Calculation method based on CASMO/SIMULATE for isotopic concentrations of fuel samples irradiated in Ringhals PWR

Tariq Zuwak
Abstract

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This is a M. Eng. degree project at Uppsala University carried out at Vattenfall Nuclear Fuel AB. The goal of it is to present a best estimate method based on the code package CASMO/SIMULATE for the purpose of calculating the isotopic concentrations of a specified number of isotopes in a fuel sample. The calculations done with the method shall produce small deviations from reliable measured values, which characterize the accuracy of CASMO/SIMULATE, but also simplicity based on the computing time and handling of the amount of data is an important factor in the development of the method.

The development of the method has been based on a sensitivity calculation with CASMO/SIMULATE on a number of relevant parameters affecting the isotope concentrations. The proposed method has then been applied on three samples irradiated in Ringhals 4 and Ringhals 3. At last the calculated isotopic concentrations have been benchmarked against measured data from Studsvik Laboratory.

The sensitivity analyzes has shown that the parameters affecting the neutron moderation are very important for calculating the isotopic concentrations. The core axial resolution is also an important factor for the samples taken from top of the rod, where the power gradient is large. The comparison of the calculated and measured values has shown that SIMULATE, in the analysed cases, simulates a lower final burnup. This has created a need to correct the final burnup in order to get better results in terms of lower relative deviations between the measured and calculated data.
Populärvetenskaplig sammanfattning

Energiproduktion från kärnkraftsreaktorer följs idag med hjälp av mätningar och avancerade simuleringsskador. Exempel på parametrar som simuleras är effekt, neutronflödet i härden, utbrännning av bränslevar samt uppbyggnad av olika isotoper.

För tryckvattenreaktorer använder Vattenfall kodpakketet CASMO/SIMULATE som är utvecklat av Studsvik Scandpower (SSP). Detta kodpaket förbättras kontinuerligt av SSP i syfte att öka nogrannheten och applikationerna. För att visa hur noga det verkliga förloppet simuleras kan koderna jämföras mot mätningar.

Målet med detta arbete är att baserat på kod-paketet CASMO/SIMULATE ta fram en metod som på ett enkelt sätt kan beräkna halter av ett specifikt antal isotoper i ett bränsleprov. Metoden skall kunna användas för att verifiera beräkningsmodellen för isotopuppbyggnad i CASMO. Den skall ge ett bra resultat, d.v.s. beräkna olika isotoper vars avvikelser från tillförlitliga uppmätta värden är rimliga och karakterisera beräkningsosäkerheten i CASMO/SIMULATE. Korta beräkningstider och enkelhet på hantering av mångden data är också viktiga faktorer i utvecklingen av metoden.

Utvecklingen av metoden har grundat sig på känslighetsanalyser av ett antal parametrar i CASMO/SIMULATE som påverkar isotopkoncentrationer. Metoden har sedan tillämpats på tre prover bestrålade i Ringhals 4 och Ringhals 3. Slutligen har de beräknade koncentrationerna jämförts med uppmätta värden från Studsvik laboratoriet.

Känslighetsanalyserna visade att de parametrar som påverkade neutronmodereringen är mycket viktiga för beräkningen av isotopkoncentrationer. Härdenäxiella upplösning är av en stor betydelse för de prover som har tagits från toppen av staven, där effektgradienten är hög. Vid jämförelsen av de beräknade isotophalterna med de uppmätta värdena, har SIMULATE i samtliga fall simulerat en lägre slutlig utbrännning. Detta har skapat behov av att korrigera den slutliga utbrännningen och därmed få bättre resultat i form av lägre relativ avvikelse gentemot uppmätt data.
Executive summary

The purpose of this project was to present a best estimate method based on the code package CASMO/SIMULATE for the purpose of calculating a specified number of isotopes in spent fuel sample.

The method presented in this report calculates the isotopic concentration with reasonable deviations from measurements, which gives a reliable view of the amount of different isotopic concentrations in spent fuel. This may be useful to know for several purposes. One, and possibly even the most important purpose may be to use the appropriate materials for the final disposal of the spent fuel.
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1 Introduction

1.1 Background
The nuclear energy production is carefully followed in the operation by measurements and calculations. The power, neutron flux, burnup and the production of different isotopes in the fuel are simulated with advanced calculation codes during the whole fuel lifetime in the reactor.

For this purpose Vattenfall uses different types of calculation codes. For the PWRs, the code package CASMO/SIMULATE (S3) supplied by Studsvik Scandpower (SSP) is used. This code package is continuously improved by SSP referring to accuracy and applications. In order to show the degree of improvement, the codes are benchmarked against other codes, but also against measurements.

In this master of diploma work the calculation of burnup and isotopic concentrations are benchmarked against measured fuel samples. However, the calculation of isotope concentrations for a certain fuel rod is not straightforward. A lot of data must be calculated and used in the right way in order to get results with high accuracy.

1.2 Goal
The goal is to present a best estimate method for comparisons of CASMO calculated vs measured isotopic concentrations. The development of the method shall be based on a sensitivity calculation with CASMO/SIMULATE on a number of relevant parameters affecting the isotope concentrations, see the project specification [1]. The calculations done with the method shall correctly calculate the isotopic concentration. The relative deviations from reliable measured values will characterize the uncertainty of CASMO/S3. But also the simplicity based on the computing time and handling of the amount of data is an important factor in the development of the method. The proposed method is applied on three samples irradiated in Ringhals 4 (R4) and Ringhals 3 (R3).
1.3 Samples

1.3.1 Ringhals 4 PWR samples

The fuel rod from where the R4 samples have been taken comes from assembly 50T. This assembly is manufactured by Framatome ANP (now AREVA) and has an initial enrichment of 3.70 w/o and contains no burnable absorbers. Details on material and geometry of 50T can be found in [2]. The assembly has been irradiated for five annual cycles between September 1998 and the end of July 2003. During that period the assembly had different position in the core, see figure 1.

![Figure 1: Position of assembly 50T during cycle 16-20.](image)

From the irradiated rod, two samples have been taken, RGU1 and RGU2. Sample RGU1 contains three pieces of identical length (each 13 mm long) cut out in the centrum of the rod. Sample RGU2 is only cut out in one piece (14 mm long) close to the top plug of the same rod. The axial position of the samples and the position of the rod within assembly 50T are presented in figure 2.
1.3.2 Ringhals 3 PWR samples

The isotope data for Ringhals 3 comes from the assembly 3V5. The sample rod was manufactured by Siemens (now AREVA) and operate for five annual cycles between July 2000 and May 2005 [3]. Figure 3 shows the position of the assembly 3V5 for each cycle.

