-year cooling, the samples were brought, dissolved and radiochemically analysed in two diferent laboratories: the SCK-CEN and the ITU (Institute for Transuranium Elements, Germany) laboratory. A total of 53 isotopes, including both long and short-lived nuclides were measured there and recorded in a technical report [23].

From the description of Gösgen reactor (geometry, nominal thermal power, fuel enrichment, etc.), the irradiation history of the fuel and the cooling of the samples have been simulated by ALEPH2, and the comparison between the measured values of the concentrations of the nuclides and their computed values from the output file is made in the present document.

1.3. Contents of the document

The present document will be divided in six separate parts: the ALEPH2 theoretical basis, the characteristics of the study case, the description of the ALEPH2 input file related to the study case, the analysis of the simulation's output, the additional studies made on the problem and the conclusion.

The chapter devoted to the theoretical basis will describe the MCNP5 code and its methods to obtain the MCNP neutron flux spectra [21], followed by the depletion methodology used in ALEPH2 [20].

The following section will be devoted to the study case description, with in particular, the description of the reactor core, the irradiation history of the samples and their cooling from the removal of the plant to the dates of the chemical analysis experiments.

Regarding the description of the input file, it will globally consist in explaining how to translate the study case into ALEPH2 code lines, thanks to MCNP's [22] and ALEPH2's [20] manuals.

The analysis of the output of the simulation will be related to the comparison between the computed concentrations of selected nuclides and their measured values.

The sixth section will then present the results of sensitivity studies in which some parameters are added or adjusted in the input file, and will show whether the accuracy of the results is improved with them or not.

Finally, a conclusion based on the results, their accuracy compared to the measured values and on the sensitivities of final concentrations to the perturbations of parameters, will be made.

Theory

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Sommaire

As stated in the introduction, ALEPH2 is a Monte-Carlo burn-up code developed in SCK-CEN, Belgium. The purpose of this document is the simulation of the neutron irradiation history in a reactor core and the depletion of selected materials inside it. In order to carry out such a task, the irradiation and post-irradiation history of these materials is first divided in several steps and, regarding whether an updated neutron flux is required during the step (irradiation step), a Monte-Carlo transport code (MCNP code) is launched and simulates neutrons everywhere in the volume of the problem. From the spatial-energy distributions of those neutrons are then calculated reaction rates and finally the depletion of the selected materials of the problem. On the contrary, when no neutron flux is needed for the step (decay step), only the depletion algorithm is applied and the calculation goes here in a single phase.

MCNP codes (there are several versions) being widely used and validated for decades, one of ALEPH2's major interests lies in the fact that its input files are simply MCNP inputs to the top of which a few ALEPH2-specific cards are added. These specific cards are in particular the materials followed in the system, their volume, the path to the Monte-Carlo code executable, the path to the folder containing neutron-induced data and the description of the irradiation or decay substeps.
To make it simple, it can be said that the ALEPH2-specific cards contain all the temporal informations of the problem - i.e. the power, the time during which this power can be assumed constant, etc. - while the part of the input file related to MCNP contains all the chemical compositions and geometric informations.

When an ALEPH2 input is run, the following calculation flow is applied:

- First of all, ALEPH2 generates a MCNP input file - called "0.i" - by removing the extra top cards and adjusting the input to the corresponding step. It means particularly that the materials which are depleted by ALEPH2's solver are identified in the geometry and that the program provides an energy binning in each of them for the subsequent calculations.
- Then, a Monte-Carlo transport calculation is launched, throughout which a lot of neutrons with different energies and velocities are created in the entire problem. The geometry of the problem is itself divided into smaller volumes called *cells* which are each filled by a material. The neutrons are then followed separately by the program

which computes all their histories from birth to death, either by escaping from the system, through absorption by an atom or through an artificial termination if the critical mode is on.
To describe each elementary interaction as accurately as possible, the code requires a lot of cross section data. Indeed, MCNP has to know what the probability will be for the neutron to be absorbed by an atom of the material where the interaction is occuring, or again if it will fission an atom and create itself new neutrons, what will be their related energy in that case, etc. This is why the path to a huge folder containing neutron-induced data - nuclides' cross sections as well as emission distributions for secondary particles (if newborn fission neutrons are created or if the kinematics of scattered particles has to be calculated) or decay data - is attached to the ALEPH2 file during all the calculation. This complete nuclear library was computed thanks to an auxiliary utility called ALEPH-DLG (Data Library Generator) [19]. This one provides both the general transport neutron data suitable for the MCNP transport code, in ACE format (A Compact ENDF - Evaluated Nuclear Data Format)[1] and the ALEPH-format activation data used for the depletion of the materials. It can be added here that, an ALEPH2's particulate feature being the full data consistency between the MCNP ACE-formatted files and the files related to the depletion in the code, they use exactly the same reaction cross sections except that the second set of data is extended to higher energies, to higher numbers of nuclides (many more nuclides actually play a role in decay chaines of the problem than there are which have a significant effect on the neutron fluxes) and reactions per target nuclide by adding the activation data libraries. In the same idea of consistency, the common part of MCNP transport data and subsequent depletion data have their cross section tables linearized on the same energy grid[2].

- Then, from the motion of each neutron, it is possible for the MCNP code to compute a certain amount of values of interest. The quantities which are collected in the study case here are the neutron track lengths inside each cell and their relative statistical weight, i.e. their importance in the problem. A track refers to each component of a source particle during its history. For instance, a neutron may move along its line of flight from a position to another one located 2[cm] apart, then undergo an elastic scattering with an atom, move again 1[cm] to another direction and finally be absorbed by an atom. In the end, there would be in that case two tracks recorded by the program, each one with its proper length.
  It can be said that every neutron's motion is different in a core since there are a lot of materials in a system and they do not interact in the same manner with the neutrons. But above all, this can be explained by the fact that probabilities play a huge role in a nuclear system. For instance, two neutrons created at exactly the same place and with the same energy will maybe never follow the same path since one of them may be absorbed directly by an atom, while the other may be scattered through several collisions to eventually escape the system.
  Finally, from these neutron track lengths, time-independent estimations of the neutron fluxes inside the cells - called F4 tallies - are computed by MCNP and written in a

[1] ACE is a data compression archive file format suitable for MCNP. It includes all the details of the ENDF representations, but in a quite different form since all the cross sections are for instance given in a single union energy grid in which linear interpolation is possible.

[2] The energy distribution of each neutron cross section is in fact made of thousands of points which are so close to each other that linear interpolation between them reproduces the evaluated distribution over the energy of the cross section within a specified tolerance; this is why it can also be called *continuous energy neutron cross section*.

MCNP tally file called ”0.m”.
In the same time, an output text file containing all the informations of the previous calculation is created and named ”0.o”.

- Once the MCNP calculation is completed, ALEPH2 uses the top cards of the input file kept in memory since the very beginning ot the step and where the irradiation history - i.e. the thermal power and the time during which this power can be assumed - of the system is described. From this power, it is possible to use the F4 tallies from the ”0.m” file to calculate physical reaction rates, since time is now part of the problem.
  At this point, the code uses these reaction rates to deplete the selected materials from their initial compositions (defined previously in the part of the input related to the MCNP calculation) in order to calculate the new compositions of the materials at the end of the time step.
  It can be understood here that one basic working assumption of ALEPH2 is the invariability of reaction rates - i.e. neutron flux and its energy spectrum - within an irradiation time step. Indeed, the depletion solver uses values which have been computed at the beginning of the time step to solve compositions at the end of it[3].

- If another irradiation time step is available in the top cards, ALEPH2 generates a new MCNP input file - called ”1.i” - with the updated compositions of the materials. Here, since there are more data available in the ALEPH-format activation data files than in the MCNP ACE files, ALEPH2 truncates the full set of nuclides which result from the previous step to those nuclides for which the general purpose nuclear data are available, in order that no error occurs during the MCNP calculation. In the same kind of idea, ALEPH2 estimates then the number of collisions which may occur on every of the remaining nuclides and, if the result is too low, the nuclide is also not considered in the material composition list provided in the file ”1.i”.
  Then, exactly the same calculation flow as above is applied, except that the tallies of the MCNP calculation are this time written in a ”1.m” tally file, and that all the nuclides from step 0 are used during the depletion calculation, since ALEPH-format activation data are available for them here.

  On the contrary, if the following step is a decay step, no MCNP calculation is launched (and thus no ”1.i” nor ”1.m” files are created) since there is no neutron flux in the core. In that case, to deduce their new isotopic compositions, only a depletion due to decays is applied on the materials.

- At the end, after that n - irradiation or decay - steps have been taken into account by ALEPH2 (and thus n ”.o” files generated), the final ALEPH2 output is created and made available to the user. This file contains in particular the neutron fluxes, the burn-up of the materials and the compositions of the materials at each time step.

The typical ALEPH2 flow explained here is shown in fig 2.1.

[3] Even if it has not been used in the present document, it has to be noted that there exists however in ALEPH2 an option which allows to solve the system of depletion equations where the coefficients are dependent on time, making it a unique worldwide feature for that kind of code.

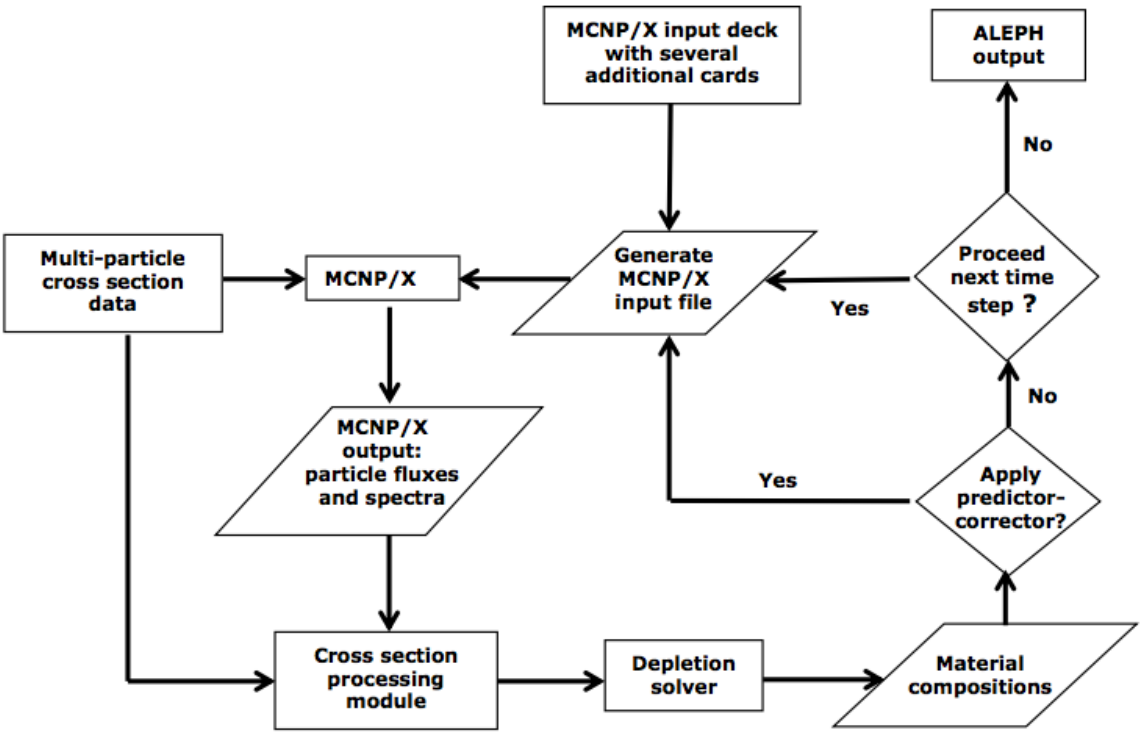

Figure 2.1.: Calculation flow of ALEPH2 [20].

It can be seen on this figure that the optional predictor-corrector algorithm is a part of the calculation flow which has not been explained above. This algorithm will be detailed later in section 6, but it can already be mentioned that it consists in taking into account the changes in neutron flux shape due to accumulation of fission products in the course of the time step, by - in general - doubling the MCNP calculations per each irradiation step.

The following section explains in a first part the theory related to the MCNP calculation and in a second part how to transform the tallies into physical neutron reaction rates and how the materials are finally depleted by the solver of ALEPH2.

2.1. 1^{st} part: Monte-Carlo transport code

2.1.1. Introduction to MCNP

MCNP - which stands for Monte-Carlo N-Particle transport code - is a code that has been originally developed by the Monte Carlo Group in the applied Physics Division at the Los Alamos National Laboratory at least since 1957, even if the roots of the method go back further. The MCNP codes are comprised of about 425 subroutines written in Fortran 90 and C even if they were previously written in other ANSI standards. There exist currently a lot of different versions of MCNP (MCNP5, MCNP6, MCNPX, etc.), some more recent than others or even upgraded versions. The one that has been used in this document is the MCNP5 code.

MCNP is a transport code which solves the Boltzmann transport equation (the interaction with matter) in several transport modes: neutron only, photon only, electron only, combined neutron/photon, neutron/photon/electron/etc. It means, for instance, that if the combined neutron/photon mode is activated, when a neutron hits a fissile isotope and a fission reaction occurs, two or three new neutrons are created and it is sometimes even possible that a photon is emitted if the energy of one of the fission product is a little bit above one of its stable energy state.
In the present document however, only the neutron transport equations are solved since the purpose of the document is to find the concentrations of the materials inside a nuclear PWR core. In that case, ionizations, photons and electrons interactions (electromagnetic, photo-electric, Compton effect or even bremsstrahlung for instance) are way too low in order to have a real impact on the neutron flux and thus on the core composition. Nevertheless, the α (helium atom emission), β (electron or positron emission) and γ (photon emission) heatings from delayed radiation due to fission products or nuclei decaying are taken into account anyway in the power balance of the core, since they represent approximately 7[%] of the thermal power.
All of this will be explained more thoroughly later, but what has to be understood here is that the only interactions taken into account in order to obtain the neutron flux in this document are between the neutrons and the matter, but α,β and γ delayed radiations are however included in the reactor power balance.

There exist two kinds of methods that solve the Boltzmann transport equation whose variables in the phase space of the problem are the neutron's position $\vec{r}$ = (x,y,z), the neutron's direction of propagation $\vec{\Omega} = (\omega_x, \omega_y, \omega_z)$[4], the energy E of the neutron and the time t: the deterministic and the probabilistic analysis [5]. While the first method solves directly the Boltzmann transport equation in a numerically approximated manner everywhere throughout a modeled system, the statistical one, also called the Monte Carlo method, models the nuclear system exactly and then solves this exact model statistically anywhere in the modeled system. This statistical method, implemented in MCNP5, possesses the advantage that there is no need to even write down the differential equations that represent the behavior of the system and that the physical system is simply described by probability density functions available in the ACE-format general transport neutron data in the library, and from which the parameters for the transport of neutrons are randomly sampled. Practically, the MCNP5 code simulates a huge number of individual neutrons at several times in snapshots of the problem[5] and computes *tallies*, "pictures" of physical values of the problem and that reflect aspects of the average behavior of the neutrons[6] in the system.

[4] The third component is not an unknown of the problem since it is derived from the fact that $\vec{\Omega}$ is a normed vector: $||\vec{\Omega}|| = 1 = \omega_x^2 + \omega_y^2 + \omega_z^2$.

[5] Each Monte-Carlo simulation is time-independent since it is computed in a picture of the problem; the time is thus in that case not a variable of the neutron phase space, but a given value.

[6] This last assertion comes from the central limit theorem which states that, when independent random variables are added, their properly normalized sum tends toward a normal distribution even if the original variables themselves are not normally distributed. From this, it is possible to create confidence intervals for the expected value of the distribution and thus reflecting the average behavior of the neutrons.

2.1.2. F4 flux tallies in MCNP5

As stated earlier, the Monte-Carlo code simulates a huge number of neutrons in the geometry of the problem and records their track lengths in order to characterize the neutron flux in each cell. To understand how the neutron track lengths can be representative of the neutron flux in a cell, a few physical values have to be first defined:

- $n\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right)$ represents the neutron angular density at the point $\left(\vec{r}, \mathrm{E}, \vec{\Omega}\right)$ of the six dimensions phase space and at the time t. It is in fact the average number of neutrons per unit of volume, solid angle and energy, situated in $\vec{r}$, with an energy equal to E and propagating in the direction $\vec{\Omega}$.
- $\mathrm{N}\left(\vec{r}, \mathrm{E}, t\right) = \int_{\Omega} n\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right) d\Omega$ is the neutron density in particles/cm^3/MeV.
- $\Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right)$ is the neutron angular flux in particles/cm^2/s/MeV/steradian[7]. This quantity is equal to the product between the scalar velocity of the neutrons $\left(v \equiv ||\vec{v}|| = \sqrt{\frac{2\mathrm{E}}{m}}\right)$ and the neutron angular density: $\Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right) = v \cdot n\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right)$.

From the definition above, it can be seen that $\Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right)$ $\mathrm{d}\Omega$ dE dt represents the total number of neutrons passing through each cm^2 of an arbitrary volume, within a solid angle $\mathrm{d}\Omega$ around the direction $\vec{\Omega}$, with an energy equal to $\mathrm{E} \pm \frac{d\mathrm{E}}{2}$ and during the time dt.
If the arbitrary volume is set to be the volume of a cell of the problem, the total number of neutrons per cm^2 in the cell is found by integrating $\Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right)$ over all the directions of propagation, the energy spectrum and during a certain time:

$$\overline{\phi}_{\mathrm{V}} = \frac{1}{\mathrm{V}} \int d\mathrm{V} \int d\mathrm{E} \int d\Omega \int \Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right) dt \tag{2.1}$$

$\overline{\phi}_{\mathrm{V}}$ is called the average neutron flux in a cell and is the physical quantity represented by the tallies used in the current document, i.e. the F4 tallies.
It is again possible to transform the equation above in order to show its relation with the neutron track lengths:

$$\begin{aligned}
\overline{\phi}_{\mathrm{V}} &= \frac{1}{\mathrm{V}} \int d\mathrm{V} \int d\mathrm{E} \int d\Omega \int \Psi\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right) dt \\
&= \frac{1}{\mathrm{V}} \int d\mathrm{V} \int d\mathrm{E} \int d\Omega \int v \cdot n\left(\vec{r}, \mathrm{E}, \vec{\Omega}, t\right) dt \\
&= \frac{1}{\mathrm{V}} \int d\mathrm{V} \int d\mathrm{E} \int v \cdot \mathrm{N}\left(\vec{r}, \mathrm{E}, t\right) dt \\
&= \frac{1}{\mathrm{V}} \int d\mathrm{V} \int d\mathrm{E} \int \mathrm{N}\left(\vec{r}, \mathrm{E}, t\right) ds \qquad ,
\end{aligned} \tag{2.2}$$

with the differential unit of neutron track length $ds = v \cdot dt$.
Here, the quantity $\mathrm{N}\left(\vec{r}, \mathrm{E}, t\right) ds$ may be thought of as a track length density. This explains thus why each neutron track length is recorded by MCNP5 in order to represent the F4 tally spectrum. The average flux in a cell can thus be estimated by summing WT_l/V for all particle tracks in the cell. The energy-dependent subdivisions of $\overline{\phi}_{\mathrm{V}}$ are here made by

[7] The steradian is a unit of solid angle, equal to the angle at the centre of a sphere subtended by a part of the surface equal in area to the square of the radius.

binning the track lengths in appropriate energy bins. In that case, the resulting $\overline{\Phi}_V(E)$ represents the number of neutrons per cm^2 that have circulated in a cell during a certain time t and whose energies were comprised in the boundaries of discrete energy bins. This is why the F4 tallies can be called time-independent estimations of the neutron fluxes inside the cells.

Practically, each time a neutron is starting a track length, the MCNP code computes the value $\frac{WT_l}{V}$ and records it with the energy associated with the neutron. In this equation, T_l represents the track length of the neutron, while W is its statistical weight. This weight can simply be seen as a tally multiplier. In a normal mode, it is equal to 1 each time a new neutron is created, and the value is progressively decreased following the interactions of the neutron with the atoms of the materials. For instance, if a neutron collides with an atom and has a 60 % probability of being captured by it, the remaining neutron will start a new track, but this time with a weight equal to 40 % of the initial value, in order to represent the fact that the neutron is more likely to be absorbed by an atom than to continue its path in the material. In that case, the two F4 tallies that MCNP would record would be $\frac{T_{l,1}}{V}$ and $\frac{0.4 \cdot T_{l,2}}{V}$, with $T_{l,1}$ different than $T_{l,2}$.

2.1.3. Physics in MCNP5

In order to calculate the neutron track lengths of the problem, the program needs to follow every newborn neutron from its birth to its death either through absorption, by escaping from the system or through an artificial termination if the critical mode is on. During this process, the neutrons will somehow be scattered or will even fission fissile atoms of the system and thus create new neutrons. To determine the outcome of each collision between a neutron and an atom, probability distributions are randomly sampled using the general neutron transport data from the folder whose path in the system is defined in the input file.

First of all, MCNP5 generates neutrons from a source selected by the user and lets them move - one after the other - everywhere in the problem. Each of the neutrons is given an energy sampled from a user-defined probability density spectrum and a direction of propagation. This one is computed by MCNP5 by sampling u, v and w the cosines of the angles between the neutron's direction of propagation and respectively the axis Ox, Oy and Oz.
From this, the program can calculate the first collision along the track of the neutron between it and an atom, using the following theory.

It is known that the probability of a collision between l and l+dl along the line of flight of a neutron of energy E with an atom is given by:

$$p(l)dl = e^{-\Sigma_t(E)l}\Sigma_t(E)dl \tag{2.3}$$

Where Σ_t is the neutron total macroscopic cross section of the medium (i.e. the sum of the macroscopic cross sections between a neutron and each nuclide of the material contained in the cell) and is interpreted as the probability per unit length of a collision between the neutron and an atom of the medium.
By setting ζ the random number on [0,1] to be:

$$\zeta = \int_0^{T_l} e^{-\Sigma_t(E)l}\Sigma_t(E)dl = 1 - e^{-\Sigma_t(E)T_l} \quad , \tag{2.4}$$

it follows that:

$$T_l = -\frac{1}{\Sigma_t(E)} ln(1-\zeta) \tag{2.5}$$

Since $(1-\zeta)$ is distributed just as ζ[8], one may replace the other. The neutron track length is thus given by:

$$T_l = -\frac{1}{\Sigma_t(E)} ln(\zeta) \tag{2.6}$$

In order to calculate the track length at each step of the neutron history, MCNP5 generates thus a random number ζ and computes the equation above at every step of the neutron lifetime. It can be seen here that, the larger the macroscopic cross section of the medium (i.e. the higher the likelihood for the neutron to interact with the medium), the smaller is the neutron track length.

After that this step has been computed, MCNP5 first identifies the nuclide which the neutron has collided with at the end of its track, and over a second phase selects the reaction that occured, according to the different cross sections - macroscopic cross sections for the nuclide identification and microscopic for the reaction identification.
However, if T_l is larger than the distance between the neutron and the border of the cell in which the neutron is moving, the track length of the neutron in the cell is set to be the distance between it and the border. Then, MCNP5 computes the path of the neutron in the next cell - filled by another material or not - from the border between the two cells, and also records the track length. In that case, the neutron has the same energy than the one in the previous cell (a neutron can not lose much of its kinetic energy by moving a few millimeters) and the same direction of propagation.

So, after calculating the track length, the collision nuclide is identified. To manage it, MCNP5 generates a random number ζ on the unit interval [0,1] (a new number, not the one generated in the neutron track length calculation) and the k^{th} on a total of n nuclides is chosen according to the following relation:

$$\sum_{i=1}^{k-1} \Sigma_{t,i} < \zeta \sum_{i=1}^{n} \Sigma_{t,i} \leq \sum_{i=1}^{k} \Sigma_{t,i} \tag{2.7}$$

The relation above can be understood with a simple example[9].
A neutron whose energy is equal to 0.025[eV] is moving in a material made of fresh fuel UO_2. The density of the material is equal to $10[g/cm^3]$ and the uranium is enriched to $5[wt.\%]$. It is supposed here that the only nuclides present in the problem are O-16 (nuclide 1), U-235 (nuclide 2) and U-238 (nuclide 3). At the energy corresponding to the one of the incident neutron, the microscopic total cross sections of the nuclides are respectively:

- O-16: $\sigma_{t,1} = 5[b]$[10] $(\sigma_{t,1} \approx \sigma_{s,1})$.

[8] If ζ is randomly chosen from a uniform distribution on [0,1], then $(1-\zeta)$ is also uniformly distributed on [0,1].

[9] Even if the example is simplified compared to reality, the values are more or less what can be found in reality in a typical PWR.

[10] 1[b] = 1[barn] = $10^{-24}[cm^2]$.

- U-235: $\sigma_{t,2} = 500[b]$ $(\sigma_{t,2} \approx \sigma_{f,2})$.
- U-238: $\sigma_{t,3} = 10[b]$ $(\sigma_{t,3} \approx (\sigma_{s,3} + \sigma_{c,3}))$.

The macroscopic total cross sections of the three nuclides are thus equal to:

- O-16: $\Sigma_{t,1} = N_{O-16} \cdot \sigma_{t,1} = 10 \cdot 0.12$[11]$\cdot \frac{6.02 \cdot 10^{23}}{16} \cdot 5 \cdot 10^{-24} = 0.226[cm^{-1}]$.
- U-235: $\Sigma_{t,2} = N_{U-235} \cdot \sigma_{t,2} = 10 \cdot 0.88 \cdot 0.05 \cdot \frac{6.02 \cdot 10^{23}}{235} \cdot 500 \cdot 10^{-24} = 0.563[cm^{-1}]$.
- U-238: $\Sigma_{,3} = N_{U-238} \cdot \sigma_{t,3} = 10 \cdot 0.88 \cdot 0.95 \cdot \frac{6.02 \cdot 10^{23}}{238} \cdot 10 \cdot 10^{-24} = 0.211[cm^{-1}]$.

Where the atomic density of nuclide i [particles/cm^3] is given by the equation:

$$N_i = \rho_{fuel} \cdot F_i \cdot 6.02 \cdot 10^{23} \cdot \frac{1}{M_{m,i}} \quad , \tag{2.8}$$

with F_i the weight fraction of nuclide i and $M_{m,i}$ its molar mass.

It is obvious from these values that the nuclide which is the most likely to be defined as the collision nuclide by MCNP5 is the U-235. Indeed, since $\sum_{i=1}^{n} \Sigma_{t,i}$ is equal to 1[12] in the present case, the equation 2.7 can be written as:

$$\sum_{i=1}^{k-1} \Sigma_{t,i} < \zeta \leq \sum_{i=1}^{k} \Sigma_{t,i} \tag{2.9}$$

It can thus be seen that the chosen nuclide k is number 1 (i.e. the O-16) if $\zeta \in$ [0,0.226]; is number 2 (i.e. the U-235) if $\zeta \in$ [0.226,0.789]; is number 3 (i.e. the U-238) if $\zeta \in$ [0.789,1]. The nuclide with the highest macroscopic total cross section is thus the one which is the most likely to be identified as the collision nuclide.

Now that the collision nuclide has been identified, the next step consists in defining which reaction has occured. There are a lot of reactions which are possible at a given energy between an atom and a neutron: fission, capture, elastic or inelastic scattering, (n,2n) reaction, etc.

The first thing that MCNP5 does is processing the absorption of the neutron by the nuclide. Indeed, as mentioned previously, when a neutron interacts with an atom and has a non zero probability to be captured by it, a fraction $\frac{\sigma_a}{\sigma_t}$ of the incident particle weight is deposited in the collision cell[13]. From this, the absorption is treated in such a way that a new statistical weight is given to the survival neutron(s), following the equation:

$$W_{new} = \left(1 - \frac{\sigma_a}{\sigma_t}\right) W_{old} \tag{2.10}$$

This means that, once the reaction and the outgoing particle(s) parameters (energy, direction of propagation, etc.) have been defined, the outgoing particle(s) start(s) a new random walk

[11] From the values above, the weight fraction of oxygen in the fuel is 12[%] and the uranium fills the remaining 88[%].

[12] It is a simple coincidence here that the value is equal to 1, this is not something that should be taken as granted when computing this part of the code.

[13] The absorption cross section σ_a is specially defined for MCNP as the sum of all (n,x) reactions cross sections, where x is anything except neutrons. This means that it does not include $\sigma_{(n,f)}$ - or shorter in this document, σ_f - as usual, here.

with a weight reduced to the value stated by the equation above.

Now that the absorption has been processed, the program selects whether the collision between the nuclide and the neutron is an elastic or a non-elastic reaction[14]. An elastic collision is an elastic scattering in which the total kinetic energy of the system is conserved, while on the contrary, a non-elastic collision does not conserve the total kinetic energy of the system. In that case, the neutron activates the nucleus, putting it into an excited, unstable, short-lived energy state which causes it to quickly emit some kind of radiation or to fission, in order to bring it back down to a stable or ground state. However - as stated before -, no electron nor photon emissions are allowed in the present document since the transport mode has been set to "neutrons only"[15].

The selection of an elastic scattering is made by MCNP5 with the probability:

$$P_{el} = \frac{\sigma_{el}}{\sigma_t - \sigma_a} = \frac{\sigma_{el}}{\sum_i \sigma_{\overline{el},i} + \sigma_{el}} \tag{2.11}$$

With i summed over all the non-elastic collision cross sections $\sigma_{\overline{el},i}$ (it includes the fission (n,f), inelastic scattering (n,n'), (n,np)[16], etc.). The selection of a non-elastic collision is then made with the remaining probability:

$$P_{\overline{el}} = 1 - P_{el} = \frac{\sum_i \sigma_{\overline{el},i}}{\sum_i \sigma_{\overline{el},i} + \sigma_{el}} \tag{2.12}$$

It is seen here that the probabilities are calculated with respect to the value $\sigma_t - \sigma_a$ and not σ_t since, from the statistical weight reduction above (eq 2.10), the absorption cross section is not part of the problem anymore.

If the collision is determined to be non-elastic, the type of reaction, n, among the N possible, is sampled in the same way than how the nuclide was selected (eq 2.7), except that macroscopic cross sections are replaced here by microscopic ones:

$$\sum_{i=1}^{n-1} \sigma_{\overline{el},i} < \zeta \sum_{i=1}^{N} \sigma_{\overline{el},i} \leq \sum_{i=1}^{n} \sigma_{\overline{el},i} \tag{2.13}$$

Where ζ is again a random number on [0,1].

For instance, if the collision nuclide of the previous example was supposed to be U-235 (it had a probability of 56[%] to be chosen, as a recall) and that its microscopic total cross section at 0.025[eV] is divided in: $\sigma_t = 500[b] = 420(\sigma_f) + 70(\sigma_a) + 10(\sigma_{el})$, MCNP5 samples the reaction in the following way.
First of all, it processes the absorption of the neutron by the atom and computes thus a new weight for the survival neutron(s), equal to $W_{new} = \left(1 - \frac{70}{500}\right) W_{old} = 0.86 W_{old}$.

[14] In the slang of nuclear physics, the term inelastic reaction often refers to the inelastic scattering reaction; this is why the opposite of elastic reaction is non-elastic reaction here.

[15] In case of an inelastic scattering, the excess of energy of the nucleus is thus simply considered as lost; this is why using the "neutrons only" mode is an approximation and does not reflect totally the reality.

[16] Even if the proton emission is not allowed in this transport simulation, the associated cross section is still used in the total cross section.

Then, MCNP5 selects the reaction to be an elastic scattering, with the probability $P_{el} = \frac{10}{420+10} = 0.02$ or a fission (the only non-elastic reaction here), with the probability $P_f = 1 - P_{el} = 0.98$.
It follows thus that when the U-235 is chosen to be the collision nuclide and that the energy of the neutron is equal to $0.025[eV]$, a fission reaction is sampled 98[%] of the time and a number $\overline{\nu}$ of fission neutrons are then created, each with a weight equal to $0.86W_{old}$.

In order to complete the theory that was just explained, it should be mentioned that in most cases, the collision between a neutron and an atom is affected by the thermal motion of the atom - and is also sometimes affected by the presence of other atoms nearby. Indeed, both the energy and the direction of propagation of the exiting neutron, values in which the user is interested by in order to calculate the tallies, are affected by this motion. From this fact, continuous energy Monte-Carlo codes have traditionally used three different models for the simulation of elastic and inelastic scatterings between a neutron and a target nuclide:

- At high neutron energies, target thermal motion is neglected, and simple target at rest elastic and inelastic scattering models are used.

- At epithermal neutron energies (a few [eV] to 10s or 100s of [eV]), while the same model as above is used for the inelastic scattering, a free gas elastic scattering model is used to account for thermal motion of the target nuclides.
  This free gas thermal theory consists in the same time in adjusting the elastic cross section and in taking into account the velocity of the target nucleus when the kinematics of a collision are being calculated.
  First of all, the elastic scattering cross section (and thus also the total cross section) is adjusted - partly during the setup of the problem - in order to correspond to the temperature of the materials in the problem, if it was not already the case (the data attached to the input file are sometimes not available at the required temperature). The elastic scattering cross section is in this case adjusted from its zero-temperature cross section by raising it by a factor $F(a)$: $\sigma_{el,temp=T} = \sigma_{el,temp=0} \cdot F(a)$, where a depends on the atomic weight of the target atom, the temperature of the target atom and on the energy of the incident neutron.
  Secondly, the free gas thermal treatment states that the incident neutrons are scattering off unbound target nuclei (free gas) that are distributed energy-wise in a Maxwell-Boltzmann distribution:

$$p(V) = \frac{4}{\pi^{1/2}} \beta^3 V^2 e^{-\beta^2 V^2} \tag{2.14}$$

  Where V represents the velocity of the nucleus and β depends here on the mass of the target nucleus and on the temperature of the material.
  To represent the elastic scattering in MCNP5 in that case, the cosine of the angle between the incident neutron velocity and the target velocity, μ, is sampled uniformly by MCNP5 on the interval [-1,1]. From this, the probability distribution $P(V, \mu)$ of target atoms with velocity V and direction of propagation given by μ is computed by transforming the Maxwell-Boltzmann distribution above in order to represent the fact that neutrons are more often elastically scattered when μ equals -1, i.e. the neutron and the target atom move in opposite direction.
  Then, it is finally possible to sample the direction of propagation of the exiting neutron and to apply the two-body kinematics (atom/neutron) to deduce its exiting energy.

- At thermal neutron energies (up to a few [eV]), a S(α,β) thermal scattering treatment is used to account for thermal motion and chemical binding effects between the atoms of the material in which the neutrons are moving. The quantities α and β standing for, respectively, the momentum and energy transfer, the S(α,β) data fully represent the thermal neutron elastic and inelastic scatterings by molecules and crystalline solids when the energy of the incident neutron is very low. In such a case, the target nuclei can not be considered unbound anymore and the scattering of a neutron is computed as the sum of a coherent and an incoherent scattering cross sections, which represent each the fact that the scattering waves in the crystalline solid or in the molecule can interfere positively or not.
  It has to be mentioned here that, when the above conditions are met (low energetic neutron and target atom bound into a crystalline or a molecule), the elastic and inelastic scattering cross sections are also taken in these S(α,β) tables from the neutron-induced data attached to the problem. This means that all the previous equations (track length calculation, collision nuclide identification, statistical weight reduction due to absorption and reaction identification) use these S(α,β) cross sections instead of the regular elastic and inelastic scattering cross sections from the library.
  Finally, if the energy of the incident neutron is low and if the target atom is unbound, a free gas model is simply used also in that range of energy.

With everything that has been explained and with the emission distributions for secondary particles also available in the tables attached to the problem (regular or S(α,β) tables), it is then possible for the program to compute all the parameters of the neutron(s) after the collision (energy, velocity and direction of propagation).
For instance, in case of:

- An elastic scattering (n,n): If the incident neutron is epithermal or thermal with the target atom unbound, MCNP5 first samples the target direction-of-flight vector, following the free gas model. If the neutron energy is high enough, the target at rest model is used and the target direction-of-flight vector is set to zero. Then, the program generates the cosine of the angle between incident and exiting neutron directions from angular distribution tables provided at a number of incident neutron energies in the collision nuclide library[17].
  On the contrary, if the energy of the neutron is low enough and if the target atom is bound into a molecule or a cristalline structure (and if the data are available), MCNP5 takes all these values from the elastic scattering part of the S(α,β) library.
  Finally, it samples the exiting energy of the neutron from a two-body kinematics which depends on the center-of-mass angle between the incident and exiting neutron directions and on the mass of the collision nuclide (for instance, if a neutron bounces on a U-235 atom, it loses less energy than if the target atom is H-1).

- An inelastic scattering (n,n'): The cosine of the angle between incident and exiting neutron directions is again sampled from angular distribution tables (see above), which may be S(α,β) values if the target atom is bound into a molecule or a crystalline and if the energy of the neutron is low enough. The energy of the exiting neutron is then

[17] The MCNP5 code generates random numbers on [0,1] to first sample a cosine bin for the cosine between the incident and exiting neutron's directions of propagation from the cumulative density function available in the library at the corresponding neutron incident energy, and secondly to determine more precisely the cosine value in this bin.

either given by a S(α,β) table, or otherwise by the following equation:

$$E_{out} = \left(\frac{A}{A+1}\right)^2 \left[E_{in} - \frac{Q(A+1)}{A}\right] \tag{2.15}$$

Where A is the mass of the target nucleus and Q is a value provided in the library as an energy distribution related to the incident neutron energy.

- A fission (n,f): MCNP5 generates an amount of neutrons which is statistically equal to the average number of neutrons per fission at the incident neutron energy, $\overline{\nu}(E)$. For instance, if a nuclide has a $\overline{\nu}(E)$ value equal to 2.65, MCNP5 first generates a number ζ on the unit interval [0,1] and then simulates 3 fission neutrons if the random value $\zeta \in$ [0,0.65], or 2 if $\zeta \in$ [0.65,1] (in that case, $\overline{\nu}(E) = 0.65 \cdot 3 + 0.35 \cdot 2$).
  Each of these fission neutrons are moreover generated with an energy sampled from an energy fission distribution specific to each nuclide: a Maxwell or a Watt spectrum, for instance.

Criticality program flow

With the previous notations and by simplifying the unknown neutron angular flux $\Psi\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right)$ to short Ψ, the time-dependent linear Boltzmann transport equation for neutrons with prompt fission source and external source is written in an arbitrary volume by [4]:

$$\begin{aligned}\frac{1}{v}\frac{\delta\Psi}{\delta t} = &\int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s\left(E', \overrightarrow{\Omega'} \rightarrow E, \overrightarrow{\Omega}\right)\Psi\left(\overrightarrow{r}, E', \overrightarrow{\Omega'}, t\right) \\ &+ \frac{\chi(E)}{4\pi}\int_0^\infty dE' \int_{4\pi} d\Omega' \nu\Sigma_f\left(\overrightarrow{r}, E'\right)\Psi\left(\overrightarrow{r}, E', \overrightarrow{\Omega'}, t\right) \\ &+ q\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right) - \overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\Psi - \Sigma_t\Psi\end{aligned} \tag{2.16}$$

This equation can be written again:

$$\frac{1}{v}\frac{\delta\Psi}{\delta t} = [S + M]\Psi + q - [L + T]\Psi \tag{2.17}$$

Where S is the scatter-in operator (i.e. the gain term from the scatterings of neutrons with direction of propagation $\overrightarrow{\Omega'}$, energy E' and exiting at the state $\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right)$), M the fission multiplication operator (i.e. the neutron gain term from fissions which result in exiting neutrons at state $\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right)$), L the leakage operator (i.e. the loss of neutrons at state $\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right)$ due to leakages from the arbitrary volume) and T the collision operator (i.e. the loss term due to the absorptions - captures and fissions - and the scatterings of neutrons whose state is $\left(\overrightarrow{r}, E, \overrightarrow{\Omega}, t\right)$).

In the particular steady-state case without any external source, this equation may be rewritten:

$$0 = ([S + M] - [L + T])\Psi \tag{2.18}$$

This homogeneous equation represents the problem which is statistically solved by MCNP5 at each step, and either has the trivial $\Psi = 0$ solution or not if the operator ([S + M] − [L + T])

is singular, i.e. admits a non-zero eigenvalue.
To solve this, the solution consists on adopting another approach and to create a static eigenvalue problem - with eigenvalue k_{eff} - from the time-dependent transport equation and by introducing k_{eff}, a scaling factor on the multiplication operator:

$$[\mathrm{L}+\mathrm{T}])\Psi = \mathrm{S}\Psi + \frac{1}{k_{eff}}\mathrm{M}\Psi \tag{2.19}$$

It can be seen here that when $k_{eff} = 1$, the equation 2.19 is exactly the same as the equation 2.18, which means that the neutron gains balance exactly the losses and that no scaling factor is needed for the multiplication factor. On the contrary, if $k_{eff} < 1$, the fission multiplication operator is here artificially increased by the scaling factor to sustain the neutron balance and an external source q would thus be necessary. Finally, if $k_{eff} > 1$, the equation above stays homogeneous (q=0) but the fission multiplication operator has to be artificially lowered from the fact that the system sustains itself by creating more and more neutrons.
The problem with MCNP5 comes thus when $k_{eff} \geq 1$, because in that case, when a neutron is dropped into the system, its history simulated by Monte Carlo becomes infinitely long: it will for instance create 2 or 3 fission neutrons, then each of them will have its own history, and due to $k_{eff} \geq 1$, they will again cause another fissions, etc. In fine, the history will never stop and the program will run infinitely. Therefore, the problem must be solved in another way; and this is why MCNP5 has a special criticality mode.

The criticality mode, or the kcode mode, consists in sampling during each calculation several cycles in which the neutron source is different and generated from the fissions of the previous cycle. In that mode, the fission is actually treated as absorption and, in order that a neutron history does not last infinitely, fission acts as a termination in the neutron random walk process (contrary to the normal case called *NPS case*, previously explained). Practically, this means that when the identification of the reaction results in fission, the same statistical weight reduction than in equation 2.10 (with σ_f instead of σ_a) is applied on the neutron weight, and the fission site is recorded in the system. With this, it is possible to take account of all the fissions that happened in the cycle, and the fission neutrons (their amount is sampled between 2 and 3, for thermal neutrons) of next cycle can then start from the fission sites recorded at the previous cycle, etc. until all cycles are completed.

Since the criticality source changes from cycle to cycle, a few additional informations are requested in a kcode calculation: the nominal number N of source histories per cycle[18], an initial guess of k_{eff}[19] for the first cycle, the total number I_t of cycles in each MCNP5 calculation and the number I_c of cycles to skip before that tallies are accumulated. Indeed, before that I_c cycles have been completed, the neutron transport is treated without any tally recording since it is important that k_{eff} reaches first an equilibrium value in order to avoid any source of statistical errors.

[18] Something here may seem illogical: it is said that the source changes from cycle to cycle in a kcode calculation, but in the same time that the same amount N of source histories per cycle are created. In fact, M = $\sum n$ (varying with cycle) source particles generated from the fission sites of previous cycle are started at each cycle, but the program gives them a weight W equal to N/M in order to make as if N rather than M particles started in each cycle.

[19] In MCNP5, k_{eff} is estimated by the program at each cycle and corresponds to:

$$k_{eff} = \frac{fission\ neutrons\ in\ cycle\ i+1}{fission\ neutrons\ in\ cycle\ i}$$

2.2. 2^d part: ALEPH2-specific theory

At this point, MCNP5 has completed the simulation of all the neutron histories everywhere in the problem. From them, it has recorded the F4 neutron flux tallies $\frac{WT_l}{V}$ each associated with the energy of the neutron in the cells filled by the materials that the user wants to deplete[20], and this forms what can be called the MCNP neutron flux spectrum $\phi^{MCNP}(E)$. Indeed, even if the neutrons are simulated in the entire geometry, it is possible that the user wants to deplete only some of the materials, and the F4 tallies are thus only computed in the cells filled by them. The next step consists thus in transforming these tallies into reaction rates, i.e. bringing the time in these unit-of-[particles/cm^2] values, with the help of the top cards of the input file related to the irradiation history. As a recall, this irradiation history is made in particular of the thermal power of (a part of) the problem and also the time during which this power can be assumed constant.

The first thing to understand here is how ALEPH2 calculates the reaction rate $R_{i,j}^{MCNP}$ of a reaction i (neutron capture, fission, etc.) occuring with a nuclide j in a cell, by using the MCNP neutron flux spectrum $\phi^{MCNP}(E)$:

$$R_{i,j}^{MCNP} = \int \sigma_{i,j}(E)\phi^{MCNP}(E)dE = \sum_{g=1}^{n} \sigma_{i,j,g}\phi_g^{MCNP} \tag{2.20}$$

Where the energy spectrum has been split in n energy bins, with $\sigma_{i,j,g}$ the microscopic reaction i cross section of the nuclide j averaged on the energy bin g and ϕ_g^{MCNP} the MCNP neutron flux spectrum integrated over the same energy bin: $\phi_g^{MCNP} = \int_{E_g-1}^{E_g} \phi^{MCNP}(E)dE$.
This $R_{i,j}^{MCNP}$ can thus be seen here as a "reaction rate" in units of number of reactions i on nuclide j per average neutron.

The next step consists in finding the neutron source rate of the system in units of $[neutrons/s]$, in order to get the physical reaction rate $R_{i,j}$ - i.e. the number of reactions i on nuclide j per second - from $R_{i,j}^{MCNP}$.

In the ALEPH-format activation neutron data files from the library, it is posssible to find the value $Q_{i,j}(E)$, i.e. the recoverable energy release in the process of type i that occured between a nuclide j and a neutron of energy E. Fission being the only reaction from those files whose recoverable energy Q_f is - very - slightly dependent on the energy of the incident neutron, it is considered in the equations hereafter that none of the recoverable energy releases is actually varying with the energy of the incident neutron[21]. Then, considering that all the physical reaction rates are known, it is thus possible to calculate the amount of energy per unit time released in a cell filled by a material k (the thermal power of the material k), by summing the contribution of each reaction rate of every nuclide in the material:

$$\dot{Q_{tot,k}} = P_k = \sum_j \sum_i N_j R_{i,j} Q_{i,j} = \sum_j N_j (R_{f,j}Q_{f,j} + R_{c,j}Q_{c,j}) \tag{2.21}$$

[20] It has to be noted that the F4 tally written in the .o file corresponds to an average value in $[cm^{-2}]$ per fission neutron: $F4 = \sum_i \frac{W_i T_{l,i}}{V} /$ (number of fission neutrons), where i is summed over all the track lengths in the corresponding cell of volume V.

[21] The energy dependence of Q_f is however taken into consideration in ALEPH2.

Where N_j is the amount (in atoms) of nuclide j in the material and $\sum_j \sum_i R_{i,j} Q_{i,j}$ is replaced by the two terms which produce energy in a material: the neutron captures ($\sum_j \sum_i R_{c,j} Q_{c,j}$) and the fissions ($\sum_j \sum_i R_{f,j} Q_{f,j}$). Indeed, the contribution of other reactions to the total energy release is found negligible for most of the systems.
It can also be seen that, as mentioned earlier, even if the emissions of α, β and γ particles were not allowed in the transport code, they are however included in the power balance here: the energy release $Q_{c,j}$ of a neutron capture in a material is indeed due to decaying nuclei, and consequently to the energy transfer of their potentially released α or β particles when they collide atoms of the material (their kinetic energy is then progressively transferred in the medium as thermal energy) or to the emission of photons (γ particles) which directly increase the thermal energy inside the material.

It is then possible to transform eq 2.21 by using $R_{i,j}^{MCNP}$ instead of $R_{i,j}$, and to calculate the neutron source rate S expressed in neutrons per second from the link between P_k and P_k^{MCNP}. Indeed, since the first one, given in a top card of the input file related to the irradiation history, has units of energy per unit time while the second is expressed in energy per average neutron, their ratio gives the neutron rate of the problem[22]

$$\begin{aligned} S = \frac{P_k}{P_k^{MCNP}} &= \frac{P_k}{C \sum_j N_j (R_{f,j}^{MCNP} Q_{f,j} + R_{c,j}^{MCNP} Q_{c,j})} \\ &= \frac{P_k}{C \sum_j N_j \sum_{g=1}^{n} \phi_g^{MCNP} (\sigma_{f,j,g} Q_{f,j} + \sigma_{c,j,g} Q_{c,j})} \end{aligned} \tag{2.22}$$

Where, since P_k is given in [MW] in the input file and $Q_{i,j}$ in [MeV] in the libraries, C denotes the conversion coefficient from [MW] to [MeV·s^{-1}], and where j is summed over all the nuclides of the material k at the beginning of the time step.
It has to be recalled that the thermal power given in the irradiation history can also be related to the total system, and not to a single material. In that case, the source strength S is then given by:

$$S = \frac{P_{tot}}{\sum_k P_k^{MCNP}} = \frac{P_{tot}}{C \sum_k \sum_j N_{j,k} \sum_{g=1}^{n} \phi_{g,k}^{MCNP} (\sigma_{f,j,g} Q_{f,j} + \sigma_{c,j,g} Q_{c,j})} \tag{2.23}$$

The thermal power is summed here over the fissions and neutron captures of each of the nuclides in every material in the sytem. It can also be seen in eq 2.23 that, since the ϕ^{MCNP} are different in each of the materials, the reaction rates in a material k are computed with the MCNP neutron flux spectrum (integrated first over the energy bin g and then summed over all the bins) related to it: $\phi_{g,k}^{MCNP}$.

With the neutron source strength S, it is then finally possible to transform the $R_{i,j,k}^{MCNP}$ into physical reaction rates in each material k of the system that has to be depleted and where tallies were previously computed:

[22] As already mentioned, the term $C \sum_j N_j R_{f,j}^{MCNP} Q_{f,j}$ of eq 2.22 is actually computed in ALEPH2 by using the energy dependence of $Q_{f,j}$:
$C \sum_j N_j \int \sigma_{i,j}(E) \phi^{MCNP}(E) Q_{f,j}(E) dE = C \sum_j N_j \sum_{g=1}^{n} \sigma_{i,j,g} \phi_g^{MCNP} Q_{f,j,g}$, where $Q_{f,j,g}$ is the energy released by the fission of the nuclide j, averaged on the energy bin g.

$$\begin{aligned} \mathrm{R}_{i,j,k}\ [s^{-1}] &= \mathrm{S}\ [neutron/s] \cdot \mathrm{R}^{\mathrm{MCNP}}_{i,j,k}\ [1/neutron] \\ &= \mathrm{S} \int \sigma_{i,j}(\mathrm{E}) \phi^{\mathrm{MCNP}}_{k}(\mathrm{E}) d\mathrm{E} \\ &= \mathrm{S} \sum_{g=1}^{n} \sigma_{i,j,g} \phi^{\mathrm{MCNP}}_{g,k} \end{aligned} \tag{2.24}$$

The depletion of each material k in the problem can eventually be achieved by creating and solving at the end of the time step, a large system of X coupled, linear, first-order ordinary differential equations with constant coefficients and similar to the following:

$$\begin{aligned} \frac{d\mathrm{N}_j}{dt} &= \sum_{\substack{n=1 \\ \neq j}}^{\mathrm{X}} l_{j,n} \lambda_n \mathrm{N}_n + \sum_{\substack{m=1 \\ \neq j}}^{\mathrm{X}} \left(f_{j,m} \mathrm{S} \int \phi^{\mathrm{MCNP}}_{k}(\mathrm{E}) \sigma_{f,m}(\mathrm{E}) d\mathrm{E} \right) \mathrm{N}_m - \left(\lambda_j + \mathrm{S} \int \phi^{\mathrm{MCNP}}_{k}(\mathrm{E}) \sigma_{a,j}(\mathrm{E}) d\mathrm{E} \right) \mathrm{N}_j \\ &= \sum_{\substack{n=1 \\ \neq j}}^{\mathrm{X}} l_{j,n} \lambda_n \mathrm{N}_n + \sum_{\substack{m=1 \\ \neq j}}^{\mathrm{X}} f_{j,m} \mathrm{S} \cdot \mathrm{R}^{\mathrm{MCNP}}_{f,m,k} \mathrm{N}_m - \left(\lambda_j + \mathrm{S} \cdot \mathrm{R}^{\mathrm{MCNP}}_{a,j,k} \right) \mathrm{N}_j \\ j &= 1, ..., \mathrm{X} \end{aligned} \tag{2.25}$$

With

- X : the number of nuclides that it is possible to find in the material k (fission products, neutron capture products and decay products included).
- $\phi^{\mathrm{MCNP}}_{k}(\mathrm{E})$: the MCNP neutron flux spectrum in material k.
- S: the source strength or source rate calculated by eq 2.22 (one material) or 2.23 (all the problem), depending on what is given as thermal power in the top cards of the input file.
- $l_{j,n}$: the fraction of radioactive decay of nuclide n which leads to the formation of nuclide j.
- λ : the radioactive decay constant (it is linked to the half-life $\mathrm{T}_{1/2}$ of a radioactive nuclide by the equation $\lambda = \frac{ln2}{\mathrm{T}_{1/2}}$).
- $f_{j,m}$: the fission product yield of the nuclide m which leads to the creation of nuclide j.
- $\sigma_{a,j} = \sigma_{c,j} + \sigma_{f,j}$: the microscopic absorption cross section of nuclide j.
- $\sum^{\mathrm{X}}_{n=1,\neq j} l_{j,n} \lambda_n \mathrm{N}_n$: the creation rate of nuclide j from the radioactive decays of the other (N-1) nuclides. If $l_{j,n}$ equals 0, it means that no nuclide j is created from the decays of nuclide n.
- $\sum^{\mathrm{X}}_{m=1,\neq j} f_{j,m} \mathrm{S} \cdot \mathrm{R}^{\mathrm{MCNP}}_{f,m,k} \mathrm{N}_m$[23]: the creation rate of nuclide j from the fission of the other (N-1) nuclides. In the same way, if $f_{j,m}$ equals 0, no nuclide j is created from the fissions of nuclide m.

[23] It should be noted that this term is computed in the same way than explained in equation 2.20: the energy spectrum is divided in energy bins in which the MCNP neutron flux spectrum $\phi^{\mathrm{MCNP}}_{k}(\mathrm{E})$ is integrated and in which an average value is calculated for $f_{j,m}$ and $\sigma_{f,m}$. What is shown in eq 2.25 is thus not totally correct since it assumes that $f_{j,m}$ is constant whatever the energy; it has been written in this way just to use the notation $\mathrm{R}^{\mathrm{MCNP}}_{f,m,k}$ as defined in eq 2.20.

- $-\lambda_j N_j$: the loss rate of nuclide j due to its radioactive decays.
- $-S \cdot R^{MCNP}_{a,j,k} N_j$: the loss rate of nuclide j due to its fissions and neutron captures.

It has to be mentioned here that, from the full data consistency between the MCNP ACE-formatted files and the ALEPH-formatted files related to the depletion of the code, the cross sections used to build the system above are exactly the same (and are linearized on the same energy grid) than the ones used in the Monte-Carlo calculation, except that they have been extended to higher energies and that the activation data files have been added in order to extend the list of nuclides where cross sections are available to all the nuclides that play a role in the depletion of the fuel (the fissile nuclides, their fission products and every nuclides of the decay chaines).

Finally, ALEPH2 can calculate the composition of each depleted material to the time corresponding to the end of the irradiation step by solving the following system:

$$\dot{N}_k = A \cdot N_k \tag{2.26}$$

With $\dot{N}_k$ a column vector Nx1 of the time derivative of the nuclides' concentrations, A a sparse (a lot of the elements are null) transition matrix NxN containing the transformation rates and N_k a column vector Nx1 of the concentrations of the nuclides.
For instance, if the material k contains only two nuclides, the system relative to it would be:

$$\begin{bmatrix} \frac{dN_1}{dt} \\ \\ \frac{dN_2}{dt} \end{bmatrix} = \begin{bmatrix} -\lambda_1 - SR^{MCNP}_{a,1} & l_{1,2}\lambda_2 + f_{1,2}SR^{MCNP}_{f,2} \\ \\ l_{2,1}\lambda_1 + f_{2,1}SR^{MCNP}_{f,1} & -\lambda_2 - SR^{MCNP}_{a,2} \end{bmatrix} \begin{bmatrix} N_1 \\ \\ N_2 \end{bmatrix} \tag{2.27}$$

All the previous theory being related to an irradiation step, it should be noted that ALEPH2 must also sometimes solve concentrations at the end of decay steps. In that case, the above system can be rewritten simply by setting the reaction rates to zero, since there is no neutron flux in the problem:

$$\begin{bmatrix} \frac{dN_1}{dt} \\ \\ \frac{dN_2}{dt} \end{bmatrix} = \begin{bmatrix} -\lambda_1 & l_{1,2}\lambda_2 \\ \\ l_{2,1}\lambda_1 & -\lambda_2 \end{bmatrix} \begin{bmatrix} N_1 \\ \\ N_2 \end{bmatrix} \tag{2.28}$$

In the former version of ALEPH, systems such as in 2.26 and that could be in the form of eq 2.27 or 2.28, were solved by the ORIGEN-2.2 code [1] which uses a matrix exponential method and where the short-lived nuclides had to be removed from the system and treated separately.
In order to gain accuracy on the results, it has been however decided in ALEPH2 to replace ORIGEN-2.2 by a built-in depletion module mode of a Runge-Kutta method of order 5 (Radau IIA, three stages) with step size control and continuous output [19].

Study case

3

Sommaire

The benchmark case studied in this document is related to the chemical composition of a spent fuel from a PWR plant located in Gösgen, Switzerland. Two adjacent samples called GU3 and GU3' have been withdrawn from one of its spent fuel rod in 1997 after approximately 3 years of irradiation, and their compositions were analysed in different laboratories. While the dissolution and radiochemical analysis of the former was performed at the ITU (Institute for Transuranium Elements, Germany), the GU3' sample was transported to the SCK-CEN.

The positions of samples GU3 and GU3' are described in the benchmark [23]: the fuel rod and the fuel assembly which they belonged to and the position with time of this assembly in the core are in particular given in the document. Nevertheless, their relative position in the fuel rod is not specified and, even if it is mentioned that both are adjacent samples from the center of the rod, it is not possible to know which one was situated above the other, leading eventually to an uncertainty in the problem's description - and eventually in the later results.

A total of 53 isotopes including long-lived isotopes such as U-235, U-238, Pu-239, some isotopes of Cs, Nd,... and also short-lived isotopes of Am, Ru, Pu, Sr,... were measured and recorded at different times in the laboratories. While long-lived isotopes do barely evolve with time, this assumption is not true for the short-lived ones; this is why a full irradiation-and-cooling history of the samples has to be described in ALEPH2 in order to compare the values from [23] with the results.

The steps towards the validation are the following:

- A general view of Gösgen core, its main characteristics and the full description of the samples' irradiation and decay history inside the core.
- A description of the ALEPH2 input file with:
  - The Monte-Carlo calculation to get the F4 neutron flux tally spectra.
  - The time-dependent part of ALEPH2 which computes the depletion of the fuel in the core.
- The analysis of the results.
- Some additional studies to analyse the sensitivity of the results to the choice of the libraries for the cross sections, to the effect of the number of particles simulated, etc.

3.1. Gösgen nuclear power plant description

The Gösgen nuclear plant is located in Däniken, Switzerland. Its commercial operation started on the 1^{st} November of 1979 and it has been progressively increased over the years from 970[MWe] to 990[MWe] and finally to 1020[MWe]. The heat source of Gösgen thermal power station is a Pressurized Water Reactor which contains an amount of 177 15-by-15 lattice type assemblies, each made up of 205 UO_2 fuel rods and 20 guide tubes used to control the criticality inside the core by supporting the control rods when they are inserted inside.
There are plenty of data related to Gösgen's core and its assemblies in [23] but the major ones that are used in the ALEPH2's input are given in table 3.1.

Reactor type	PWR
Nominal thermal power [MW]	3002
Global yield of the plant [%]	33.98
Primary system pressure [bar]	150.04
Coolant average temperature [°C]	309.0
Number of assemblies	177
Lattice type	15x15
Number of fuel rods	205
Pellet diameter [cm]	0.911
Cladding material	Zr-4
Clad outer diameter [cm]	1.075
Clad inner diameter [cm]	0.93
Number of guide tubes	20
Guide tube material	Zr-4
Guide tube outer diamater [cm]	1.38
Guide tube inner diameter [cm]	1.24
Lattice pitch [cm]	1.43
Active fuel length [cm]	355

Table 3.1.: Characteristics of Gösgen's core and its assemblies.

3.2. Position and irradiation history of sample GU3 inside the core

As explained earlier, GU3 and GU3' relative positions inside the core are not recorded in the report. Due to this, everything that will follow will be related to a sample which includes both of them at the same time and whose height is thus twice the one of GU3 or GU3'. In the interest of simplification, this "global" sample will be called hereafter GU3 and - if not clearly specified - will always stand for the two samples at the same time.

GU3 is a 10-cm-high sample taken out from the middle of a fuel rod (more precisely cut between 122.42 and 132.42[cm] from the bottom end of the active fuel) which was irradiated during three fuel cycles: cycles 16, 17 and 18.
At the beginning of Gösgen's cycle 16 in 1994, the rod belonged to the fresh fuel assembly 1601. Afterwards, this assembly was moved to another location in the core at the beginning of cycle 17. Finally, at the beginning of cycle 18, the rod which GU3 belonged to was removed from the assembly 1601 and put inside the assembly 1701 which had already been burnt till

17.70[MWd/kgU][1].
Fig 3.1 presents the positions of sample GU3 in the core during its 3-years irradiation from assembly 1601 to 1701.

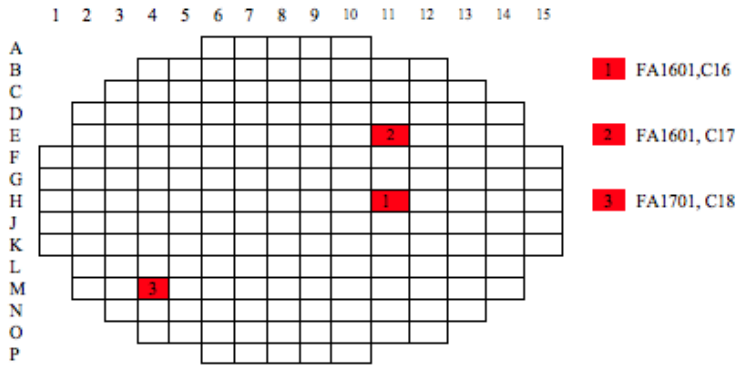

Figure 3.1.: Irradiation position of GU3: from assembly 1601 at H11 during cycle 16 to assembly 1601 at E11 during cycle 17 and finally to assembly 1701 at M4 during cycle 18 [23].
The assemblies here should be squared and not rectangular so that the core looks cylindrical as it is in reality.

Even if the positions of the assemblies which contain the sample GU3 during the three cycles are known, there is no information at all about the other assemblies of the core. For example, one may ask which burn-up level the neighbouring assemblies of 1601 and 1701 were already burnt at during the irradiation, whether they were made of fresh fuel or not, etc. All these unanswered questions are relevant and necessary in case of a complete description of the core. It was thus not possible to fully represent Gösgen's core in ALEPH2 and this explains why all the description of the problem that will follow in this report is done on a single assembly and not on the entire core and its 177 assemblies[2].
Nevertheless, working with only one assembly could lead to large errors on GU3's final composition because the neutron flux (ϕ(E) integrated over all the energy spectrum) is not uniform everywhere in the core. Indeed, a good approximation of the neutron flux ϕ inside a cylindrical core is given by

$$\phi(r,z) = \phi_0 \cdot cos\left(\frac{\pi \cdot z}{H+2\lambda}\right) \cdot J_0\left(2.40491 \cdot \frac{r}{R+\lambda}\right) \tag{3.1}$$

With z the distance from the centre of the core, H the active length of the fuel rods (355[cm] here), λ the extrapolated length which represents the fact that the flux is not equal to zero at the border of the core, r the radial coordinate, R the radius of the cylinder and J_0 is the Bessel function of order 0.
This equation is an approximation since in the real case, the neutron flux is not as easily defined due to local variations of burnable poisons (Gd_2O_3 pellet or Integrated Fuel Burnable Absorber), small power peaking or channel factor changes, the presence of metallic grids in

[1] The [MWd/kgU] is a unit a depletion which represents the fraction of fuel atoms that underwent fission. 1 [MWd/kgU] corresponds to the depletion of 1 kg of uranium (not UO_2) when it is burnt under a power of 1[MW] during 1 day.

[2] Informations in benchmarks are actually often relative to a single assembly because it is currently not possible to model entire core problems by the majority of codes: for instance, keeping allways k_{eff} to 1 - which would be the only correct way to reproduce the real functionning of the reactor - is something technically almost impossible to achieve.

the core which locally drop the power since there is no neutron emission, etc.
In the assemblies 1601 and 1701, GU3 keeps the same z coordinate but its radial coordinate increases from cycle 16 to 18 since it moves away from the center of the core. The neutron flux in GU3 is thus larger at the beginning of the irradiation than it is in the end. This explains why an error in GU3's composition may be induced by working with a single assembly.
The solution to avoid this problem consists in working with the sample's irradiation history only. Indeed, it has been seen that the reaction rates in an element can be deduced in ALEPH2 from both the MCNP neutron flux spectrum from MCNP5 and the thermal power of the element (see eq 2.22 and 2.24). So, if the user computes a tally spectrum inside the sample's geometry and uses GU3's thermal power history during all the irradiation, the neutron flux inside the sample will be defined as accurately as it is possible to do it with the data from the benchmark, no matter how GU3 moves inside the core.
Table 3.2 presents the sample's irradiation history during cycles 16 to 18.

Cycle	Operation time (EFPD)	Sample thermal power [kW]	Sample burn-up [MWd/kgU]
16			
	0	3.763	0
	6	3.985	0.403
	150	3.692	10.171
	320	3.464	20.796
	336.8	2.981	21.771
17			
	0	3.002	21.771
	6	3.143	22.096
	150	2.955	29.872
	299.5	2.874	37.461
	328.7	2.345	38.866
18			
	0	2.808	38.866
	6	2.736	39.149
	150	2.367	45.417
	301.2	2.308	51.400
	331.6	1.932	52.504

Table 3.2.: GU3's irradiation history of cycles 16, 17 and 18.

Another point to take into account is the fact that GU3's positions in the two assemblies were not the same. Indeed, when it was moved to the other assembly at the beginning of cycle 18, GU3's fuel rod was also given a different location inside it. As it can be seen in fig 3.2 and 3.3 (in red), its place in the lattice changed from P7 to R11.

As explained above by eq 3.1, the power, and so the neutron flux, on the sample's location decreases due to the position of the assembly in the core, but each rod inside the assembly does also not experience the same flux. For instance during the cycles 16 and 17, the effect of the guide tube (which is just a hollow tube filled by water) in P6 did affect more the power of the sample than the guide tube at P10 did during cycle 18 because this one was not a direct neighbour of GU3.
Fortunately, the solution to this problem is exactly the same as above since it only requires to

work with the sample's irradiation history and not with the history of the entire assembly. In this way, all the movements of the assemblies which GU3 belongs to, but also the movements of the rods inside them are no longer problems.

It can be seen in fig 3.3 that the rod containing GU3 was not the only one that moved from assembly 1601 to 1701 since three others took place at positions N9, N12 and S13; they are represented by blue squares. The assembly 1701 was thus filled in total by 20 guide tubes, 201 fuel rods burnt until 17.70[MWd/kgU] and 4 fuel rods which already experienced 2 irradiation cycles.

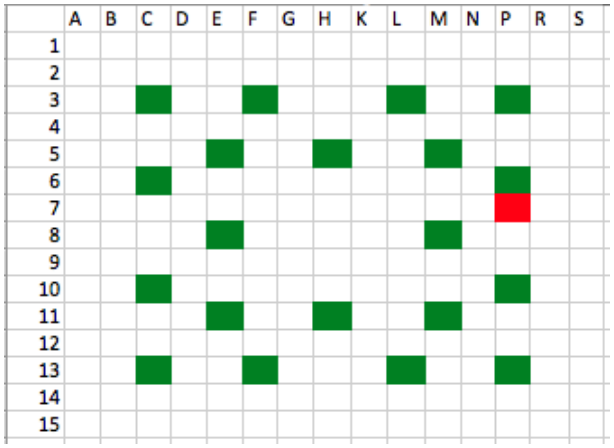

Figure 3.2.: Assembly 1601, cycles 16 and 17. GU3 sample is the red square. In these figures, the green squares represent the guide tubes of the assembly while the white ones are the fuel rods.

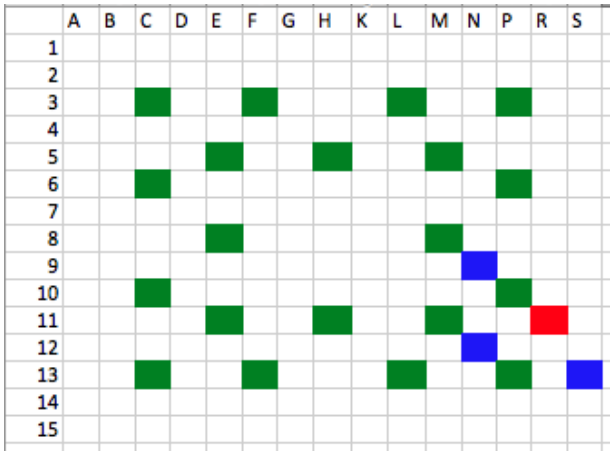

Figure 3.3.: Assembly 1701, cycle 18. GU3 sample is the red square and the blue ones are the other rods that come from assembly 1601.

3.3. Decay history of sample GU3

Before that their concentrations have been analysed, samples GU3 and GU3' have been transported to the laboratories, stored and chemically prepared. During this time, there was no neutron flux inside the core and the changes in the chemical compositions of the samples were

only due to radioactive decays.
So, it is as important as it was for the irradiation history to accurately describe the decay of the samples. As explained earlier, this is even more true in the case of the short-lived isotopes since their concentration decreases very quickly with the time.

Table 3.3 gives the measurement cooling dates associated with the isotopes and to the laboratory where they were performed.

Date	Laboratory	Isotopes
28/01/1999	ITU	U, Pu
26/03/1999	ITU	Nd, I-129
04/05/1999	ITU	Sm, Eu, Cs, Ce-144, Pm-147
16/06/1999	ITU	Cm, Am-241, Am-243, Np-237
01/07/1999	SCK-CEN	Cs, Eu, Ce-144, Ru-106, Sb-125
06/10/1999	ITU	Gd-155, Sr-90, Mo-95, Tc-99, Ru-101, Ru-106, Rh-103
12/10/1999	SCK-CEN	U, Pu
24/11/1999	SCK-CEN	Nd
01/12/1999	SCK-CEN	Gd-155
13/12/1999	SCK-CEN	Sm
21/12/1999	SCK-CEN	Am, Np-237
24/12/1999	SCK-CEN	I-129
03/03/2000	SCK-CEN	Pm-147
10/04/2000	SCK-CEN	Mo-95, Tc-99, Ru-101, Rh-103, Ag-109
16/05/2000	SCK-CEN	Sr-90

Table 3.3.: Cooling dates corresponding to the measurements of the isotopes in the two laboratories.

To these information must be added the dates of the cycles 16, 17 and 18 of the operating power plant. Indeed, there was during these cycles also some time during which the reactor was stopped and thus not irradiated by the neutrons anymore. Moreover, the end of the cycle 18 is required since it is necessary in order to determine the total duration from the end of GU3's irradiation to the beginning of the measurements in the laboratories.
Table 3.4 gives hereafter the dates of the start-up and the shutdown of cycles 16 to 18.

Cycle	Beginning	End
16	29/06/1994	10/06/1995
17	05/07/1995	08/06/1996
18	30/06/1996	07/06/1997

Table 3.4.: Operation dates of Gösgen from cycle 16 to 18.

It can be seen here that there is a certain amount of time between the end of a cycle and the beginning of the next cycle. This can be explained by the fact that the replacement of spent uranium rods by fresh fuel ones requires a certain amount of time. The decay time of GU3 from cycle 16 to cycle 17 is 25 days while it is 22 days between cycle 17 and cycle 18.

ALEPH2 input file

4

Sommaire

It has been explained in section 2 that the ALEPH2 burn-up code is able to compute the depletion of materials when they are being irradiated by a neutron flux, or not - as it was the case with sample GU3 in Gösgen's core -. Indeed, when the sample does not experience any neutron flux, the chemical concentrations of the materials just evolve due to radioactive decay processes, and it does not change anything to the way ALEPH2 works (see eq 2.25, with ϕ_k^{MCNP} set to 0).

First of all, a general Monte-Carlo transport code computes the tallies in all the cells of the studied problem in order to get "snapshots" of the neutron fluxes inside them. These values are indeed not real fluxes since they do not have units of $[neutrons/cm^2s]$ yet because the time has not been taken into account so far in the problem (the neutrons are moving in what can be called a frozen version of the core at a certain time). After this, the thermal power - generated by the fissions and the radioactive decays - of the sample is used by the program to calculate a neutron source rate which allow to transform the $R_{i,j}^{MCNP}$ (see eq 2.20) into real reaction rates which are valid during all the period where the power produced in the sample is assumed constant. The depletion of all the materials in which the user has an interest can then be successfully achieved.

A general ALEPH2 input can thus be seen as a two-part input - with each part separated by a "END" or a "MESSAGE" keyword[1]. The first part is related to the irradiation and decay history of the sample, while the second part is the Monte-carlo transport which calculates the neutron flux tallies inside the cells of the problem, whenever a new time step instruction begins in the first part.
The structure of an ALEPH2 input can be visualized in fig 4.1.

[1] Since "MESSAGE" keyword is the header of the MCNP part of the input file, the "END" message, only used to inform ALEPH2 where the ALEPH-specific cards end and where the MCNP5 cards begin, is not requested if the "MESSAGE" keyword is present.

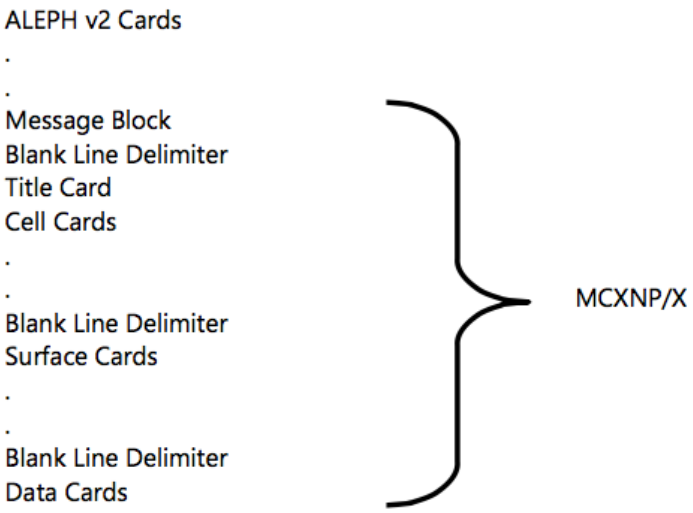

Figure 4.1.: Structure of ALEPH2 input file [20].

The folllowing section will describe in two distinct parts the ALEPH2 input file related to the sample GU3. The MCNP5 part of the code will first be explained, followed by the ALEPH2-specific elements - even if the two parts are presented in the opposite way in the structure of an ALEPH2 input, see figure above.

4.1. 1^{st} part: MCNP5 cards

It can be seen in fig 4.1 that the part of the ALEPH2's input file related to MCNP5 is itself divided into three general parts: the cell cards, the surface cards and the data cards.
First of all, the surface cards are the code lines which describe finite or infinite geometric surfaces in a 3-D space. Then, from a combination (intersections and unions) of the different parts of the space defined by these surfaces, the cells of the problem are defined. A density, a temperature and a material number are finally assigned to each of the cells in order to form what are called the cell cards.
The last part - i.e the data cards - are the lines which contain the following informations:

- The material cards, i.e. the isotopic compositions of the materials which fill the cells and their related neutron interaction tables - containing all the cross sections and emission distributions for secondary particles -.
- The source cards, i.e. the general description (position, energy spectrum) of the source used to generate the neutrons which move inside the problem during the simulation.
- The tallies cards, i.e. the choice of tallies that the program has to compute and the associated cells (for instance, a user may request that MCNP5 computes tallies in only one cell if the material inside it is the only part of the system in which the user is interested to know the chemical composition over the time).

Nevertheless, in order to help the reader to understand clearly the MCNP5 part of the input file, the subsection hereafter is not presented in the same order than in fig 4.1, but in the following way:

- First, a description of the materials in the assemblies and their related material cards.

- Second, an explanation about the problem's division into cells and the description of all the cell cards with in particular their geometric description from the surface cards.
- Third, the source cards (with a related kcode criticality calculation).
- And finally, the tallies cards.

4.1.1. Material cards

In an operating core, if the metallic grid - which holds every fuel rods and guide tubes together - is neglected, only a few materials are present: fresh and burnt uranium oxide, zircaloy cladding, helium and water.

Regarding the fuel rods, they are made of cylindrical UO_2 pellets, surrounded by a cylindrical zircaloy cladding - which represents the first barrier in case of the melting of the fuel - and between them, a gap is filled by pressurized helium.

On the other hand, the guide tubes are simply hollow tubes of zircaloy filled by water or by control rods in case of a reactivity control. During all the simulation, they are however filled only by water because the power plant is supposed to be working at full power all the time. This means that the control rods are supposed to be in their safety stand-by position at the top of the core, ready to be injected but never filling the guide tubes.

The material cards are the code lines which define as well the initial isotopic concentrations of the materials in the problem as the reference of their neutron interaction tables. All the materials from these cards will fill at least a cell of the problem at a certain time, but only some of them - according to the choices of the user - will be depleted by the solver of ALEPH2. These selected materials will thus have a different composition each time a new MCNP5 calculation - corresponding to a new step of the sample history (irradiation or decay step) - will be run.

Ii should be noted that in MCNP5, the different isotopes are defined by their Z number and atomic mass A in what is called the "ZAID". From this, they are always written in accordance with a generic notation ZZZAAA, where the first zeros are not necessary. For instance, the isotope H-1 is recognized in the files by the notation 001001, or 1001 since the first zeros can be omitted. In the same way, O-16 is written 008016 (or 8016), U-235: 092235 (or 92235), etc.

Regarding the neutron interaction tables of the material cards, they are all selected from the ACE-formatted general transport neutron data generated by the auxiliary utility ALEPH-DLG. To select the temperature which corresponds to the neutron interaction table of a nuclide, the user must simply provide the isotope in its ZZZAAA form and attach to it the suffix ".nnc", where nn is related to the temperature in kelvins and the letter c stands for the choice to use continuous-energy neutron tables. For instance, the continuous-energy neutron interaction table of U-235 at 1000[K] is given by 92235.10c, the table of H-1 at a temperature of 600[K] is given by 1001.06c, etc.[2]
It should be noted that the neutron data are not processed for all the temperatures, but only at selected ones. What was done in practice is that experiments were made at several neutron

[2]If all the isotopes of a material have the same temperature, they can also be listed and simply be preceded by the code line "nlib=nnc".

discrete energies and then combined with the predictions of nuclear model calculations in order to extract the true value at 0[K]. The utility ALEPH-DLG increased then the temperature of the target nuclides by steps of 50[K], in order to compute the temperature-dependent data such as some cross sections. For instance, the Doppler broadening in the epithermal range of energy for the fission, capture and elastic cross sections was each time processed at the new temperature, and the elastic scattering cross sections were also multiplied by a factor F(T) (thermal free gas elastic scattering treatment, see section 2). The ACE-formatted, relative to the temperature and suitable for MCNP calculation, general transport neutron data, were then finally processed at 0, 50, 100, 150, etc. [K].

From this, if the temperature of a material is not the same as one at which ALEPH-DLG processed data, the user has to provide to MCNP5 a temperature as close as possible from it, sometimes 20 or 30[K] above or below.
Table 4.1 provides the mean temperature of each of the material in the core and the closest temperature to which a neutron interaction table is available for each of them[3].

Material	Mean temperature [K]	Temperature chosen in library [K]
Oxyde uranium	1000	1000
Helium	700	700
Zirconium	600	600
Zirconium in guide tubes	570	600
Water	575	600
Water in guide tubes	566	600

Table 4.1.: Mean temperatures of the materials and closest temperatures where a neutron interaction data is available in the files.

Due to the Doppler and the moderator temperature effects, the most important temperatures of the problem are certainly the ones related to the UO_2 and to the water moderator.
Indeed, the Doppler temperature effect explains in particular the fact that, when the temperature of the target U-238 atoms of the UO_2 increases, the relative speed of the neutron with respect to the nucleus is somewhat uncertain, and this translates into a broadening of the resonances in the U-238 capture cross section. On the other hand, an increase of the moderator's temperature has a double influence: the thermal spectrum of the neutrons shifts toward a higher temperature - where σ_f of U-235 is smaller - and in the same time the water density decreases, leading to less neutron moderations. In each case, the moderation of the neutron flux in the core is altered; this is why the two temperatures in question have to be very accurately provided by the user of the program.

To conclude here, a material card Mn is simply made of code lines composed of the identification of an isotope and its neutron interaction table in the ZZZAAA.nnc form, followed by a value corresponding to the fraction of the isotope in question in the material's composition. In the case of a mass fraction, this value is moreover preceded by a minus sign, in order to make the difference with an atomic fraction.

[3]It should be mentioned that the temperatures of the UO_2 and water come from [23], but the ones related to the helium and the zirconium have been approximately deduced from them.

Fresh uranium oxide

At the beginning of cycle 16, all the fuel rods of assembly 1601 are made of fresh UO_2 enriched to 4.1[$wt.\%$]. This means that for 100[g] of uranium, 4.1[g] is here U-235. The other parts of the uranium in the fresh pellet are U-234, 0.042[$wt.\%$] and U-238, 95.858[$wt.\%$]. The total mass fraction of uranium in the fuel is thus equal to 88.14[$wt.\%$], and the remaining fraction composed of oxygen.
With the molar composition of natural oxygen given by [16]: [O-16] = 99.76[%], [O-17] = 0.04[%] and [O-18] = 0.2[%], table 4.2 is a summary of all the isotopes' mass fractions in the fresh UO_2 that can be found in Gösgen power plant.