The axial position and the position of the sample rod within assembly 3V5 are presented in figure 4.
1.4 Measurements

The isotope concentrations for these samples are experimentally determined at Studsvik Laboratory. The contents of the different isotopes are measured by different methods and some nuclides are analyzed with more than one method. Here are the methods, which have been used in the analysis [2]:

- Isotope Dilution Analysis (IDA)
- Gamma Scan
- ICP-MS Analysis with Separately Determined Response Factors
- Analyses with external calibration
- Residue Analysis

Only two of them are here below shortly presented, IDA and Gamma scan, since almost all the measured data come from these two methods. For details about the other methods, please, see [2].

1.4.1 Isotope Dilution Analysis

The Isotope Dilution Analysis is used for most of the isotopes. This method is based on addition of a known amount of an enriched isotope, called "spike", to a sample. Isotopic ratios between the added isotope and the isotope to be analysed are determined by mass spectrometry. And then the amount of the isotope to be determined in the sample can be calculated according to following formula [2]:

\[ N^S_b = N^S_a \cdot \frac{1 - R_M}{R_S - R_M} \]

where

\( a = \text{Spike isotope} \)
Once the isotope \( b \) has been determined, all other isotopes of the same element can be determined by the isotopic ratios measured by mass spectrometry.

The measured accuracy for the isotopes analyzed with the IDA is estimated to 1-5\%. However, the uncertainty for \(^{142}\text{Ce}\) is above 30\% for RGU1 and for \(^{241}\text{Am}\) and \(^{243}\text{Am}\) 25 and 22\%, respectively for RGU2.

### 1.4.2 Gamma Scan

Axial gamma scanning was performed applying the technique of closely spaced point measurements. Instrument for the measurements, a high-purity germanium detector behind a 0.5 mm tungsten collimator was used. The detector and collimator system was adjusted to give photon energy independent activity values for a fuel rod with a certain diameter. The activities were decay corrected to the end of irradiation. A well-characterized reference rod segment (F3F6) was scanned together with the segments [2].

The main idea behind this method is to identify a number of correction factors in order to determine the absolute activity of the sample. The contributions of all these parameters are summarized in a general formula for determining of the absolute activity see equation 2.

\[
a = \frac{a - \bar{a} \cdot c}{f(E_\gamma) \cdot g \cdot d}
\]

(2)

where

- \( a \) = Absolute activity [Bq/mm]
- \( \bar{a} \) = Apparent (measured) activity [Bq/mm]
- \( f \) = Absorption factor
- \( E_\gamma \) = Energy peak
- \( g \) = Geometry factor
- \( d \) = Dead time correction factor
- \( c = \frac{137\text{Cs reference rod correction}}{a_{\text{ref}}} \)

\[
a_{\text{ref}}(t_{\text{ref}}) \]

\[
a_{\text{ref}}(t_{\text{ref}}) \]

\[
a_{\text{ref}}(t_{\text{ref}}) \]
\( a_{RR} = \text{Activity of reference rod} \)

\( a_{AR} = \text{Apparent (measured) activity of reference rod} \)

\( t_{ref} = \text{Time at end of irradiation of rod of concern} \)

For RGU1 and RGU2 the isotopes \(^{103}\text{Ru}, \, ^{106}\text{Ru}, \, ^{134}\text{Cs}, \, ^{137}\text{Cs}\) and \(^{154}\text{Eu}\) have been analyzed with this method. All these isotopes have accuracy of about 5\%, except \(^{154}\text{Eu}\), which has accuracy of about 20\%.

Also, the prediction of the sample burnup was done using the gamma activity results for \(^{137}\text{Cs}\). In addition to this gamma activity CASMO is used to determine the final burnup.

### 1.5 Calculation tools

#### 1.5.1 SIMULATE

SIMULATE (S3) is a three-dimensional calculation program used for both the PWR- and BWR cores. In the calculation, the neutron flux are divided into high-energy flux (fast) and thermal flux, and the core is divided into a specific set of nodes. For example a fuel assembly is divided in 24 axial and four radial nodes, which means 96 nodes per fuel assembly. Simply, this means that SIMULATE solves a three-dimensional diffusion equation for the neutron flux at each node and connect the solutions between the different nodes with boundary conditions in order to describe the entire fuel core. Necessary input to SIMULATE is cross-sectional data describing the fuel design calculated by CASMO and is accessed through a linking program, CMSLINK. As further input to SIMULATE, core operating data as well as specification of the included fuel assemblies with their burnout histories can be mentioned.

#### 1.5.2 CASMO and CMSLINK

CASMO is a two-dimensional depletion transport theory code designed for fuel rods inside a fuel assembly. The idea behind this program is to place the fuel assembly in an infinite lattice in order to simulate the neutron transport inside and around the assembly. CASMO computes a multi-dimensional neutron flux distributions by solving the neutron transport eigenvalue problem. The solutions are used to compute different types of reactor physics’ parameters such as neutron flux, cross-sections, neutron age, buckling, isotope concentrations etc. CASMO contains a library of microscopic cross-section for a large number of nuclides. The input-data is given to CASMO via a file, which specifies lattice data (the fuel geometry, construction material, fuel enrichment and density), and boron level, power, fuel temperature, moderator density and temperature. The output consists of a large amount of data; the most important for this study is the isotope concentrations of the predefined nuclides.

CMSLINK is a tool to convert the cross-sections from CASMO to a table used by SIMULATE.
2 Calculation method

The idea behind the development of the method of calculating isotopic concentrations is to use CASMO. It uses reflective boundary conditions, which means that only the same types of fuel assemblies are simulated during the depletion history. In the reality the fuel assembly with its rod sample is positioned together with other assemblies with different lattice data and burnup status. Therefore the unique operation (irradiation) data for the specific fuel assembly sample must be calculated with the 3D code SIMULATE before CASMO is used. This calculation method is schematically presented in figure 5 and can simply be described in three steps:

1. The reactor operation and the irradiation of the sample is simulated by SIMULATE. The input and output parameters are described in chapter 2.1.