Atom	Isotope	ZAID	Composition [$wt.\%$]
Oxygen	O-16	8016	11.83
	O-17	8017	5.04E-03
	O-18	8018	2.67E-02
Uranium	U-234	92234	3.70E-02
	U-235	92235	3.61
	U-238	92238	84.49

Table 4.2.: Fresh UO_2 weight composition.

In MCNP5, the material card M2 (this number means just that the material is the second material described in the input file[4]) of fresh UO_2 at 1000[K] is thus given by the following lines where the minus sign - as a recall - stands for a mass fraction:

```
M2 nlib=10c
8016  -0.118317732
8017  -4.50680E-05
8018  -2.37200E-04
92234 -3.70188E-04
92235 -0.036137400
92238 -0.844892412
```

Burnt uranium oxide

As explained in section 3, most of the assembly 1701 in cycle 18 is filled by fuel pins previously burnt until 17.70[MWd/kgU]. Since they will have a large effect on the neutron flux - and thus on GU3's final composition - during the last cycle of irradiation, it is necessary to know accurately the chemical composition of such pins. In order to get it, a simplified ALEPH2 input file - which will be detailed later - representing one single fuel pin being irradiated until the correct burn-up has been computed in ALEPH2.

Pressurized helium

Because of its high thermal conductivity and its stable state under radiation, helium has been chosen to fill the gap between the pellet and its cladding, which is needed to prevent

[4]The code lines which are presented in all the section come from the real input file, see appendix A.1.

the thermal expansion of the fuel. From this, it means that the heat generated in the UO_2 is transfered to the water in a way that the temperature profile is rather smooth (the temperature gradients from the UO_2 to the water are actually small enough to be suppoprted by the materials) and that the composition of the helium stays rather constant during all the irradiation. Moreover, this gas is pressurized to approximately 30[bar] in order to counteract the primary water pressure on the cladding (more than 150[bar], see table 3.1).
In its natural conditions, the helium is composed of only 2 isotopes, He-3 and He-4, in according with the proportions given by [13], written in table 4.3.

Atom	Isotope	ZAID	Composition [%]
Helium	He-3	2003	1.34E-04
	He-4	2004	99.99

Table 4.3.: Natural helium atomic composition.

The MCNP5 material card of the 700[K] helium is thus:

```
M3 nlib=07c
2003 1.3400E-6
2004 0.99999866
```

Zircaloy cladding

The zircaloy-4 (also called Zr-4) cladding is the surrounding material of both guide tubes and fuel pins. The choice of such a material for the cladding has been done because of its low neutron absorption cross section σ_a, leading to a small decrease of the thermal neutron flux when the neutrons come back in the fuel rod after their thermalization in the moderator.
The Zr-4 is mainly composed of zirconium (98.23[%]) but contains small fractions of tin (1.45[%]), iron (0.21[%]), chromium (0.1[%]) and hafnium (0.01[%]). With the natural concentrations of those five atoms given respectively by [18], [17], [15], [11] and [12], the final isotopic composition of Zr-4 is given in table 4.4.

Atom	Isotope	ZAID	Composition [%]
Zirconium	Zr-90	40090	50.54
	Zr-91	40091	11.02
	Zr-92	40092	16.85
	Zr-94	40094	17.07
	Zr-96	40096	2.75
Tin	Sn-112	50112	1.41E-02
	Sn-114	50114	9.57E-03
	Sn-115	50115	4.93E-03
	Sn-116	50116	2.11E-01
	Sn-117	50117	1.11E-01
	Sn-118	50118	3.51E-01
	Sn-119	50119	1.25E-01
	Sn-120	50120	4.72E-01
	Sn-122	50122	6.71E-02
	Sn-124	50124	8.40E-02

Atom	Isotope	ZAID	Composition [%]
Iron	Fe-54	26054	1.23E-02
	Fe-56	26056	1.93E-01
	Fe-57	26057	4.45E-03
	Fe-58	26058	5.88E-04
Chromium	Cr-50	24050	4.31E-03
	Cr-52	24052	8.38E-02
	Cr-53	24053	9.50E-03
	Cr-54	24054	2.36E-03
Hafnium	Hf-174	72174	1.62E-05
	Hf-176	72176	5.21E-04
	Hf-177	72177	1.86E-03
	Hf-178	72178	2.73E-03
	Hf-179	72179	1.36E-03
	Hf-180	72180	3.51E-03

Table 4.4.: Zr-4 cladding atomic composition.

Again here, the MCNP5 material card is the following:

```
M1 nlib=06c
40090 .50539335
40091 .11021406
40092 .16846445
40094 .17072374
40096 .02750440
50112 1.40650E-4
...
```

Water moderator

The water in a PWR core fulfills two distinct functions: first, it cools down the reactor by taking out the heat generated in the pellet which is then exchanged in the steam generator; and secondly, it moderates the fast fission neutrons in order that their interactions with the U-235 atoms result statistically in a lot of fissions (the neutron energy is decreased by inelastic scatterings until $\sigma_{f,\mathrm{U-235}}(\mathrm{E}) > (\sigma_{t,\mathrm{U-235}} - \sigma_{f,\mathrm{U-235}})(\mathrm{E})$).

Since the reactivity in the core at the beginning of a cycle is above zero[5] to compensate the negative - and evolving over the fuel cycle - terms of the reactivity balance (the xenon and samarium effects, the moderator temperature coefficient which, when the temperature of the water and when the fuel burn-up increase, lessens the neutron flux by shifting its thermal spectrum towards higher energies where in particular the capture reasonances of Pu-240 are larger, and the doppler coefficient which also lessens the number of neutrons by broadening the resonance peaks of $\sigma_{c,\mathrm{U-238}}$ when the fuel temperature increases), some burnable poison has to be also added in the water, in order that it captures itself the excess neutrons in the reactor; and this, more rapidly than the fission products can do it. The neutron absorption

[5] This is what is called the initial fuel excess of reactivity.

rate is therefore reduced in time and it is then possible to always keep the reactivity ρ to zero.
In the case of Gösgen's reactor, the chosen poison is boric acid (H_3BO_3) because of the huge neutron capture cross section of B-10. The boron being progressively consumed during a cycle, its concentration is constantly evolving in the nuclear core (it decreases exponentially and then suddenly rises at the beginning of the following cycle due to a refill in H_3BO_3 in order to counteract the sudden increase of the neutron production rate in the vessel due to the fresh fuel replacement). Since the user is here only interested in the fuel compositions but not in how the concentration of H_3BO_3 evolves during the simulation, the boron has thus not to be put in any material card of the MCNP5 part of the ALEPH2 input and it will simply be added at each irradiation step in the top cards[6]: the material card relative to the water in MCNP5 is thus only composed of hydrogen and oxygen.
Table 4.5 gives the water composition as it is found in the MCNP5's part of the input. The decompositions of both oxygen and hydrogen in their natural isotopes were taken from [16] and [14].

Atom	Isotope	ZAID	Composition [%]
Hydrogen	H-1	1001	66.66
	H-2	1002	7.67e-3
Oxygen	O-16	8016	33.25
	O-17	8017	1.27e-2
	O-18	8018	6.67e-2

Table 4.5.: Water moderator atomic composition.

The MCNP5 material card corresponding to the water is then:

```
M4 nlib=06c
1001 0.66659
1002 7.6666667E-5
8016 0.33254
8017 1.2666667E-4
8018 6.6666667E-4
MT4 lwtr.62t
```

It can be seen here that another material thermal card "MT4 lwtr.62t" is also attached to the material. This card corresponds to a thermal neutron interaction table S(α,β) (the data which describe very precisely the thermal neutron scatterings by molecules and crystalline solids when the energy of the incident neutron is low, see section 2) available in the general transport neutron data file. Indeed, the "lwtr.62t" provides here the scattering data at 600[K] between a neutron and a H-1 atom, which is the main isotope in the core responsible for the neutron flux thermalization by inelastic scatterings[7].

[6] In a perfect case, the user would not have to change it manually at each time step since ALEPH2 should normally calculate it accurately. Indeed, from the power of the sample, the program computes a neutron flux in the water, then the depletion solver is applied on every nuclide that it is possible to find in the water and a new boron concentration is computed. Nevertheless, this new value is never the same as the one measured experimentally - due certainly to imprecisions in the benchmark data - and the boron concentration has to be corrected every time a new irradiation step is computed.

[7] The less the weight of the atom which the neutron collides with, the more is its loss of energy.

4.1.2. Cell and surface cards

Division of the problem in materials (and the related cells)

As explained earlier, the tallies are the time-independent values returned by the Monte-Carlo calculation, and which can be seen as pictures of physical quantities in the core. For instance, the F4 tallies are the one that has been used in this study case and which are a representation of the neutron fluxes in the cells. As a reminder, such a tally is calculated inside a cell for each neutron by multiplying its track length by its relative weight and dividing the value by the volume of the cell. This explains why it is important to correctly define the parameters of the cells of the problem as well as their geometry: in one hand, their volumes are needed in the F4 calculation and in the other hand, the code should know if a neutron crosses the border of the cell or not (i.e. if the track length is larger than the cell) because in that case, the neutron also contributes to F4 tallies in the next cell.

It has to be understood that the user does not require that MCNP5 calculates the F4 tallies everywhere in the assembly since it would take a lot of useless time. Indeed, only the neutron flux inside the cells which have an important impact on the final GU3's composition will be computed. For instance, the F4 tallies in a cell filled by the helium situated between a fuel rod and its cladding will not be requested by the user since helium is rather stable under neutron irradiation and only fills a very small volume of the problem. This means that even if tallies were calculated in that cell, that the tally spectrum made possible to calculate reaction rates thanks to the estimate power of the sample GU3 and that the depletion solver of ALEPH2 was then applied on the helium, the new composition of this material would not be different enough from the initial helium to impact significantly the neutron flux in GU3.

Besides, sample GU3 and the rest of the fuel inside the reactor can not be considered as cells filled by a same material. Indeed, as explained by eq 3.1, the neutron flux in a reactor is not constant and depends both on the radial position and the z coordinate. Since all the fuel rods do not have the same radial position in the assembly, computing a global neutron flux for all the fuel would amount to saying that the compositions of GU3 and the one of the rest of the assembly are the same during all the irradiation history. This choice would lead to significant errors on GU3's composition at the end of the three cycles and can thus not be used here to compare the results with the benchmark values.
In the same kind of idea, it is useful to isolate the neighbouring fuel rods of GU3 in separate materials since they will impact the composition of GU3 more than the other fuel rods of the core. By doing this, the Monte-Carlo transport code will calculate in each of the neighbouring cells a different tally neutron flux spectrum and all of these fluxes will be given to ALEPH2's depletion solver which will calculate a new concentration, slightly different from the others, for each of the neighbouring materials. If a next irradiation step is then required, a new MCNP5 input file is created with the updated material compositions, and the process is computed again. At each time step, the effect of a neighbouring fuel rod on the sample GU3 will thus be a little bit different compared to the others. For instance, if one of the neighbours experiences a neutron flux a little bit larger than what the others do, its new composition will contain less U-235 atoms at the end of the irradiation time. So, in the next MCNP5 transport calculation, less neutrons will fly from this neighbour than from the other fuel rods towards sample GU3, since there will be less fissions in this one.
Separating the fuel rods in cells filled by different materials allows thus to better describe the behaviour of the core. Separating each of all the fuel rods would however result in a huge

loss of calculation time, since a lot of them are located too far away from GU3 to have a significant effect on its composition.

Before going further in the separation of the problem in materials, a good point to remember here is the link between the MCNP5 cells and the materials which are burnt in the ALEPH2 cards. First of all, geometric cells are created in MCNP5 and are filled by some materials. Then, the Monte-Carlo calculation simulates neutrons everywhere in the core in order to describe its behaviour as much as possible and F4 tallies in some cells are finally computed and given to ALEPH2 in order to proceed to the time-dependent neutron irradiation. At this point, ALEPH2 does not look anymore at the geometry of the problem. From the thermal power of sample GU3, it calculate a source strength (in particles per second), then reaction rates in the materials, and finally, from their initial composition and the reaction rates deduced, the depletion solver computes their burn-up. The materials are thus just chemical compositions of the cells relative to the current time step, and are not, in any way, linked to them for the entire simulation.
It can be understood here that, in order to help the user to better model the irradiation history, it is possible to exchange the material which fills a cell by another material at the beginning of a time step (in the ALEPH2 top cards) without any problem. In that case, the F4 calculations in MCNP5 are then computed in the same geometry (i.e cell) but with a different chemical composition (i.e. material), and the depletion solver simply depletes this new material. In practice, it is thus also even possible to switch two materials of the problem together - when two fuel rods switch position in an assembly, for instance.
However, if the exchange of a material is made with a new material which was not already burnt by the neutron flux in the core (i.e. was not present in the problem yet), the old material is then removed from the system and the only terms that are allowed in the evolution of its composition are radioactive decays, since it is not irradiated anymore by the neutron flux.

What has just been explained is very useful for Gösgen study case, since it makes possible to describe the problem stated in section 3 with only one assembly, which will represent in a first time the assembly 1601 (cycles 16 and 17) and then in a second time the assembly 1701 (cycle 18). The only thing to do in that case is to permute materials inside the assembly at the beginning of cycle 18 (and making sure that they are related to same volumes). At the beginning of the time step, ALEPH2 will then assume that other materials (some of which were ”waiting” outside of the system since they were not irradiated in assembly 1601 during cycles 16 and 17) fill the already defined cells. The only thing that the user has to provide in this case in the ALEPH2 cards of the input file are the numbers of the materials - defined in the material cards - that will be switched together.
With this, it makes for instance possible to exchange GU3 in P7 (see fig 3.2) by a fuel rod of same volume but already burnt until 17.7[MWd/kgU] (which was ”waiting” outside) and in the same time to exchange the fuel rod in R11 which was burnt during cycles 16 and 17, by the sample GU3 (see fig 3.3). The total volume of the materials in the system remains then constant, since one new fuel rod burnt until 17.7[MWd/kgU] replaces the sample GU3, which itself fills now the cell of a fuel rod burnt during cycles 16 and 17 and now removed of the system.

All of this explains why it was chosen to divide the fuel UO_2 in separate materials, and why the related cells in the lattice have thus all a different cell card.
In practice, the fuel of the assembly has to be divided in the following way:

- The UO_2 fuel rod which fills GU3's position of cycles 16 and 17, P7.
- The UO_2 fuel rod which fills GU3's position of cycle 18, R11.
- Each of the seven neighbouring fuel rods of GU3 in cycles 16 and 17 (not eight neighbours, because P6 is a guide tube) in positions N6, N7, N8, P8, R6, R7 and R8.
- Each of the seven neighbouring fuel rods of GU3 in cycle 18 (the neighbour in P10 is also a guide tube) in positions P11, P12, R10, R12, S10, S11 and S12.
- The three fuel rods located in N9, N12 and S13 which moved with GU3 from assembly 1601 to assembly 1701. In fact, they are the only cells which will be filled by the same material during all the simulation, since all the other cells will be filled at the beginning of cycle 18 either by "new" fuel burnt until 17.7[MWd/kgU] or by the sample GU3.
- The rest of the assembly's fuel rods.

Fig 4.2 is a representation of what the assembly's decomposition in materials and cells looks like.

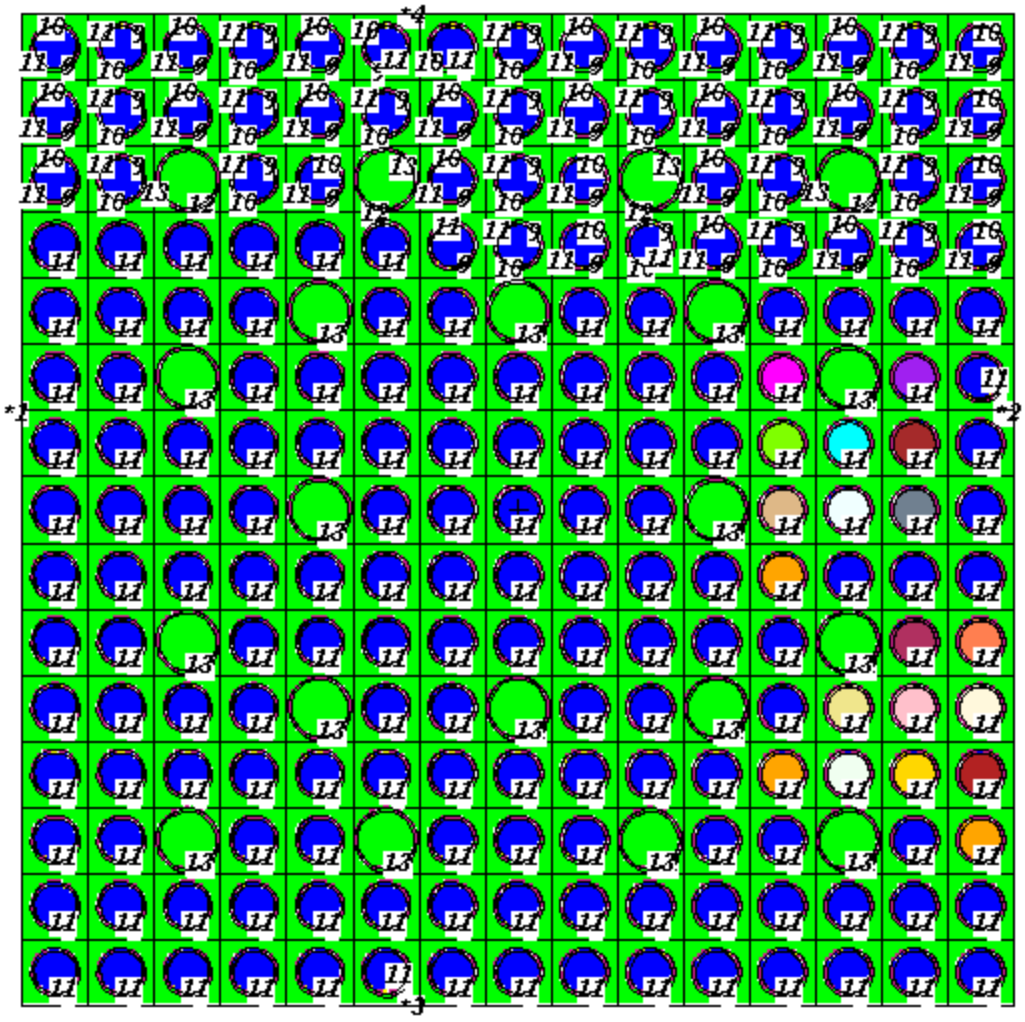

Figure 4.2.: Picture of the assembly with the different materials and their related cells, from MCNP5 geometry plotting function (numbers have here nothing to see with the material decomposition).

In the figure, the large circles represent the guide tubes and the small ones the fuel rods. Regarding the colors, they all correspond to a material which fills a cell or a group of cells. Indeed, the green is the water (the guide tubes are also filled by water, as a recall), the red around the fuel rods and in the guide tubes is the Zr-4 cladding and the other colors represent the different fuel materials:

- Light blue, GU3's position in cycles 16 and 17.
- Light pink, GU3's position in cycle 18.
- Orange, The three fuel rods others than GU3 common to assemblies 1601 and 1701.
- Navy blue, all the fuel rods except the ones described just above and the fourteen neighbours of GU3.
- Remaining colors, the fourteen neighbours of GU3 during the three cycles.

Description of the cells in MCNP5

Now that the decomposition of the problem in separate materials and their related cells has been described, it is time to write it in MCNP5 code lines.
First of all, it has to be known that a cell is defined by the following parameters, all of them separated by at least one blank:

- Its cell number.
- Its cell material number (i.e the identification number of the material which fills the cell, from the material cards).
- Its cell material density. If this one is preceded by a minus sign, it means that the density is given in terms of $[g/cm^3]$, while a positive entry can be interpreted as an atom density in units of $[10^{24}\ atoms/cm^3]$.
- The complete description of its geometry from the surface cards.
- All its other parameters: the temperature of the material which fills the cell, the statistical weight of a newborn fission neutron inside it, etc.

Since the neutron track lengths and the choice of the collision nuclide are computed with the help of the macroscopic total cross section of the material Σ_t in which the neutron is flying, the material density is very important in the neutron transport code. Indeed, with the composition of the material from the material card and with the material density, MCNP5 can calculate the concentration of each isotope. From this, the neutron track length of eq 2.6 is given by:

$$T_l = \sum_i \left(\frac{-1}{\Sigma_{t,i}} \right) ln(\zeta) = \sum_i \left(\frac{-1}{\rho \cdot F_i \cdot \frac{6.02 \cdot 10^{23}}{M_{m,i}} \cdot \sigma_{t,i}} \right) ln(\zeta) \tag{4.1}$$

With i summed over all the nuclides of the material, ρ is the density of the material in $[g/cm^3]$, F_i the weight fraction of nuclide i in the medium (from the material's card) and $M_{m,i}$ is its molar mass.
Table 4.6 presents hereafter the densities of the materials present in the assembly.

Material	Density $[g/cm^3]$
UO_2	10.4
He	0.0020907
Zr-4	6.5093
Zr-4 in guide tubes	6.5093
Water	0.723
Water in guide tubes	0.743

Table 4.6.: Densities of the materials present in an assembly.

The densities of the moderator and the UO_2 above come directly from [23], while the one of the cladding has been computed from its chemical composition (see table 4.4) and the density of the helium comes from the perfect gas law:

$$\rho = \frac{p}{R^* \cdot T} = \frac{30 \cdot 101325}{\frac{8.3145}{4.003} \cdot 700} \cdot \frac{1}{10^6} = 0.0020907[g/cm^3] \tag{4.2}$$

Prior to defining all the cells of Gösgen's assembly, the following part is first an explanation - emphasized by a few examples - on how the geometry of a problem is generally defined in MCNP5 thanks to the surface cards.

A volume - or a cell - is defined in MCNP5 by the intersections of 2D and/or 3D surfaces in a three-dimensional space. For instance, creating a cube centered on (0,0,0) requires six 2D surfaces or planes each of them corresponding to one side of the cube. In that case, the cell defining the inner part[8] of the cube is given by the formula:

$$\text{left}(x - D = 0) \cap \text{right}(x + D = 0) \cap \text{left}(y - D = 0) \cap \text{right}(y + D = 0) \cap \text{left}(z - D = 0) \cap \text{right}(z + D = 0)$$

Where $\text{left}(x - D = 0)$ represents the left side of the plane whose equation is $x = D$ (also called the negative side of the surface, since it represents the space located in the direction of the decreasing x coordinate) and $\text{right}(x + D = 0)$ is simply the space to the right of the plane $x = -D$ (also called the positive side of the surface).
In MCNP5, such regions are described and combined by boolean operators, with in particular:

- Left(): a simple minus sign.
- Right(): a plus sign (or nothing).
- The intersection of regions: a blank between the surfaces which represent the regions.
- The union of regions: a ":" symbol between the surfaces.

There exist also in MCNP5 surfaces and volumes cards in order to represent the surfaces used to define the cells.
For instance, the plane $(x - D = 0)$ is written "PX D", while $(x + D = 0)$ is given by "PX -D". Another useful example is "CZ R", to define a cylinder with axis O_z and radius R.

The former cube example can then be written in MCNP5 code lines by:

[8] The outer part of a volume is also considered as a cell, even if it is not filled by any material (i.e. if it is a void cell).

```
c here begin the cell cards[9]
1 MAT_ID MAT_DENS -1 2 -3 4 -5 6
2 MAT_ID MAT_DENS  1:-2:3:-4:5:-6
c here end the cell cards

c here begin the surface cards
1 PX  D
2 PX -D
3 PY  D
4 PY -D
5 PZ  D
6 PZ -D
c here end the surface cards
```

The first four lines of this code represent the description of the cells, while the last ones are the surface cards which are used to define their geometry.
Here, the cell number 1 represents the cube since "-1 2 -3 4 -5 6" is exactly the same as what was written previously to define it. Indeed, it correponds to the intersections of the negative sides of the surfaces 1 (x-D=0), 3 (y-D=0) and 5 (z-D=0) with the positive sides of the surfaces 2 (x+D=0), 4 (y+D=0) and 6 (z+D=0). The second cell whose geometry is given by "1:-2:3:-4:5:-6" represents on the other hand everything in the 3D space except the cube, since it is described by the union of the positive sides of surfaces 1, 3, 5 with the negative sides of surfaces 2, 4, 6, i.e. exactly the contrary of the first cell's geometry.

Another small and very useful example corresponds to a single fuel rod similar to the ones which form the assemblies of Gösgen reactor. From the values of table 3.1 and by limiting the height of the rod to 10[cm] - as GU3's height -, it is possible to create fig 4.3 with the help of the geometry plotting function of MCNP5.
The colors correspond here respectively to: green, the water; pink/red, the Zr-4 cladding; blue, the helium and yellow, the UO_2.

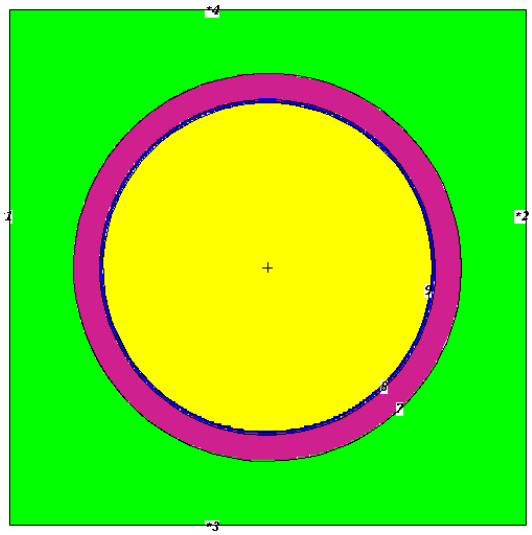

Figure 4.3.: Picture of a single fuel rod that can be found in Gösgen's core, with the water around it (MCNP5 geometry plotting function).

[9] A line that begins by a "c" followed by a blank is a comment line and is always neglected by the code.

The MCNP5 code lines used to create fig 4.3 are the followings:

```
c beginning of cell cards
1 1 -10.40     -9                      $ Fuel UO2
2 2 -0.0020907 -8 9                    $ He gap
3 3 -6.5093    -7 8                    $ Zr-4 cladding
4 4 -0.723     -1 2 -3 4 -5 6 7        $ Water
5 0             1:-2:3:-4:5:-6         $ Void space around everything[10]
c end of cell cards

c beginning of surfaces (in [cm])
1 PX  0.715
2 PX -0.715
3 PY  0.715
4 PY -0.715
5 PZ  5
6 PZ -5
c end of surfaces
c beginning of cylinders (in [cm])
7 CZ 0.5375                            $ ZR4 outer cylinder
8 CZ 0.4650                            $ ZR4 inner cylinder
9 CZ 0.4555                            $ UO2 cylinder
c end of cylinders
```

There are here five cells which describe the problem:

- The cell number 1 which is the fuel UO_2 defined by the negative side (the central part) of the surface number 9, a vertical cylinder of radius 0.4555[cm].
- The cell number 2 which is the helium defined by the intersection between the positive side (the external part) of the surface 9 and the negative side of the surface 8, i.e. the volume between two vertical cylinders of radius 0.4555[cm] and 0.465[cm].
- The cell number 3 which is the Zr-4 defined by the intersection between the external part of the surface 8, a vertical cylinder of radius 0.465[cm] and the internal part of the surface 7, a vertical cylinder of radius 0.5375[cm].
- The cell number 4 which is the water defined by the intersection of the internal part of a 10-centimeter-high rectangular parallelepiped of 1.43[cm]-by-1.43[cm] square section (”-1 2 -3 4 -5 6”) and 7, the external part of a cylinder of radius 0.5375[cm].
- The cell number 5 which is the void cell around the problem, defined as the inverse of ”-1 2 -3 4 -5 6”.

Since the geometries of the fuel rods and the guide tubes in Gösgen's assembly are always the same, it is obvious that the user will not have to describe each of them separately. There exist some tools in MCNP5 which allow to duplicate as much as wanted by the user a single geometry in a larger volume. These tools are known by the keywords *universe*, *fill* and *lattice* in MCNP5, and help to create what are called the repeated structures cards. Such cards allow the user to mention that a cell has to be filled by something called a universe. This universe can be a cell, multiple cells or even a lattice.

[10] If a cell is void, it has no material density and its material number is 0.

To make it simple:

- When the *universe* card is attached to a cell, it means that this cell belongs to this universe.
- When the *fill* card is attached to a cell, it specifies with which universe the cell is filled.
- When the *lattice* card is attached to a cell, it means that this cell - which can already belong to a universe - is made of an array of either hexahedra (solids with six faces) or hexagonal prisms (solids with eight faces).

The solution to represent Gösgen's assembly as it was defined in fig 4.2 is the following. First of all, a huge cell the size of the entire assembly has to be defined. To this cell has to be attached the keyword "fill=1", which means that this cell is filled by the universe number 1. Then, the user must specify that this universe 1 is a lattice made of fuel rods identical to the one of fig 4.3 and of guide tubes. Each of the elements of the lattice must then be associated with an universe number which represents either a guide tube or a fuel rod (there will be a lot of different universe numbers for the fuel rods since a distinction is required between a lot of them: two positions of GU3, neighbours, etc.). Finally, the cells that belong to these universes must be each defined in a generic cell card.

To simplify the explanation, the MCNP5 code description of the assembly is divided hereafter in two parts. First, the following code lines are related to the description of the global cell filled by the universe 1, which is itself a lattice of universes:

```
c cell cards
1 0 1 -2 3 -4 5 -6           fill=1
2 0 77 -7 88 -8    u=1 lat=1 fill= -7:7 -7:7 0:0

  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  3  2  2  3  2  2  2  3  2  2  3  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  3  2  2  3  2  2  3  2  2  2  2
  2  8  3  14 2  2  2  2  2  2  2  2  3  2  2
  2  9  5  13 2  2  2  2  2  2  2  2  2  2  2
  2  10 11 12 3  2  2  2  2  2  3  2  2  2  2
  2  2  2  6  2  2  2  2  2  2  2  2  2  2  2
  15 21 3  2  2  2  2  2  2  2  2  2  3  2  2
  16 7  20 2  3  2  2  3  2  2  3  2  2  2  2
  17 18 19 6  2  2  2  2  2  2  2  2  2  2  2
  6  2  3  2  2  3  2  2  2  3  2  2  3  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2

c surface cards
1  PX -10.725
2  PX  10.725
3  PY -10.725
4  PY  10.725
5  PZ -5
```

```
6  PZ  5
77 PX -0.715
7  PX  0.715
88 PY -0.715
8  PY  0.715
```

The first line of this code represents the "parent" cell, i.e. the assembly whose geometry is defined as the intersections of six planes described in the surface cards: 1, -2, 3, -4, 5 and -6. This cell should be considered as a void cell (material number equal to zero and material density neglected) since the materials that fill the assembly are all going to be defined later in their own cell cards. Here, the card "fill=1" attached to this cell means that it is filled by the universe number 1.

The cell number 2 belongs to this universe 1 since it has the card "u=1" attached to it; it fills thus the first cell just described. Moreover, the fact that this cell also possesses the card "lat=1" means that the universe 1 is a lattice of hexaedra[11]. To divide the universe 1 in a lattice, the user must provide the geometry of one element to MCNP5 and the program will duplicate it as much as possible inside the borders of the assembly.
The single element is simply here a small rectangular parallelepiped (the distinction between the fuel rods and the guide tubes inside the elements will be done later, according to their universes) as the one defined by the borders of fig 4.3 and whose geometry is given by the card "77 -7 88 -8", the intersection of four vertical planes. Here, the top and the bottom surfaces do not have to be given to MCNP5 because the elements of the lattice are limited by the cell that they fill, i.e. the asssembly. The program knows therefore by itself that the missing planes to close the shape of the element are $z = -5$ and $z = 5$.

At that point, the user must provide the universes that fill all the elements of the lattice. Some of these universes may fill a lot of elements, while some others may just fill one. For instance, all the guide tubes of the assembly belong to the same universe (they are all exactly the same and do not require to be separated), which means that this one will fill 20 elements of the lattice. Regarding the fuel rods, the case is diferent since some of them must have their own universe. For instance, the two positions of GU3 have to be filled by two distinct universes because the cells filled by these universes must be separate in order that it will be possible at one time to change the fuel material inside them. For the same reason, each of the neighbouring elements of these two positions in the lattice need its own universe. As it can be understood here, the division in universes of the fuel elements in the lattice needs to follow the same division that was explained before and which is presented in fig 4.2.

For MCNP5 to be able to correctly fill the elements with their universe, the user needs to provide the initial element (0,0) and in which directions in the lattice he wants the two lattice indices to increase. Here, the position of the element (0,0) has already been chosen because it is in fact given by "77 -7 88 8", the intersection of the negative sides of the surfaces number 7 and 8 and the positive sides of the surfaces number 77 and 88. This corresponds thus to the central element of the lattice (location H8) since by definition, both this element and the lattice are centered on the origin of the 3D space. Regarding the directions in which the user wants the indices in the lattice to increase, the rule is the following: for a hexahedral lattice cell, beyond the first surface listed in the geometry of the single element is the (1,0) element, beyond the second surface listed is the (-1,0) element, then the (0,1) and (0,-1) lattice

[11] If the card had been "lat=2", the elements of the lattice would then have been hexagonal prims.

elements in that order. In this case, the element (1,0) is the element situated in G8 because the first surface listed is the surface number 77 which corresponds to the plane of equation $x = -0.715$. This means that the element of the lattice which has this plane in common with the element (0,0) is considered as the element (1,0). In the same way, the element (-1,0) is the element in K8 since it is located just at the right of the surface 7 of equation $x = 0.715$. Finally, the element (0,1) is situated in H9 and the element (0,-1) is located in H7.

Fig 4.4 presents hereafter the elements of the lattice associated with their indices.

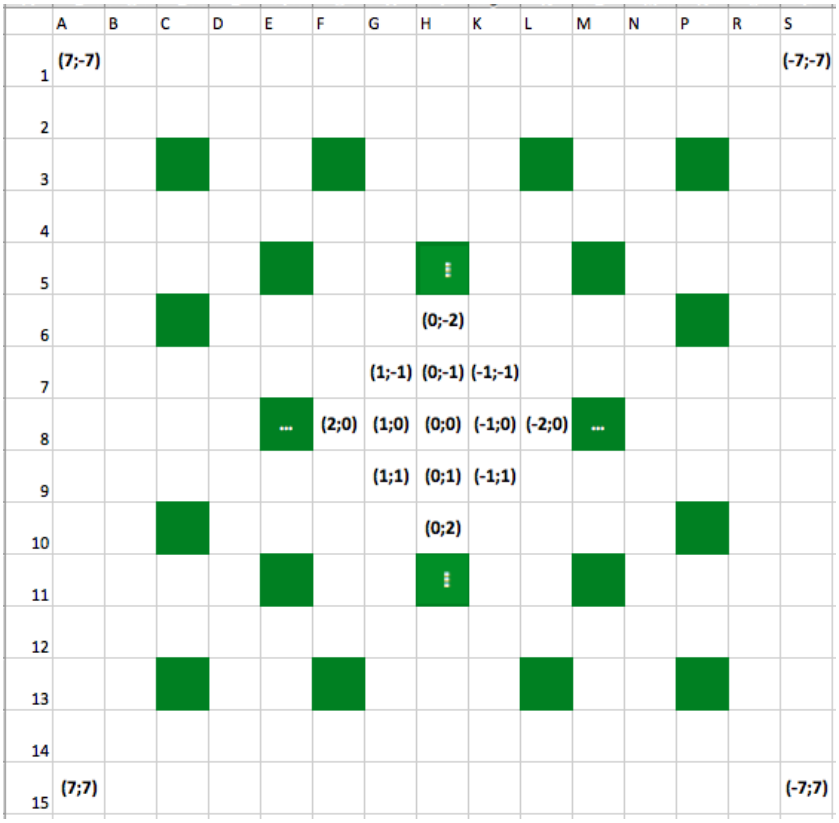

Figure 4.4.: Elements of the assembly and their indices in the lattice.

With the card "fill: -7:7 -7:7 0:0"[12], the elements of the lattice are successively filled by their universe. The first one being filled is situated at the upper right corner in S1, since it corresponds to the element (-7,-7). The universe associated to this element is the universe number 2 since it corresponds to the first number in the array of the code above. Then, the first indice is increased and the second element (-6,-7), at position R1 is filled also by the universe 2, and so on. When the first indice has increased until 7, it goes back to the value -7 and the second indice moves from -7 to -6. The same process as above is repeated again, but the row of the lattice which is this time filled by the universes is the second one.
For example, it can be seen in the code that the universe 5 in the lattice possesses the indices (-5,-1). Since this corresponds to the location P7 in the assembly, this universe is thus the one which the cells of the fuel rod GU3 during cycles 16 and 17 belong to (see fig 3.2).
As a conclusion here, even if the lattice's decomposition described by the array of the code

[12]It is possible to represent 3D lattices with the "fill" card, which is the reason why three indices are present here. Nevertheless, the fact that the third indice varies from 0 to 0 means that there is only one element in the vertical direction and that the lattice is only 2D here.

above looks reverse compared to the one in fig 4.2 (because the lattice is filled from right to left and from top to bottom), the filling of the elements by the universes follows exactly the same principle.

Finally, the second part of the cell cards in MCNP5 consists in creating generic cells and attaching to them the correct universe from the lattice to which they belong. In the array above, the universes correspond respectively to:

- 2, the universe of the cells which form all the fuel rods and the water around them, and which are different from what is defined by the universes 5 to 21.
- 3, the universe of the cells which form all the guide tubes and the water around and inside them.
- 5, the universe of the cells which form the fuel rod GU3 during the cycles 16 and 17 and its water.
- 6, the universe of the cells which form the three other fuel rods common to the assemblies 1601 and 1701, with the water around them.
- 7, the universe of the cells which form the fuel rod GU3 during the cycle 18 and its water.
- 8 to 21, the universe of the cells which form the fourteen neighbours of GU3 during the three cycles (seven before the cycle 18 and seven after) and their water.

For instance, the description of the cells which belong to the universes 2, 3 and 5 are given in the following lines:

```
c cell cards
3  1 -6.5093     -9 10  u=2          $ Zr-4 around UO2
4  2 -10.40      -11    u=2          $ Fuel UO2
5  3 -0.0020907  -10 11 u=2          $ He between Zr-4 and UO2
6  4 -0.723       9     u=2          $ Water around UO2
c
7  1 -6.5093     -12 13 u=3          $ Zr-4 guide tube
8  4 -0.743      -13    u=3          $ Water in guide tube
9  4 -0.723       12    u=3          $ Water around guide tube
c
c cells related to the first position of GU3 (P7)
10 1 -6.5093     -9 10  u=5          $ Zr-4 around UO2
11 5 -10.40      -11    u=5          $ Fuel UO2
12 3 -0.0020907  -10 11 u=5          $ He between Zr-4 and UO2
13 4 -0.723       9     u=5          $ Water around UO2

...

78 0 -1:2:-3:4:-5:6[13]
```

[13] Another cell which represents the volume around the assembly is also defined here: cell 78. Exactly as the cell number 1 which represents the global volume of the assembly in the previous code lines, the cell 78 does not belong to any universe, and is void.

```
c cylinders cards
9  CZ .5375                          $ Zr-4 cladding outer cylinder
10 CZ .465                           $ Zr-4 cladding inner cylinder
11 CZ .4555                          $ UO2 cylinder
12 CZ .69                            $ ZR-4 guide tube outer cylinder
13 CZ .62                            $ Zr-4 guide tube inner cylinder
```

Regarding the code lines of the universe 2 for instance, the major difference compared to the one represented in fig 4.3, is the definition of the cell filled by the water which does not require the rectangular parallelepiped's sides to be intersected by the external part of the Zr-4 outer cylinder in the geometry description. Indeed, since the elementary element of the lattice has been already defined, saying that the water is only defined by the positive side "9" of the Zr-4 outer cylinder is correct because this volume is already limited by the sides of this element.
Moreover, it can be seen here that, since their material number - i.e. number 1 - is the same, the cells 3, 7 and 10 are made of the same Zr-4 material. So, if this material was given in the ALEPH2 top cards in order to be depleted, its composition would change after each irradiation step and the three cells would be filled by a new but identical for all, composition. This means that during all the problem, it will not be possible that the composition of one of those cells differs from the others. In the same way, cells 6, 8, 9 and 13 are thus filled by the same water composition (material number 4) and cells 5 and 12 by the same helium (material number 3). On the other hand, the cells cooresponding to the fuel UO_2 have to be filled by different materials, as explained earlier. This explains why the cell number 4 - related to the fuel of the universe 2 - is filled by the material 2, while the cell number 11 - related to the universe 5 - is filled by the material 5[14].
It should be added here that the initial chemical composition of the fuel materials (materials number 2, 5, 6, 7, etc. and 21) is exactly the same as what has been detailed earlier in the material card of the fresh UO_2. They have thus all the same cell card, apart from their identification and material numbers.

The cells of the other 18 universes of the lattice are created exactly in the same way (with a unique material number for their fuel) than what is done for universe 5. They are thus not detailed here, but the reader can find them in the appendix section A.1, related to the final ALEPH2 input file.

It was mentioned earlier that there exist other parameters than its number, its density, its material number and its geometric description in a cell card description. The universe to which the cell belongs, if the cell is made of a lattice or not, how to fill its elements if the cell is indeed a lattice,... are some of those - now well known - extra parameters.
There are however two remaining parameters which are rather important in the study case here: the temperature of the material which fills the cell and the "importance" of the cell.