2. The isotope concentrations are calculated by CASMO. Input data to CASMO consists of results from SIMULATE together with lattice data, see chapter 2.2.

3. In the last step (CMPR), results of the calculated isotopic concentrations are analysed and compared with measured values, see chapter 2.3.

The following versions of the programs have been used in this study:

- SIMULATE-3 version 6.08.05_VAT_9
- CASMO-4 version 2.10.21P_VAT -0 with the unadjusted JEF-2.2 based nuclear data library (J20200)
- CMSLINK version 1.26.02
Figure 5. Schematic view of the calculation method.
2.1 SIMULATE

The simulation of the operation for the 5 cycles require a number of cycle specific input data as:

- Cycle length
- Core operation power
- Core loading pattern
- Assembly burnup history data
- Core cooling flux

The core follow operation and cooling flux values are measured by Ringhals with certain uncertainties, and consequently they can affect the calculation simulation of the core cycles. They are used as best estimated values and are not included in the sensitivity analysis of this study.

Instead, the following input parameters are included in the sensitivity calculation, and hence the development of the isotopic concentration calculation method:

- Control rod bank position
- Core inlet water temperature
- Depletion steps
- Number of axial nodes

Both the control rod bank position and core inlet water temperature are functions of the depletion. As more depletions steps are used, more different bank positions and temperatures must be given.

The number of axial nodes affects the resolution of the results. A large number of axial nodes and depletions steps create a large number of data and long computing time.

Simulation with S3 gives following output parameters:

- Nodal power density (3RPD)
- Nodal fuel temperature (3TFU)
- Nodal assembly exposure (3EXP)
- Nodal density and reactor temperature of the moderator (3DEN and TM0)
- Nodal flux of both high-energy and thermal neutrons (3FLX, group 1 and 2)
2.1.1 MATLAB

The output-file from SIMULATE contains a huge amount of data for all assemblies, at all nodes and for all parameters. MATLAB has been used for the purpose of reading the relevant parameters at the specific sample node for the specific assembly. The author has designed a script, exjobb_tz, used for this purpose. See Attachment C.

Exjobb_tz is based on the script read_cms, which was first designed by Studsvik Scandpower. Read_cms reads the output-file from SIMULATE into Matlab.

Exjobb_tz is divided into three parts.
- In the first part, the relevant parameters at the specific node for the specific assembly are read.
- In the second part boron values for each cycle are read and written.
- In the last part an input-file including all the parameters necessary for CASMO is generated.

2.2 CASMO

When calculating the isotope concentrations with CASMO, all the output parameters (except nodal flux) from SIMULATE listed in chapter 2.1 are used as input, completed with:

- Initial lattice data (fuel enrichment, material and geometry)
- Isotope specification

Using these parameters as input, CASMO calculates isotopic concentrations as function of nodal pin (sample) burnup.

2.3 CMPR

Comparison of the calculated and measured concentrations has been done by calculating the relative deviation for each isotope, according to the following formula:

\[
Relative_{\text{deviation}} = \frac{\text{Calculated} - \text{Measured}}{\text{Measured}}
\]  

The analysis is done in an excel-file, “Analysis-of-Isotope-concentrations.xls”.
2.4 Correction of burnup

In order to make a fair comparison of the CASMO calculated and the measured isotopic concentrations, the concentrations must be compared at the same burnup level. There are a number of ways to do this correction.

One way is to use the fact that some isotopes are very well known to be both calculated and measured with high accuracy. For example the Neodymium (Nd) isotopes are often used in this type of studies. They are good burnup indicators also because of their weak neutron spectrum dependence and their none migration quality. By matching (linear regression) the calculated concentrations of the Nd-isotopes to their measured concentrations, the final burnup value can be corrected, see figure 6.

The 8 last calculated burnup values are presented in the figure with dots connected with a line. The measured values are presented with big dots at the final burnup value based on the $^{137}$Cs measured gamma profile.

![Figure 6. Regression lines of the calculated concentrations and measured values](image)

Every Nd-isotope contributes to the burnup value by its weight, which is dependent on the slope of its burnup dependence and the accuracy of the measurement of that isotope. The weight is proportional to the slope and inversed proportional to the measurement uncertainty. For example, the weight will be high for isotope curves with steep slopes and small measured uncertainties, for details see Attachment B.
Another way to determine the S3 final burnup is to use the final burnup value based on the measurement of the $^{137}$Cs gamma profile. Using equation 2, in section 1.4.2, the absolute gamma activity can be calculated. CASMO is then used in order to calculate the number of fissions, and hence the final burnup. Figure 7 shows the $^{137}$Cs based burnup profile for RGU1 and RGU2 from bottom to top of the sample rod.

![Figure 7. Cs-137 based burnup profile of rod with position of RGU samples.](image_url)
2.5 **Sensitivity Analysis**

As mentioned in section 2.1-2.3 a large number of parameters are input to both SIMULATE and CASMO. Each parameter has a different impact on the results. To find out how these parameters affect the isotopic concentrations and thus are important for the accuracy, a sensitivity analysis for some of the most important parameters is done, table 9.

Table 1. Sensitivity parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Reference</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of depleted steps (NDS)</td>
<td>Best estimate</td>
<td>Standard</td>
</tr>
<tr>
<td>Number of axial nodes (NAN)</td>
<td>12</td>
<td>24</td>
</tr>
<tr>
<td>Number of boron values (NBV)</td>
<td>1 value/depl.step</td>
<td>1 value/cycle</td>
</tr>
<tr>
<td>Uranium enrichment (UE)</td>
<td>Nominal</td>
<td>+0,05 w/o (+1.4 %)</td>
</tr>
<tr>
<td>Fuel temperature (FT)</td>
<td>1 value/depl.step</td>
<td>+50 K (+6 %)</td>
</tr>
<tr>
<td>Uranium density (UD)</td>
<td>Nominal</td>
<td>+0,1 g/cm3 (≈ +1%)</td>
</tr>
<tr>
<td>Moderator density (MD)</td>
<td>1 value/depl.step</td>
<td>+0,05 g/cm3 (≈ +7%)</td>
</tr>
<tr>
<td>Inlet moderator temp.</td>
<td>Best estimate</td>
<td>+2 K</td>
</tr>
<tr>
<td>Water gap (WG)</td>
<td>Nominal</td>
<td>0,01 cm (≈ +1,5 % volume water fuel ratio)</td>
</tr>
</tbody>
</table>

The sensitivity has been calculated by dividing the isotope concentrations for each case with the reference values, according to the following formula:

\[
Sensitivity = \frac{[A]'-[A]_{ref}}{[A]_{ref}} \quad (4)
\]

Where

\([A]' = \) Concentration of isotope A in the sensitivity case

\([A]_{ref} = \) Concentration of isotope A in the reference case
It should be noted that in this sensitivity study, no measured values are involved.