The temperature of the material in the cell - as mentioned previously in section 2 - is used in the epithermal range of energy of the neutrons, with the free gas thermal treatment. This

[14] It can be seen here that it was chosen, in order to simplify the understanding of the code, to give the same number to the fuel material than to the universe to which the related cell belongs. This explains why the universe number 4 was omitted in the code above, since the material 4 was already chosen to be the water (see the previous material cards).

one consists in a first time in adjusting the zero-temperature elastic cross section to the temperature of the target material, and in a second time in taking into account the velocity of the target nucleus when the kinematics of a collision is being calculated. Nevertheless, if the neutron data in the library files were already associated with the correct temperature in the material cards, there is no need to adjust their elastic cross sections and only the velocities of the target nucleus are then computed, using the temperature. In the example here, the Zr-4 in the guide tubes and the water are the only materials in the core where the elastic cross sections are transformed, since the other materials have already been associated with the correct neutron data, see table 4.1.
The temperatures are given in the cell cards following the keyword *tmp*. They are not expressed in any unit of temperature, but in term of energy, in [MeV]. This can be explained thanks to the equation 2.14 which gave the probability density function for the Maxwellian distribution of target velocities.
From this equation, it can be shown that the most probable scalar velocity V of the target nuclei is equal to $1/\beta$, with β defined as

$$\beta = \left(\frac{M_n}{2k_B T}\right)^{\frac{1}{2}} \tag{4.3}$$

Where Mn is the mass of the target nucleus in $[MeV \cdot sh^2/cm^2]$, T is its temperature in [K] and $k_B = 8.617e^{-11}$[MeV/K] is the Boltzmann's constant.
The kinetic energy related to the most probable velocity of the target nucleus is thus equal to $1/2 \cdot M_n \cdot V^2 = 1/2 \cdot M_n \cdot \beta^{-2} = k_B T$.
The value $k_B T$ is called the equilibrium temperature of the target nuclei in [MeV] and is the number that has to be attached to the *tmp* keyword in the cell card to express its temperature. Table 4.7 presents thus the temperature of each material expressed in [K] and their $k_B T$ value in [MeV].

Material	Temperature [K]	$k_B T$ [MeV]
UO_2	1000	8.617E−08
He	700	6.032E−08
Zr-4	600	5.170E−08
Zr-4 in guide tubes	570	4.912E−08
Water	575	4.955E−08
Water in guide tubes	566	4.877E−08

Table 4.7.: Temperature of the materials and average kinetic energy of their nuclei.

The last parameter of the cell is called the importance and is represented by a number associated to the keyword *imp:n*[15]. This parameter is used to say whether a cell is important in the studied case or not and to help particles to move to the most important regions of the geometry. It is also used to terminate the particles history if the importance is zero. In fact, if the importance of a cell is equal to 1, the statistical weight of a newborn particle is 1, if the importance is 2, then the W equals 0.5 (the initial particle is split in two, each weighting 0.5), etc.

[15] The "n" stands for neutrons since they are the simulated particles. If the problem also allowed photon emissions, it would have been possible to find "imp:p" or "imp:n,p" (if both had the same statistical weight) keywords, for instance.

In Gösgen's case, each cell except the void cell which represents the outside of the assembly and where the neutrons are not allowed to go (this would be a loss of time and accuracy for the user) has the same importance. This explains why all the cells of the assembly have an importance equal to one, while the value is zero for the outside cell.

In the end, for instance, the complete cell card of the UO_2 which belongs to the universe 5 and whose cell number is 11, is the following:

```
11  5  -10.40  -11  imp:n=1  u=5  tmp=8.617E-08
```

Another example here is the cell card of the cell 78, the outside of the assembly:

```
78  0  -1:2:-3:4:-5:6  imp:n=0
```

4.1.3. Source cards

Before that MCNP5 can compute any tallies of the problem, it requires a neutron generation source inside its geometry. From this source, the program will generate neutrons and then proceed to the general transport calculation, i.e. following each of many particles from the source throughout its life to its death in some terminal category. Then, the neutron flux in a cell of volume V is estimated by the F4 tallies, using the neutron track length $T_{l,i}$ and the relative weight W_i of each neutron:

$$F4_i = \frac{W_i T_{l,i}}{V} [n_0^1 / cm^2] \tag{4.4}$$

It has been seen that problems occur in a simulation if the eigenvalue k_{eff} of the time-dependent transport equation is equal or above 1 since in that case, when a neutron is dropped into the system, its history simulated by Monte Carlo becomes infinitely long. The solution to this problem consists in creating a criticality source since, unlike fixed source problems where the source being sampled throughout the problem never changes, the criticality source changes from cycle to cycle and is each time generated from the fission sites of the previous cycle.
It has been seen in section 2 that a criticality calculation requires a couple of things: a kcode card and an initial spatial distribution of fission points for the first cycle.

There exist different ways to define the initial distribution of fission points: either the coordinates of each point are given to MCNP5 from a KSRC card, or a general volume distribution source SDEF card is created. However, whatever the choice here, the fission source will converge to the same distribution sooner or later. Here, the option that has been chosen is the SDEF card made up of a cylindrical volume distribution source surrounding - nearly all - the assembly, since it allows k_{eff} and the flux spectra to converge faster than with the KSRC card.

A cylindrical volume distribution source is defined by the variables ERG, POS, AXS, RAD, and EXT in the following way. The axis of the cylinder passes through the point POS in the direction AXS. The positions of the particles are then sampled uniformly on a circle whose radius is RAD, centered on the axis of the cylinder. The circle lies in a plane perpendicular to AXS at a distance from POS which is the sampled value of EXT. Regarding ERG, its meaning will be explained later.

In the case here, POS is the center of the assembly, AXS is the vertical axis of the asssembly, RAD is a values corresponding to half the side of the assembly and EXT corresponds to the height.
Since a circle with a radius half the side of a square does not totally include this square inside its borders, it can be asked why the radius of the cylindrical volume distribution was not chosen to be $\sqrt{2}$ times larger. This is simply because the MCNP5 code samples fission sites only inside the fissionable materials and thus, a larger number of random trials would be needed inside the cylinder in order to find some of them if part of the cylinder was created in the void space around the assembly. On the contrary, a too small radius RAD is also not acceptable since the time that it would take for k_{eff} and the flux spectra to converge would be in that case way too large.
In MCNP5 code lines, the POS, AXS, RAD and EXT cards of the volume source are written in the following way:

```
axs=0 0 1 pos= 0 0 0 rad=d2 ext=d3
si2 0 10.7
si3 -4.95 4.95
```

In can be seen here that POS is equal to the coordinate (0,0,0) which is the center of the assembly, and that AXS = (0,0,1) corresponds to a vector parallel to the z axis. Regarding RAD and EXT cards, they are each time sampled from a probability distribution Dn given in the corresponding card SIn. Here, the values SIn correpond to the bin boundaries for histogram distributions: 0 to 10.7[cm] for RAD, the sampled radial coordinate and -4.95 to 4.95[cm] for EXT, the sampled axial coordinate.
Here, it has been decided that the virtual volume of the neutron source does not lie on any of the defined surfaces of the assembly's geometry, and it was thus defined to be just included inside it. This is the reason why the EXT card is defined here with the values ± 4.95 instead of ± 5 which are the geometric limits of the assembly. In the same way, the outer radius of the RAD card is 10.7 and not 10.725[16].

The final card used to define the cylindrical volume distribution source here is the ERG card. This one is related to the energy of every source particle of the first cycle. This energy is each time selected from a generic Watt thermal fission distribution since the energy of the fission neutrons in a nuclear core follows approximately this particular probability density spectrum:

$$p(\mathrm{E}) = \mathrm{C} \cdot e^{(\frac{-\mathrm{E}}{a})} \cdot sinh(b\mathrm{E})^{\frac{1}{2}} \tag{4.5}$$

With a and b the parameters of the sprectrum and C a constant so that the distribution respects the fundamental probability equation $\int_0^\infty p(\mathrm{E})d\mathrm{E} = 1$.
Here, the parameters have been set to the values a = 0.988 and b = 2.249 in order to correspond to the U-235 fission spectrum since this one is the most likely atom to fission in a PWR. From this, the constant C is equal to 0.4396 and the Watt fission energy distribution is given at fig 4.5.

[16] With the lattice pitch value and the number of elements per row of the assembly from table 3.1, the half of the side of an assembly is given by $\frac{1.43 \cdot 15}{2} = 10.725$.

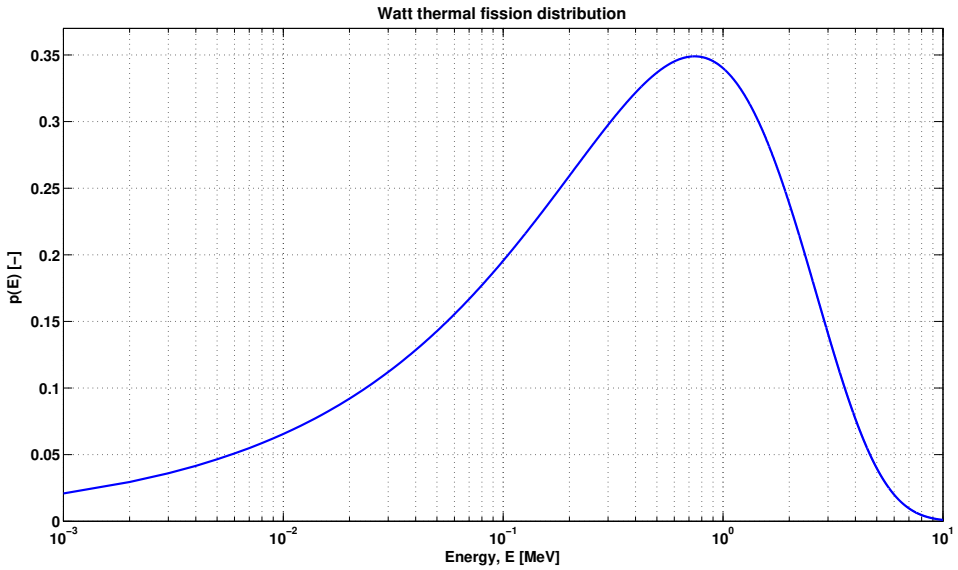

Figure 4.5.: Watt thermal fission energy distribution of the neutron generation source for the first cycle of the criticality code: $p(\mathrm{E}) = 0.4396 \cdot e^{(-\mathrm{E}/0.988)} \cdot sinh((2.249\mathrm{E})^{0.5})$.

In MCNP5, the Watt distribution parameters a and b of the source are given to the ERG card through an intermediate source probability card:

```
erg=d1
sp1 -3 0.988 2.249
```

Here, the "-3" parameter is used to specify that the distribution follows the Watt fission spectrum and not a Gaussian or Maxwell spectrum, for instance.

In the end, the source distribution is thus given in MCNP5 in the following way:

```
sdef erg=d1 axs=0 0 1 pos= 0 0 0 rad=d2 ext=d3
sp1 -3 0.988 2.249
si2 0 10.7
si3 -4.95 4.95
```

Now that the initial spatial distribution of fission points for the first cycle has been defined, the remaining part of the criticality calculation is the kcode card. As a reminder, such a card requires the following informations:

- The nominal number of source histories, N, per k_{eff} cycle.
- An initial guess of k_{eff}.
- The number of source cycles, Ic, to skip before k_{eff} and tallies accumulation.
- The total number of cycles, It, in the problem.

It has been chosen here to work with 100 effective and 30 inactive cycles, i.e. Ic = 30 and It = 130. This means that after the first 30 cycles, the fission source spatial distribution is assumed to have achieved equilibrium and that active cycles begin, leading to k_{eff} and tallies accumulation. Regarding the initial guess of k_{eff}, it has been set to 1.0, since the only consequence of a too low or too high value is that the number of fission sites written as source points for the next cycle will be, respectively, too high or too low relative to the desired nominal number N.

The last parameter of the kcode card is the nominal number of histories, N, per k_{eff} cycle. There is here no magic trick to choose this value, but it is easily understandable that a too small value requires a quasi-infinite number of cycles to converge and a too high, a lot of memory and also a huge calculation time.
In order to decide which value to choose, a few ALEPH2 calculations with a varying number N have been run on a single irradiation step of the sample, and the following parameters have been compared:

- The relative error of the tallies (given by the output file of the MCNP5 calculation).
- The U-235 fission reaction rate in the sample:

$$R_{U-235}\ [cm^{-3}\cdot s^{-1}] = \phi\ [cm^{-2}\cdot s^{-1}]\cdot \sigma_f\ [cm^2]\cdot N_{U-235}\ [cm^{-3}] \tag{4.6}$$

  With ϕ the neutron flux spectrum in the sample integrated over the entire energy range (found in the ALEPH2's output file), σ_f the average microscopic U-235 fission cross section (found in a cross section file generated during the run) and N_{U-235} the volumic concentration of U-235 atoms in the sample (deduced from the densities of each isotopes given in the ALEPH2's output file).

- The total calculation time which is the sum of the processing of the neutron induced data, the Monte-Carlo transport code, the buiding of the K[17] systems of first-order ordinary differential equations and their resolution.

The goal here is to find a value N such that the U-235 fission reaction rate in a cell is considered constant (it does not vary with N) and with a calculation time and a relative tally error sufficiently low. Then, if this value is chosen wisely - small, but not too small -, a lot of computation time will be gained and the tallies will be still accurate enough.
Fig 4.6, 4.7 and 4.8 present the relation between the nominal number of source histories, N and respectively the U-235 fission reaction rate in GU3, the relative tally error and the computation time.

From them, the value N has been set to 50000 because R_{U-235} seems to be more or less constant from the value 20000 (even if it fluctuates again a little bit at N equal to 60000), the tally error is very small (≈ 0.2[%]) and the calculation time is less than 400[s][18]. Moreover, a chapter of section 6 will study the impact of this parameter on the accuracy of the results.

[17] K is here the number of materials to deplete.

[18] The calculation time has to be taken carefully here since it represents the time that it takes to proceed to the first ALEPH2 step, where only a few nuclides are present in a material's composition. This time may be multiplied by 3 or 4 for the next cycles since, with decay of nuclides, with the neutron absorption of "newborn" nuclides resulting in nuclides not present yet, etc., the composition of each material becomes way more extended and so does the system which defines the time evolution of every nuclide.

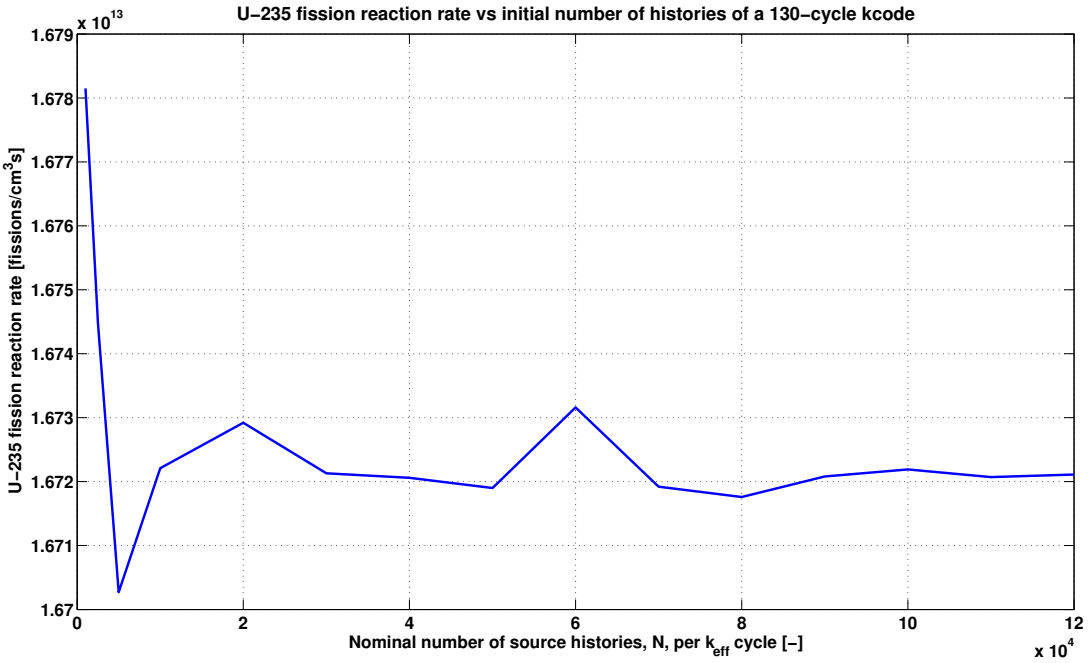

Figure 4.6.: U-235 fission reaction rate in GU3 in function of N.

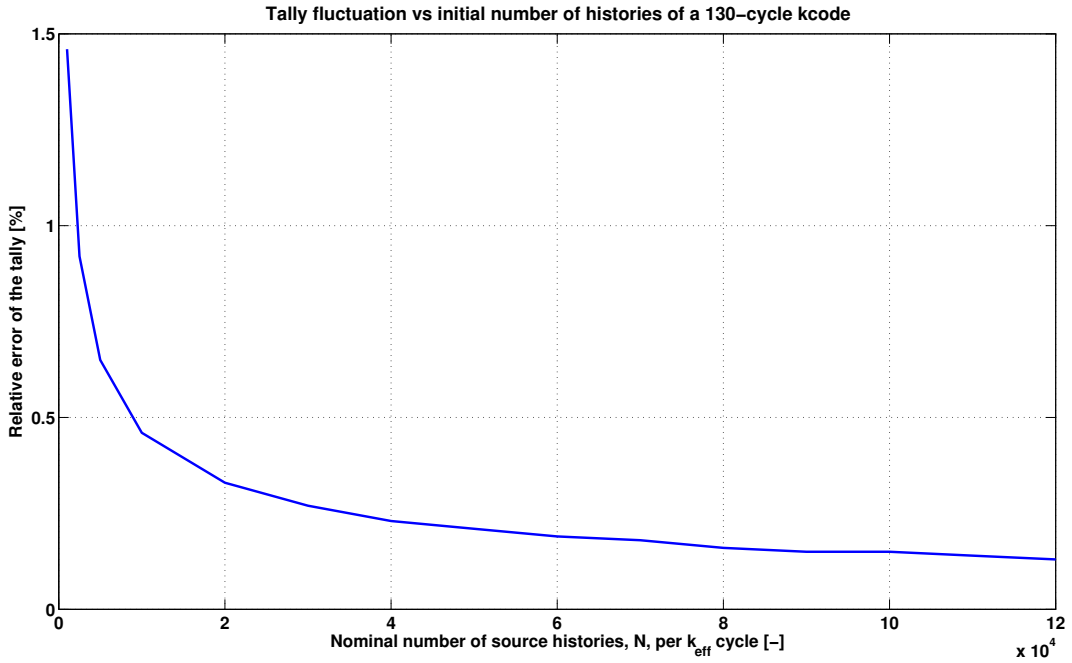

Figure 4.7.: Relative F4 tally error in function of N.

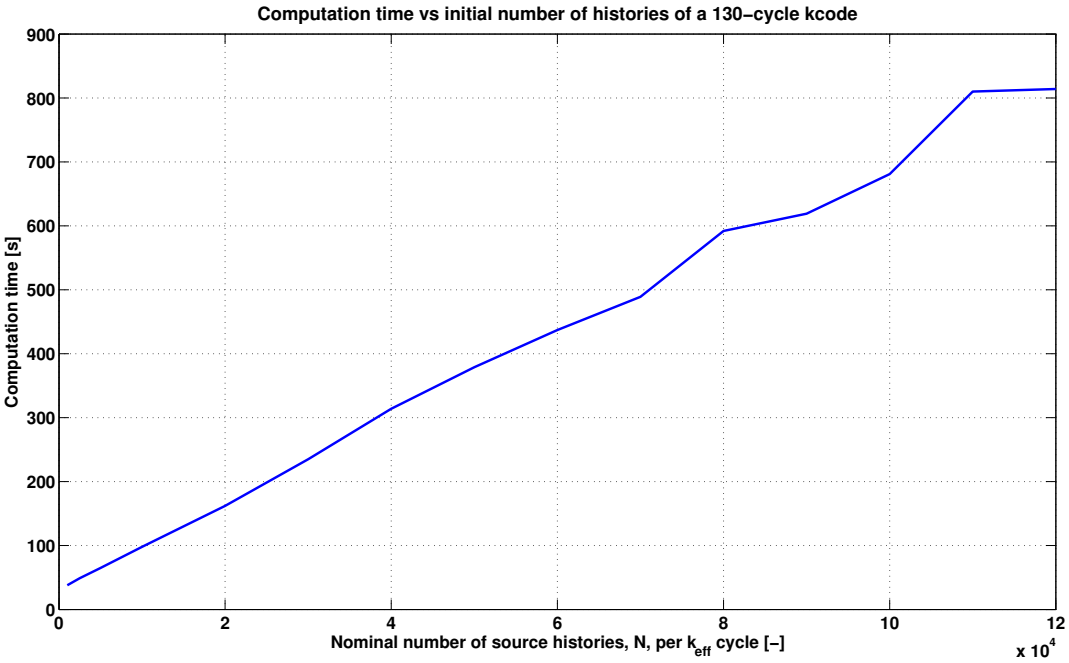

Figure 4.8.: Computation time of 1 step in function of N.

Finally, the MCNP5 total source card is the following:

```
kcode 50000 1.00 30 130
totnu
c
sdef erg=d1 axs=0 0 1 pos= 0 0 0 rad=d2 ext=d3
sp1 -3 0.988 2.249
si2 0 10.7
si3 -4.95 4.95
```

Where "totnu" represents the fact that the total number of fission neutrons (prompt and delayed) is used in the kcode for the computation of the fission sites of the next cycles.

4.1.4. Tallies cards

So far, the composition of the materials and the cells that they fill have been defined in MCNP5. As explained, not every of these materials have to be depleted by the solver of ALEPH2 if the evolution of their chemical composition does not influence significantly the sample GU3. This explains thus why no F4 tallies are requested here in the cells filled by the helium and the Zr-4. On the contrary, tallies have to be computed in all the UO_2 fuel cells, but they must be separated as explained earlier: a tally spectrum for the cell corresponding to the sample's position in cyles 16 and 17, another for the cell of GU3's position in cycle 18, fourteen others for each of the fourteen neighbouring fuel rods, etc. In total, eighteen tally spectra have thus to be computed by MCNP5 in the fuel. Moreover, since it is sometimes difficult for the program to calculate the total volume of the cell(s) in which a tally spectrum must be computed and since this value is used in each F4 tally calculation, the user must also provide each of these volumes in the code.

For instance, in order to specify that the program needs to calculate a single tally spectrum in all the fuel rods which belong to the universe 2, the user must only give the number of the generic cell duplicated in every element of the lattice associated with this universe - i.e. the cell number 4 (see code line above: "4 2 -10.40 -11 u=2 *Fuel UO2*") - and the total volume of these cells, 1212.38[cm^3].
In the same way, the MCNP neutron flux spectrum computed in the fuel cell which belongs to universe 5 (the first position of GU3 during its irradiation) is done by giving to MCNP5 the cell number 11 (see code line above: "11 5 -10.40 -11 u=5 $ *Fuel UO2*) and the volume 6.5182[cm^3] (the volume of a 10-[cm]-high fuel pellet).

It should be mentioned that since the boron concentration in the water is added in the ALEPH2 top cards at each step, a tally spectrum in the water has to be computed as well. Indeed, it is not possible in ALEPH2 to change manually the concentration of any material without depleting it. In conclusion, a single tally spectrum is requested in all the cells filled by the water and which belong either to all the fuel rods universes (u = 2, 5, 7,..., 21) or to the guide tubes universe (u = 3), for a total volume of 2682.77[cm^3].

The MCNP5 code hereafter presents thus all the nineteen (eighteen for the fuel and one for the water) F4 tally spectra defined by their cell number(s) and the associated volume. The cell numbers related to a tally spectrum are written on a same line of the code following the keyword *f4:n*, while the associated volumes are written after all of them, in the same order and following the keyword *sd4*:

```
f4:n 11                          $ UO2, GU3's position 1:  P7 (M5 then M23)[19]
      4                          $ UO2, remaining pins (M2 then M22)
     (6 8 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77)
                                 $ Water (M4)
     15                          $ UO2, 3 fuel pins common to both assemblies (M6)
     19                          $ UO2, GU3's position 2:  R11 (M7 then M5)
     23                          $ UO2, GU3's neighbour C16/17:  R6 (M8 then M24)

     ...                         $ UO2, GU3's 13 other neighbours C16/17/18

sd4 6.5182 1212.38 2682.77 19.5545 6.5182 6.5182 6.5182 6.5182 6.5182
    6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182
```

It can be seen here that each tally spectrum in a fuel material requires only one generic cell, while the one in the water requires the combination of a lot of them ("(6 8 9 13 ... 77)"), since it has been decided to work with the same water composition in all the assembly - and thus in all the universes -.

[19]The comment "M5 then M23" represents here the fact that during the cycles 16 and 17, the tallies are computed in a cell filled by the material 5, while during the cycle 18, the material is changed and the cell is then filled by the material 23, UO_2 fuel burnt until 17.7[MWd/kgU].

4.2. 2^d part: ALEPH2 cards

The second part of an ALEPH2 input file is related to the sample's irradiation history. Indeed, it has been explained in section 3 that, since the sample is moving during its irradiation (to another assembly and to another location inside), the best and accurate way to calculate its composition was to work with its own thermal power.
It has been seen in table 3.2 that the thermal power of the sample and its burn-up are known five times during each cycle. It has to be mentioned here that each thermal power of the sample in this table is a value that has been measured at a given time and that can thus not be assumed constant during all the timespan defined by the Δt between the two successive lines of the table. To solve this problem, it has then been chosen to work with the sample's burn-up and to deduce from it an average thermal power that can be assumed constant during all the duration of the time step Δt:

$$\overline{P}_{sample} = \frac{\rho \cdot F_U \cdot V_{sample} \cdot \Delta BU_{sample}}{\Delta t} \tag{4.7}$$

With ρ the density of the UO_2 in [g/cm^3], F_U the mass fraction of uranium in UO_2, V_{sample} equal to 6.5182 [cm^3] and ΔBU_{sample} defined as the difference between the burn-ups of GU3 at the end and the beginning of the step.
For instance, the average power of GU3 during the 6 first days of the cycle 16 is given by $\overline{P}_{sample} = \frac{10.4 \cdot 0.8814 \cdot 6.5182 \cdot 0.403}{6} = 4.013[kW]$.

Table 4.8 presents thus the average powers of GU3 during the 3 cycles. It can be seen here that there is a total of fourteen irradiation steps for the cycles 16 and 18, and thirteen steps for the cycle 17. To manage this from table 3.2, the irradiation steps of the table have simply be divided and the burn-ups of the sample have then been linearly interpolated at the associated times.
As stated earlier, another important value used at each irradiation step is the boron weight concentration in [ppm] in the water. Again here, it is possible to find theses values in [23] at the same five times than in table 3.2. The boron concentrations of the new steps have thus also simply been linearly interpolated from these values.

Cycle	Operation time (EFPD)	BU_{sample} [MWd/kgU]	$\overline{P}_{sample}$ [kW]	[B] [ppm]
16				
	0	0	4.013	1705
	6	0.403	4.127	1347
	20	1.353	4.105	1283
	40	2.710	4.085	1192
	60	4.066	4.068	1100
	90	6.101	4.046	963
	120	8.136	3.955	827
	150	10.171	3.833	690
	180	12.046	3.789	569
	210	13.921	3.728	448
	240	15.796	3.703	327
	270	17.671	3.678	207
	300	19.546	3.646	86

Cycle	Operation time (EFPD)	BU_{sample} [MWd/kgU]	$\overline{P}_{sample}$ [kW]	[B] [ppm]
	320	20.796	3.468	5
	336.8	21.771	/	5
17				
	0	21.771	3.236	1601
	6	22.096	3.284	1247
	20	22.852	3.271	1184
	40	23.932	3.247	1095
	60	25.012	3.232	1005
	90	26.632	3.214	871
	120	28.252	3.163	736
	150	29.872	3.083	602
	180	31.395	3.059	483
	210	32.918	3.018	364
	240	34.441	3.008	245
	270	35.964	2.996	126
	299.5	37.461	2.875	9
	328.7	38.866	/	9
18				
	0	38.866	2.818	1675
	6	39.149	2.750	1300
	20	39.758	2.709	1235
	40	40.629	2.659	1142
	60	41.499	2.602	1049
	90	42.805	2.549	910
	120	44.111	2.472	770
	150	45.417	2.418	631
	180	46.604	2.388	509
	210	47.791	2.350	387
	240	48.978	2.339	266
	270	50.165	2.328	144
	300	51.353	2.323	22
	301.2	51.400	2.170	17
	331.6	52.504	/	17

Table 4.8.: Extended sample irradiation history of cycles 16, 17 and 18. $\overline{P}_{sample}$ is here a power which can be assumed constant during the Δt defined by the difference between the operating times of the line in which it is written and the following one.

Prior to defining each of the irradiation steps, the first ALEPH2-specific cards which are mandatory in an input file are related to the materials which are followed in the problem (i.e. depleted by the solver) and their volume.

Regarding the materials that are followed by the problem, they are composed first of the ones that fill the cells of the assembly during the two first cycles, and then of the ones which fill it during the cycle 18. In order to help the reader to easily associate each MCNP neutron flux to the correct material, the material numbers have been written here in the same order than what has been done for the cell(s) that they fill in the tallies cards of the MCNP5

calculation.
For instance, it has been seen earlier that the first tally spectrum which is calculated corresponds to the tallies in the cell number 11 - the first position of GU3 in the assembly - filled by the material 5 during the cycles 16 and 17. The first material number written in the ALEPH2 top cards is thus the material number 5. The second, third, fourth and fifth ones are respectively the materials 2, 4, 6 and 7 - the major part of the fuel UO_2, the water, the three fuel pins which are common to the three cycles and the second position of GU3 in the assembly -, and the fourteen next are the fourteen neighbouring fuel rods of GU3 during its irradiation. Next to those material numbers are the numbers related to the materials which replace the first ones at the beginning of the cycle 18 and which have a chemical composition corresponding to UO_2 depleted until 17.7[MWd/kgU]. Since there are eighteen different fuel materials at the beginning of the irradiation and that only two of them stay in the core during the three cycles (the sample GU3, M5 and three other fuel rods common to the three cycles, M6), a total of sixteen materials are thus added here.

Finally, regarding the volumes of the materials, the requested values are exactly the same as in the tallies cards and are thus given in the same order than their associated material above.

The MCNP5 code lines hereafter present thus the followed materials - BURN card - and their volume - VOL card:

```
BURN 5 2 4 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
     22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
VOL 6.5182 1212.38 2682.77 19.5545 6.5182 6.5182 6.5182 6.5182 6.5182
    6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182
```

It can be seen in the code here that, while there are thirty-five materials followed by ALEPH2, only nineteen volumes are entered in the VOL card. This allows in fact the program to understand clearly that every material whose index is above nineteen is a material which will only play a role later in the problem.

The final step consists then in defining all the irradiation-and-decay history of the sample GU3 inside and outside the reactor. Each irradiation step is described by the thermal power of the sample, the step duration and the boron concentration in the water.

An irradiation step of constant power is given by the card "IRP S MAT_{ID} $\overline{P}_{sample}$ D DURATION", where $\overline{P}_{sample}$ is the thermal power in [MW] of the selected (the S stands for selected) material whose material number is MAT_{ID} and which can be assumed constant during a number of days (the D stands for days) equal to DURATION[20].
For instance, the first irradiation step is given by:

```
IRP s 5 4.01316E-03 d 6
```

Besides, a decay step - i.e. the decay of nuclides in the materials listed in the BURN keyword when there is no neutron flux in the core - is given by the card "DEC D DURATION NO".

[20] It has been explained in section 2 that it is also possible to deduce the source strength S from the total power of the system. In that case, an irradiation step of constant power is given by the card "IRP T $\overline{P}_{tot}$ D DURATION", where the T stands for total.

Here, the D stands again for days and the NO is used so that no MCNP5 calculation is launched at the beginning of this step (no tally spectrum is required in such a step) since by default, this is normally the case in order to continuously know the evolution of k_{eff}.
For instance, the decay step which corresponds to the time between the cycles 16 and 17 is given by:

```
DEC d 25 no
```

Regarding the boron concentration in the water, it is provided by the card "PPM MAT_{ID} ZZZAAAm VALUE", where VALUE (negative value if weight [ppm], and positive if atomic [ppm]) is the concentration in PPM of the nuclide whose ZAID is given by the notation ZZZAAAm, in the material whose number is MAT_{ID}. Here, the ZZZAAAm corresponding to the natural boron (made of B-10 and B-11) is 0050000 (or 50000). The last 0 represents here the fact that the nuclide is in a stable state, while a 1 would have represented a metastable state[21].
For instance, the boron concentration card which corresponds to the beginning of the first irradiation step is given by:

```
PPM 4 50000 -1705
```

Finally, from the values of table 4.8 and the decay timespans of table 3.4, the cards of the first two cycles are given by the following code lines:

```
c Irradiation history
c Cycle 16
c
IRP s 5 4.01316E-03 d 6
PPM 4 50000 -1705
IRP s 5 4.12651E-03 d 14
PPM 4 50000 -1347
IRP s 5 4.10534E-03 d 20
PPM 4 50000 -1283

...                  $ Other irradiation sub steps of cycle 16

IRP s 5 3.46758E-03 d 16.8
PPM 4 50000 -5
DEC d 25 no
c
c Cycle 17
c
IRP s 5 3.23640E-03 d 6
PPM 4 50000 -1601
IRP s 5 3.28359E-03 d 14
```

[21] The notation is thus here a little bit different than in MCNP where nuclides were defined only by ZZZAAA. In that case, the metastable state of a nuclide defined by ZZZAAA is thus represented in MCNP by another ZZZAAA notation: for instance, U-236 is idendified by 92236 and U-236m by 92632 (since a nuclide with a Z number of 92 and an atomic mass of 632 does not exist, the user understands clearly here when he sees it that it represents a metastable state of uranium)

```
PPM 4 50000 -1247
IRP s 5 3.27060E-03 d 20
PPM 4 50000 -1184

...                    $ Other irradiation sub steps of cycle 17

IRP s 5 2.87491E-03 d 29.2
PPM 4 50000 -9
DEC d 22 no
```

At this point, nearly all the depleted fuel has to be replaced by the composition of another material corresponding to UO_2 burnt until 17.7[MWd/kgU]. Managing this in ALEPH2 is easily feasible since there exist change material cards "CHM OLDMAT NEWMAT" which only need the two material numbers that have to be exchanged, i.e. the old and the new materials which fill the associated cell or group of cells.
For instance, the material number 2 which fills all the cells which belong to the fuel of universe 2 in the lattice can be exchanged by a new material number 22 (one of the "extra" materials in the BURN keyword) with the code line:

```
CHM 2 22
```

In the same way, it is possible to change the material number 5 inside the rod which corresponds to the first position of GU3 by a new fuel material number 23 burnt until 17.7[MWd/kgU], and in the same time to replace the fuel material in position R11 (2^d position of GU3) by GU3's material number 5. Here, the code is then:

```
CHM 5 23
CHM 7 5
```

The last CHM instructions consist then in replacing the material in each of the fourteen neighbouring fuel rods of GU3 by, again, a new depleted-to-17.7[MWd/kgU] fuel material. Finally, the density of each new material needs to be also defined in the problem through a "CHMD DENSITY" card, where DENSITY can be provided either in [g/cm^3] (negative entry) or in [atoms/(barn·cm] (positive entry).
For instance, the density of the material number 22 is defined by the code line:

```
CHMD 22 7.006526620156E-02
```

Where the value 7.0065E-02[atoms/(barn·cm] corresponds approximately to 10.399[g/cm^3].

The irradiation steps of cycle 18 and the decay steps which correspond to the time between each measurement cooling dates (see table 3.3) are then given by the following code lines:

```
c Cycle 18
c
IRP s 5 2.81816E-03 d 6
CHM 2 22
CHM 5 23
```

```
CHM 7 5
CHM 8 24
CHM 9 25
CHM 10 26
CHM 11 27
CHM 12 28
CHM 13 29
CHM 14 30
CHM 15 31
CHM 16 32
CHM 17 33
CHM 18 34
CHM 19 35
CHM 20 36
CHM 21 37
CHMD 22 7.006526620156E-02
CHMD 23 7.006526620156E-02

...                 $ CHMD cards of the other new materials

CHMD 37 7.006526620156E-02
PPM 4 50000 -1675
IRP s 5 2.75044E-03 d 14
PPM 4 50000 -1300
IRP s 5 2.70854E-03 d 20
PPM 4 50000 -1235

...                 $ Other irradiation sub steps of cycle 18

IRP s 5 2.16983E-03 d 30.4
PPM 4 50000 -17
c
c Decay until experiments at SCK and ITU
DEC d 600.  no      $ U, Pu :  ITU (from 07/06/1997 to 28/01/1999)
DEC d 57.   no      $ Nd, I-129 :  ITU
DEC d 39.   no      $ Sm, Eu, Cs, Ce-144, Pm-147 :  ITU
DEC d 43.   no      $ Cm, Am-241, Am-243, Np-237 :  ITU
DEC d 15.   no      $ Cu, Cs, Eu, Ce-144, Ru-106, Sb-125 :  SCK
DEC d 97.   no      $ Gd-155, Sr-90, Mo-95, Tc-99, Ru-101, Ru-106, Rh-103 :  ITU
DEC d 6.    no      $ U, Pu :  SCK
DEC d 43.   no      $ Nd :  SCK
DEC d 7.    no      $ Gd-155 :  SCK
DEC d 12.   no      $ Sm :  SCK
DEC d 8.    no      $ Am, Np-237 :  SCK
DEC d 3.    no      $ I-129 :  SCK
DEC d 70.   no      $ Pm-147 :  SCK
DEC d 38.   no      $ Mo-95, Tc-99, Ru-101, Rh-103, Ag-109 :  SCK
DEC d 36.   no      $ Sr-90 :  SCK
```

Here, the CHM and CHMD cards are associated with the IRP card "IRP s 5 2.81816E-03 d 6" right above. Technically, the materials are thus first changed and then the MCNP calculation is launched.

4.3. ALEPH2 final input file

The final ALEPH2 input file with, on top, the ALEPH2-specific cards and below them the part of the code related to the MCNP5 calculation is given in appendix A.1.

Here, everything in the input has already be explained, apart from a few things:

- The DATN card at the beginning of the input file is used to specify the path to the folder containing the neutron activation data files in ALEPH format prepared by the ALEPH-DLG utility and used for the depletion of the materials.
- Regarding the ACE-format general transport neutron data folder used in the Monte-Carlo calculation, its path in the system is given in the first line of a *xsdir* file attached to the problem and defined through the *message* directive at the beginning of the MCNP5 part of the input file. For instance here, the code line "message: xsdir = xsdir32a" of the input file (see appendix A.1) states that the xsdir directory file is related to data from the library JEFF-3.2 [3], and not from another library.
  In addition to the path to the general transport neutron data folder in the system, the xsdir directory file also contains a list of every nuclide for which such data (cross sections, spectra, angular distributions, etc.) are available and where is attached the name of the file in the general folder in which they are actually located. With this list, the user can check that the material cards that he provided in the input file do not contain any nuclide for which general transport neutron data are not available, and can thus avoid errors. In the same idea, when a new time step begins and that a ".i" file is created by ALEPH2, the code relies on the xsdir file to truncate the full set of nuclides resulting from the previous step to those nuclides for which the general purpose transport data are available.
- The MCNP top card "MCNP /srv/clu/sci/bin/mcnp5_c740.sh 16" of the input file is used to first give the full path to the MCNP5 executable to be used by ALEPH2, and secondly to specify that 16 CPUs are requested for the MCNP5 execution in parallel mode.
- The composition of the fuel burnt until 17.7[MWd/kgU] and its density (used for the replacement material cards, M22 to M37) have been computed with an ALEPH2 input file given in appendix A.2. Its main characteristics are: the geometry of a single fuel rod (the same than in fig 4.3), four irradiation steps of 84.2 days each, a boron concentration evolution in the water approximately the same as in the cycles 16 to 18 (from 1700 [ppm] to $\approx$ 0 [ppm]) and a constant power equal to $\overline{P} = \frac{10.4 \cdot 0.8814 \cdot 6.5182 \cdot 17.7}{84.2 \cdot 4} = 3.14[kW]$.
- The surface cards related to the six planes of the border of the assembly have all a "+" sign written before their identification number in order to specify that these borders are "white borders". These borders are used in order to prevent the neutrons from leaving the assembly during the transport code. They are then reflected by a border with a cosine density distribution, $p(\zeta) = \zeta$, relative to the surface normal, where ζ is a random number on [0,1]. This allows thus the neutrons to go back in the assembly with random

new directions of propagation when they hit the border of the assembly. This represents the idea that, if the entire core had been described in the input file, neutrons would have entered the assembly from the adjacent assemblies, as it is the case in reality[22].

[22] This simplification is a good compromise between the calculation time and the quality of the results: even if they are a little bit less accurate, the time required to compute the general Monte-Carlo transport code in a single assembly is a lot smaller than in a geometry where all the assemblies of the core would have been described.