2.5.1 Number of depleted steps
In order to carefully (with high resolution) follow the operation the number of depletion steps and operation data will be very high and hence the amount of data difficult to be handled. The aim of this calculation is to study the sensitivity on the results for a standard resolution compared to high resolution depletion steps. It is known that at the beginning and end of each cycle, the power gradient is high. This study investigates if more depletion steps, at the beginning and end of each cycle affect the results.

2.5.2 Number of axial nodes
This part of the sensitivity analysis refers to core axial resolution. In the reference case, the core is divided into 12 axial nodes. In this part the sensitivity of changing the axial nodes to 24 is studied.

2.5.3 Number of boron values
Usually, the boron depletion is simulated during the cycles. This means that a new boron value is used for each depletion step. In the sensitivity case only one average boron value is used for each cycle.

2.5.4 Uranium enrichment
The suppliers deliver reliable fuel. However, there are still small uncertainties due to manufacturing reasons. The uncertainty in the $^{235}$U enrichment is typically less than 0.05 w/o. The initial enrichment level of the assembly 50T was 3.70 w/o with tolerance limit of ± 0.05 w/o. In this sensitivity case the enrichment level is increased to 3.75 w/o.

2.5.5 Fuel temperature
Benchmarking of computer code predictions against measured fuel temperatures indicates that there is considerable uncertainty in calculated values. The resonance escape probability factor decreases with the fuel temperature, which in turn decreases the reactivity. However, the reactivity decrease will be partly compensated for by larger plutonium build up. In order to study how this phenomenon affects the isotope concentrations, a sensitivity analysis has been done for a 50 K higher fuel temperature.

2.5.6 Uranium density
In this sensitivity case 0.1 g/cm³ higher uranium density than nominal has been studied. Besides the effect on the isotope concentrations, it is also interesting to compare the results with the corresponding results from the enrichment increase.

2.5.7 Moderator density and inlet water temperature
The moderator density affects the neutron spectrum, which in turn affects the burnup and the build up of the different isotopes. The inlet water temperature, the water flux with its distribution inside the vessel, the control rod bank and the
power are the operation parameters, which are of great importance in the calculation of the local moderator density. Another source of error in order to predict the true moderator density is the calculation method itself with the interaction between S3 and CASMO. By comparing the neutron spectrum calculated by S3 and CASMO, this code interaction effect on the moderator density can be estimated.

In this study two different calculations showing the sensitivity results for the uncertainties of the reactor operation parameters have been done. The first calculation aim to study the sensitivity results for the inlet water temperature, which is here increased by +2 K.

The second calculation takes care of the rest of the input operation parameter uncertainties. The parameters affect each other in different degrees, which make the calculation difficult to perform. By assuming that the accumulated effect of the uncertainties of the input parameters affect the SIMULATE output of the moderator density with a certain value, the final effect of the CASMO isotopic concentration can be calculated. In this case, the accumulated value has been estimated to 0.05 g/cm³, which means about 7 % higher moderator density. This is however a very high density increase, which is based on the largest possible input error.

2.5.8 Water gap

An important design parameter is the water gap between fuel assemblies. Experience from measurement of assemblies shows that the fuel assembly tends to be bend more or less. Both assembly bowing and rod bowing are well know, which means that the distance between the fuel rods in the assembly or the assemblies itselfes are changed. This bowing phenomena gives rise to water gaps between rods and assemblies which deviate from nominal values. Figure 8 shows the cross-section of an ideal fuel assembly where the distance between two fuel rods is defined (pin pitch).
In the sensitivity case the pin pitch is increased to 1.265 cm, which in turn makes the whole assembly little wider and consequently the channel between the fuel assemblies little smaller. The increased pin pitch makes the moderator to fuel volume of the assembly to be 1.5 % larger.
3 Results

3.1 Sensitivity Analysis

In order to clearly present the results, they are presented in two groups, with 5 and 4 sensitivity parameters in each group, respectively. The results are presented in figures 9-12 and in table 2 and 3.

3.1.1 Group one

Group one consists of the following sensitivity parameters:

- Moderator density
- Number of boron values
- Number of depleted steps
- Inlet temperature
- Number of axial nodes

Figure 9 shows clearly that number of depleted steps, boron values, axial nodes and inlet water temperature have very low sensitivity for RGU1. The small inlet water temperature increase (0.8 %) affects the moderator density 0.5 % and hence affects the isotopic concentration very little. However, the second calculation with the 7 % higher moderator density affects the isotopic concentration very much, especially the actinides; $^{235}$U and $^{239}$Pu, which are the most important isotopes. The isotopes $^{235}$U and $^{239}$Pu have decreased by 11 % and 6 %, respectively. This is was also expected due to the exaggerated increase of the moderator density.
According to figure 10, the number of axial nodes has a larger impact on the results for the majority of the isotopes, especially for $^{235}$U, which has increased by over 10%. The impact on $^{239}$Pu is, however, insignificant.

The number of depleted steps and boron values and inlet water temperature has negligible impact on the results.

Sensitivity of the moderator density is similar for RGU2 as RGU1. The isotopes $^{235}$U and $^{239}$Pu are decreased by 9% and 7% respectively.
3.1.2 Group two

Group two contains the remaining parameters, which are:

- Uranium enrichment
- Fuel temperature
- Uranium density
- Water gap

![Figure 11. Sensitivity of uranium enrichment, fuel temperature, uranium density and water gap for RGU1.](image)

The sensitivity of uranium enrichment for RGU1 is relatively low for most of the isotopes including the actinides according to figure 11. Influence of this parameter is negligible for Pu isotopes and about 1% for $^{235}$U.

Fuel temperature has also a low sensitivity for majority of the isotopes, except $^{235}$U, which has sensitivity of about -1%. The impact on Pu isotopes is less than 1%.

Uranium density and water gap are the parameters, which have largest sensitivity for most of the isotopes. Increasing uranium density and the volume ratio between moderator and fuel give less amount of $^{235}$U left, -3% and -4% respectively. For $^{239}$Pu the corresponding figures are +1.5% and -1.0% respectively.
Figure 12. Sensitivity of the uranium enrichment, uranium density, fuel temperature and water gap for RGU2.

Sensitivity of all the parameters for RGU2 shown in figure 12 looks almost the same as for RGU1. The uncertainty in uranium enrichment has a little influence on the fission products and the plutonium isotopes. The $^{235}\text{U}$ left, is however, increased by about 3%.

Fuel temperature has a different sensitivity for RGU2 than for RGU1. For most of the isotopes the results are small negative values. However, the $^{235}\text{U}$ has increased by 1 %.

Notable parameters are still the uranium density and water gap. The $^{235}\text{U}$ is decreased by 2% and 3% respectively. The $^{239}\text{Pu}$ is increased by 1% and 0.25%, for uranium density and water gap respectively.

In table 2 and 3, all the sensitivity analyses of all parameters for different isotopes are presented for both RGU1 and RGU2. Total uncertainty is calculated for the parameters in group 2, by taking the square root of the quadratic sum of the parameters. All these parameters values without the fuel temperature contain uncertainties, which are impossible to avoid. Only the vendors of the fuel can minimize the tolerances by their own manufacturing process.
<table>
<thead>
<tr>
<th>Isotopes</th>
<th>GROUP 1</th>
<th>GROUP 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo95</td>
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Table 2. Sensitivity analysis of group one parameter, RGU1.
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<td>Cm245</td>
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<td>1.04%</td>
</tr>
</tbody>
</table>
3.1.3 The best estimated method

It can be noticed from the sensitivity analysis that number of boron values and the depleted steps do not have remarkable effect on the results for both samples. Therefore it is enough accurate and simple to use the boron values and depletion data from the core follow standard calculation. Here simplicity and data handling have higher priority than calculation accuracy.

The sensitivity analysis also shows that number of axial nodes has a significant influence on isotope concentrations for RGU2. Therefore In order to produce accurate results the method shall contain at least 24 axial nodes. It indicates that a high axial resolution is needed for samples close to the top and bottom nodes of the fuel.

The sensitivity results of the moderator density indicate its large impact on the calculation of isotope concentrations. The input operation data to S3 affect that mostly, but also the way S3 and CASMO interact with each other might affect the results. By comparing the results of the neutron flux spectrum from the two codes, the calculation method can be studied. For all the 5 cycles the neutron flux ratio between fast and thermal neutrons from both S3 and CASMO were exactly the same, thereby confirming that the interaction between SIMULATE and CASMO for this aspect is excellent. One can conclude that the uncertainties coupled to moderator density are connected only to the input operation data and the calculation procedure in S3/CASMO codes themselves.

Therefore, no correcting of the moderator density is needed and the best estimate values calculated by Simulate are good enough.

Except fuel temperature, all the other parameters from group two are related to manufacturing with certain tolerance limits. There is a number of advanced fuel temperature codes, but all of them contain significant uncertainties. Benchmarking of these codes against measured fuel temperature indicates that there is a considerable uncertainty in calculated values (about 100 K). It is nowadays difficult to find a code with uncertainty less than 50 K. For that reason the results of fuel temperature sensitivity analysis are included in the manufacturing product tolerances and a total impact of these uncertainties on the isotope concentrations are calculated. For $^{235}$U and $^{239}$Pu for RGU1 the total impact are 7 % and 2 %, respectively. The corresponding figures for RGU2 are 5 % and 2 %, respectively.
3.2 Isotope concentrations of the assembly 50T and 3V5

3.2.1 Correction of burnup

For the correction of the final burnup, both methods described in section 2.4 have been studied. The method based on neodymium isotopes was first attempted, which for 50T-RGU1 and -RGU2 gave little higher burnup than S3 calculated, but lower than measured, based on gamma profile of $^{137}$Cs, as shown in table 4. For 3V5, the method of neodymium isotopes gave the lowest burnup compared to the other burnup values.

Table 4. The S3 calculated, corrected and measured burnup.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Assembly</th>
<th>Sample</th>
<th>The corrected burnup, based on Nd-isotopes</th>
<th>Measured burnup, based on gamma scan of $^{137}$Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>50T-RGU1</td>
<td>61.3</td>
<td>63.3</td>
<td>63.8</td>
<td>65.9</td>
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<td>57.1</td>
<td>57.6</td>
<td>59.6</td>
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<tr>
<td>3V5</td>
<td>61.5</td>
<td>63.5</td>
<td>58</td>
<td>59</td>
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</table>

In this study the best agreement between the calculated and measured concentrations are achieved by adjusting the S3 final burnup value to the $^{137}$Cs gamma profile based value. All the comparison between measured and calculated isotope concentrations are presented before and after burnup correction, table 5-7.

3.2.2 Comparison of the calculated and measured concentrations

The results in terms of relative deviation between the calculated and measured concentrations are presented in figure 13 and table 5, 6 and 7 for RGU1, RGU2 and 3V5 respectively.

![Comparison measured vs calculated values](image_url)  
Figure 13. Comparison of calculated and measured values.
Figure 13 aims to show the agreement between the results from measurements and calculation, but also identify the points positioned far outside the “zero deviation” line for all three cases. The points with high values far from the line, here defined as outlayers, are clearly seen in this type of plot. The out layers are $^{99}$Tc, $^{239}$Pu, $^{240}$Pu, $^{242}$Pu and $^{142}$Ce for RGU1, $^{236}$U and $^{140}$Ce for RGU2 and $^{140}$Ce, $^{235}$U, $^{236}$U, $^{239}$Pu and $^{240}$Pu for 3V5.

The relative deviation between calculated and measured values is shown in table 5, 6 and 7. For the absolute values, please see attachment D. It can be noticed that for some fission products the deviation between calculated and measured values increases after burnup correction. However, the most important nuclides, which are the actinides, generally give best results after burnup correction. For $^{235}$U, the deviation before the correction was 31.3 %, 24.8 % and 21.8 %, which decreased to -0.5 %, -1.7 % and 5.5 % for RGU1, RGU2 and 3V5 respectively. For $^{239}$Pu, the deviation before the correction was 12.0 %, 3.6 % and 7.5 %, which decreased to 9.3 %, 2.0 % and 2.5 % for RGU1, RGU2 and 3V5 respectively.