Results

5

After that all the irradiation and the decay steps have been processed, an ALEPH2 output file is generated by the program, in which the composition of every followed material is given for each step. Since the list of isotopes per material, the number of time steps and the number of materials are huge, the output file is also rather big and necessitates to process the results in an automatic way.
Figure 5.1 presents hereafter a part of the output file related to the material number 5, i.e. the sample GU3. It can be seen here that the first row is the time, the first and second columns are the nuclides and their ZAID and that all the other elements are the nuclides' concentrations at each time step.

```
*******************************************************************************
*--- Table  1 --- Evolution of nuclide concentrations (g/cm3)                  *
*******************************************************************************

*****   Material       5
                Time   (days)     0.000000E+00  6.000000E+00  2.000000E+01  4.000000E+01  6.000000E+01

 Nuclide         ALEPH ID
  1-H-1           10010           0.000000E+00  1.713755E-10  7.382367E-10  1.240690E-09  1.764842E-09
  1-H-2           10020           0.000000E+00  3.590823E-11  1.658690E-10  2.940509E-10  4.078913E-10
  1-H-3           10030           0.000000E+00  9.012741E-17  3.633114E-14  1.150682E-13  1.192367E-13
  2-He-3          20030           0.000000E+00  7.712506E-20  3.637754E-17  2.313044E-16  4.771656E-16
  2-He-4          20040           0.000000E+00  6.937687E-12  8.133430E-11  3.630479E-10  8.766256E-10
  2-He-6          20060           0.000000E+00  0.000000E+00  1.890147E-24  3.802427E-24  4.844230E-24
  3-Li-6          30060           0.000000E+00  6.122733E-19  7.913133E-18  3.091379E-17  6.670710E-17
  3-Li-7          30070           0.000000E+00  3.850585E-13  1.402734E-12  2.863232E-12  4.292167E-12
  3-Li-8          30080           0.000000E+00  6.254866E-24  2.402115E-23  4.495864E-23  6.604664E-23
  4-Be-7          40070           0.000000E+00  4.944010E-14  8.787876E-14  9.320281E-14  9.208978E-14
  4-Be-9          40090           0.000000E+00  3.174216E-16  1.696058E-13  3.819098E-13  3.983464E-13
  4-Be-10         40100           0.000000E+00  2.498596E-16  3.110591E-15  1.181638E-14  2.494546E-14
  4-Be-11         40110           0.000000E+00  3.585150E-24  1.382168E-23  2.556132E-23  3.749627E-23
  5-B-10          50100           0.000000E+00  6.691092E-18  7.811087E-17  2.860695E-16  5.894036E-16
  5-B-11          50110           0.000000E+00  1.436695E-16  1.707971E-15  6.672692E-15  1.485977E-14
  5-B-12          50120           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  5-B-13          50130           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  6-C-11          60110           0.000000E+00  3.509633E-20  1.355624E-19  2.507702E-19  3.677910E-19
  6-C-12          60120           0.000000E+00  2.010623E-09  9.037478E-09  1.584185E-08  2.236833E-08
  6-C-13          60130           0.000000E+00  6.629748E-07  2.259327E-06  4.484001E-06  6.725011E-06
  6-C-14          60140           0.000000E+00  1.385780E-13  1.619892E-12  6.512254E-12  1.466805E-11
  6-C-15          60150           0.000000E+00  0.000000E+00  1.063577E-23  1.514877E-23  1.957722E-23
  7-N-13          70130           0.000000E+00  7.170179E-17  7.468401E-17  7.254532E-17  7.064687E-17
  7-N-14          70140           0.000000E+00  1.225732E-12  4.359026E-12  8.841019E-12  1.286589E-11
  7-N-15          70150           0.000000E+00  2.895898E-10  1.407383E-09  2.459964E-09  3.402029E-09
  7-N-16          70160           0.000000E+00  5.353399E-14  7.518435E-14  4.683636E-14  4.886223E-14
  7-N-17          70170           0.000000E+00  2.701375E-22  1.319142E-21  1.948515E-21  2.739353E-21
  8-O-14          80140           0.000000E+00  2.409921E-16  2.510154E-16  2.438272E-16  2.374464E-16
  8-O-15          80150           0.000000E+00  0.000000E+00  1.066347E-16  1.123358E-16  0.000000E+00
  8-O-16          80160           1.233440E+00  1.233439E+00  1.233437E+00  1.233434E+00  1.233431E+00
  8-O-17          80170           0.000000E+00  2.396763E-08  8.219975E-08  1.649218E-07  2.471755E-07
  8-O-18          80180           0.000000E+00  1.116710E-15  1.302724E-14  5.230775E-14  1.174195E-13
  8-O-19          80190           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  9-F-19          90190           0.000000E+00  0.000000E+00  1.648725E-22  1.363372E-21  4.578076E-21
 10-Ne-20        100200           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
 24-Cr-66        240660           0.000000E+00  9.303032E-23  9.552148E-23  9.316923E-23  9.322690E-23
 24-Cr-67        240670           0.000000E+00  1.038989E-22  1.067233E-22  1.043562E-22  1.046959E-22
 25-Mn-66        250660           0.000000E+00  8.224552E-20  8.459721E-20  8.268331E-20  8.289777E-20
 25-Mn-67        250670           0.000000E+00  3.695943E-20  3.801532E-20  3.725359E-20  3.744379E-20
 25-Mn-68        250680           0.000000E+00  5.311201E-21  5.468665E-21  5.359670E-21  5.389177E-21
 25-Mn-69        250690           0.000000E+00  4.048912E-22  4.168302E-22  4.080917E-22  4.099239E-22
 26-Fe-56        260560           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
 26-Fe-57        260570           0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

Figure 5.1.: Part of the ALEPH2 output file, related to sample GU3.

In order to quickly get the informations from the file, a Matlab function has thus been developed. This one can be found in appendix A.3 and, to make it simple, works in this way:

- First, the part of the output file related to the material 5 (i.e. GU3) is loaded in Matlab.
- Then, the Matlab function reads the first column in order to find the row which corresponds to the selected nuclide. For instance, if the user is interested by the U-235, the program compares each element of the first column until it finds the correct string "92-U-235". It knows thus here the row it is going to work with.
- From the irradition-and-decay history, the Matlab function takes the value from the column which corresponds to the measurement cooling date associated with the nuclide (see table 3.3).
- Finally, since the composition of every nuclide has been expressed in [mg/g-fuel] at the ITU and SCK-CEN laboratories, while they are printed out in units of [g/cm^3] in the output file, the value of the output file is multiplied by 1000 and divided by the initial density of GU3.

In order to find with which one the results are the closest to experimental, the ALEPH2 input file has been run with three different neutron interaction data libraries: the US ENDFB-VII.1 [8] [7] library and the European JEFF libraries (Nuclear Energy Agency), JEFF-3.2 [3] and JEFF-3.3T3[1].

Moreover, the values are also compared to the results from the technical report [23] and which have been computed by another depletion code, MONTEBURNS [2] and by SCALE code system [10] run with KENO-VI Monte-Carlo code and its proper depletion code named TRITON. The characteristics of these two calculations are approximately the same than what has been done in ALEPH2, except that each cycle was represented by seven time steps for full power, one step for reduced power and one step for the shutdown period between the end of a cycle and the beginning of the next one; and that ten and four cooling time steps have been performed for decay and built-up calculations for SCK-CEN and ITU measurements, respectively. Moreover, the neutron data library attached to the MONTEBURNS' calculation is JEFF-3.1 [9] and is ENDFB-VII [6] for SCALE.

The results are presented for the major long and short-lived nuclides of GU3's final composition, in appendix A.4 (tables) and in fig 5.2 and 5.3 (charts) hereafter. They are shown in terms of the percentage difference between the calculated value and the measured one: if a (C/E - 1) value is below 0, this means that the calculated composition is smaller than the measured one, while it is larger if the result is above 0.

[1]The JEFF-3.3 library was still a beta version under development in the time this document was written, which means that no reference is available for this library up to now.

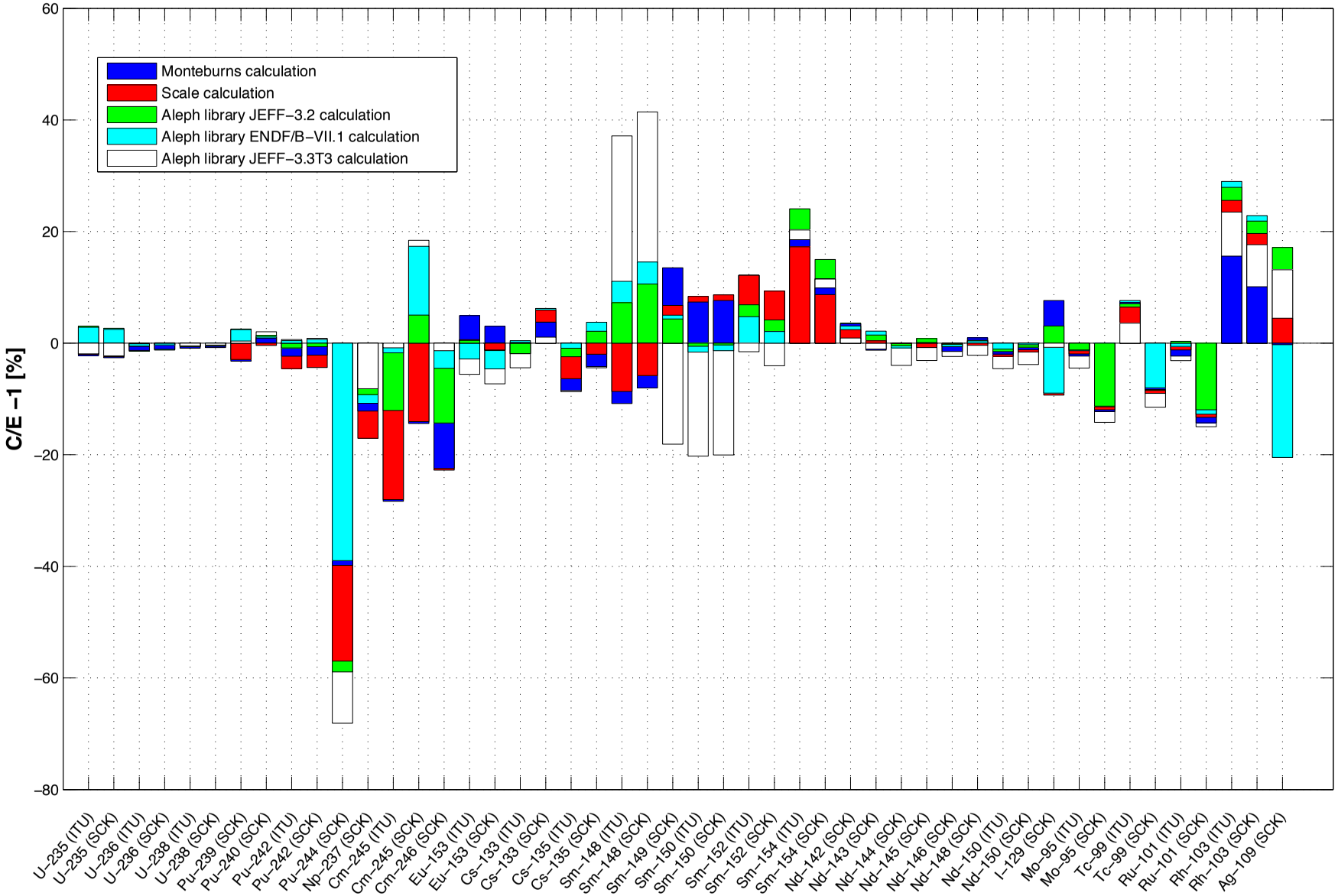

Figure 5.2.: Long-lived isotopes: comparison between the results obtained with three different neutron data libraries in ALEPH2 and with a MONTEBURNS and a SCALE calculations.

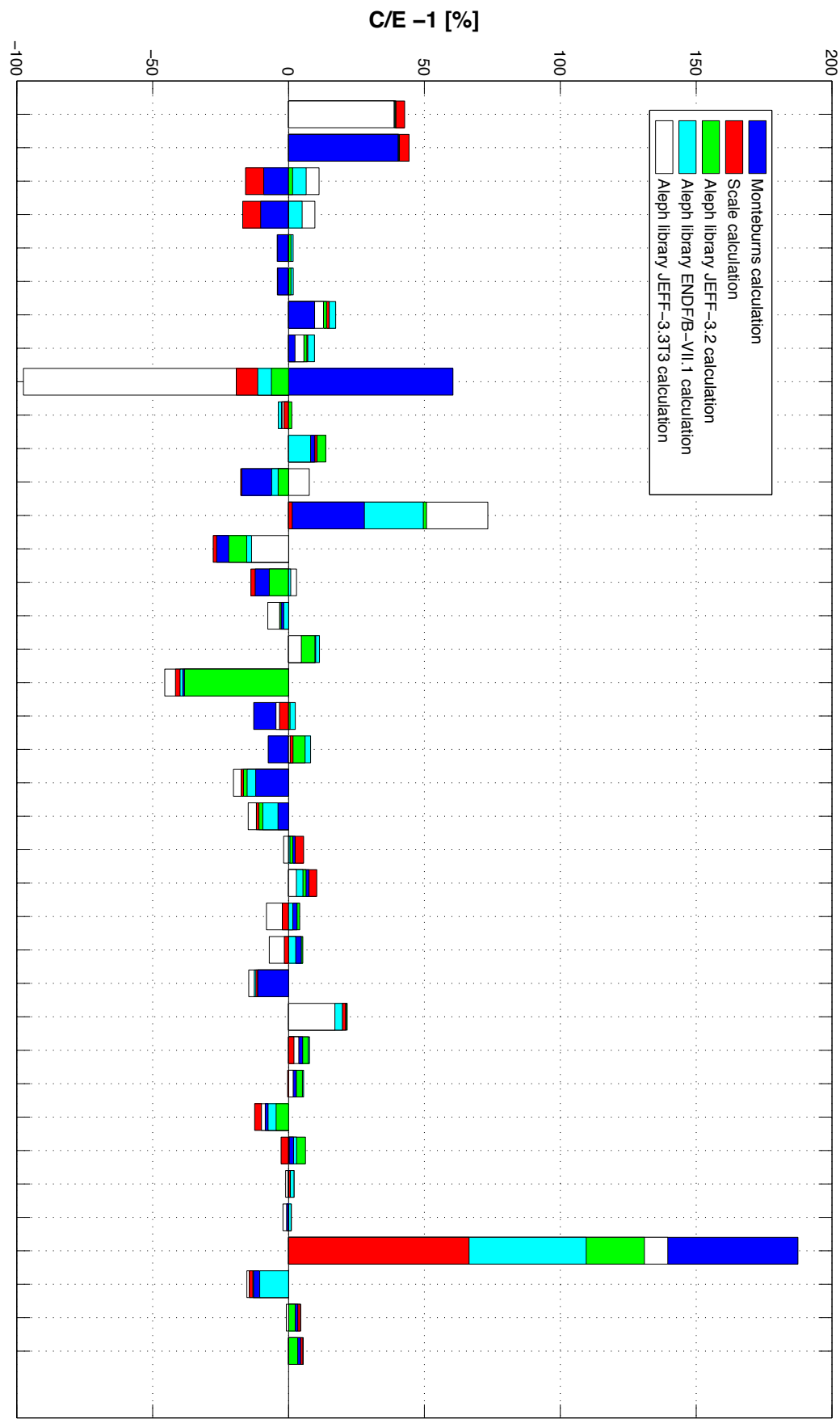

Figure 5.3.: Short-lived isotopes: comparison between the results obtained with three different neutron data libraries in ALEPH2 and with a MONTEBURNS and a SCALE calculations.

It can be seen in tables from A.4 and from fig 5.2 and 5.3 that the nuclides which have the largest concentrations in GU3 are very well computed by ALEPH2, since the difference between them and the theoretical values is below 3-4[%] for the long-lived nuclides (main isotopes: U-238, U-235, U-236, Pu-239 and Pu-240) and below 4-5[%] for the short-lived (main isotopes: Cs-137, Pu-241 and Sr-90). On the contrary, the computed concentrations of the nuclides which form minor parts of GU3's composition are prone to be situated far from their measured values, since a small error (measured or computed) leads immediatly to a large difference between them. For the long-lived isotopes, this is the case for Pu-244 or Sm-154 which have respectively a measured concentration of 1.63E-04[mg/g-fuel] and 5.0E-02[mg/g-fuel] (average value between ITU and SCK-CEN measurements). For the short-lived isotopes, this is for instance the case for Am-242m, Cm-243, Eu-151 and Sb-125 and their respective measured concentration equal to 8.10E-04, 5.23E-04, 3.70E-04 and 6.61E-03[mg/g-fuel].

It can also be noted that, in general, when a calculated concentration is approximately correct compared to the measured value, this observation can be extended to the four other calculations either made with another neutron data library or by another code. For instance, for the long-lived nuclides, the Nd isotopes are always accurately calculated; and this is also the case for the Ce or Cs isotopes regarding the short-lived ones. This is certainly due to the fact that the neutron interaction data are in that case very well described in the literature and thus approximatively the same whatever the library. In the same way, if a computed nuclide's concentration is very far away from the measured value, the similar observation is often made for the other results related to the same nuclide. This can be seen for instance for Pu-244 (nuclide with long $T_{1/2}$) or Sb-125 (nuclide with short $T_{1/2}$).

Since it is more difficult to experimentally measure the concentration of a short-lived nuclide, it seems natural that the differences between their computed and measured concentrations are often larger than the ones related to the long-lived nuclides. Even if the scale is not the same for the two graphs - meaning that it is difficult to compare the two together -, this assumption can be verified in fig 5.2 and 5.3.

Regarding the results of ALEPH2 compared to the ones computed with MONTEBURNS and SCALE, they seem on average identically accurate: they are sometimes better (such as for Cm-246), sometimes worse (as for Ag-109), but often more or less the same.
Two parameters have thus been calculated in order to compare them more precisely: the average accuracies $|(1-C/E)|_{av}$ and the chi-squared factors $\chi^2 = \sum_{i=1}^{N} \frac{(C_i - E_i)^2}{E_i}$ of both long and short-lived nuclides, where C_i is the computed concentration of a nuclide in GU3's composition and E_i its expected value from the technical report [23].
Table 5.1 presents thus hereafter these parameters for the MONTEBURNS, the SCALE and the three ALEPH2 calculations.

Code	Library	$\lvert(1-C/E)\rvert_{av}$ [%]		χ^2	
		Long $T_{1/2}$	Short $T_{1/2}$	Long $T_{1/2}$	Short $T_{1/2}$
MONT.	JEFF-3.1	7.295	16.882	0.2815	0.1145
SCALE	ENFB-VII	7.698	12.959	0.2516	0.1111
ALEPH2	JEFF-3.2	6.656	13.707	0.2004	0.0817
	JEFF-3.3T3	9.197	17.113	0.2712	0.0832
	ENDFB-VII.1	6.428	13.264	0.1977	0.0772

Table 5.1.: Comparison between the mean errors and the χ^2 factors of the MONTEBURNS, SCALE and ALEPH2 calculations.

While $\lvert(1-C/E)\rvert_{av}$ gives the average error of the calculation, the χ^2 factor, also related to the differences between the expected and the computed values since it is constructed from a sum of squared errors, reflects the non-uniform dispersion of the values around the E_i and gives the idea that some C_i may be situated far away from them if its value is rather large. Comparing the results between them in order to find the best ones necessitates thus to take into account both $\lvert(1-C/E)\rvert_{av}$ and χ^2 parameters and to try finding a compromise where they are globally the smallest.
From table 5.1, it can thus be seen that the results in ALEPH2 - except with the libary JEFF-3.3T3 - are better than the ones obtained with MONTEBURNS and SCALE, since both their average error and χ^2 factors are a little bit smaller.
Moreover, as it can be seen in the table above and in fig 5.2 and 5.3, the library in ALEPH2 where the worst results are observed with, is the JEFF-3.3T3 library. For instance, nuclides such as Pu-244, Sm-148, Sm-149, Sm-150, Am-242m or Cm-243 have in that case their concentration situated a lot much farther away from their measured value than the ones obtained with the libraries JEFF-3.2 and ENDFB-VII.1.

To conclude here, the concentrations computed by ALEPH2 are globally correct - and even better than the ones obtained with the two other codes - compared to the experimental values. Nevertheless, they show worse results with the short-lived nuclides than with the long ones, due certainly to the experimental errors induced by their smaller lifetime. Moreover, the concentrations of some nuclides are sometimes situated very far away from the measured values, whatever the library or the code used. The problem is in that case either due to inaccurate decay data related to these nuclides (or to the ones whose decays create them), or more likely to a global problem in the input file which results in imprecisions for every code and every library.

Additional studies 6

Sommaire

6.1. FPY: Selection of interpolation scheme for fission product yields

It has been seen in section 2 that the composition of each material k is found by solving at each time step a system made of X coupled, linear, first-order ordinary differential equations with constant coefficients and similar to the following:

$$\frac{dN_j}{dt} = \sum_{\substack{n=1 \\ \neq j}}^{X} l_{j,n}\lambda_n N_n + \sum_{\substack{m=1 \\ \neq j}}^{X} \left(S \int f_{j,m}(E)\phi_k^{MCNP}(E)\sigma_{f,m}(E)dE \right) N_m - \left(\lambda_j + S \int \phi_k^{MCNP}(E)\sigma_{a,j}(E)dE \right) N_j \tag{6.1}$$

Where the second term is the creation rate of nuclide j from the fission of nuclide m, and is computed in the way that the energy spectrum is divided in energy bins in which the neutron flux spectrum $\phi_k(E)$ is integrated and in which average values are calculated for $f_{j,m}$ and $\sigma_{f,m}$.

The problem here is that, while cross sections are linearized on very fine energy grid, the energy dependence of fission yields ($f_{j,m}(E)$ in the equation above) is represented in fission product yield libraries by only a few points. Indeed, the different libraries often contain independent fission product yields only at thermal energy (0.0253[eV]), at energy characteristic to fast spectrum (400-500[keV]) and at very fast energies (2 or 14[MeV]) which have been evaluated based on experimental informations on different fissioning systems. From this, it can be undertood that it is difficult to measure a lot of points of the energetic spectrum of $f_{j,m}(E)$ since it requires each time to set up an experiment using a mono-energetic neutron beam that will fission certain target nuclide. The problem is that anyhow, in the volume of a target, neutrons will be spread in energy - and so will be the resulting yields - because before that they arrive to the nuclei which they will fission, they will already have lost a part of their energy on other nuclei via inelastic interactions and thus, the energies at which the fissions actually occur become somewhat uncertain. In this way, the results are associated with the average energy typical either to thermal, to fast or to very fast energy even if the energies of the incident neutrons are actually spread around these values.
By default, ALEPH2 uses the interpolation scheme provided in the fission product yield data

files, where all above points can be connected using linear or histogram interpolation. Thus, when the code calculates the second term of eq 6.1, it first converts the cross section $\sigma_{f,m}$ and the fission yield $f_{j,m}$ into the energy grid of the flux spectrum, assuming that in between energy boundaries of each bin of the flux spectrum, an average value is used for them, and then integrates inside each energy bin the MCNP neutron flux multiplied by these $f_{j,m,av}$ and $\sigma_{f,m,av}$.
With only three points for $f_{j,m}$, it can be however understood here that a linear interpolation between them may not be the most accurate way of estimating the fission product yields for all energies. This results thus in an uncertainty that can be a source of errors during the depletion of the materials. From this, there exists in ALEPH2 another way of defining $f_{j,m}(E)$ which consists in saying that below a certain energy threshold, the thermal fission product yield is used, above it and up to 2 or 14[MeV] (depending on the nuclide), the fast fission product yield applies and for the remaining energies, the very fast fission product yield is used: the "FPY SPECTRUM VALUE" card (a top card in the input file). This one allows in fact the user to define the transition energy corresponding to VALUE in [MeV] between the thermal and fast parts of the spectrum: if the neutron energy is below it, the fission yields defined at 0.0253[eV] will be used, and the fast yields defined at 400 or 500[keV] will be picked up in the case where the neutron energy is above it, but lower than 2 or 14[MeV]. For instance, the card "FPY spectrum 1E-03" sets the transition value between thermal and fast spectrum to 1[keV].

The first advanced study is thus here related to the selection of an interpolation scheme for fission product yields. Calculations have been completed with the fpy parameter varying from 10[eV] to 1[keV] for the library JEFF-3.3T3 and from 10[eV] to 100[keV] for the library ENDFB-VII.1, in order to see the effect on the results obtained with the worst and the best libraries (see table 5.1).

The results are presented hereafter in fig 6.1, 6.2, 6.3, 6.4, 6.5 and 6.6 where the calculated concentrations are compared to the values obtained with the default fpy parameter, and in the form of absolute values in the tables of appendix A.5. Since they correspond to $|(1-C/E)_{default\ fpy}| - |(1-C/E)_{fpy=x}|$, the values in these graphs are given relative to the previous results where no FPY card was added in the input file. This means that, for instance, if the concentration of a nuclide with the default fpy parameter was equal to 1.05 times the measured value, and equal to 1.02 times it with the fpy parameter set to any value, the number associated with this nuclide in the graph is $|1-1.05| - |1-1.02| = 3$[%]. On the contrary, if the new value is 0.94, the value associated with that nuclide is $|1-1.05| - |1-0.94|$ = -1[%], which means that the accuracy is worse than before.
In such graphs, it is then easily possible to see whether a nuclide's concentration is more accurate or not compared to the results of section 5. Indeed, if the value which it corresponds to in the graph is above 0, the resulting concentration is in this case closer to the measured value than before, and if the value is below 0, this is the contrary. For instance, it can be seen in fig 6.1 that the concentration of U-235 is $\approx$ 0.5[%] better when the fpy parameter is varying (whatever the value), or again that the concentration of Cm-246 is 2.5, 3 and 3.5[%] worse with the fpy parameter equal to respectively 10, 100 and 1000[eV].

It should also be noted that the figures 6.3 and 6.6 are the same than, respectively, fig 6.2 and fig 6.5, but where the value associated with Sb-125 was removed. This nuclide is in fact rejected here because the gain obtained by using the FPY card is so large ($\approx$ 45[%] for the two libraries) that it becomes difficult to see the effect on the other nuclides.

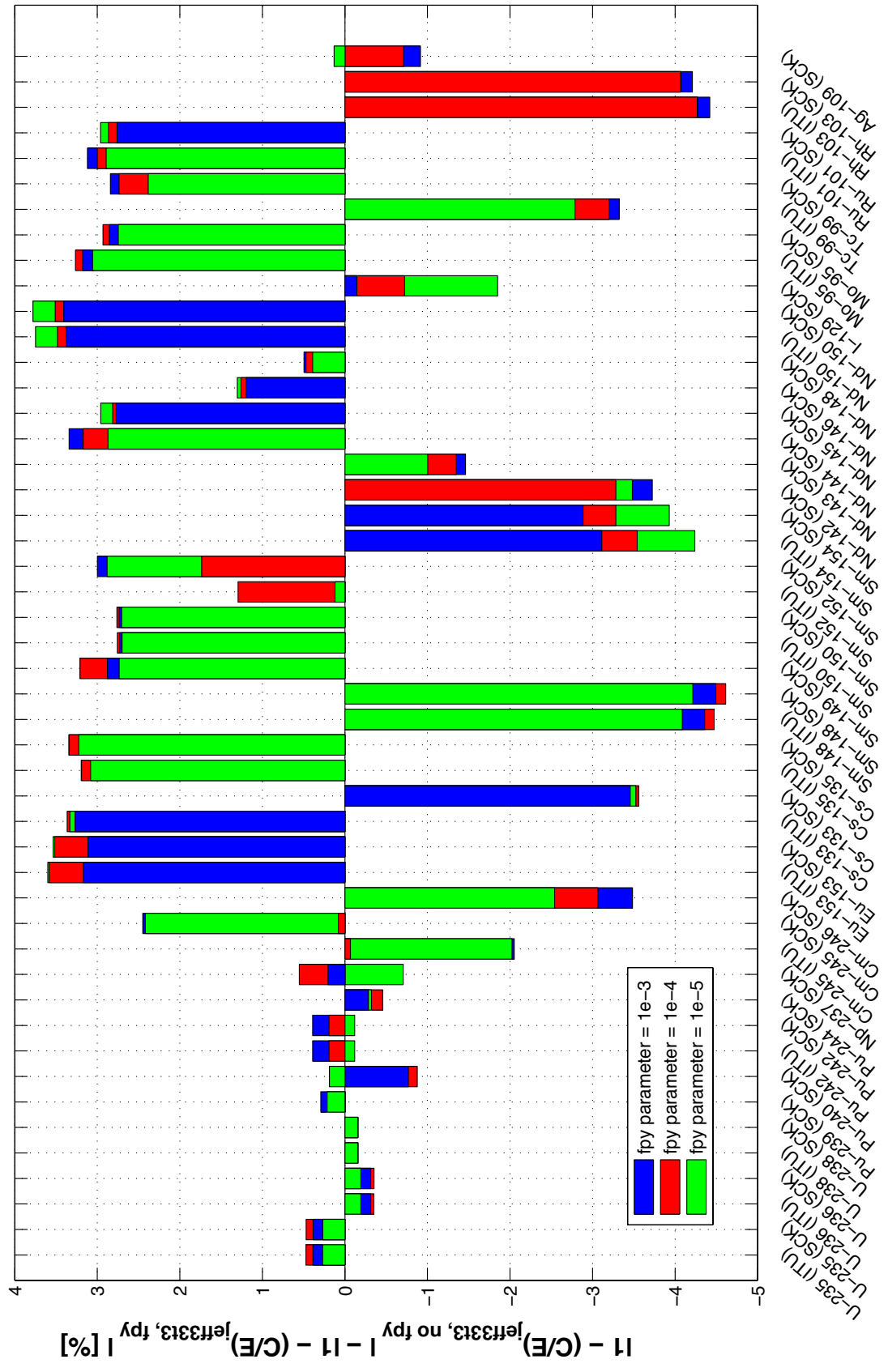

Figure 6.1.: Long-lived isotopes, library JEFF3.3T3: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 1[keV].

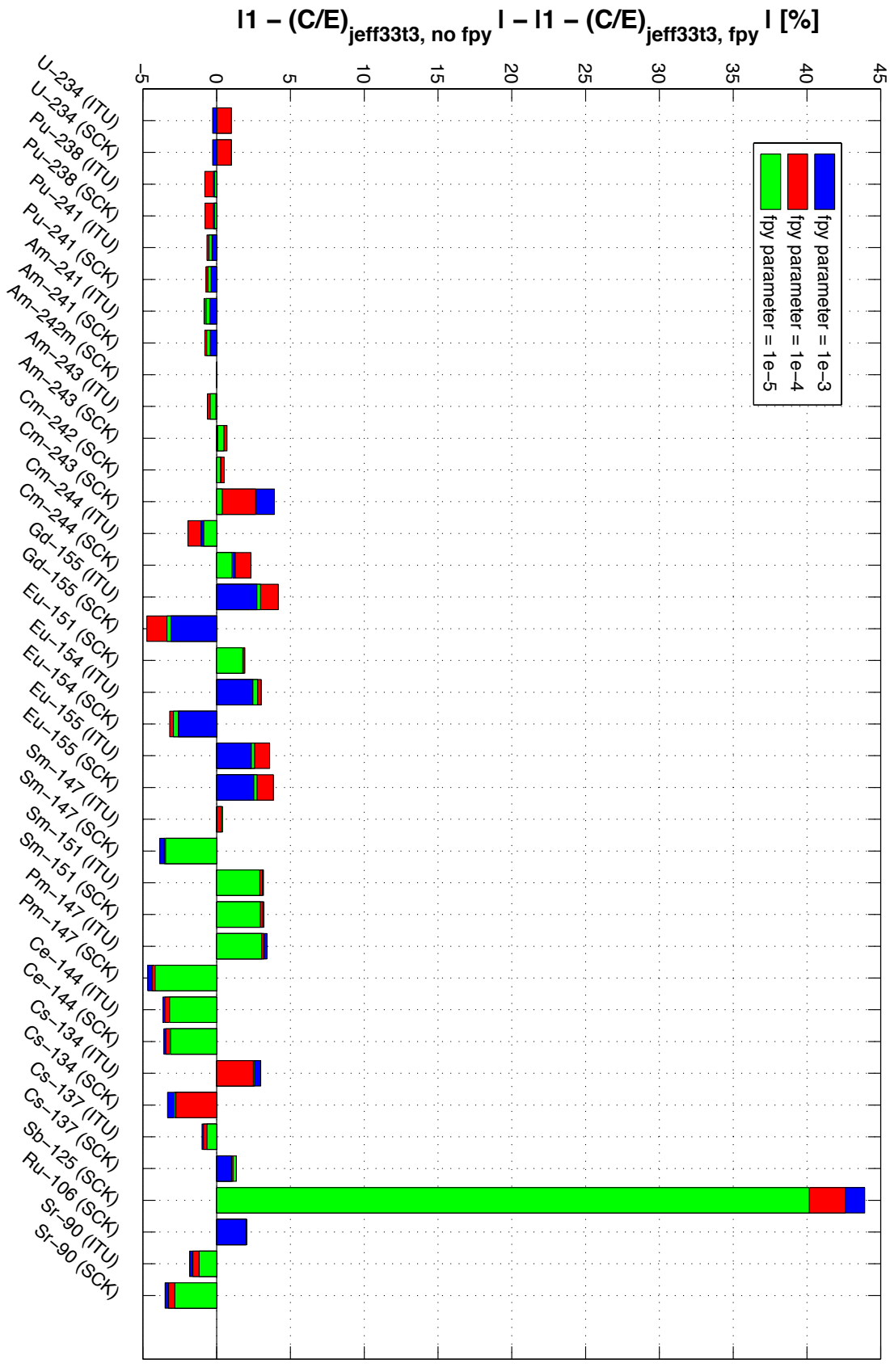

Figure 6.2.: Short-lived isotopes, library JEFF3.3T3: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 1[keV].

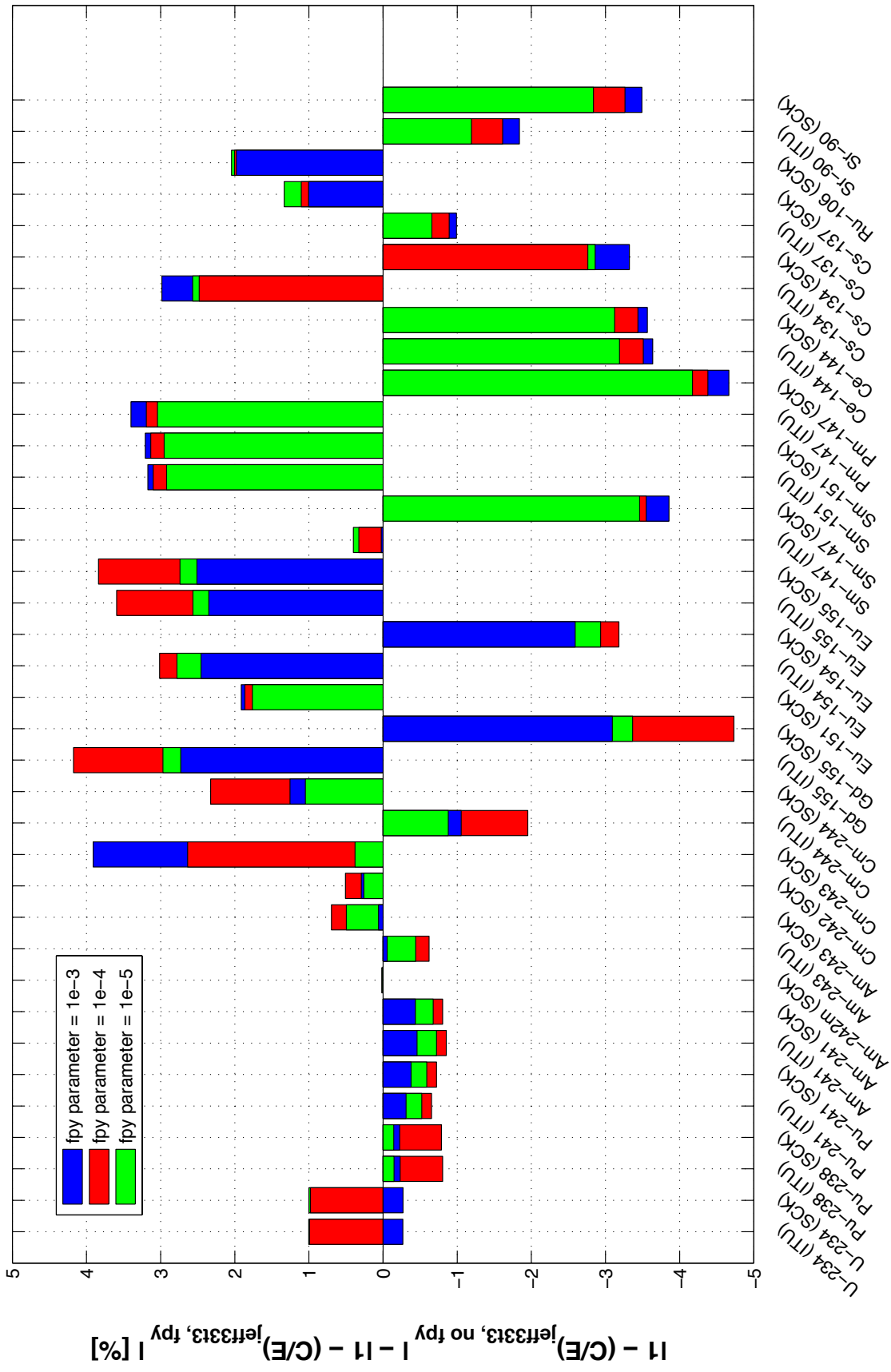

Figure 6.3.: Short-lived isotopes, library JEFF3.3T3: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 1[keV], without the Sb-125.

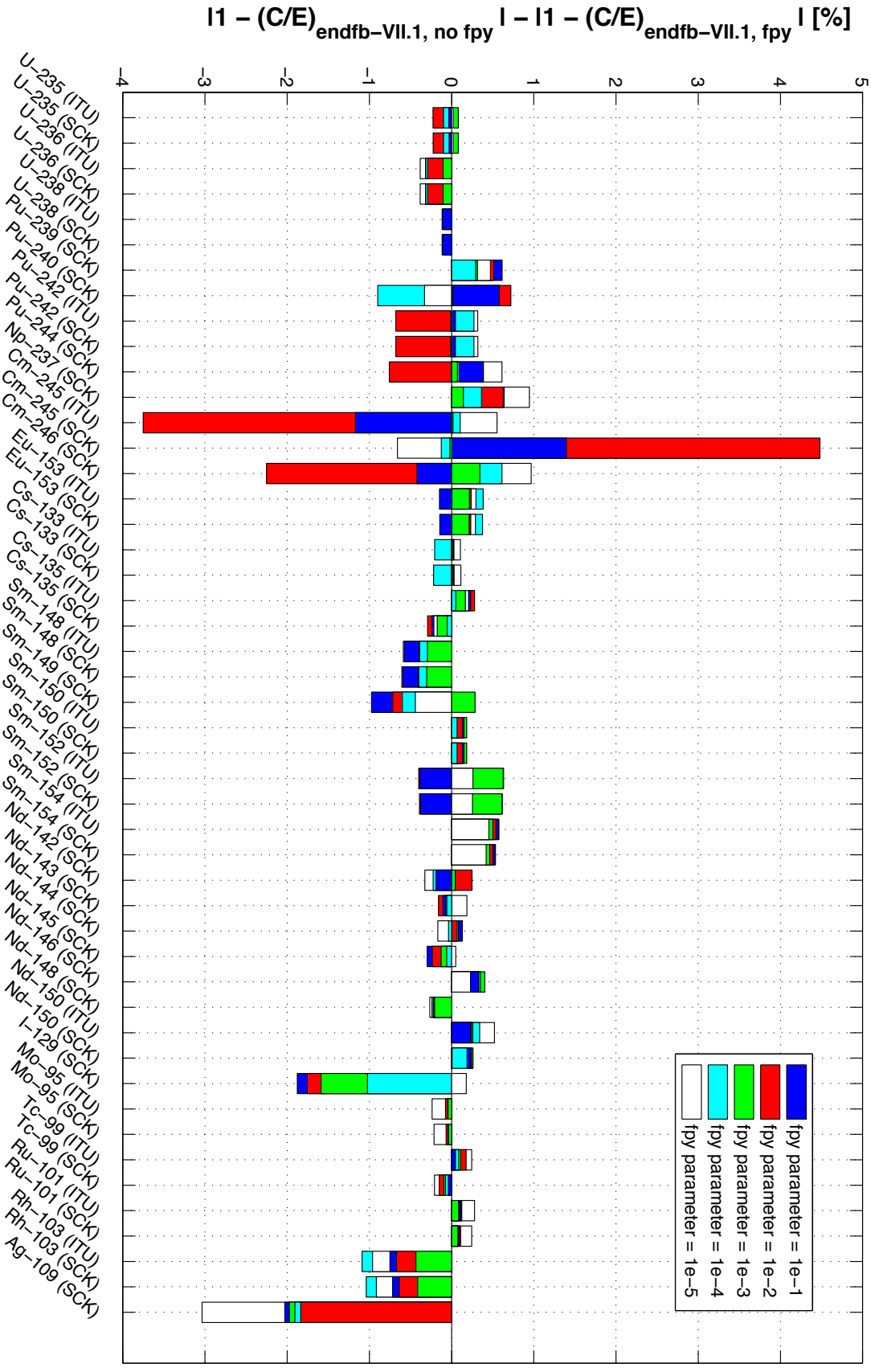

Figure 6.4.: Long-lived isotopes, library ENDFB-VII.1: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 100[keV].

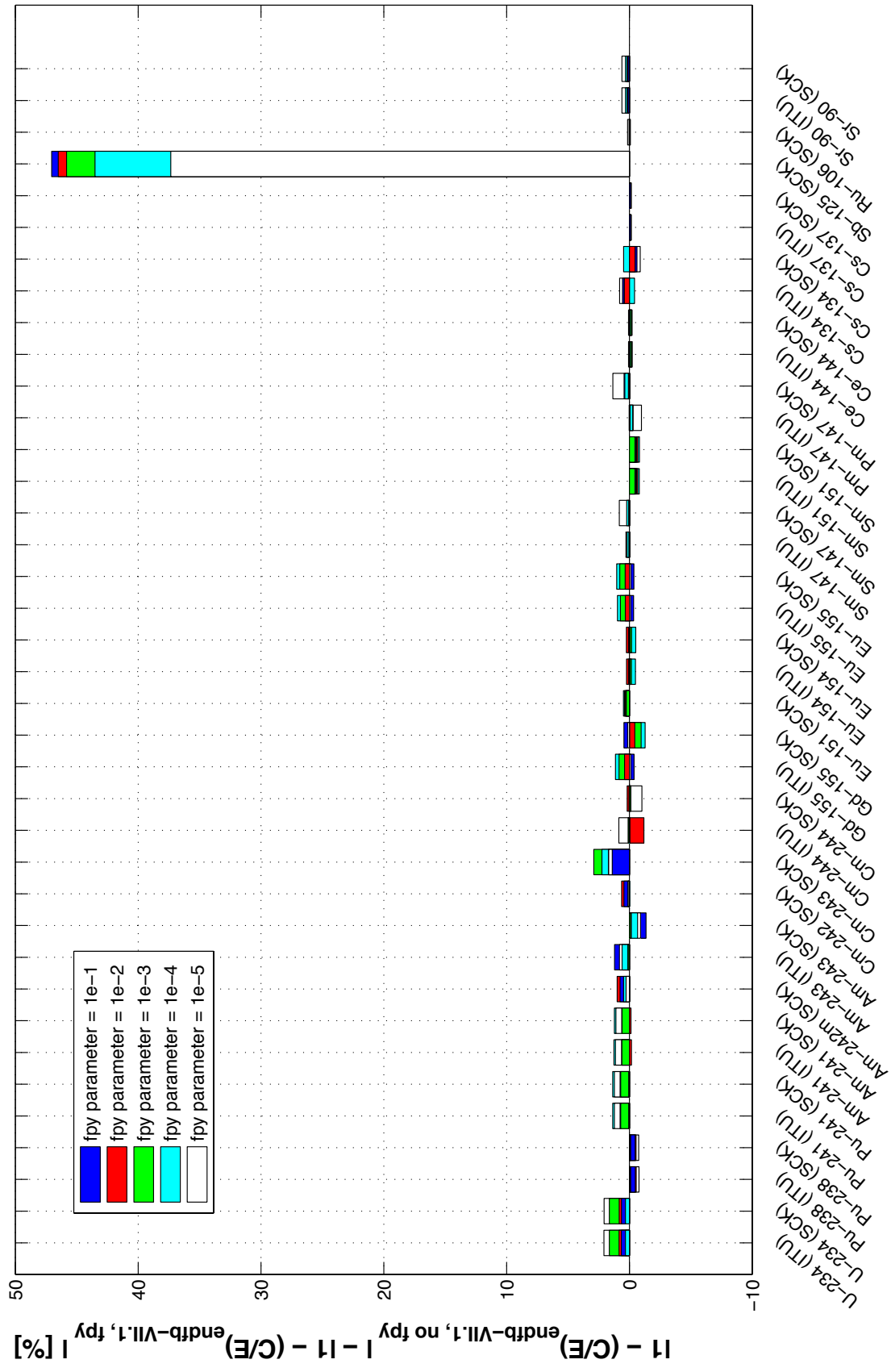

Figure 6.5.: Short-lived isotopes, library ENDFB-VII.1: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 100[keV].

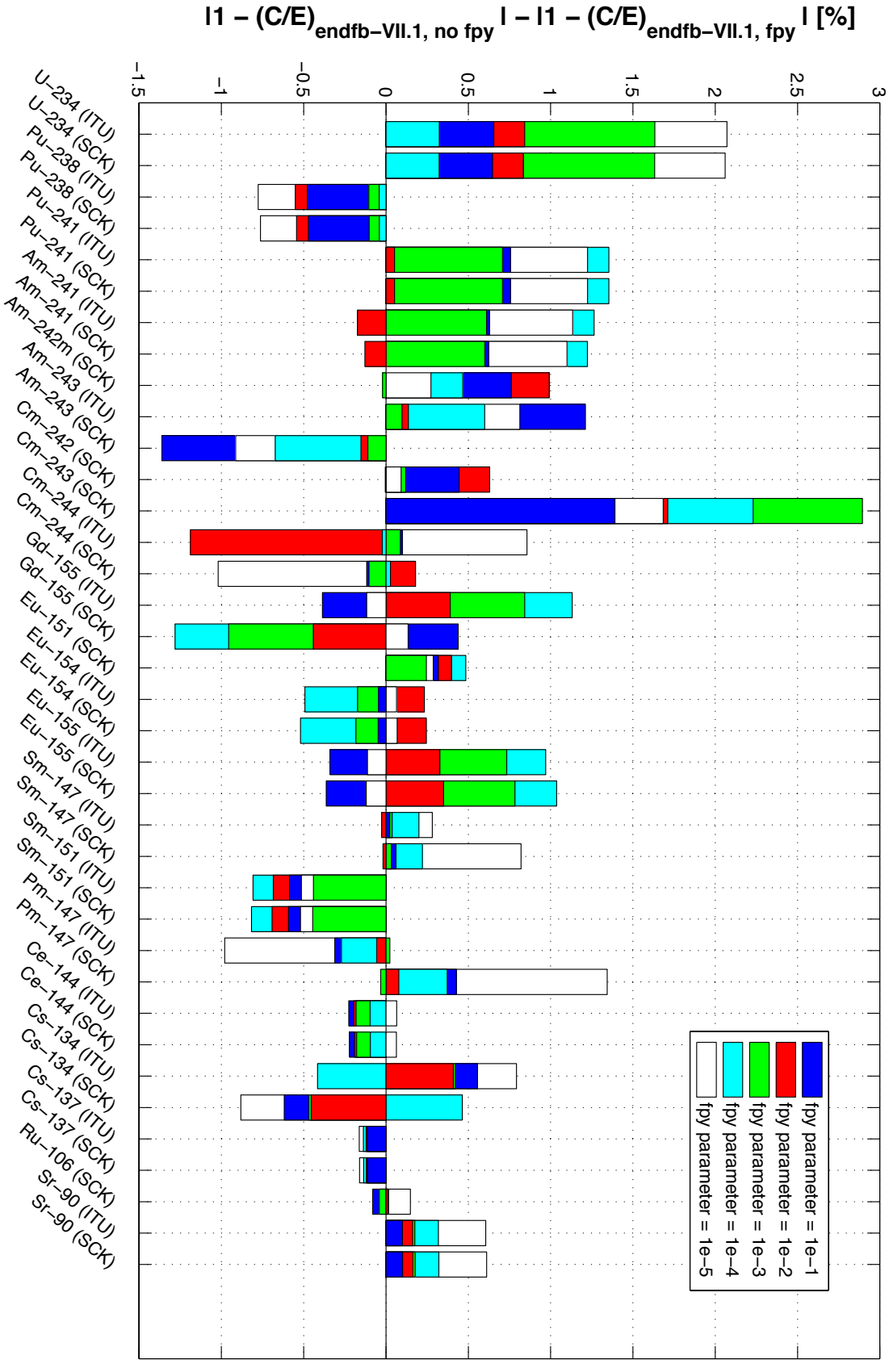

Figure 6.6.: Short-lived isotopes, library ENDFB-VII.1: comparison between the results obtained with the default fpy parameter and with values from 10[eV] to 100[keV], without the Sb-125.

It can be seen in these graphs that there are on average, when the FPY card is used, as many nuclides where the accuracy is improved as there are where it is not the case. It is thus difficult to see whether the global accuracy of an output has increased or not compared to the previous results.
Due to this, the average values $|(1-C/E)|_{av}$ and χ^2 have again been computed in table 6.1 for the long-lived and the short-lived isotopes for each fpy parameter and library.

Code	Library	fpy parameter [MeV]	$\|(1-C/E)\|_{av}$ [%] Long $T_{1/2}$ nuclides	$\|(1-C/E)\|_{av}$ [%] Short $T_{1/2}$ nuclides
MONT.	JEFF-3.1	/	7.295	16.882
SCALE	ENFB-VII	/	7.698	12.959
ALEPH2	JEFF-3.2	default	6.656	13.707
	JEFF-3.3T3	default	9.197	17.113
		1E-03	8.837	15.997
		1E-04	8.829	15.953
		1E-05	8.853	16.047
	ENDFB-VII.1	default	6.428	13.264
		1E-01	6.546	11.933
		1E-02	6.590	11.975
		1E-03	6.435	11.827
		1E-04	6.497	11.886
		1E-05	6.455	11.998

Code	Library	fpy parameter [MeV]	χ^2 Long $T_{1/2}$ nuclides	χ^2 Short $T_{1/2}$ nuclides
MONT.	JEFF-3.1	/	0.2815	0.1145
SCALE	ENFB-VII	/	0.2516	0.1111
ALEPH2	JEFF-3.2	default	0.2004	0.0817
	JEFF-3.3T3	default	0.2712	0.0832
		1E-03	0.2922	0.0781
		1E-04	0.2918	0.0768
		1E-05	0.2905	0.0751
	ENDFB-VII.1	default	0.1977	0.0772
		1E-01	0.2213	0.0700
		1E-02	0.2227	0.0712
		1E-03	0.2204	0.0676
		1E-04	0.2259	0.0694
		1E-05	0.2220	0.6665

Table 6.1.: Mean error and χ^2 related to 13 calculations of the problem.

From the tables above, it appears that the use of the interpolation scheme which sets the energy transition between the thermal and fast parts of $f_{j,m}(E)$, results in a global improvement on the short-lived nuclides, since both $|(1-C/E)|_{av}$ and χ^2 have significantly decreased.
Regarding the best results, it can be said that they are obtained with the ENDFB-VII.1 library and the fpy parameter equal to 1E-03[MeV] because, even if the values $|(1-C/E)|_{av}$ and χ^2 have increased a little bit for the long-lived nuclides compared to the ones obtained with the same library and the default fpy, they are globally way better for the short-lived nuclides. Moreover, as already stated in section 5, it can be seen that the worst ALEPH2 results are again obtained with the JEFF3.3T3 library.

Following all these observations, the upcoming simulations of the current section have been completed with the library ENDFB-VII.1 and the fpy parameter set to 1E-03[MeV].

6.2. Predictor-corrector

It has been seen in fig 2.1 that it is possible to invoke a predictor-corrector algorithm in an ALEPH2 calculation flow. It is used in order to reflect the neutron flux changes within a given time step. Indeed, since the basic working assumption of ALEPH2 in the default mode is the invariability of the reaction rates within each step (the depletion solver uses reaction rates which have been computed with the initial compositions of the materials at the beginning of the time step to compute their final composition at the end of the step), this hypothesis does not represent the real functioning of a nuclear reactor because fission products are progressively built up and, many of them being strong neutron absorbers, the neutron population in the core actually becomes more and more poisoned, and the neutron spectrum, harder with time.
To solve this problem, several predictor-corrector mechanisms exist in ALEPH2 in order to model the changes during each time step, and the one which has been used in this study is the default one, invoked by the card "CORR 1". In this algorithm, the neutron flux spectrum ϕ(E) is calculated at the beginning of the time step, and the concentrations are then obtained at the middle of this time step, $N_{i+1/2}$. Then, using these ones, ϕ(E) is recalculated and the concentrations are finally solved from the beginning to the end of the time step using this middle-step neutron flux spectrum, $\phi_{i+1/2}$(E).
It should be noted that the drawback of such a mechanism is that it doubles in general[1] the calculation time, since MCNP5 is launched twice at every irradiation step.
The predictor-corrector algorithm used in this study is shown hereafter in fig 6.7.

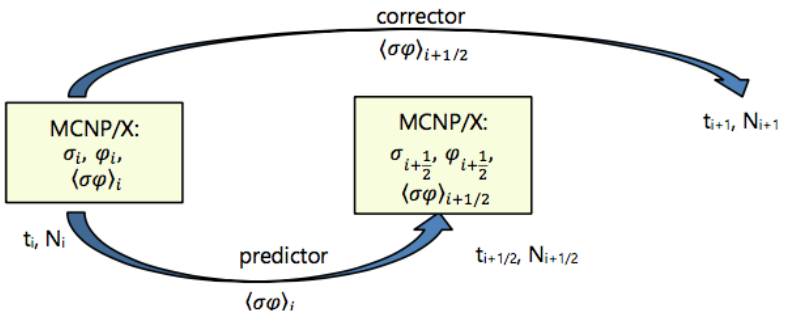

Figure 6.7.: Predictor-corrector algorithm [20].

The results of the calculation made with this additional predictor-corrector card can then be found in appendix A.6.

6.3. Variable fuel temperature

It was also explained previously that the temperature of the fuel is an important parameter in the problem, due to the Doppler effect which lessens the neutron thermalization (the

[1] It is possible to apply this algorithm only at selected time steps.

epithermal neutron absorptions by U-238 atoms increase) and thus the amount of U-235 fissions, when the temperature of the fuel increases.
In the previous ALEPH2 input file, the average pin fuel temperature was chosen to be constant and equal to 1000[K] (see tables 4.1 and 4.7). Nevertheless, this hypothesis does not represent accurately the real problem since, during the irradiation of UO_2, the U-235 concentration decreases with the burn-up. This, consequently, leads to the decrease of the power produced by the fuel and thus finally, also to the decrease of its temperature. In conclusion, the temperature of UO_2 may be equal on average to 1000[K] during its irradiation, but its absolute temperature has to be larger at the beginning and then must progressively decrease to reach 800-850[K] at the end.
It is then possible in ALEPH2 to change the temperature of a selected material at the beginning of a time step, thanks to a CHMT card. For instance, if the user wants to set the temperature of GU3 (material number 5) to 1250[K] at the beginning of a step, he can do it by simply adding a "CHMT 5 1250" card in the input file at the corresponding step.
From the temperature of GU3 given for each of the steps defined in table 3.2 [23] and by linearly interpolating values for the substeps, the evolution of the average pin fuel temperature has been described in ALEPH2. However, it has been chosen in this study to adjust this temperature only at the time steps which correspond to global decreases of 50[K] in order to limit the additional code lines to steps where meaningful effects can be observed. From this choice, the following GU3's temperature history has been coded in the ALEPH2 input file:

Cycle	Operation time (EFPD)	GU3's temperature [K]
16	0	1250
	150	1200
	336.8	1150
17	0	1050
	180	1000
	299.5	950
18	60	900
	120	850
	331.6	800

Table 6.2.: Evolution of the sample's temperature during the three irradiation cycles.

The results of the calculation made with these additional CHMT cards can be found in appendix A.7.

6.4. KCODE card: number of source neutrons per cycle doubled

The last study is relative to a part of the input file which was mentioned earlier in section 4: the nominal number of source histories, N, per keff cycle. In the input file, it was decided to set it to the value 50000 in order not to lose too much time in calculations, even if the U-235 fission reaction rate did not reach totally its equilibrium value yet (see fig 4.6).
Due to this, another ALEPH2 calculation has been run with a value N doubled compared to the initial case, i.e. whith N equal to 100000 and the resulting GU3's composition can then be found in appendix A.8.

6.5. Observations from the additional studies

In order to see whether the accuracy has been globally improved or not, the results of the three last studies (predictor-corrector algorithm, temperature of GU3 and number of source neutrons per cycle doubled in kcode card) have been compared to the previous values, obtained with the library ENDFB-VII.1 and the fpy parameter set to 1E-03[MeV].
The resulting values $|(1-\mathrm{C/E})_{\mathrm{ENDFB-VII.1},\ py=1\mathrm{E}-03}| - |(1-\mathrm{C/E})_{\mathrm{ENDFB-VII.1},\ py=1\mathrm{E}-03,\ option}|$ are then shown in fig 6.8 and fig 6.9 for respectively the long and the short-lived nuclides.

Again here, because the values in these two figures are sometimes above 0, sometimes under 0, it is difficult to say whether the concentrations fit globally better the measured values than previously or not. Moreover, it can be observed that, for some nuclides and whatever the chosen study, the results have been improved compared to the measured value of one laboratory, but not compared to the other. This is for instance the case for Cm-245 or Nd-150 (long-lived nuclides), or Am-243, Cm-244 or Cs-134 (short-lived nuclides). For those nuclides, it is thus impossible to say whether the "predictor-corrector", the" varying fuel temperature" or the "doubled N value" options improved the results of the simulation or not.
For these reasons, the average values $|(1-\mathrm{C/E})|_{av}$ and the χ^2 parameters have thus again been computed for the long and the short-lived isotopes, for each of the three cases.
The results are shown hereafter in table 6.3.

Library	fpy parameter [MeV]	option	$\lvert(1-\mathrm{C/E})\rvert_{av}$ [%] Long $T_{1/2}$ nuclides	$\lvert(1-\mathrm{C/E})\rvert_{av}$ [%] Short $T_{1/2}$ nuclides
ENDFB-VII.1	1E-03	/	6.435	11.827
		pred-corr	6.526	12.146
		UO_2 temp.	6.578	11.948
		N doubled	6.522	11.896
Library	fpy parameter [MeV]	option	χ^2 Long $T_{1/2}$ nuclides	χ^2 Short $T_{1/2}$ nuclides
ENDFB-VII.1	1E-03	/	0.2204	0.0676
		pred-corr	0.2205	0.0710
		UO_2 temp.	0.2281	0.0705
		N doubled	0.2186	0.0697

Table 6.3.: Comparison between the 4 calculations computed with minor changes in the input file (additional top cards).

The results here being neither worse nor really better, it can not be said that the use of a predictor-corrector algorithm, of a variable fuel temperature description or of a larger number of particles simulated per each cycle of a kcode calculation brings accuracy in the outputs of Gösgen study case.
It can simply be concluded that the optimum values of the step length, the average pin fuel temperature and the number of neutrons per kcode batch were already found in the previous input files and that the remaining uncertainties of the results are therefore associated with deficiencies of the model itself or with nuclear data.

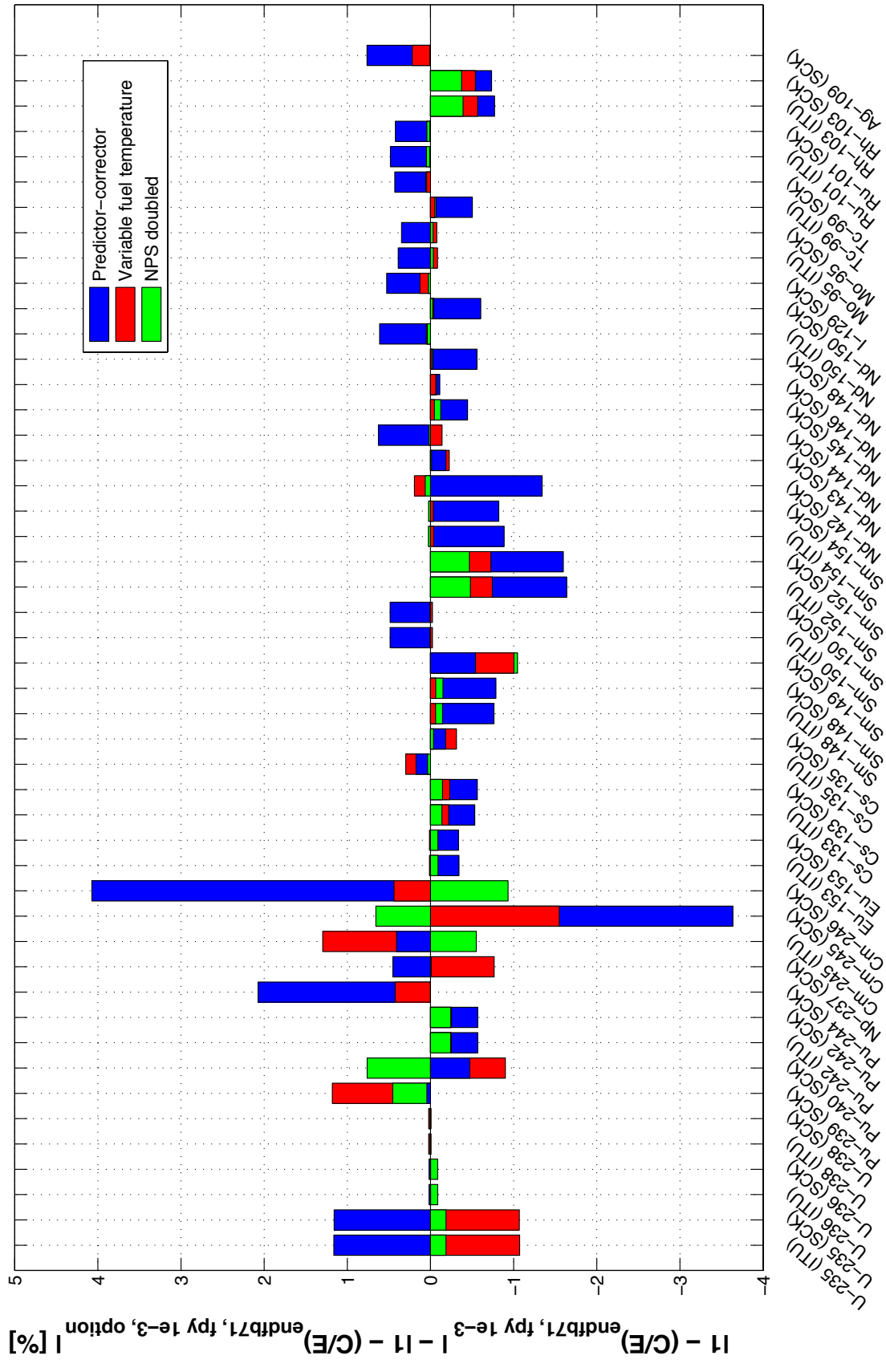

Figure 6.8.: Long-lived isotopes, library ENDFB-VII.1, fpy parameter = 1[keV]: comparison between the results obtained with a predictor-corrector algorithm, a varying fuel temperature or a doubled number of particles simulated per kcode, and the results without any of these cards.

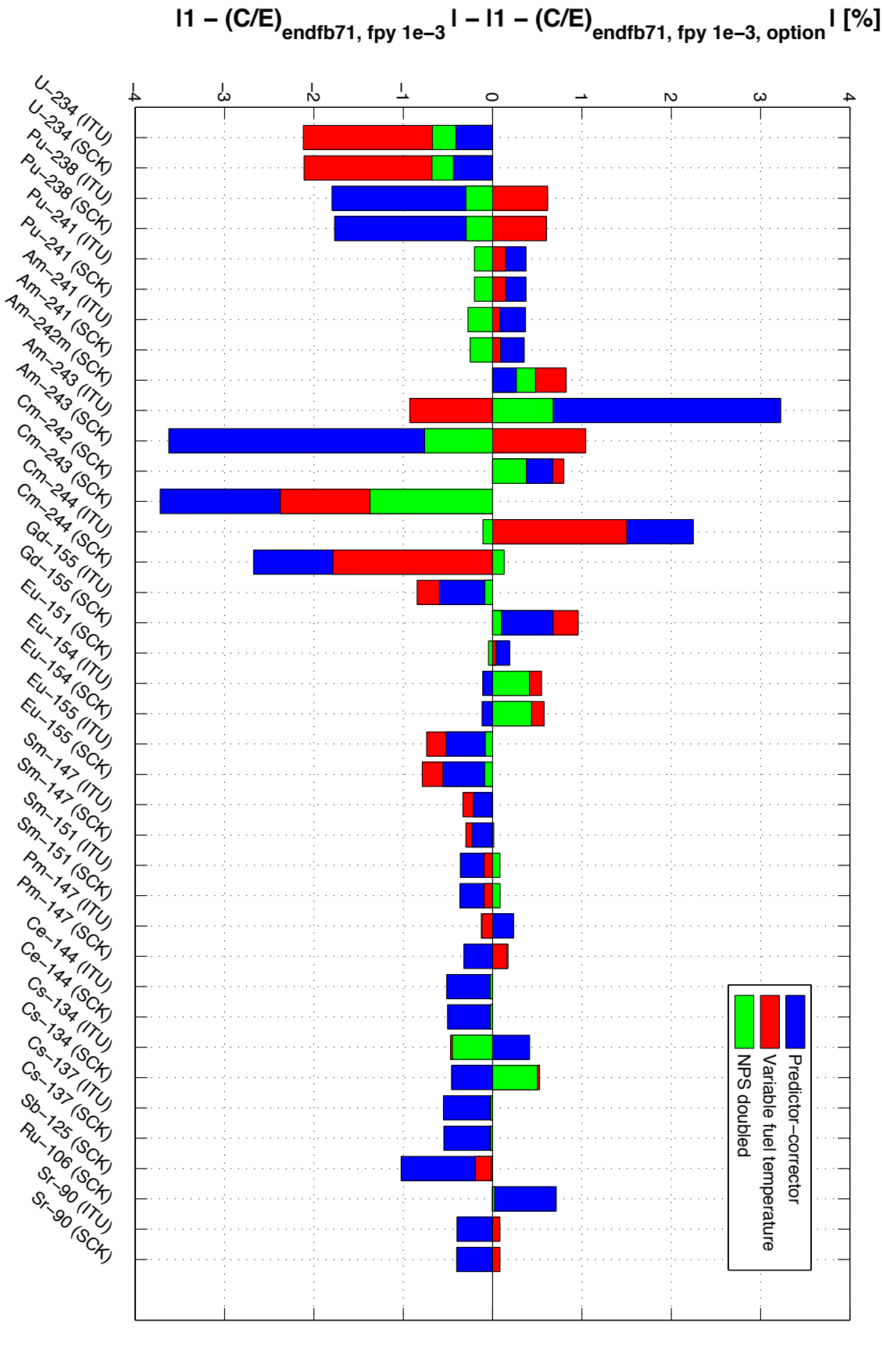

Figure 6.9.: Short-lived isotopes, library ENDFB-VII.1, fpy parameter = 1[keV]: comparison between the results obtained with a predictor-corrector algorithm, a varying fuel temperature or a doubled number of particles simulated per kcode, and the results without any of these cards.

Conclusion

7

The purpose of this master thesis was the comparison between the measured spent fuel isotopic content of two samples - GU3 and GU3' - irradiated in Gösgen PWR core, Switzerland and the concentrations obtained using the ALEPH2 depletion code on this benchmark case.

The first part of this document was related to the theory inherent to the ALEPH2 code, and was separated in two distinct parts.
First of all, the MCNP5 Monte-Carlo transport of particles that occurs at the beginning of each time step was explained, with the history flow of each neutron from birth to death: how to calculate the neutron flux tallies thanks to the neutron track lengths, how the collision nuclides and the reactions in which the neutron is involved are sampled, how to calculate the parameters of the neutron after the collision, etc. are some of the points which were described in details in the report.
From this, the second part of the theory was the description of the depletion of the materials, with the creation of systems of first-order ordinary differential equations whose constant coefficients are either decay terms or reaction rates calculated thanks to the link between the above MCNP5 neutron flux tallies and the irradiation history of the problem which brings time in the Monte-Carlo time-independent problem by deducing a neutron source rate at each step.

The study case was then translated in ALEPH2 code lines, using both MCNP5 cards for the description of the assembly's geometry and the division in cells, the initial composition of the materials in them, the creation of an initial neutron source in the problem or again for the choice of the output tallies, and ALEPH2-specific cards for the selection of the materials which are depleted, the possible exchanges of materials inside some cells during the irradiation, the adjustement of the boron concentration in the water, the description of the irradiation history and the cooling of GU3 and GU3', etc.

From this, the calculation of the samples' final compositions has been done and the concentrations of 53 nuclides have been compared to their measured values.
The results were rather correct since the calculated concentrations of the long-lived isotopes were situated on average at 6[%] from the measured values (with some nuclides, such as Pu-244, whose concentration is situated at more than 60[%]) and the calculated concentration of the short-lived isotopes on average at 12[%] (with some nuclides, such as Sb-125, whose concentration is situated at more than 150[%]). The long-lived isotopes were indeed more accurately described than the short ones because of the fact that they are easier to measure (due to their larger $T_{1/2}$), meaning that their concentration can be assumed rather constant during the entire experiment.

It has also to be noted that ALEPH2 showed globally better results than two other codes (MONTEBURNS and SCALE) related to the same problem did; and this, particularly when the neutron interaction data library was ENDFB-VII.1 and when the transition energy between the thermal and the fast spectrum for the fission product yields was set to 1E-03[MeV], and no more linearly interpolated from very few values.

Finally, advanced studies have been made in order to see the effects on the results of the use of a predictor-corrector algorithm, of a variable fuel temperature description and of a larger number of particles simulated per each cycle of a criticality calculation. These studies did however not bring any significant improvement. But, this is not especially a bad thing and may simply mean that optimum values of the step length, the average pin fuel temperature and the number of fission neutrons per batch were already found previously, and that the remaining uncertainties of the results can therefore only be associated with deficiencies of the benchmark model itself or with nuclear data.

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Annexes

A

A.1. ALEPH2 final input