Most of the fission product isotopes have been improved after burnup correction in the three cases.

The relative deviations of the isotopes $^{140}$Ce and $^{142}$Ce for RGU1, after burnup correction, are 54 % and 57 %, which are quite unreasonable. The corresponding values for RGU2 are 20.1% and 10.9 % and for 3V5 10.2 and 2.9 %, respectively.

The burnup correction has resulted in a higher relative deviation for the isotopes $^{147}$Pm, $^{152}$Sm, $^{153}$Eu, $^{154}$Eu, $^{158}$Gd, $^{234}$U, $^{244}$Cm and $^{245}$Cm. Common for these isotopes is that they are in small quantities and in some cases combined with a larger uncertainty in measured data. However, it can be mentioned that 18 of 42 isotopes has resulted in a lower relative deviation for RGU1. The corresponding values for RGU2 and 3V5 are 23 of 42 and 18 of 34 isotopes, respectively.

The isotopic concentrations as function of burnup at the end of the cycle are shown in attachment A for all three cases. It can be mentioned that some isotopes are more or less dependent on the burnup, depending on how steep the slope of the curve is. The steeper the slope curve has, the stronger the dependence and vice versa. The $^{235}$U is strongly dependent on burnup while $^{234}$U, which is almost constant and not affected at all.
Table 5. Relative deviations of the RGU1 sample before and after burnup correction.

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<td>Before burnup correction</td>
<td>After burnup correction</td>
</tr>
<tr>
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<td>Relative deviation [%]</td>
<td>Relative deviation [%]</td>
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</table>
Table 6. Relative deviations of the RGU2 sample before and after burnup correction.

<table>
<thead>
<tr>
<th>Isotopes</th>
<th>X/238U, weight %</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Before burnup correction</td>
<td>After burnup correction</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Relative deviation [%]</td>
<td>Relative deviation [%]</td>
<td></td>
</tr>
<tr>
<td>Mo95</td>
<td>10,3</td>
<td>18,1</td>
<td></td>
</tr>
<tr>
<td>Tc99</td>
<td>4,1</td>
<td>10,8</td>
<td></td>
</tr>
<tr>
<td>Ru101</td>
<td>-5,4</td>
<td>2,4</td>
<td></td>
</tr>
<tr>
<td>Ru103</td>
<td>-10,9</td>
<td>-7,4</td>
<td></td>
</tr>
<tr>
<td>Ru106</td>
<td>-6,3</td>
<td>0,5</td>
<td></td>
</tr>
<tr>
<td>Rh103</td>
<td>-5,2</td>
<td>-0,9</td>
<td></td>
</tr>
<tr>
<td>Ag109</td>
<td>-3,6</td>
<td>6,1</td>
<td></td>
</tr>
<tr>
<td>Cs133</td>
<td>-6,5</td>
<td>-1,1</td>
<td></td>
</tr>
<tr>
<td>Cs134</td>
<td>-9,1</td>
<td>2,5</td>
<td></td>
</tr>
<tr>
<td>Cs135</td>
<td>-5,6</td>
<td>2,4</td>
<td></td>
</tr>
<tr>
<td>Cs137</td>
<td>-7,8</td>
<td>-0,3</td>
<td></td>
</tr>
<tr>
<td>La139</td>
<td>-8,7</td>
<td>-1,6</td>
<td></td>
</tr>
<tr>
<td>Ce140</td>
<td>10,6</td>
<td>20,1</td>
<td></td>
</tr>
<tr>
<td>Ce142</td>
<td>2,4</td>
<td>10,9</td>
<td></td>
</tr>
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<td>Pr141</td>
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<td></td>
</tr>
<tr>
<td>Nd142</td>
<td>-7,8</td>
<td>11,2</td>
<td></td>
</tr>
<tr>
<td>Nd143</td>
<td>4,6</td>
<td>6,3</td>
<td></td>
</tr>
<tr>
<td>Nd144</td>
<td>-11,2</td>
<td>-0,1</td>
<td></td>
</tr>
<tr>
<td>Nd145</td>
<td>3,2</td>
<td>9,4</td>
<td></td>
</tr>
<tr>
<td>Nd146</td>
<td>-7,0</td>
<td>2,3</td>
<td></td>
</tr>
<tr>
<td>Nd148</td>
<td>-1,8</td>
<td>6,6</td>
<td></td>
</tr>
<tr>
<td>Nd150</td>
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<td></td>
</tr>
<tr>
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</tr>
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<td>-11,2</td>
<td></td>
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<tr>
<td>Sm150</td>
<td>-4,0</td>
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<td></td>
</tr>
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<td>Sm152</td>
<td>21,2</td>
<td>28,4</td>
<td></td>
</tr>
<tr>
<td>Sm154</td>
<td>-3,1</td>
<td>8,3</td>
<td></td>
</tr>
<tr>
<td>Eu153</td>
<td>23,4</td>
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</tr>
<tr>
<td>Eu154</td>
<td>-7,1</td>
<td>1,0</td>
<td></td>
</tr>
<tr>
<td>Gd156</td>
<td>-12,7</td>
<td>7,3</td>
<td></td>
</tr>
<tr>
<td>Gd158</td>
<td>36,6</td>
<td>65,4</td>
<td></td>
</tr>
<tr>
<td>U234</td>
<td>-15,1</td>
<td>-21,8</td>
<td></td>
</tr>
<tr>
<td>U235</td>
<td>24,8</td>
<td>-1,7</td>
<td></td>
</tr>
<tr>
<td>U236</td>
<td>-7,5</td>
<td>-6,9</td>
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</tr>
<tr>
<td>Np237</td>
<td>-12,1</td>
<td>-6,2</td>
<td></td>
</tr>
<tr>
<td>Pu238</td>
<td>-21,6</td>
<td>-9,2</td>
<td></td>
</tr>
<tr>
<td>Pu239</td>
<td>3,6</td>
<td>2,0</td>
<td></td>
</tr>
<tr>
<td>Pu240</td>
<td>-3,1</td>
<td>0,6</td>
<td></td>
</tr>
<tr>
<td>Pu241</td>
<td>0,3</td>
<td>2,0</td>
<td></td>
</tr>
<tr>
<td>Pu242</td>
<td>-11,0</td>
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</tr>
<tr>
<td>Am243</td>
<td>-15,3</td>
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<td></td>
</tr>
<tr>
<td>Cm244</td>
<td>22,2</td>
<td>63,3</td>
<td></td>
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<tr>
<td>Cm245</td>
<td>1,8</td>
<td>39,1</td>
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</table>
Table 7. Relative deviation of the 3V5 sample before and after burnup correction.