```
TIT Evaluation of Gösgen GU3 sample
DATN /srv/clu/sci/pack/mcnp/xs_aleph_testing/aleph2/libn/jeff32a
BURN 5 2 4 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
     22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
VOL 6.5182 1212.38 2682.77 19.5545 6.5182 6.5182 6.5182 6.5182 6.5182
    6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182
TAL 4
MCNP /srv/clu/sci/bin/mcnp5_c740.sh 16       $ MCNP5 is run on 16 CPUs
OUT lib

c Irradiation history
c Cycle 16
c
IRP s 5 4.01316E-03 d 6
PPM 4 50000 -1705
IRP s 5 4.12651E-03 d 14
PPM 4 50000 -1347
IRP s 5 4.10534E-03 d 20
PPM 4 50000 -1283
IRP s 5 4.08471E-03 d 20
PPM 4 50000 -1192
IRP s 5 4.06788E-03 d 30
PPM 4 50000 -1100
IRP s 5 4.04617E-03 d 30
PPM 4 50000 -963
IRP s 5 3.95464E-03 d 30
PPM 4 50000 -827
IRP s 5 3.83269E-03 d 30
PPM 4 50000 -690
IRP s 5 3.78937E-03 d 30
PPM 4 50000 -569
IRP s 5 3.72786E-03 d 30
PPM 4 50000 -448
IRP s 5 3.70326E-03 d 30
PPM 4 50000 -327
IRP s 5 3.67758E-03 d 30
PPM 4 50000 -207
IRP s 5 3.64576E-03 d 20
PPM 4 50000 -86
IRP s 5 3.46758E-03 d 16.8
```

```
PPM 4 50000 -5
DEC d 25 no
c
c Cycle 17
c
IRP s 5 3.23640E-03 d 6
PPM 4 50000 -1601
IRP s 5 3.28359E-03 d 14
PPM 4 50000 -1247
IRP s 5 3.27060E-03 d 20
PPM 4 50000 -1184
IRP s 5 3.24734E-03 d 20
PPM 4 50000 -1095
IRP s 5 3.23220E-03 d 30
PPM 4 50000 -1005
IRP s 5 3.21435E-03 d 30
PPM 4 50000 -871
IRP s 5 3.16288E-03 d 30
PPM 4 50000 -736
IRP s 5 3.08312E-03 d 30
PPM 4 50000 -602
IRP s 5 3.05891E-03 d 30
PPM 4 50000 -483
IRP s 5 3.01804E-03 d 30
PPM 4 50000 -364
IRP s 5 3.00836E-03 d 30
PPM 4 50000 -245
IRP s 5 2.99613E-03 d 29.5
PPM 4 50000 -126
IRP s 5 2.87491E-03 d 29.2
PPM 4 50000 -9
DEC d 22.  no
c
c Cycle 18
c
IRP s 5 2.81816E-03 d 6
CHM 2 22
CHM 5 23
CHM 7 5
CHM 8 24
CHM 9 25
CHM 10 26
CHM 11 27
CHM 12 28
CHM 13 29
CHM 14 30
CHM 15 31
CHM 16 32
CHM 17 33
```

```
CHM 18 34
CHM 19 35
CHM 20 36
CHM 21 37
CHMD 23 7.006526620156E-02
CHMD 24 7.006526620156E-02
CHMD 25 7.006526620156E-02
CHMD 26 7.006526620156E-02
CHMD 27 7.006526620156E-02
CHMD 28 7.006526620156E-02
CHMD 29 7.006526620156E-02
CHMD 30 7.006526620156E-02
CHMD 31 7.006526620156E-02
CHMD 32 7.006526620156E-02
CHMD 33 7.006526620156E-02
CHMD 34 7.006526620156E-02
CHMD 35 7.006526620156E-02
CHMD 36 7.006526620156E-02
CHMD 37 7.006526620156E-02
PPM 4 50000 -1675
IRP s 5 2.75044E-03 d 14
PPM 4 50000 -1300
IRP s 5 2.70854E-03 d 20
PPM 4 50000 -1235
IRP s 5 2.65852E-03 d 20
PPM 4 50000 -1142
IRP s 5 2.60165E-03 d 30
PPM 4 50000 -1049
IRP s 5 2.54864E-03 d 30
PPM 4 50000 -910
IRP s 5 2.47179E-03 d 30
PPM 4 50000 -770
IRP s 5 2.41762E-03 d 30
PPM 4 50000 -631
IRP s 5 2.38813E-03 d 30
PPM 4 50000 -509
IRP s 5 2.35009E-03 d 30
PPM 4 50000 -387
IRP s 5 2.33897E-03 d 30
PPM 4 50000 -266
IRP s 5 2.32829E-03 d 30
PPM 4 50000 -144
IRP s 5 2.32337E-03 d 1.2
PPM 4 50000 -22
IRP s 5 2.16983E-03 d 30.4
PPM 4 50000 -17
c
c Decay until experiments at SCK and ITU
DEC d 600.  no       $ U, Pu :  ITU
```

```
DEC d 57.   no       $ Nd, I-129 :  ITU
DEC d 39.   no       $ Sm, Eu, Cs, Ce-144, Pm-147 :  ITU
DEC d 43.   no       $ Cm, Am-241, Am-243, Np-237 :  ITU
DEC d 15.   no       $ Cu, Cs, Eu, Ce-144, Ru-106, Sb-125 :  SCK
DEC d 97.   no       $ Gd-155, Sr-90, Mo-95, Tc-99, Ru-101, Ru-106, Rh-103 :  ITU
DEC d 6.    no       $ U, Pu :  SCK
DEC d 43.   no       $ Nd :  SCK
DEC d 7.    no       $ Gd-155 :  SCK
DEC d 12.   no       $ Sm :  SCK
DEC d 8.    no       $ Am, Np-237 :  SCK
DEC d 3.    no       $ I-129 :  SCK
DEC d 70.   no       $ Pm-147 :  SCK
DEC d 38.   no       $ Mo-95, Tc-99, Ru-101, Rh-103, Ag-109 :  SCK
DEC d 36.   no       $ Sr-90 :  SCK


c MCNP5 part of the aleph input file
message:  xsdir=xsdir32a

c TITLE: GOSGEN ASSEMBLY DESCRIPTION
c
c
c cell cards
1 0 1 -2 3 -4 5 -6           fill=1
2 0 77 -7 88 -8    u=1 lat=1 fill= -7:7 -7:7 0:0
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  3  2  2  3  2  2  2  3  2  2  3  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  3  2  2  3  2  2  3  2  2  2  2
  2  8  3  14 2  2  2  2  2  2  2  2  3  2  2
  2  9  5  13 2  2  2  2  2  2  2  2  2  2  2
  2  10 11 12 3  2  2  2  2  2  3  2  2  2  2
  2  2  2  6  2  2  2  2  2  2  2  2  2  2  2
  15 21 3  2  2  2  2  2  2  2  2  2  3  2  2
  16 7  20 2  3  2  2  3  2  2  3  2  2  2  2
  17 18 19 6  2  2  2  2  2  2  2  2  2  2  2
  6  2  3  2  2  3  2  2  2  3  2  2  3  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
c
3  1  -6.5093     -9 10  imp:n=1   u=2     tmp=5.170E-08    $ Zr4 around UO2
4  2  -10.40      -11    imp:n=1   u=2     tmp=8.617E-08    $ Fuel UO2
5  3  -0.0020907  -10 11 imp:n=1   u=2     tmp=6.032E-08    $ He |b| Zr4 and UO2
6  4  -0.723       9     imp:n=1   u=2     tmp=4.955E-08    $ Water around UO2
c
7  1  -6.5093     -12 13 imp:n=1   u=3     tmp=4.912E-08    $ Zr4 GT
8  4  -0.743      -13    imp:n=1   u=3     tmp=4.877E-08    $ Water in GT
9  4  -0.723       12    imp:n=1   u=3     tmp=4.955E-08    $ Water around GT
```

```
c
c cells related to the first position of GU3 (P7)
10 1  -6.5093     -9 10  imp:n=1   u=5     tmp=5.170E-08    $ Zr4 around UO2
11 5  -10.40      -11    imp:n=1   u=5     tmp=8.617E-08    $ Fuel UO2
12 3  -0.0020907  -10 11 imp:n=1   u=5     tmp=6.032E-08    $ He |b| Zr4 and UO2
13 4  -0.723       9     imp:n=1   u=5     tmp=4.955E-08    $ Water around UO2
c
c
c cells related to the 3 fuel pins common to the 3 cycles (N9, N12, S13)
14 1  -6.5093     -9 10  imp:n=1   u=6     tmp=5.170E-08    $ Zr4 around UO2
15 6  -10.40      -11    imp:n=1   u=6     tmp=8.617E-08    $ Fuel UO2
16 3  -0.0020907  -10 11 imp:n=1   u=6     tmp=6.032E-08    $ He |b| Zr4 and UO2
17 4  -0.723       9     imp:n=1   u=6     tmp=4.955E-08    $ Water around UO2
c
c
c cells related to the second position of GU3 (R11)
18 1  -6.5093     -9 10  imp:n=1   u=7     tmp=5.170E-08    $ Zr4 around UO2
19 7  -10.40      -11    imp:n=1   u=7     tmp=8.617E-08    $ Fuel UO2
20 3  -0.0020907  -10 11 imp:n=1   u=7     tmp=6.032E-08    $ He |b| Zr4 and UO2
21 4  -0.723       9     imp:n=1   u=7     tmp=4.955E-08    $ Water around UO2
c
c
c cells related to GU3's neighbours in cycles 16/17
22 1  -6.5093     -9 10  imp:n=1   u=8     tmp=5.170E-08    $ Zr4 around UO2
23 8  -10.40      -11    imp:n=1   u=8     tmp=8.617E-08    $ Fuel UO2
24 3  -0.0020907  -10 11 imp:n=1   u=8     tmp=6.032E-08    $ He |b| Zr4 and UO2
25 4  -0.723       9     imp:n=1   u=8     tmp=4.955E-08    $ Water around UO2
c
26 1  -6.5093     -9 10  imp:n=1   u=9     tmp=5.170E-08    $ Zr4 around UO2
27 9  -10.40      -11    imp:n=1   u=9     tmp=8.617E-08    $ Fuel UO2
28 3  -0.0020907  -10 11 imp:n=1   u=9     tmp=6.032E-08    $ He |b| Zr4 and UO2
29 4  -0.723       9     imp:n=1   u=9     tmp=4.955E-08    $ Water around UO2
c
30 1  -6.5093     -9 10  imp:n=1   u=10    tmp=5.170E-08    $ Zr4 around UO2
31 10 -10.40      -11    imp:n=1   u=10    tmp=8.617E-08    $ Fuel UO2
32 3  -0.0020907  -10 11 imp:n=1   u=10    tmp=6.032E-08    $ He |b| Zr4 and UO2
33 4  -0.723       9     imp:n=1   u=10    tmp=4.955E-08    $ Water around UO2
c
34 1  -6.5093     -9 10  imp:n=1   u=11    tmp=5.170E-08    $ Zr4 around UO2
35 11 -10.40      -11    imp:n=1   u=11    tmp=8.617E-08    $ Fuel UO2
36 3  -0.0020907  -10 11 imp:n=1   u=11    tmp=6.032E-08    $ He |b| Zr4 and UO2
37 4  -0.723       9     imp:n=1   u=11    tmp=4.955E-08    $ Water around UO2
c
38 1  -6.5093     -9 10  imp:n=1   u=12    tmp=5.170E-08    $ Zr4 around UO2
39 12 -10.40      -11    imp:n=1   u=12    tmp=8.617E-08    $ Fuel UO2
40 3  -0.0020907  -10 11 imp:n=1   u=12    tmp=6.032E-08    $ He |b| Zr4 and UO2
41 4  -0.723       9     imp:n=1   u=12    tmp=4.955E-08    $ Water around UO2
c
42 1  -6.5093     -9 10  imp:n=1   u=13    tmp=5.170E-08    $ Zr4 around UO2
```

```
43 13 -10.40      -11     imp:n=1   u=13    tmp=8.617E-08    $ Fuel UO2
44 3  -0.0020907  -10 11 imp:n=1   u=13    tmp=6.032E-08    $ He |b| Zr4 and UO2
45 4  -0.723       9      imp:n=1   u=13    tmp=4.955E-08    $ Water around UO2
c
46 1  -6.5093     -9 10  imp:n=1   u=14    tmp=5.170E-08    $ Zr4 around UO2
47 14 -10.40      -11     imp:n=1   u=14    tmp=8.617E-08    $ Fuel UO2
48 3  -0.0020907  -10 11 imp:n=1   u=14    tmp=6.032E-08    $ He |b| Zr4 and UO2
49 4  -0.723       9      imp:n=1   u=14    tmp=4.955E-08    $ Water around UO2
c
c
c cells related to GU3's neighbours in cycle 18
50 1  -6.5093     -9 10  imp:n=1   u=15    tmp=5.170E-08    $ Zr4 around UO2
51 15 -10.40      -11     imp:n=1   u=15    tmp=8.617E-08    $ Fuel UO2
52 3  -0.0020907  -10 11 imp:n=1   u=15    tmp=6.032E-08    $ He |b| Zr4 and UO2
53 4  -0.723       9      imp:n=1   u=15    tmp=4.955E-08    $ Water around UO2
c
54 1  -6.5093     -9 10  imp:n=1   u=16    tmp=5.170E-08    $ Zr4 around UO2
55 16 -10.40      -11     imp:n=1   u=16    tmp=8.617E-08    $ Fuel UO2
56 3  -0.0020907  -10 11 imp:n=1   u=16    tmp=6.032E-08    $ He |b| Zr4 and UO2
57 4  -0.723       9      imp:n=1   u=16    tmp=4.955E-08    $ Water around UO2
c
58 1  -6.5093     -9 10  imp:n=1   u=17    tmp=5.170E-08    $ Zr4 around UO2
59 17 -10.40      -11     imp:n=1   u=17    tmp=8.617E-08    $ Fuel UO2
60 3  -0.0020907  -10 11 imp:n=1   u=17    tmp=6.032E-08    $ He |b| Zr4 and UO2
61 4  -0.723       9      imp:n=1   u=17    tmp=4.955E-08    $ Water around UO2
c
62 1  -6.5093     -9 10  imp:n=1   u=18    tmp=5.170E-08    $ Zr4 around UO2
63 18 -10.40      -11     imp:n=1   u=18    tmp=8.617E-08    $ Fuel UO2
64 3  -0.0020907  -10 11 imp:n=1   u=18    tmp=6.032E-08    $ He |b| Zr4 and UO2
65 4  -0.723       9      imp:n=1   u=18    tmp=4.955E-08    $ Water around UO2
c
66 1  -6.5093     -9 10  imp:n=1   u=19    tmp=5.170E-08    $ Zr4 around UO2
67 19 -10.40      -11     imp:n=1   u=19    tmp=8.617E-08    $ Fuel UO2
68 3  -0.0020907  -10 11 imp:n=1   u=19    tmp=6.032E-08    $ He |b| Zr4 and UO2
69 4  -0.723       9      imp:n=1   u=19    tmp=4.955E-08    $ Water around UO2
c
70 1  -6.5093     -9 10  imp:n=1   u=20    tmp=5.170E-08    $ Zr4 around UO2
71 20 -10.40      -11     imp:n=1   u=20    tmp=8.617E-08    $ Fuel UO2
72 3  -0.0020907  -10 11 imp:n=1   u=20    tmp=6.032E-08    $ He |b| Zr4 and UO2
73 4  -0.723       9      imp:n=1   u=20    tmp=4.955E-08    $ Water around UO2
c
74 1  -6.5093     -9 10  imp:n=1   u=21    tmp=5.170E-08    $ Zr4 around UO2
75 21 -10.40      -11     imp:n=1   u=21    tmp=8.617E-08    $ Fuel UO2
76 3  -0.0020907  -10 11 imp:n=1   u=21    tmp=6.032E-08    $ He |b| Zr4 and UO2
77 4  -0.723       9      imp:n=1   u=21    tmp=4.955E-08    $ Water around UO2
c
c 78  0           -1:2:-3:4:-5:6 imp:n=0
c end of cell cards for sample problem
```

```
c surface cards
+1 PX -10.725
+2 PX  10.725
+3 PY -10.725
+4 PY  10.725
+5 PZ -5
+6 PZ  5
77 PX -0.715
7  PX  0.715
88 PY -0.715
8  PY  0.715
c cylinders cards
9  CZ .5375                          $ Zr4 cladding outer cylinder
10 CZ .465                           $ Zr4 cladding inner cylinder
11 CZ .4555                          $ UO2 cylinder
12 CZ .69                            $ ZR4 guide tube outer cylinder
13 CZ .62                            $ Zr4 guide tube inner cylinder

c Material cards
c
M1  nlib=06c          $ Zr4
   40090 .50539335
   40091 .11021406
   40092 .16846445
   40094 .17072374
   40096 .02750440
   50112 1.40650E-4
   50114 9.57000E-5
   50115 4.93000E-5
   50116 2.10830E-3
   50117 1.11360E-3
   50118 3.51190E-3
   50119 1.24555E-3
   50120 4.72410E-3
   50122 6.71350E-4
   50124 8.39550E-4
   26054 1.22640E-4
   26056 1.92675E-3
   26057 4.45200E-5
   26058 5.88000E-6
   24050 4.31000E-5
   24052 8.37890E-4
   24053 9.50100E-5
   24054 2.36500E-5
   72174 1.62000E-7
   72176 5.20600E-6
   72177 1.86060E-5
   72178 2.72970E-5
   72179 1.36290E-5
```

```
   72180 3.51000E-5
c
c
M2  nlib=10c          $ UO2
   8016 -0.118317732
   8017 -4.50680E-5
   8018 -2.37200E-4
   92234 -3.70188E-4
   92235 -0.036137400
   92238 -0.844892412
c
c
M3  nlib=07c          $ Helium
   2003 1.3400E-6
   2004 .99999866
c
c
M4  nlib=06c          $ Water
   1001 0.66659
   1002 7.6666667E-5
   8016 0.33254
   8017 1.2666667E-4
   8018 6.6666667E-4
MT4  lwtr.62t
c
c
M5  nlib=10c          $ UO2 sample GU3
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M6  nlib=10c          $ UO2 3 other fuel rods common to the 3 cycles
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M7  nlib=10c          $ UO2 fuel rod corr.  to 2d position of GU3
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
```

```
  92235 -0.036137400
  92238 -0.844892412
c
c
c All the neighbouring fuel rods' materials
M8  nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M9  nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M10 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M11 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M12 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
```

```
c
M13 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M14 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M15 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M16 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M17 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M18 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
```

```
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M19 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M20 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c
M21 nlib=10c          $ UO2
  8016 -0.118317732
  8017 -4.50680E-5
  8018 -2.37200E-4
  92234 -3.70188E-4
  92235 -0.036137400
  92238 -0.844892412
c
c All the fuel materials already burnt until 17.7[MWd/kgU]
c
M22                   $ UO2
  1001.10c 2.413217772243E-07
  1002.10c 6.708256479922E-08
  1003.10c 7.416289143603E-07
  2003.10c 1.026226384459E-08
  2004.10c 1.152802173453E-05
  3006.10c 1.202785136660E-07
  3007.10c 1.785781174997E-08
  6000.10c 9.280288760154E-08
  6013.10c 2.532310775076E-05
  8016.10c 6.610026206252E-01
  8017.10c 2.649101440512E-04
  8018.10c 1.324875865722E-03
  32073.10c 1.401010587080E-08
  32074.10c 3.489279152779E-08
```

```
32076.10c 2.864034501377E-07
33075.10c 7.321351776097E-08
34077.10c 5.101425765584E-07
34078.10c 1.345669907419E-06
34079.10c 2.991962686068E-06
34080.10c 7.348228885875E-06
34082.10c 1.880071372669E-05
35081.10c 1.156793624731E-05
36082.10c 1.742541534056E-07
36083.10c 2.805353708227E-05
36084.10c 5.868595772694E-05
36085.10c 1.496161754184E-05
36086.10c 1.066564749277E-04
37085.10c 5.571130270345E-05
37087.10c 1.383144194247E-04
38086.10c 1.326450875765E-07
38088.10c 1.890439231036E-04
38089.10c 3.449832907768E-05
38090.10c 2.949431143641E-04
39089.10c 2.125678673389E-04
39090.10c 7.493560630187E-08
39091.10c 5.373542970243E-05
40090.10c 3.970810207934E-06
40091.10c 2.596134532095E-04
40092.10c 3.308209420030E-04
40093.10c 3.616531095442E-04
40094.10c 3.664437344800E-04
40095.10c 7.427993564884E-05
40096.10c 3.716414771713E-04
41095.10c 4.986368134462E-05
42095.10c 2.485359658468E-04
42096.10c 5.058499450151E-06
42097.10c 3.608424081097E-04
42098.10c 3.576724183543E-04
42099.10c 7.933288723027E-09
42100.10c 3.943911499242E-04
43099.10c 3.627637959947E-04
44099.10c 1.271255898545E-08
44100.10c 1.834583297337E-05
44101.10c 3.311158038065E-04
44102.10c 3.009893500975E-04
44103.10c 2.901828050112E-05
44104.10c 1.809707610920E-04
44106.10c 6.076527087516E-05
45103.10c 1.894804943927E-04
45105.10c 8.796434063876E-12
46104.10c 3.142563658675E-05
46105.10c 1.166705830580E-04
46106.10c 3.410180709330E-05
```

```
46107.10c 5.348560957040E-05
46108.10c 3.271998934278E-05
46110.10c 1.128857057793E-05
47109.10c 2.147037924150E-05
47110.47c 1.833175142974E-08
47111.10c 2.615009886322E-08
48110.10c 4.025068932500E-06
48111.10c 5.907337753605E-06
48112.10c 3.327868941339E-06
48113.10c 1.029285775356E-07
48114.10c 4.955271945191E-06
48115.47c 1.313320844584E-08
48116.10c 2.344846566220E-06
49115.10c 4.528495658099E-07
50115.10c 9.753082195621E-08
50116.10c 1.495757257220E-06
50117.10c 2.141511193834E-06
50118.10c 2.203784976612E-06
50119.10c 1.828348961897E-06
50120.10c 2.314953232289E-06
50122.10c 2.871139540351E-06
50123.10c 1.612303313883E-07
50124.10c 4.247566814811E-06
50125.10c 1.287183323382E-08
50126.10c 7.278322751476E-06
51121.10c 2.148995869845E-06
51123.10c 2.851488978883E-06
51124.10c 1.945360246934E-08
51125.10c 3.481250682988E-06
52122.10c 6.642797016626E-08
52124.10c 6.088232296733E-08
52125.10c 4.057130317740E-07
52126.10c 1.013303916210E-06
52127.47c 8.558936650374E-07
52128.10c 2.781120034020E-05
52129.47c 1.597177802655E-06
52130.10c 1.230843171557E-04
52132.10c 1.689782228797E-08
53127.10c 1.206225319451E-05
53129.10c 5.073717939223E-05
53131.10c 7.854063003061E-07
53135.10c 3.234697340847E-18
54128.10c 2.848477231187E-07
54130.10c 7.774042395154E-07
54131.10c 1.620493360500E-04
54132.10c 3.084532181356E-04
54133.10c 4.093400758223E-07
54134.10c 4.698182523005E-04
54135.10c 7.401035485629E-18
```

```
54136.10c 7.161712791822E-04
55133.10c 3.859296719366E-04
55134.10c 2.297198054322E-05
55135.10c 1.158299438359E-04
55136.10c 6.768933051860E-08
55137.10c 3.844753765693E-04
56134.10c 3.032575709666E-06
56136.10c 3.044340447789E-06
56137.10c 4.811094076589E-06
56138.10c 4.061474869265E-04
56139.10c 9.571506777251E-19
56140.10c 5.072219874869E-06
57139.10c 3.848949819847E-04
57140.10c 7.679427223220E-07
58140.10c 3.735906706042E-04
58141.10c 2.789870353961E-05
58142.10c 3.511782449137E-04
58143.10c 6.531701548675E-12
58144.10c 1.999260262690E-04
59141.10c 3.220381347532E-04
59143.10c 5.827976022964E-06
60142.10c 1.947011131140E-06
60144.10c 1.503652098022E-04
60145.10c 2.212875436333E-04
60146.10c 1.933757705525E-04
60147.10c 1.270919667936E-06
60148.10c 1.082041437505E-04
60150.10c 4.694010865104E-05
61147.10c 8.985483469070E-05
61148.10c 3.396289840573E-08
61148.47c 3.979807105569E-07
61149.10c 3.342149125953E-10
61151.10c 7.683702120667E-14
62147.10c 1.200045249848E-05
62148.10c 2.290597107774E-05
62149.10c 2.390200584358E-06
62150.10c 7.404519567338E-05
62151.10c 6.886835119023E-06
62152.10c 3.279426049248E-05
62153.10c 5.108140321958E-11
63151.10c 1.055376604332E-08
63153.10c 2.402901751588E-05
63154.10c 3.654729062220E-06
63155.10c 1.319012921423E-06
63156.10c 2.763260690718E-07
64154.10c 1.072227631942E-07
64155.10c 2.318205378977E-08
64156.10c 7.264448471448E-06
64157.10c 4.526685344875E-08
```

```
  64158.10c 2.518358638734E-06
  64160.10c 2.285299225625E-07
  65159.10c 4.311546480140E-07
  66161.10c 1.079273477882E-07
  66162.10c 7.610281708822E-08
  66163.10c 4.773746598986E-08
  66164.10c 1.838585930033E-08
  67165.10c 1.613532216272E-08
  92234.10c 1.104730778305E-04
  92235.10c 8.737698867510E-03
  92236.10c 1.074475376009E-03
  92237.10c 2.627068050661E-07
  92238.10c 3.126028393077E-01
  93237.10c 6.766983755815E-05
  93238.10c 6.515006090516E-11
  93239.10c 2.274427461998E-08
  94238.10c 9.924799618889E-06
  94239.10c 1.753203159696E-03
  94240.10c 3.383350298961E-04
  94241.10c 2.069850033807E-04
  94242.10c 2.608314172353E-05
  95241.10c 3.019510871766E-06
  95242.47c 3.857718231882E-08
  95243.10c 2.434125684809E-06
  96242.10c 4.870767178637E-07
  96244.10c 3.123727835823E-07
  96245.10c 1.001377005783E-08

...            The "extra" materials 23 to 37 have the same comp.  than mat.  22

c
c source cards
c
print -85 -128 140
prdmp 0 0 1 0 0
kcode 50000 1.00 30 130
totnu
c
sdef erg=d1 axs=0 0 1 pos= 0 0 0 rad=d2 ext=d3
sp1 -3 0.988 2.249
si2  0 10.7
si3 -4.95 4.95
c
c tallies cards
c
fc4 flux
f4:n 11
      4
      (6 8 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77)
```

```
      15
      19
      23
      27
      31
      35
      39
      43
      47
      51
      55
      59
      63
      67
      71
      75
sd4 6.5182 1212.38 2682.77 19.5545 6.5182 6.5182 6.5182 6.5182 6.5182
    6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182 6.5182
fq4 E F
c
```

A.2. ALEPH2 single pin input (in order to calculate the composition of the fuel UO_2 burnt until 17.7[MWd/kgU])

```
TIT Fuel pin burnt until burn-up of 17.70 [MWd/kgU]
DATN /srv/clu/sci/pack/mcnp/xs_aleph_testing/aleph2/libn/jeff32a
BURN 3 4
VOL 6.5182 11.373
TAL 4
MCNP /srv/clu/sci/bin/mcnp5_c740.sh 16
OUT lib tpd aci

c Irradiation history
c
c
IRP s 3 3.140041178E-03 d 84.2
PPM 4 50000 1700
IRP s 3 3.140041178E-03 d 84.2
PPM 4 50000 1000
IRP s 3 3.140041178E-03 d 84.2
PPM 4 50000 600
IRP s 3 3.140041178E-03 d 84.2
PPM 4 50000 100
DEC d 25.
DEC d 1.  no

c MCNP5 part of the aleph input file
```

```
message:  xsdir=xsdir32a

c
c cell cards for fuel pin problem
1 0             1 -2 3 -4 5 -6 imp:n=1 fill=1
2 1 -6.5093    -7 8            imp:n=1 u=1     tmp=5.170E-08
3 2 -0.0020907 -8 9            imp:n=1 u=1     tmp=6.032E-08
4 3 -10.40     -9              imp:n=1 u=1     tmp=8.617E-08
5 4 -0.7046     7              imp:n=1 u=1     tmp=4.955E-08
6 0            -1:2:-3:4:-5:6  imp:n=0
c end of cell cards for fuel pin problem

c beginning of surfaces
+1 PX -0.715
+2 PX 0.715
+3 PY -0.715
+4 PY 0.715
+5 PZ -5
+6 PZ 5
7 CZ 0.5375
8 CZ 0.465
9 CZ 0.4555
c end of surfaces

c Material cards
c
M1  nlib=06c          $ Zr4
   40090 .50539335
   40091 .11021406
   40092 .16846445
   40094 .17072374
   40096 .02750440
   50112 1.40650E-4
   50114 9.57000E-5
   50115 4.93000E-5
   50116 2.10830E-3
   50117 1.11360E-3
   50118 3.51190E-3
   50119 1.24555E-3
   50120 4.72410E-3
   50122 6.71350E-4
   50124 8.39550E-4
   26054 1.22640E-4
   26056 1.92675E-3
   26057 4.45200E-5
   26058 5.88000E-6
   24050 4.31000E-5
   24052 8.37890E-4
   24053 9.50100E-5
```

```
   24054 2.36500E-5
   72174 1.62000E-7
   72176 5.20600E-6
   72177 1.86060E-5
   72178 2.72970E-5
   72179 1.36290E-5
   72180 3.51000E-5
c
c
M2  nlib=10c          $ UO2
    8016 -0.118317732
    8017 -4.50680E-5
    8018 -2.37200E-4
   92234 -3.70188E-4
   92235 -0.036137400
   92238 -0.844892412
c
c
M3  nlib=07c          $ Helium
   2003 1.3400E-6
   2004 .99999866
c
c
M4  nlib=06c          $ Water
   1001 0.66659
   1002 7.6666667E-5
   8016 0.33254
   8017 1.2666667E-4
   8018 6.6666667E-4
MT4  lwtr.62t
c
c source cards
c
print -85 -128 140
prdmp 0 0 1 0 0
kcode 50000 1.00 30 130
totnu
c
sdef erg=d1 axs=0 0 1 pos= 0 0 0 rad=d2 ext=d3
sp1 -3 0.988 2.249
si2  0 0.4555
si3 -4.95 4.95
c
c tallies cards
c
fc4 flux
f4:n (4<1)
     (5<1)
sd4 6.5182 11.373
```

```
fq4 E F
c
```

A.3. Matlab function used to read the ALEPH2 output files

```
function [C_E_long,C_E_short] = thesis_script_output_files(filename,density)

fileID = fopen(filename);
M5_original = textscan(fileID,'%s %u %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64
%f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64
%f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64
%f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64 %f64
%f64 %f64 %f64 %f64 %f64 %f64');
fclose(fileID);
format long;

C_E_long = zeros(1,48);
C_E_short = zeros(1,38);

% U-235
for i=1:length(M5_original{1})
  if strcmp(M5_original{1}(i),'92-U-235')
     U_235_ITU = M5_original{47}(i)*1000/density
     U_235_ITU_meas = 5.31;
     C_E_long(1,1) = U_235_ITU/U_235_ITU_meas;
     U_235_SCK = M5_original{53}(i)*1000/density;
     U_235_SCK_meas = 5.33;
     C_E_long(1,2) = U_235_SCK/U_235_SCK_meas;
  end
end

% U-236
for i=1:length(M5_original{1})
  if strcmp(M5_original{1}(i),'92-U-236')
     U_236_ITU = M5_original{47}(i)*1000/density
     U_236_ITU_meas = 4.99;
     C_E_long(1,3) = U_236_ITU/U_236_ITU_meas;
     U_236_SCK = M5_original{53}(i)*1000/density;
     U_236_SCK_meas = 4.98;
     C_E_long(1,4) = U_236_SCK/U_236_SCK_meas;
  end
end