<table>
<thead>
<tr>
<th>Isotopes</th>
<th>Calculations, X/238U, weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Before burnup correction</td>
</tr>
<tr>
<td></td>
<td>Deviation [%]</td>
</tr>
<tr>
<td>Cs133</td>
<td>-7,7</td>
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<tr>
<td>Cs134</td>
<td>26,1</td>
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<td>Cs135</td>
<td>-8,6</td>
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<td>Cs137</td>
<td>-5,7</td>
</tr>
<tr>
<td>La139</td>
<td>-4,2</td>
</tr>
<tr>
<td>Ce140</td>
<td>7,1</td>
</tr>
<tr>
<td>Ce142</td>
<td>0,6</td>
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<td>Nd142</td>
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</tr>
<tr>
<td>Nd143</td>
<td>10,6</td>
</tr>
<tr>
<td>Nd144</td>
<td>-4,1</td>
</tr>
<tr>
<td>Nd145</td>
<td>6,3</td>
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<tr>
<td>Nd146</td>
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<td>Nd148</td>
<td>0,2</td>
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<tr>
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<td>2,2</td>
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<td>-16,1</td>
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<td>-1,1</td>
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<td>20,9</td>
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<td>Eu153</td>
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<td>73,4</td>
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</tr>
<tr>
<td>Gd158</td>
<td>59,9</td>
</tr>
<tr>
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</tr>
<tr>
<td>U236</td>
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<td>Np237</td>
<td>-4,6</td>
</tr>
<tr>
<td>Pu238</td>
<td>-9,0</td>
</tr>
<tr>
<td>Pu239</td>
<td>7,5</td>
</tr>
<tr>
<td>Pu240</td>
<td>2,6</td>
</tr>
<tr>
<td>Pu241</td>
<td>10,0</td>
</tr>
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<td>Pu242</td>
<td>1,3</td>
</tr>
<tr>
<td>Am241</td>
<td>-35,3</td>
</tr>
<tr>
<td>Am243</td>
<td>-15,0</td>
</tr>
</tbody>
</table>
4 Discussion

The fresh nuclear fuel consists only of the uranium isotopes. The actinides, Pu, Cm, Np and Am, as well as the fission products are produced during the operation. The neptunium isotopes and $^{238}$Pu originate from neutron capturing of $^{235}$U while the other actinides are a result of neutron capturing of $^{238}$U. The isotopes $^{235}$U, $^{239}$Pu and $^{241}$Pu make the major contribution to the energy release and maintenance of the chain reaction.

Some actinides, which are build-up faster than they decay, will increase along with burnup. Other isotopes, which are created as fast as they decay, achieve a balance and will remain constant along with burnup. However, $^{235}$U, which makes the major contribution to the energy release and is not build-up during the operation, will obviously decrease along with burnup. This means that the final burnup of a fuel is an important parameter for the concentrations of the isotopes highly influenced by burnup, for example $^{235}$U, $^{144}$Nd, $^{150}$Sm, $^{237}$Np, $^{152}$Sm and $^{137}$Cs. It is also confirmed by the burnup correction giving better results for these types of isotopes, except the isotopes $^{140}$Ce and $^{142}$Ce, which have a positive gradient along with burnup and the measured value is much lower than calculated for both RGU1 and RGU2. In this case, the measured concentrations of these isotopes must be uncertain. The other isotopes giving worse results after burnup correction are usually in small amounts and combined with greater uncertainties.

Increasing the uranium enrichment in the sensitivity analyzes, was a good example of a parameter affecting the final burnup. An increase in uranium enrichment means increasing the fissile nuclei, $^{235}$U. Since there are increasing number of $^{235}$U, it means there should be relatively more $^{235}$U left at the end of the cycle, as demonstrated by sensitivity analysis. For RGU1 the increase of $^{235}$U was about 1 % and the corresponding value for RGU2 was almost 3 %. The $^{239}$Pu was decreased by about 1 % for RGU1 and for RGU2 the isotope was increased by 0.4 %. This may be due to better moderating at the position of RGU1, which caused more fission of $^{235}$U and less build up of $^{239}$Pu. At position of RGU2, the moderator density is lower, which means that the neutron spectrum is harder and consequently the more $^{239}$Pu are built up.

Another phenomenon affecting the isotopic concentrations is the neutron spectrum in the core. The neutron spectrum affects not only the build up of plutonium but also the distribution of the fissions products from $^{235}$U and $^{239}$Pu. This will affect the isotopic concentrations because these isotopes have slightly different fission product yields, and hence tendency to form some isotopes more than others. This is the second main phenomenon that affects the isotopic concentration and appears in some of the sensitivity analyzes.

Moderator density is a good example of the parameter causing a change in the neutron spectrum. For the RGU1 sample the isotopes $^{235}$U and $^{239}$Pu has decreased by 11 % and 6 % due to higher value of the moderator density. A higher moderator density means that more neutrons are slowed down to
thermal energy, which in turn increases the fissions of $^{235}$U and decreases the build up of $^{239}$Pu. This explains the decrease of $^{235}$U and $^{239}$Pu concentrations. Furthermore, it should also be noted that in this sensitivity analysis the moderator density was changed by +0.05 g/cm$^3$, which is a high perturbation. It may be compared with the sensitivity analysis of inlet water temperature, which was changed only by 2 degrees resulting in a change in moderator density of only -0.004 g/cm$^3$. Even that little change could affect $^{235}$U about -1 % and +1 % for RGU1 and RGU2 respectively.

Increasing the pin pitch 0.01 cm made the moderator to fuel volume ratio 1.5 % larger. This is another example on the parameter causing a change in the neutron spectrum. A higher moderator to fuel volume ratio increases the resonance passage factor (p) because of increasing the probability for the neutron to be slowed down to thermal energy before being captured in $^{238}$U. On the other hand, the thermal utilization factor (f) is decreased by a larger volume ratio of moderator and fuel, because of increasing probability for the neutron capture in the moderator. Since these two parameters are included in the four-factor formula, the product of these parameters gives the optima. For PWR reactors, which are in general undermoderated an increased moderator to fuel volume ratio means an increased reactivity level. The results from this analysis show a decrease of 4 % and 3 % of $^{235}$U for RGU1 and RGU2 respectively, indicating on a softer neutron spectrum and less $^{239}$Pu buildup.