...    % % % % % Same for all the other nuclides

end
```

A.4. Comparison between three data libraries

A.4.1. Library JEFF-3.2

Isotope	True value (mg/g-fuel)	ALEPH (JEFF-3.2) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.472	1.03	0.98	0.98
U-235(SCK)	5.33	5.472	1.03	0.97	0.98
U-236(ITU)	4.99	4.918	0.99	0.99	1.00
U-236(SCK)	4.98	4.918	0.99	0.99	1.00
U-238(ITU)	817.0	811.62	0.99	0.99	0.99
U-238(SCK)	816.0	811.62	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.250	1.03	0.97	0.97
Pu-240(SCK)	2.50	2.535	1.01	1.01	1.00
Pu-242(ITU)	0.895	0.887	0.99	0.98	0.95
Pu-242(SCK)	0.893	0.887	0.99	0.98	0.96
Pu-244(SCK)	1.63E-04	6.70E-05	0.41	0.60	0.43
Np-237(SCK)	0.715	0.649	0.91	0.88	0.83
Cm-245(ITU)	1.02E-02	8.97E-03	0.88	0.72	0.72
Cm-245(SCK)	8.54E-03	8.97E-03	1.05	0.86	0.86
Cm-246(SCK)	1.27E-03	1.09E-03	0.86	0.78	0.77
Eu-153(ITU)	0.162	0.163	1.01	1.05	1.01
Eu-153(SCK)	0.165	0.163	0.99	1.03	0.99
Cs-133(ITU)	1.47	1.44	0.98	0.98	1.00
Cs-133(SCK)	1.39	1.44	1.04	1.04	1.06
Cs-135(ITU)	0.424	0.414	0.98	0.91	0.94
Cs-135(SCK)	0.405	0.414	1.02	0.96	0.98
Sm-148(ITU)	0.231	0.248	1.07	0.89	0.91
Sm-148(SCK)	0.224	0.248	1.11	0.92	0.94
Sm-149(SCK)	2.96E-03	3.09E-03	1.04	1.13	1.07
Sm-150(ITU)	0.394	0.392	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.392	1.00	1.08	1.09
Sm-152(ITU)	0.115	0.123	1.07	1.12	1.12
Sm-152(SCK)	0.118	0.123	1.04	1.09	1.09
Sm-154(ITU)	4.69E-02	5.82E-02	1.24	1.19	1.17
Sm-154(SCK)	5.06E-02	5.82E-02	1.15	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.04	1.03	1.02
Nd-143(SCK)	0.945	0.959	1.01	0.99	1.00
Nd-144(SCK)	1.89	1.88	1.00	0.99	1.00
Nd-145(SCK)	0.872	0.879	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.250	0.98	0.98	0.98
Nd-150(SCK)	0.252	0.250	0.99	1.00	0.98
I-129(SCK)	0.236	0.243	1.03	1.07	0.91
Mo-95(ITU)	1.030	1.018	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.018	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.048	1.07	1.07	1.07
Tc-99(SCK)	1.143	1.048	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.076	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.076	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.602	1.28	1.16	1.26
Rh-103(SCK)	0.494	0.602	1.22	1.10	1.20
Ag-109(SCK)	0.1053	0.1235	1.17	1.00	1.05

Table A.1.: Long-lived isotopes, library JEFF-3.2.

Isotope	True value (mg/g-fuel)	ALEPH (JEFF-3.2) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.173	1.39	1.39	1.43
U-234(SCK)	0.124	0.175	1.41	1.40	1.44
Pu-238(ITU)	0.328	0.333	1.02	0.91	0.84
Pu-238(SCK)	0.332	0.332	1.00	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.190	1.14	1.09	1.15
Am-241(SCK)	0.212	0.226	1.07	1.02	1.07
Am-242m(SCK)	8.10E-04	7.59E-04	0.94	1.60	0.81
Am-243(ITU)	0.236	0.239	1.01	0.97	0.98
Am-243(SCK)	0.210	0.239	1.14	1.10	1.10
Cm-242(SCK)	9.82E-04	9.44E-04	0.96	0.83	0.82
Cm-243(SCK)	5.23E-04	7.89E-04	1.51	1.28	1.01
Cm-244(ITU)	0.136	0.106	0.78	0.74	0.72
Cm-244(SCK)	0.114	0.106	0.93	0.88	0.86
Gd-155(ITU)	3.67E-03	3.56E-03	0.97	0.97	0.97
Gd-155(SCK)	3.41E-03	3.74E-03	1.10	1.10	1.10
Eu-151(SCK)	3.70E-04	2.28E-04	0.62	0.61	0.58
Eu-154(ITU)	3.27E-02	3.29E-02	1.01	0.87	0.97
Eu-154(SCK)	3.06E-02	3.25E-02	1.06	0.92	1.02
Eu-155(ITU)	1.09E-02	9.09E-03	0.83	0.88	0.83
Eu-155(SCK)	9.97E-03	8.83E-03	0.89	0.96	0.88
Sm-147(ITU)	0.163	0.166	1.02	1.02	1.06
Sm-147(SCK)	0.173	0.184	1.06	1.07	1.10
Sm-151(ITU)	1.29E-02	1.34E-02	1.04	1.03	0.98
Sm-151(SCK)	1.27E-02	1.34E-02	1.05	1.04	0.98
Pm-147(ITU)	0.141	0.125	0.89	0.89	0.88
Pm-147(SCK)	8.25E-02	0.100	1.22	1.22	1.21
Ce-144(ITU)	7.13E-02	7.65E-02	1.07	1.05	1.02
Ce-144(SCK)	6.32E-02	6.64E-02	1.05	1.03	1.00
Cs-134(ITU)	0.128	0.122	0.95	0.91	0.87
Cs-134(SCK)	0.109	0.116	1.06	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.53E-02	2.31	2.87	1.66
Ru-106(SCK)	0.256	0.222	0.87	0.87	0.86
Sr-90(ITU)	0.645	0.661	1.02	1.03	1.04
Sr-90(SCK)	0.630	0.651	1.03	1.04	1.05

Table A.2.: Short-lived isotopes, library JEFF-3.2.

A.4.2. Library ENDF/B-VII.1

Isotope	True value (mg/g-fuel)	ALEPH (ENDF/B-VII.1) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.462	1.03	0.98	0.98
U-235(SCK)	5.33	5.462	1.02	0.97	0.98
U-236(ITU)	4.99	4.964	0.99	0.99	1.00
U-236(SCK)	4.98	4.964	1.00	0.99	1.00
U-238(ITU)	817.0	812.47	0.99	0.99	0.99
U-238(SCK)	816.0	812.47	1.00	0.99	1.00
Pu-239(SCK)	5.12	5.244	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.527	1.01	1.01	1.00
Pu-242(ITU)	0.895	0.899	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.899	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	9.95E-05	0.61	0.60	0.43
Np-237(SCK)	0.715	0.638	0.89	0.88	0.83
Cm-245(ITU)	1.02E-02	1.00E-02	0.98	0.72	0.72
Cm-245(SCK)	8.54E-03	1.00E-02	1.17	0.86	0.86
Cm-246(SCK)	1.27E-03	1.21E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.157	0.97	1.05	1.01
Eu-153(SCK)	0.165	0.157	0.95	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.00	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.420	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.420	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.257	1.11	0.89	0.91
Sm-148(SCK)	0.224	0.257	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.11E-03	1.05	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.98	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.120	1.05	1.12	1.12
Sm-152(SCK)	0.118	0.120	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.64E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.64E-02	1.12	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.965	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.880	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.00	0.99	0.99	1.00
Nd-148(SCK)	0.517	0.519	1.00	1.01	1.00
Nd-150(ITU)	0.254	0.251	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.251	1.00	1.00	0.98
I-129(SCK)	0.236	0.215	0.91	1.07	0.91
Mo-95(ITU)	1.030	1.016	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.016	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.052	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.052	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.066	0.99	0.98	0.99
Ru-101(SCK)	1.221	1.066	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.607	1.29	1.16	1.26
Rh-103(SCK)	0.494	0.607	1.23	1.10	1.20
Ag-109(SCK)	0.1053	8.37E-02	0.80	1.00	1.05

Table A.3.: Long-lived isotopes, library ENDF/B-VII.1.

Isotope	True value (mg/g-fuel)	ALEPH (ENDF/B-VII.1) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.172	1.39	1.39	1.43
U-234(SCK)	0.124	0.174	1.41	1.40	1.44
Pu-238(ITU)	0.328	0.349	1.06	0.91	0.84
Pu-238(SCK)	0.332	0.349	1.05	0.90	0.83
Pu-241(ITU)	1.48	1.51	1.02	0.96	0.96
Pu-241(SCK)	1.43	1.45	1.02	0.90	0.96
Am-241(ITU)	0.167	0.196	1.17	1.09	1.15
Am-241(SCK)	0.212	0.232	1.10	1.02	1.07
Am-242m(SCK)	8.10E-04	7.18E-04	0.89	1.60	0.81
Am-243(ITU)	0.236	0.227	0.96	0.97	0.98
Am-243(SCK)	0.210	0.227	1.08	1.10	1.10
Cm-242(SCK)	9.82E-04	9.21E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.82E-04	1.50	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.61E-03	0.98	0.97	0.97
Gd-155(SCK)	3.41E-03	3.80E-03	1.11	1.10	1.10
Eu-151(SCK)	3.70E-04	2.22E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.35E-02	1.02	0.87	0.97
Eu-154(SCK)	3.06E-02	3.31E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.24E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.03E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.01	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.31E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.30E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.89E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.68E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.67E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.118	0.92	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.39E-02	2.10	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.674	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.664	1.05	1.04	1.05

Table A.4.: Short-lived isotopes, library ENDF/B-VII.1.

A.4.3. Library JEFF-3.3T3

Isotope	True value (mg/g-fuel)	ALEPH (JEFF-3.3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.21	0.98	0.98	0.98
U-235(SCK)	5.33	5.21	0.98	0.97	0.98
U-236(ITU)	4.99	4.961	0.99	0.99	1.00
U-236(SCK)	4.98	4.961	1.00	0.99	1.00
U-238(ITU)	817.0	813.18	1.00	0.99	0.99
U-238(SCK)	816.0	813.18	1.00	0.99	1.00
Pu-239(SCK)	5.12	5.139	1.00	0.97	0.97
Pu-240(SCK)	2.50	2.55	1.02	1.01	1.00
Pu-242(ITU)	0.895	0.901	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.901	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	5.20E-05	0.32	0.60	0.43
Np-237(SCK)	0.715	0.657	0.92	0.88	0.83
Cm-245(ITU)	1.02E-02	1.01E-02	0.99	0.72	0.72
Cm-245(SCK)	8.54E-03	1.01E-02	1.18	0.86	0.86
Cm-246(SCK)	1.27E-03	1.25E-03	0.99	0.78	0.77
Eu-153(ITU)	0.162	0.153	0.94	1.05	1.01
Eu-153(SCK)	0.165	0.153	0.93	1.03	0.99
Cs-133(ITU)	1.47	1.41	0.96	0.98	1.00
Cs-133(SCK)	1.39	1.41	1.01	1.04	1.06
Cs-135(ITU)	0.424	0.387	0.91	0.91	0.94
Cs-135(SCK)	0.405	0.387	0.96	0.96	0.98
Sm-148(ITU)	0.231	0.317	1.37	0.89	0.91
Sm-148(SCK)	0.224	0.317	1.41	0.92	0.94
Sm-149(SCK)	2.96E-03	2.42E-03	0.82	1.13	1.07
Sm-150(ITU)	0.394	0.314	0.80	1.07	1.08
Sm-150(SCK)	0.393	0.314	0.80	1.08	1.09
Sm-152(ITU)	0.115	0.113	0.98	1.12	1.12
Sm-152(SCK)	0.118	0.113	0.96	1.09	1.09
Sm-154(ITU)	4.69E-02	5.64E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.64E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.037	1.01	1.03	1.02
Nd-143(SCK)	0.945	0.935	0.99	0.99	1.00
Nd-144(SCK)	1.89	1.81	0.96	0.99	1.00
Nd-145(SCK)	0.872	0.845	0.97	1.00	0.99
Nd-146(SCK)	1.01	0.986	0.98	0.99	1.00
Nd-148(SCK)	0.517	0.506	0.98	1.01	1.00
Nd-150(ITU)	0.254	0.242	0.95	0.98	0.98
Nd-150(SCK)	0.252	0.242	0.96	1.00	0.98
I-129(SCK)	0.236	0.234	0.99	1.07	0.91
Mo-95(ITU)	1.030	0.984	0.96	0.98	0.98
Mo-95(SCK)	1.147	0.984	0.86	0.88	0.88
Tc-99(ITU)	0.977	1.012	1.04	1.07	1.07
Tc-99(SCK)	1.143	1.012	0.89	0.92	0.91
Ru-101(ITU)	1.072	1.038	0.97	0.98	0.99
Ru-101(SCK)	1.221	1.038	0.85	0.86	0.87
Rh-103(ITU)	0.471	0.581	1.23	1.16	1.26
Rh-103(SCK)	0.494	0.581	1.18	1.10	1.20
Ag-109(SCK)	0.1053	0.1191	1.13	1.00	1.05

Table A.5.: Long-lived isotopes, library JEFF-3.3T3.

Isotope	True value (mg/g-fuel)	ALEPH (JEFF-3.3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.172	1.39	1.39	1.43
U-234(SCK)	0.124	0.174	1.40	1.40	1.44
Pu-238(ITU)	0.328	0.365	1.11	0.91	0.84
Pu-238(SCK)	0.332	0.364	1.10	0.90	0.83
Pu-241(ITU)	1.48	1.48	1.00	0.96	0.96
Pu-241(SCK)	1.43	1.43	1.00	0.90	0.96
Am-241(ITU)	0.167	0.188	1.13	1.09	1.15
Am-241(SCK)	0.212	0.224	1.06	1.02	1.07
Am-242m(SCK)	8.10E-04	1.96E-05	0.02	1.60	0.81
Am-243(ITU)	0.236	0.230	0.98	0.97	0.98
Am-243(SCK)	0.210	0.230	1.10	1.10	1.10
Cm-242(SCK)	9.82E-04	1.06E-03	1.08	0.83	0.82
Cm-243(SCK)	5.23E-04	9.07E-04	1.73	1.28	1.01
Cm-244(ITU)	0.136	0.118	0.87	0.74	0.72
Cm-244(SCK)	0.114	0.117	1.03	0.88	0.86
Gd-155(ITU)	3.67E-03	3.39E-03	0.92	0.97	0.97
Gd-155(SCK)	3.41E-03	3.57E-03	1.05	1.10	1.10
Eu-151(SCK)	3.70E-04	2.01E-04	0.54	0.61	0.58
Eu-154(ITU)	3.27E-02	3.12E-02	0.95	0.87	0.97
Eu-154(SCK)	3.06E-02	3.08E-02	1.01	0.92	1.02
Eu-155(ITU)	1.09E-02	8.69E-03	0.80	0.88	0.83
Eu-155(SCK)	9.97E-03	8.49E-03	0.85	0.96	0.88
Sm-147(ITU)	0.163	0.160	0.98	1.02	1.06
Sm-147(SCK)	0.173	0.178	1.03	1.07	1.10
Sm-151(ITU)	1.29E-02	1.19E-02	0.92	1.03	0.98
Sm-151(SCK)	1.27E-02	1.18E-02	0.93	1.04	0.98
Pm-147(ITU)	0.141	0.120	0.85	0.89	0.88
Pm-147(SCK)	8.25E-02	9.66E-02	1.17	1.22	1.21
Ce-144(ITU)	7.13E-02	7.40E-02	1.04	1.05	1.02
Ce-144(SCK)	6.32E-02	6.43E-02	1.02	1.03	1.00
Cs-134(ITU)	0.128	0.115	0.90	0.91	0.87
Cs-134(SCK)	0.109	0.109	1.00	1.02	0.97
Cs-137(ITU)	1.58	1.56	0.99	1.00	1.01
Cs-137(SCK)	1.59	1.56	0.98	0.99	1.00
Sb-125(SCK)	6.61E-03	1.58E-02	2.40	2.87	1.66
Ru-106(SCK)	0.256	0.217	0.85	0.87	0.86
Sr-90(ITU)	0.645	0.640	0.99	1.03	1.04
Sr-90(SCK)	0.630	0.630	1.00	1.04	1.05

Table A.6.: Short-lived isotopes, library JEFF-3.3T3.

A.5. Selection of interpolation scheme for fission product yields

A.5.1. Library JEFF-3.3T3: Transition between thermal and fast parts of the spectrum from 1e-3 to 1e-5 [Mev]

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.229	0.98	0.98	0.98
U-235(SCK)	5.33	5.229	0.98	0.97	0.98
U-236(ITU)	4.99	4.946	0.99	0.99	1.00
U-236(SCK)	4.98	4.946	0.99	0.99	1.00
U-238(ITU)	817.0	811.90	0.99	0.99	0.99
U-238(SCK)	816.0	811.90	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.125	1.00	0.97	0.97
Pu-240(SCK)	2.50	2.57	1.03	1.01	1.00
Pu-242(ITU)	0.895	0.897	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.897	1.00	0.98	0.96
Pu-244(SCK)	1.63E-04	5.15E-05	0.32	0.60	0.43
Np-237(SCK)	0.715	0.658	0.92	0.88	0.83
Cm-245(ITU)	1.02E-02	9.91E-03	0.97	0.72	0.72
Cm-245(SCK)	8.54E-03	9.91E-03	1.16	0.86	0.86
Cm-246(SCK)	1.27E-03	1.21E-03	0.95	0.78	0.77
Eu-153(ITU)	0.162	0.158	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.158	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.45	0.99	0.98	1.00
Cs-133(SCK)	1.39	1.45	1.05	1.04	1.06
Cs-135(ITU)	0.424	0.401	0.94	0.91	0.94
Cs-135(SCK)	0.405	0.401	0.99	0.96	0.98
Sm-148(ITU)	0.231	0.327	1.41	0.89	0.91
Sm-148(SCK)	0.224	0.327	1.46	0.92	0.94
Sm-149(SCK)	2.96E-03	2.51E-03	0.85	1.13	1.07
Sm-150(ITU)	0.394	0.325	0.82	1.07	1.08
Sm-150(SCK)	0.393	0.325	0.83	1.08	1.09
Sm-152(ITU)	0.115	0.117	1.02	1.12	1.12
Sm-152(SCK)	0.118	0.117	0.99	1.09	1.09
Sm-154(ITU)	4.69E-02	5.79E-02	1.23	1.19	1.17
Sm-154(SCK)	5.06E-02	5.79E-02	1.14	1.10	1.09
Nd-142(SCK)	0.037	0.039	1.05	1.03	1.02
Nd-143(SCK)	0.945	0.969	1.03	0.99	1.00
Nd-144(SCK)	1.89	1.88	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.875	1.00	1.00	0.99
Nd-146(SCK)	1.01	1.02	1.01	0.99	1.00
Nd-148(SCK)	0.517	0.526	1.02	1.01	1.00
Nd-150(ITU)	0.254	0.251	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.251	1.00	1.00	0.98
I-129(SCK)	0.236	0.238	1.01	1.07	0.91
Mo-95(ITU)	1.030	1.017	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.017	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.044	1.07	1.07	1.07
Tc-99(SCK)	1.143	1.044	0.91	0.92	0.91
Ru-101(ITU)	1.072	1.072	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.072	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.602	1.28	1.16	1.26
Rh-103(SCK)	0.494	0.602	1.22	1.10	1.20
Ag-109(SCK)	0.1053	0.1201	1.14	1.00	1.05

Table A.7.: Long-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-3 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.172	1.39	1.39	1.43
U-234(SCK)	0.124	0.174	1.41	1.40	1.44
Pu-238(ITU)	0.328	0.366	1.11	0.91	0.84
Pu-238(SCK)	0.332	0.365	1.10	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.00	0.90	0.96
Am-241(ITU)	0.167	0.189	1.13	1.09	1.15
Am-241(SCK)	0.212	0.225	1.06	1.02	1.07
Am-242m(SCK)	8.10E-04	1.96E-05	0.02	1.60	0.81
Am-243(ITU)	0.236	0.230	0.98	0.97	0.98
Am-243(SCK)	0.210	0.230	1.10	1.10	1.10
Cm-242(SCK)	9.82E-04	1.05E-03	1.07	0.83	0.82
Cm-243(SCK)	5.23E-04	8.86E-04	1.69	1.28	1.01
Cm-244(ITU)	0.136	0.116	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.116	1.02	0.88	0.86
Gd-155(ITU)	3.67E-03	3.49E-03	0.95	0.97	0.97
Gd-155(SCK)	3.41E-03	3.68E-03	1.08	1.10	1.10
Eu-151(SCK)	3.70E-04	2.09E-04	0.56	0.61	0.58
Eu-154(ITU)	3.27E-02	3.20E-02	0.98	0.87	0.97
Eu-154(SCK)	3.06E-02	3.16E-02	1.03	0.92	1.02
Eu-155(ITU)	1.09E-02	8.95E-03	0.82	0.88	0.83
Eu-155(SCK)	9.97E-03	8.74E-03	0.88	0.96	0.88
Sm-147(ITU)	0.163	0.166	1.02	1.02	1.06
Sm-147(SCK)	0.173	0.185	1.07	1.07	1.10
Sm-151(ITU)	1.29E-02	1.23E-02	0.95	1.03	0.98
Sm-151(SCK)	1.27E-02	1.22E-02	0.96	1.04	0.98
Pm-147(ITU)	0.141	0.125	0.89	0.89	0.88
Pm-147(SCK)	8.25E-02	0.100	1.22	1.22	1.21
Ce-144(ITU)	7.13E-02	7.66E-02	1.07	1.05	1.02
Ce-144(SCK)	6.32E-02	6.65E-02	1.05	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.04	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.29E-02	1.96	2.87	1.66
Ru-106(SCK)	0.256	0.222	0.87	0.87	0.86
Sr-90(ITU)	0.645	0.662	1.03	1.03	1.04
Sr-90(SCK)	0.630	0.652	1.04	1.04	1.05

Table A.8.: Short-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-3 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-4) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.234	0.99	0.98	0.98
U-235(SCK)	5.33	5.234	0.98	0.97	0.98
U-236(ITU)	4.99	4.944	0.99	0.99	1.00
U-236(SCK)	4.98	4.944	0.99	0.99	1.00
U-238(ITU)	817.0	811.87	0.99	0.99	0.99
U-238(SCK)	816.0	811.87	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.14	1.00	0.97	0.97
Pu-240(SCK)	2.50	2.57	1.03	1.01	1.00
Pu-242(ITU)	0.895	0.899	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.899	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	5.12E-05	0.31	0.60	0.43
Np-237(SCK)	0.715	0.661	0.92	0.88	0.83
Cm-245(ITU)	1.02E-02	1.01E-02	0.99	0.72	0.72
Cm-245(SCK)	8.54E-03	1.01E-02	1.18	0.86	0.86
Cm-246(SCK)	1.27E-03	1.21E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.45	0.99	0.98	1.00
Cs-133(SCK)	1.39	1.45	1.05	1.04	1.06
Cs-135(ITU)	0.424	0.401	0.94	0.91	0.94
Cs-135(SCK)	0.405	0.401	0.99	0.96	0.98
Sm-148(ITU)	0.231	0.327	1.42	0.89	0.91
Sm-148(SCK)	0.224	0.327	1.46	0.92	0.94
Sm-149(SCK)	2.96E-03	2.52E-03	0.85	1.13	1.07
Sm-150(ITU)	0.394	0.325	0.83	1.07	1.08
Sm-150(SCK)	0.393	0.325	0.83	1.08	1.09
Sm-152(ITU)	0.115	0.115	1.00	1.12	1.12
Sm-152(SCK)	0.118	0.115	0.98	1.09	1.09
Sm-154(ITU)	4.69E-02	5.81E-02	1.24	1.19	1.17
Sm-154(SCK)	5.06E-02	5.81E-02	1.15	1.10	1.09
Nd-142(SCK)	0.037	0.039	1.04	1.03	1.02
Nd-143(SCK)	0.945	0.968	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.875	1.00	1.00	0.99
Nd-146(SCK)	1.01	1.02	1.01	0.99	1.00
Nd-148(SCK)	0.517	0.526	1.02	1.01	1.00
Nd-150(ITU)	0.254	0.251	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.251	1.00	1.00	0.98
I-129(SCK)	0.236	0.239	1.01	1.07	0.91
Mo-95(ITU)	1.030	1.018	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.018	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.043	1.07	1.07	1.07
Tc-99(SCK)	1.143	1.043	0.91	0.92	0.91
Ru-101(ITU)	1.072	1.073	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.073	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.601	1.28	1.16	1.26
Rh-103(SCK)	0.494	0.601	1.22	1.10	1.20
Ag-109(SCK)	0.1053	0.1199	1.14	1.00	1.05

Table A.9.: Long-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-4 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-4) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.171	1.38	1.39	1.43
U-234(SCK)	0.124	0.173	1.39	1.40	1.44
Pu-238(ITU)	0.328	0.367	1.12	0.91	0.84
Pu-238(SCK)	0.332	0.367	1.10	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.190	1.14	1.09	1.15
Am-241(SCK)	0.212	0.226	1.06	1.02	1.07
Am-242m(SCK)	8.10E-04	1.98E-05	0.02	1.60	0.81
Am-243(ITU)	0.236	0.229	0.97	0.97	0.98
Am-243(SCK)	0.210	0.229	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	1.05E-03	1.07	0.83	0.82
Cm-243(SCK)	5.23E-04	8.93E-04	1.71	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.84	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.54E-03	0.97	0.97	0.97
Gd-155(SCK)	3.41E-03	3.73E-03	1.09	1.10	1.10
Eu-151(SCK)	3.70E-04	2.08E-04	0.56	0.61	0.58
Eu-154(ITU)	3.27E-02	3.20E-02	0.98	0.87	0.97
Eu-154(SCK)	3.06E-02	3.18E-02	1.04	0.92	1.02
Eu-155(ITU)	1.09E-02	9.08E-03	0.83	0.88	0.83
Eu-155(SCK)	9.97E-03	8.87E-03	0.89	0.96	0.88
Sm-147(ITU)	0.163	0.165	1.02	1.02	1.06
Sm-147(SCK)	0.173	0.184	1.06	1.07	1.10
Sm-151(ITU)	1.29E-02	1.23E-02	0.95	1.03	0.98
Sm-151(SCK)	1.27E-02	1.22E-02	0.96	1.04	0.98
Pm-147(ITU)	0.141	0.125	0.89	0.89	0.88
Pm-147(SCK)	8.25E-02	0.100	1.21	1.22	1.21
Ce-144(ITU)	7.13E-02	7.65E-02	1.07	1.05	1.02
Ce-144(SCK)	6.32E-02	6.64E-02	1.05	1.03	1.00
Cs-134(ITU)	0.128	0.118	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.30E-02	1.97	2.87	1.66
Ru-106(SCK)	0.256	0.222	0.87	0.87	0.86
Sr-90(ITU)	0.645	0.661	1.02	1.03	1.04
Sr-90(SCK)	0.630	0.651	1.03	1.04	1.05

Table A.10.: Short-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-4 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-5) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.223	0.99	0.98	0.98
U-235(SCK)	5.33	5.223	0.98	0.97	0.98
U-236(ITU)	4.99	4.952	0.99	0.99	1.00
U-236(SCK)	4.98	4.952	0.99	0.99	1.00
U-238(ITU)	817.0	811.92	0.99	0.99	0.99
U-238(SCK)	816.0	811.92	1.00	0.99	1.00
Pu-239(SCK)	5.12	5.13	1.00	0.97	0.97
Pu-240(SCK)	2.50	2.55	1.02	1.01	1.00
Pu-242(ITU)	0.895	0.902	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.902	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	5.14E-05	0.32	0.60	0.43
Np-237(SCK)	0.715	0.652	0.91	0.88	0.83
Cm-245(ITU)	1.02E-02	9.91E-03	0.97	0.72	0.72
Cm-245(SCK)	8.54E-03	9.91E-03	1.16	0.86	0.86
Cm-246(SCK)	1.27E-03	1.22E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.45	0.99	0.98	1.00
Cs-133(SCK)	1.39	1.45	1.05	1.04	1.06
Cs-135(ITU)	0.424	0.400	0.94	0.91	0.94
Cs-135(SCK)	0.405	0.400	0.99	0.96	0.98
Sm-148(ITU)	0.231	0.326	1.41	0.89	0.91
Sm-148(SCK)	0.224	0.326	1.46	0.92	0.94
Sm-149(SCK)	2.96E-03	2.50E-03	0.85	1.13	1.07
Sm-150(ITU)	0.394	0.325	0.82	1.07	1.08
Sm-150(SCK)	0.393	0.325	0.83	1.08	1.09
Sm-152(ITU)	0.115	0.117	1.01	1.12	1.12
Sm-152(SCK)	0.118	0.117	0.99	1.09	1.09
Sm-154(ITU)	4.69E-02	5.84E-02	1.25	1.19	1.17
Sm-154(SCK)	5.06E-02	5.84E-02	1.15	1.10	1.09
Nd-142(SCK)	0.037	0.039	1.04	1.03	1.02
Nd-143(SCK)	0.945	0.964	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.873	1.00	1.00	0.99
Nd-146(SCK)	1.01	1.02	1.01	0.99	1.00
Nd-148(SCK)	0.517	0.526	1.02	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.242	1.03	1.07	0.91
Mo-95(ITU)	1.030	1.016	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.016	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.039	1.06	1.07	1.07
Tc-99(SCK)	1.143	1.039	0.91	0.92	0.91
Ru-101(ITU)	1.072	1.075	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.075	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.601	1.28	1.16	1.26
Rh-103(SCK)	0.494	0.601	1.22	1.10	1.20
Ag-109(SCK)	0.1053	0.1190	1.13	1.00	1.05

Table A.11.: Long-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-5 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-5) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.171	1.38	1.39	1.43
U-234(SCK)	0.124	0.173	1.39	1.40	1.44
Pu-238(ITU)	0.328	0.365	1.11	0.91	0.84
Pu-238(SCK)	0.332	0.365	1.10	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.190	1.14	1.09	1.15
Am-241(SCK)	0.212	0.225	1.06	1.02	1.07
Am-242m(SCK)	8.10E-04	1.98E-05	0.02	1.60	0.81
Am-243(ITU)	0.236	0.229	0.97	0.97	0.98
Am-243(SCK)	0.210	0.229	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	1.05E-03	1.07	0.83	0.82
Cm-243(SCK)	5.23E-04	9.05E-04	1.73	1.28	1.01
Cm-244(ITU)	0.136	0.116	0.86	0.74	0.72
Cm-244(SCK)	0.114	0.116	1.02	0.88	0.86
Gd-155(ITU)	3.67E-03	3.50E-03	0.95	0.97	0.97
Gd-155(SCK)	3.41E-03	3.69E-03	1.08	1.10	1.10
Eu-151(SCK)	3.70E-04	2.08E-04	0.56	0.61	0.58
Eu-154(ITU)	3.27E-02	3.21E-02	0.98	0.87	0.97
Eu-154(SCK)	3.06E-02	3.17E-02	1.04	0.92	1.02
Eu-155(ITU)	1.09E-02	8.97E-03	0.82	0.88	0.83
Eu-155(SCK)	9.97E-03	8.76E-03	0.88	0.96	0.88
Sm-147(ITU)	0.163	0.165	1.01	1.02	1.06
Sm-147(SCK)	0.173	0.184	1.06	1.07	1.10
Sm-151(ITU)	1.29E-02	1.22E-02	0.95	1.03	0.98
Sm-151(SCK)	1.27E-02	1.22E-02	0.96	1.04	0.98
Pm-147(ITU)	0.141	0.125	0.88	0.89	0.88
Pm-147(SCK)	8.25E-02	0.100	1.21	1.22	1.21
Ce-144(ITU)	7.13E-02	7.63E-02	1.07	1.05	1.02
Ce-144(SCK)	6.32E-02	6.62E-02	1.05	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.60	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.32E-02	1.99	2.87	1.66
Ru-106(SCK)	0.256	0.222	0.87	0.87	0.86
Sr-90(ITU)	0.645	0.658	1.02	1.03	1.04
Sr-90(SCK)	0.630	0.648	1.03	1.04	1.05

Table A.12.: Short-lived isotopes, library JEFF-3.3T3 and FPY transition = 1e-5 [MeV].

A.5.2. Library ENDF/B-VII.1: Transition between thermal and fast parts of the spectrum from 1e-1 to 1e-5 [Mev]

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-1) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.463	1.03	0.98	0.98
U-235(SCK)	5.33	5.463	1.02	0.97	0.98
U-236(ITU)	4.99	4.948	0.99	0.99	1.00
U-236(SCK)	4.98	4.948	0.99	0.99	1.00
U-238(ITU)	817.0	811.57	0.99	0.99	0.99
U-238(SCK)	816.0	811.57	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.21	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.51	1.01	1.01	1.00
Pu-242(ITU)	0.895	0.899	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.899	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	1.00E-04	0.61	0.60	0.43
Np-237(SCK)	0.715	0.643	0.90	0.88	0.83
Cm-245(ITU)	1.02E-02	9.90E-03	0.97	0.72	0.72
Cm-245(SCK)	8.54E-03	9.90E-03	1.16	0.86	0.86
Cm-246(SCK)	1.27E-03	1.21E-03	0.95	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.00	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.421	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.421	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.258	1.12	0.89	0.91
Sm-148(SCK)	0.224	0.258	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.14E-03	1.06	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.121	1.05	1.12	1.12
Sm-152(SCK)	0.118	0.121	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.966	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.88	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.882	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.210	0.89	1.07	0.91
Mo-95(ITU)	1.030	1.016	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.016	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.051	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.051	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.611	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.611	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0816	0.77	1.00	1.05

Table A.13.: Long-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-1 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-1) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.172	1.38	1.39	1.43
U-234(SCK)	0.124	0.174	1.40	1.40	1.44
Pu-238(ITU)	0.328	0.351	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.350	1.05	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.195	1.17	1.09	1.15
Am-241(SCK)	0.212	0.231	1.09	1.02	1.07
Am-242m(SCK)	8.10E-04	7.24E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.230	0.97	0.97	0.98
Am-243(SCK)	0.210	0.230	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	9.25E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.75E-04	1.48	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.59E-03	0.98	0.97	0.97
Gd-155(SCK)	3.41E-03	3.78E-03	1.11	1.10	1.10
Eu-151(SCK)	3.70E-04	2.23E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.35E-02	1.03	0.87	0.97
Eu-154(SCK)	3.06E-02	3.31E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.20E-03	0.84	0.88	0.83
Eu-155(SCK)	9.97E-03	8.99E-03	0.90	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.00	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.85E-02	1.19	1.22	1.21
Ce-144(ITU)	7.13E-02	7.70E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.04	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.07E-02	1.63	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.673	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.663	1.05	1.04	1.05

Table A.14.: Short-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-1 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-2) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.473	1.03	0.98	0.98
U-235(SCK)	5.33	5.474	1.03	0.97	0.98
U-236(ITU)	4.99	4.950	0.99	0.99	1.00
U-236(SCK)	4.98	4.950	0.99	0.99	1.00
U-238(ITU)	817.0	811.55	0.99	0.99	0.99
U-238(SCK)	816.0	811.55	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.22	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.51	1.00	1.01	1.00
Pu-242(ITU)	0.895	0.905	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.905	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	9.82E-05	0.60	0.60	0.43
Np-237(SCK)	0.715	0.642	0.90	0.88	0.83
Cm-245(ITU)	1.02E-02	9.64E-03	0.95	0.72	0.72
Cm-245(SCK)	8.54E-03	9.64E-03	1.13	0.86	0.86
Cm-246(SCK)	1.27E-03	1.18E-03	0.93	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.00	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.421	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.421	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.257	1.11	0.89	0.91
Sm-148(SCK)	0.224	0.257	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.13E-03	1.06	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.121	1.05	1.12	1.12
Sm-152(SCK)	0.118	0.121	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.967	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.88	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.882	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.211	0.89	1.07	0.91
Mo-95(ITU)	1.030	1.015	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.015	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.050	1.07	1.07	1.07
Tc-99(SCK)	1.143	1.050	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.610	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.610	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0818	0.78	1.00	1.05

Table A.15.: Long-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-2 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-2) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.171	1.38	1.39	1.43
U-234(SCK)	0.124	0.173	1.40	1.40	1.44
Pu-238(ITU)	0.328	0.351	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.350	1.06	0.90	0.83
Pu-241(ITU)	1.48	1.50	1.02	0.96	0.96
Pu-241(SCK)	1.43	1.45	1.02	0.90	0.96
Am-241(ITU)	0.167	0.196	1.18	1.09	1.15
Am-241(SCK)	0.212	0.232	1.10	1.02	1.07
Am-242m(SCK)	8.10E-04	7.26E-05	0.90	1.60	0.81
Am-243(ITU)	0.236	0.227	0.96	0.97	0.98
Am-243(SCK)	0.210	0.227	1.08	1.10	1.10
Cm-242(SCK)	9.82E-04	9.27E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.73E-04	1.48	1.28	1.01
Cm-244(ITU)	0.136	0.113	0.83	0.74	0.72
Cm-244(SCK)	0.114	0.113	0.99	0.88	0.86
Gd-155(ITU)	3.67E-03	3.62E-03	0.99	0.97	0.97
Gd-155(SCK)	3.41E-03	3.81E-03	1.12	1.10	1.10
Eu-151(SCK)	3.70E-04	2.24E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.34E-02	1.02	0.87	0.97
Eu-154(SCK)	3.06E-02	3.30E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.27E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.06E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.01	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.88E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.69E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.08E-02	1.63	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.673	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.663	1.05	1.04	1.05

Table A.16.: Short-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-2 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.457	1.03	0.98	0.98
U-235(SCK)	5.33	5.457	1.02	0.97	0.98
U-236(ITU)	4.99	4.959	0.99	0.99	1.00
U-236(SCK)	4.98	4.959	1.00	0.99	1.00
U-238(ITU)	817.0	811.55	0.99	0.99	0.99
U-238(SCK)	816.0	811.55	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.23	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.53	1.01	1.01	1.00
Pu-242(ITU)	0.895	0.899	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.899	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	9.96E-05	0.61	0.60	0.43
Np-237(SCK)	0.715	0.639	0.89	0.88	0.83
Cm-245(ITU)	1.02E-02	1.00E-02	0.98	0.72	0.72
Cm-245(SCK)	8.54E-03	1.00E-02	1.17	0.86	0.86
Cm-246(SCK)	1.27E-03	1.22E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.00	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.421	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.421	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.257	1.11	0.89	0.91
Sm-148(SCK)	0.224	0.257	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.10E-03	1.05	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.119	1.04	1.12	1.12
Sm-152(SCK)	0.118	0.119	1.01	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.966	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.88	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.881	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.211	0.89	1.07	0.91
Mo-95(ITU)	1.030	1.016	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.016	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.051	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.051	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.610	1.29	1.16	1.26
Rh-103(SCK)	0.494	0.610	1.23	1.10	1.20
Ag-109(SCK)	0.1053	0.0816	0.78	1.00	1.05

Table A.17.: Long-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-3 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-3) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.170	1.37	1.39	1.43
U-234(SCK)	0.124	0.172	1.39	1.40	1.44
Pu-238(ITU)	0.328	0.350	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.349	1.06	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.195	1.17	1.09	1.15
Am-241(SCK)	0.212	0.231	1.09	1.02	1.07
Am-242m(SCK)	8.10E-04	7.18E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.227	0.96	0.97	0.98
Am-243(SCK)	0.210	0.227	1.08	1.10	1.10
Cm-242(SCK)	9.82E-04	9.22E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.67E-04	1.47	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.64E-03	0.99	0.97	0.97
Gd-155(SCK)	3.41E-03	3.83E-03	1.12	1.10	1.10
Eu-151(SCK)	3.70E-04	2.23E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.36E-02	1.03	0.87	0.97
Eu-154(SCK)	3.06E-02	3.31E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.32E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.10E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.00	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.89E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.69E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.08E-02	1.64	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.673	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.663	1.05	1.04	1.05

Table A.18.: Short-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-3 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-4) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.467	1.03	0.98	0.98
U-235(SCK)	5.33	5.467	1.03	0.97	0.98
U-236(ITU)	4.99	4.948	0.99	0.99	1.00
U-236(SCK)	4.98	4.949	0.99	0.99	1.00
U-238(ITU)	817.0	811.53	0.99	0.99	0.99
U-238(SCK)	816.0	811.53	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.23	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.55	1.02	1.01	1.00
Pu-242(ITU)	0.895	0.897	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.897	1.00	0.98	0.96
Pu-244(SCK)	1.63E-04	9.96E-05	0.61	0.60	0.43
Np-237(SCK)	0.715	0.641	0.90	0.88	0.83
Cm-245(ITU)	1.02E-02	1.00E-02	0.98	0.72	0.72
Cm-245(SCK)	8.54E-03	1.00E-02	1.17	0.86	0.86
Cm-246(SCK)	1.27E-03	1.22E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.01	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.420	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.420	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.257	1.11	0.89	0.91
Sm-148(SCK)	0.224	0.257	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.13E-03	1.06	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.98	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.120	1.04	1.12	1.12
Sm-152(SCK)	0.118	0.120	1.01	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.18	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.966	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.880	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.212	0.90	1.07	0.91
Mo-95(ITU)	1.030	1.016	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.016	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.051	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.051	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.612	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.612	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0817	0.78	1.00	1.05

Table A.19.: Long-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-4 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-4) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.172	1.39	1.39	1.43
U-234(SCK)	0.124	0.172	1.40	1.40	1.44
Pu-238(ITU)	0.328	0.349	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.349	1.05	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.00	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.00	0.90	0.96
Am-241(ITU)	0.167	0.194	1.16	1.09	1.15
Am-241(SCK)	0.212	0.230	1.08	1.02	1.07
Am-242m(SCK)	8.10E-04	7.22E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.228	0.97	0.97	0.98
Am-243(SCK)	0.210	0.228	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	9.21E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.71E-04	1.47	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.65E-03	0.99	0.97	0.97
Gd-155(SCK)	3.41E-03	3.84E-03	1.13	1.10	1.10
Eu-151(SCK)	3.70E-04	2.24E-04	0.61	0.61	0.58
Eu-154(ITU)	3.27E-02	3.37E-02	1.03	0.87	0.97
Eu-154(SCK)	3.06E-02	3.32E-02	1.09	0.92	1.02
Eu-155(ITU)	1.09E-02	9.34E-03	0.86	0.88	0.83
Eu-155(SCK)	9.97E-03	9.13E-03	0.92	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.00	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.86E-02	1.19	1.22	1.21
Ce-144(ITU)	7.13E-02	7.69E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.118	0.92	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.02	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.10E-02	1.66	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.672	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.662	1.06	1.04	1.05

Table A.20.: Short-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-4 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-5) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.460	1.03	0.98	0.98
U-235(SCK)	5.33	5.460	1.02	0.97	0.98
U-236(ITU)	4.99	4.945	0.99	0.99	1.00
U-236(SCK)	4.98	4.945	0.99	0.99	1.00
U-238(ITU)	817.0	811.56	0.99	0.99	0.99
U-238(SCK)	816.0	811.56	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.22	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.54	1.01	1.01	1.00
Pu-242(ITU)	0.895	0.896	1.00	0.98	0.95
Pu-242(SCK)	0.893	0.896	1.00	0.98	0.96
Pu-244(SCK)	1.63E-04	1.00E-04	0.62	0.60	0.43
Np-237(SCK)	0.715	0.645	0.90	0.88	0.83
Cm-245(ITU)	1.02E-02	1.01E-02	0.99	0.72	0.72
Cm-245(SCK)	8.54E-03	1.01E-02	1.18	0.86	0.86
Cm-246(SCK)	1.27E-03	1.23E-03	0.97	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.47	1.00	0.98	1.00
Cs-133(SCK)	1.39	1.47	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.421	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.421	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.258	1.12	0.89	0.91
Sm-148(SCK)	0.224	0.258	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.12E-03	1.05	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.120	1.04	1.12	1.12
Sm-152(SCK)	0.118	0.120	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.964	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.880	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.253	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.253	1.00	1.00	0.98
I-129(SCK)	0.236	0.215	0.91	1.07	0.91
Mo-95(ITU)	1.030	1.014	0.98	0.98	0.98
Mo-95(SCK)	1.147	1.014	0.88	0.88	0.88
Tc-99(ITU)	0.977	1.049	1.07	1.07	1.07
Tc-99(SCK)	1.143	1.049	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.069	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.069	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.612	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.612	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0805	0.76	1.00	1.05

Table A.21.: Long-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-5 [MeV].

Isotope	True value (mg/g-fuel)	ALEPH (FPY:1e-5) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.170	1.37	1.39	1.43
U-234(SCK)	0.124	0.172	1.39	1.40	1.44
Pu-238(ITU)	0.328	0.352	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.351	1.06	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.00	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.00	0.90	0.96
Am-241(ITU)	0.167	0.194	1.16	1.09	1.15
Am-241(SCK)	0.212	0.230	1.08	1.02	1.07
Am-242m(SCK)	8.10E-04	7.20E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.229	0.97	0.97	0.98
Am-243(SCK)	0.210	0.229	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	9.22E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.73E-04	1.48	1.28	1.01
Cm-244(ITU)	0.136	0.116	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.116	1.02	0.88	0.86
Gd-155(ITU)	3.67E-03	3.60E-03	0.98	0.97	0.97
Gd-155(SCK)	3.41E-03	3.79E-03	1.11	1.10	1.10
Eu-151(SCK)	3.70E-04	2.23E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.35E-02	1.02	0.87	0.97
Eu-154(SCK)	3.06E-02	3.31E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.22E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.01E-03	0.90	0.96	0.88
Sm-147(ITU)	0.163	0.163	1.00	1.02	1.06
Sm-147(SCK)	0.173	0.181	1.04	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.122	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.77E-02	1.18	1.22	1.21
Ce-144(ITU)	7.13E-02	7.68E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.66E-02	1.05	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.04	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.14E-02	1.72	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.90	0.87	0.86
Sr-90(ITU)	0.645	0.670	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.660	1.05	1.04	1.05

Table A.22.: Short-lived isotopes, library ENDF/B-VII.1 and FPY transition = 1e-5 [MeV].

A.6. Predictor-corrector algorithm

Isotope	True value (mg/g-fuel)	ALEPH (pred-correc.) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.395	1.02	0.98	0.98
U-235(SCK)	5.33	5.396	1.01	0.97	0.98
U-236(ITU)	4.99	4.96	0.99	0.99	1.00
U-236(SCK)	4.98	4.96	1.00	0.99	1.00
U-238(ITU)	817.0	811.49	0.99	0.99	0.99
U-238(SCK)	816.0	811.49	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.23	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.54	1.02	1.01	1.00
Pu-242(ITU)	0.895	0.904	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.904	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	1.03E-04	0.63	0.60	0.43
Np-237(SCK)	0.715	0.642	0.90	0.88	0.83
Cm-245(ITU)	1.02E-02	1.03E-02	1.01	0.72	0.72
Cm-245(SCK)	8.54E-03	1.03E-02	1.21	0.86	0.86
Cm-246(SCK)	1.27E-03	1.27E-03	1.00	0.78	0.77
Eu-153(ITU)	0.162	0.159	0.98	1.05	1.01
Eu-153(SCK)	0.165	0.159	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.01	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.07	1.04	1.06
Cs-135(ITU)	0.424	0.422	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.422	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.259	1.12	0.89	0.91
Sm-148(SCK)	0.224	0.259	1.16	0.92	0.94
Sm-149(SCK)	2.96E-03	3.12E-03	1.05	1.13	1.07
Sm-150(ITU)	0.394	0.390	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.390	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.122	1.06	1.12	1.12
Sm-152(SCK)	0.118	0.122	1.03	1.09	1.09
Sm-154(ITU)	4.69E-02	5.66E-02	1.21	1.19	1.17
Sm-154(SCK)	5.06E-02	5.66E-02	1.12	1.10	1.09
Nd-142(SCK)	0.037	0.039	1.04	1.03	1.02
Nd-143(SCK)	0.945	0.968	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.89	1.00	0.99	1.00
Nd-145(SCK)	0.872	0.885	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.523	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.254	1.00	0.98	0.98
Nd-150(SCK)	0.252	0.254	1.01	1.00	0.98
I-129(SCK)	0.236	0.212	0.90	1.07	0.91
Mo-95(ITU)	1.030	1.020	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.020	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.055	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.055	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.072	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.072	0.88	0.86	0.87
Rh-103(ITU)	0.471	0.613	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.613	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0824	0.78	1.00	1.05

Table A.23.: Long-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and predictor-corrector algorithm.

Isotope	True value (mg/g-fuel)	ALEPH (pred-correc.) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.171	1.38	1.39	1.43
U-234(SCK)	0.124	0.173	1.39	1.40	1.44
Pu-238(ITU)	0.328	0.356	1.08	0.91	0.84
Pu-238(SCK)	0.332	0.355	1.07	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.194	1.16	1.09	1.15
Am-241(SCK)	0.212	0.230	1.09	1.02	1.07
Am-242m(SCK)	8.10E-04	7.20E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.235	1.00	0.97	0.98
Am-243(SCK)	0.210	0.235	1.12	1.10	1.10
Cm-242(SCK)	9.82E-04	9.29E-04	0.95	0.83	0.82
Cm-243(SCK)	5.23E-04	7.87E-04	1.50	1.28	1.01
Cm-244(ITU)	0.136	0.118	0.87	0.74	0.72
Cm-244(SCK)	0.114	0.118	1.04	0.88	0.86
Gd-155(ITU)	3.67E-03	3.61E-03	0.98	0.97	0.97
Gd-155(SCK)	3.41E-03	3.81E-03	1.12	1.10	1.10
Eu-151(SCK)	3.70E-04	2.24E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.36E-02	1.03	0.87	0.97
Eu-154(SCK)	3.06E-02	3.31E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.26E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.05E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.01	1.02	1.06
Sm-147(SCK)	0.173	0.183	1.06	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.124	0.88	0.89	0.88
Pm-147(SCK)	8.25E-02	9.91E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.73E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.71E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.119	0.93	0.91	0.87
Cs-134(SCK)	0.109	0.113	1.04	1.02	0.97
Cs-137(ITU)	1.58	1.62	1.03	1.00	1.01
Cs-137(SCK)	1.59	1.62	1.02	0.99	1.00
Sb-125(SCK)	6.61E-03	1.09E-02	1.65	2.87	1.66
Ru-106(SCK)	0.256	0.231	0.90	0.87	0.86
Sr-90(ITU)	0.645	0.675	1.05	1.03	1.04
Sr-90(SCK)	0.630	0.665	1.06	1.04	1.05

Table A.24.: Short-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and predictor-corrector algorithm.

A.7. Variable fuel temperature

Isotope	True value (mg/g-fuel)	ALEPH (var. fuel temp) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.514	1.04	0.98	0.98
U-235(SCK)	5.33	5.514	1.03	0.97	0.98
U-236(ITU)	4.99	4.96	0.99	0.99	1.00
U-236(SCK)	4.98	4.96	1.00	0.99	1.00
U-238(ITU)	817.0	811.68	0.99	0.99	0.99
U-238(SCK)	816.0	811.68	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.17	1.01	0.97	0.97
Pu-240(SCK)	2.50	2.55	1.02	1.01	1.00
Pu-242(ITU)	0.895	0.901	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.901	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	1.00E-04	0.62	0.60	0.43
Np-237(SCK)	0.715	0.634	0.89	0.88	0.83
Cm-245(ITU)	1.02E-02	1.02E-02	1.00	0.72	0.72
Cm-245(SCK)	8.54E-03	1.02E-02	1.19	0.86	0.86
Cm-246(SCK)	1.27E-03	1.22E-03	0.96	0.78	0.77
Eu-153(ITU)	0.162	0.158	0.97	1.05	1.01
Eu-153(SCK)	0.165	0.158	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.01	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.422	1.00	0.91	0.94
Cs-135(SCK)	0.405	0.422	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.257	1.11	0.89	0.91
Sm-148(SCK)	0.224	0.257	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.13E-03	1.06	1.13	1.07
Sm-150(ITU)	0.394	0.388	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.388	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.121	1.05	1.12	1.12
Sm-152(SCK)	0.118	0.121	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.968	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.87	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.881	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.211	0.90	1.07	0.91
Mo-95(ITU)	1.030	1.015	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.015	0.88	0.88	0.88
Tc-99(ITU)	0.977	1.051	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.051	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.612	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.612	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0819	0.78	1.00	1.05

Table A.25.: Long-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and variable fuel temperature.

Isotope	True value (mg/g-fuel)	ALEPH (var. fuel temp) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.173	1.40	1.39	1.43
U-234(SCK)	0.124	0.175	1.41	1.40	1.44
Pu-238(ITU)	0.328	0.348	1.06	0.91	0.84
Pu-238(SCK)	0.332	0.347	1.04	0.90	0.83
Pu-241(ITU)	1.48	1.49	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.44	1.01	0.90	0.96
Am-241(ITU)	0.167	0.195	1.17	1.09	1.15
Am-241(SCK)	0.212	0.231	1.09	1.02	1.07
Am-242m(SCK)	8.10E-04	7.25E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.225	0.95	0.97	0.98
Am-243(SCK)	0.210	0.225	1.07	1.10	1.10
Cm-242(SCK)	9.82E-04	9.30E-04	0.95	0.83	0.82
Cm-243(SCK)	5.23E-04	7.80E-04	1.49	1.28	1.01
Cm-244(ITU)	0.136	0.117	0.86	0.74	0.72
Cm-244(SCK)	0.114	0.117	1.03	0.88	0.86
Gd-155(ITU)	3.67E-03	3.61E-03	0.98	0.97	0.97
Gd-155(SCK)	3.41E-03	3.80E-03	1.11	1.10	1.10
Eu-151(SCK)	3.70E-04	2.23E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.34E-02	1.02	0.87	0.97
Eu-154(SCK)	3.06E-02	3.30E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.24E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.03E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.01	1.02	1.06
Sm-147(SCK)	0.173	0.183	1.06	1.07	1.10
Sm-151(ITU)	1.29E-02	1.32E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.87E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.69E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.118	0.92	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.08E-02	1.64	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.672	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.662	1.05	1.04	1.05

Table A.26.: Short-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and variable fuel temperature.

A.8. KCODE card: number of source neutrons per cycle doubled

Isotope	True value (mg/g-fuel)	ALEPH (NPS doubled) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-235(ITU)	5.31	5.467	1.03	0.98	0.98
U-235(SCK)	5.33	5.467	1.03	0.97	0.98
U-236(ITU)	4.99	4.96	0.99	0.99	1.00
U-236(SCK)	4.98	4.95	1.00	0.99	1.00
U-238(ITU)	817.0	811.73	0.99	0.99	0.99
U-238(SCK)	816.0	811.73	0.99	0.99	1.00
Pu-239(SCK)	5.12	5.20	1.02	0.97	0.97
Pu-240(SCK)	2.50	2.51	1.00	1.01	1.00
Pu-242(ITU)	0.895	0.901	1.01	0.98	0.95
Pu-242(SCK)	0.893	0.901	1.01	0.98	0.96
Pu-244(SCK)	1.63E-04	9.96E-05	0.61	0.60	0.43
Np-237(SCK)	0.715	0.634	0.89	0.88	0.83
Cm-245(ITU)	1.02E-02	9.97E-03	0.98	0.72	0.72
Cm-245(SCK)	8.54E-03	9.97E-03	1.17	0.86	0.86
Cm-246(SCK)	1.27E-03	1.21E-03	0.95	0.78	0.77
Eu-153(ITU)	0.162	0.158	0.97	1.05	1.01
Eu-153(SCK)	0.165	0.158	0.96	1.03	0.99
Cs-133(ITU)	1.47	1.48	1.01	0.98	1.00
Cs-133(SCK)	1.39	1.48	1.06	1.04	1.06
Cs-135(ITU)	0.424	0.421	0.99	0.91	0.94
Cs-135(SCK)	0.405	0.421	1.04	0.96	0.98
Sm-148(ITU)	0.231	0.258	1.12	0.89	0.91
Sm-148(SCK)	0.224	0.258	1.15	0.92	0.94
Sm-149(SCK)	2.96E-03	3.13E-03	1.06	1.13	1.07
Sm-150(ITU)	0.394	0.389	0.99	1.07	1.08
Sm-150(SCK)	0.393	0.389	0.99	1.08	1.09
Sm-152(ITU)	0.115	0.120	1.05	1.12	1.12
Sm-152(SCK)	0.118	0.120	1.02	1.09	1.09
Sm-154(ITU)	4.69E-02	5.62E-02	1.20	1.19	1.17
Sm-154(SCK)	5.06E-02	5.62E-02	1.11	1.10	1.09
Nd-142(SCK)	0.037	0.038	1.03	1.03	1.02
Nd-143(SCK)	0.945	0.967	1.02	0.99	1.00
Nd-144(SCK)	1.89	1.88	0.99	0.99	1.00
Nd-145(SCK)	0.872	0.882	1.01	1.00	0.99
Nd-146(SCK)	1.01	1.01	1.00	0.99	1.00
Nd-148(SCK)	0.517	0.520	1.01	1.01	1.00
Nd-150(ITU)	0.254	0.252	0.99	0.98	0.98
Nd-150(SCK)	0.252	0.252	1.00	1.00	0.98
I-129(SCK)	0.236	0.211	0.89	1.07	0.91
Mo-95(ITU)	1.030	1.015	0.99	0.98	0.98
Mo-95(SCK)	1.147	1.015	0.89	0.88	0.88
Tc-99(ITU)	0.977	1.051	1.08	1.07	1.07
Tc-99(SCK)	1.143	1.051	0.92	0.92	0.91
Ru-101(ITU)	1.072	1.067	1.00	0.98	0.99
Ru-101(SCK)	1.221	1.067	0.87	0.86	0.87
Rh-103(ITU)	0.471	0.611	1.30	1.16	1.26
Rh-103(SCK)	0.494	0.611	1.24	1.10	1.20
Ag-109(SCK)	0.1053	0.0816	0.78	1.00	1.05

Table A.27.: Long-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and number of particles simulated during each kcode doubled.

Isotope	True value (mg/g-fuel)	ALEPH (NPS doubled) (mg/g-fuel)	C/E (ALEPH)	C/E (MONT.)	C/E (SCALE)
U-234(ITU)	0.124	0.171	1.38	1.39	1.43
U-234(SCK)	0.124	0.173	1.40	1.40	1.44
Pu-238(ITU)	0.328	0.351	1.07	0.91	0.84
Pu-238(SCK)	0.332	0.350	1.05	0.90	0.83
Pu-241(ITU)	1.48	1.50	1.01	0.96	0.96
Pu-241(SCK)	1.43	1.45	1.01	0.90	0.96
Am-241(ITU)	0.167	0.195	1.17	1.09	1.15
Am-241(SCK)	0.212	0.231	1.09	1.02	1.07
Am-242m(SCK)	8.10E-04	7.22E-05	0.89	1.60	0.81
Am-243(ITU)	0.236	0.229	0.97	0.97	0.98
Am-243(SCK)	0.210	0.229	1.09	1.10	1.10
Cm-242(SCK)	9.82E-04	9.26E-04	0.94	0.83	0.82
Cm-243(SCK)	5.23E-04	7.74E-04	1.48	1.28	1.01
Cm-244(ITU)	0.136	0.115	0.85	0.74	0.72
Cm-244(SCK)	0.114	0.115	1.01	0.88	0.86
Gd-155(ITU)	3.67E-03	3.63E-03	0.99	0.97	0.97
Gd-155(SCK)	3.41E-03	3.83E-03	1.12	1.10	1.10
Eu-151(SCK)	3.70E-04	2.23E-04	0.60	0.61	0.58
Eu-154(ITU)	3.27E-02	3.34E-02	1.02	0.87	0.97
Eu-154(SCK)	3.06E-02	3.30E-02	1.08	0.92	1.02
Eu-155(ITU)	1.09E-02	9.31E-03	0.85	0.88	0.83
Eu-155(SCK)	9.97E-03	9.10E-03	0.91	0.96	0.88
Sm-147(ITU)	0.163	0.164	1.00	1.02	1.06
Sm-147(SCK)	0.173	0.182	1.05	1.07	1.10
Sm-151(ITU)	1.29E-02	1.31E-02	1.02	1.03	0.98
Sm-151(SCK)	1.27E-02	1.31E-02	1.03	1.04	0.98
Pm-147(ITU)	0.141	0.123	0.87	0.89	0.88
Pm-147(SCK)	8.25E-02	9.87E-02	1.20	1.22	1.21
Ce-144(ITU)	7.13E-02	7.69E-02	1.08	1.05	1.02
Ce-144(SCK)	6.32E-02	6.68E-02	1.06	1.03	1.00
Cs-134(ITU)	0.128	0.118	0.92	0.91	0.87
Cs-134(SCK)	0.109	0.112	1.03	1.02	0.97
Cs-137(ITU)	1.58	1.61	1.02	1.00	1.01
Cs-137(SCK)	1.59	1.61	1.01	0.99	1.00
Sb-125(SCK)	6.61E-03	1.08E-02	1.64	2.87	1.66
Ru-106(SCK)	0.256	0.229	0.89	0.87	0.86
Sr-90(ITU)	0.645	0.673	1.04	1.03	1.04
Sr-90(SCK)	0.630	0.663	1.05	1.04	1.05

Table A.28.: Short-lived isotopes, library ENDF/B-VII.1, FPY transition = 1e-3 [MeV] and number of particles simulated during each kcode doubled.

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