The sensitivity analyses of the depletion steps showed not much impact on the isotopic concentrations. This is because SIMULATE follows the operation curve well enough, which means that there is no need for additional depletion steps.

The number of axial nodes was an important parameter for the samples taken from top and bottom of the rod where the power gradient is large. A large number of axial nodes means a better resolution that gives more accurate information about the core. The RGU2 sample that was taken from a quite high level of the rod is an excellent example showing a high sensitivity for $^{235}$U, which was 11 %. The corresponding value for RGU1 sample, where the power is quite constant, was -1 %.

The sensitivity analysis of boron values has shown no remarkable impact on isotopic concentrations. This is because the average boron values remains the same for all five cycles, hence there is no change in the neutron spectra.
5 Conclusions

Benchmarking the calculated data against measured is not that easy since there are a lot of parameters inducing uncertainties. The uncertainties could be involved at the measured data as well as the calculated, which makes it difficult to point out what is wrong. But calculation of the relative deviation is still a good indicator. Based on this, the following conclusions are drawn:

• The results of the comparison between measured and calculated isotopic concentrations show good agreement on the most important isotopes, which indicates that the calculation method (CASMO/S3) is accurate. For example $^{235}$U and $^{239}$Pu.

• The isotopes with small measured amount and with small burnup dependence show large deviation. For example $^{241}$Am, $^{152}$Sm, $^{153}$Eu, $^{244}$Cm and $^{158}$Gd.

• The core axial resolution is very important parameters for a sample taken from top or bottom of the rod, where the power gradient is large.

• The accuracy of the results is very much dependent on correct sample burnup and correct simulation of the neutron spectrum. A large part of these uncertainties have their origin in the input parameters of the calculation method. The combined impact of tolerances for fuel temperature, enrichment, uranium density and standard rod/assembly bowing are for $^{235}$U and $^{239}$Pu 5-7 % and 2 % respectively.

• The calculation procedure for isotopic comparisons is fast and more or less automatic. SIMULATE runs the reactor simulation, CASMO calculates the different isotope concentrations and CMPR analyses the data and make table and figures. The data between the different programs are easily handled by scripts in MATLAB.

• The goal of the project has been achieved by presenting a best estimate method for comparisons of CASMO calculated vs measured isotopic concentrations. The calculations done with the method calculates the isotopic concentration correctly and the relative deviations from reliable measured values characterize the uncertainty of CASMO/S3.
6 Acknowledgments

I would like to express my most sincere thanks to my supervisor at Vattenfall Nuclear Fuel AB, Klaes-Håkan Beijmer. He has assisted me throughout the entire project and given me lots of good advices. I have always felt welcome to him with any question and he has answered in a very friendly manner, which is something I have really appreciated.

I can also not forget some professional advices I have received from Ewa Kurcyusz-Ohlofsson at Vattenfall Nuclear Fuel AB. Her advices have been very crucial in some situations.

Furthermore I want to thank Thomas Smed at Studsvik Scandpower who has helped me with loading files into MATLAB. My script is based on some functions in his script, which has been of crucial importance to the execution of the project. Hans-Urs Zwicky and Michael Granfors at Studsvik invited my supervisor and I to the Studsvik Laboratory, where they described the methods of measurements and I am very grateful for their contribution to this project.
7 Bibliography


Attachments

A. *Isotope concentrations as function of burnup*

![Comparison of calculated and measured isotope concentrations as a function of burnup for different reactor units.](image)
Comparison Calculated Measured

Burnup [MWd/kgU]

n/X238U [wt%]

Comparison Calculated Measured

Burnup [MWd/kgU]

n/X238U [wt%]

Comparison Calculated Measured

Burnup [MWd/kgU]

n/X238U [wt%]
B Calculation of burnup correction with Nd-isotopes

Assume that the adjusted burnup value, Xm (matching value), has small impact on the calculated shape of the isotopic concentration curve (as a function of burnup). Use only those isotopes, which are, based on experience, easy to calculate and measure with high accuracy.

The burnup for a certain isotope, $X_i$, can be given as a function of the calculated concentration and the shape. Instead of the calculated concentration, use the measured one, $Y_i$. The new burnup value, $X_{m_i}$ is then;

$$X_{m_i} = X_{m_i}(Y_i, S_i) \text{ and } X_{1m_i} = X_{1m_i}((Y_i + D_i), S_i) \text{ (determined with regression analysis)}$$

Where;

- $Y_i = \text{the measured value for the matching isotope } i$, $D$ is the measured accuracy for that isotope.

- $S_i = \text{the calculated shape, which for a line is characterized by the slope and a constant. The slope is inverse proportional to the burnup and the constant is proportional.}$

The weight for this isotope can then be calculated as;

$$W_i = 1/(X_{1m_i} - X_{m_i})$$

The adjusted burnup is calculated as;

$$X_m = S_i \left( X_{m_i} * W_i \right) / S W_i$$
### C. Script

%% Denna script används för att låta utvärdera utvärderutvalda parametrar i en specifik nod och i x antal cyklar, från en cms-fil.
% Scripten består av 3 delar, uppdela i 3 kapitel.
% Del 1 hänvisar data från en cms fil och visar slutresultat enligt tidigare beskrivning i matrisen 'Resultat'.

%% Del 2 hänvisar borvårdena och utvärderingar från en csv-fil och ritar en regressionslinje så att man kan bemäktiga borvårde utifrån ett valfritt värde på utvärderning.

%% Del 3 skriver ut utvärderade parametrar och förbereder en textfil som sedan ska köras i CASMO.

%% 1.1 Hittar rätt mapp till filen och lagrar till path-filerna som användiga för att kunna anropa CMSREAD-metoden

clear all
clc

cd /home/pwr/Projekt/Isotopber-2011/Exjobb-2012/sim3/
% hitta rätt mapp till filen
% aligg till path-filerna
addpath /home/user/tzuw/Mfiler
addpath /home/prog/dvlp/CMSCODES/CMSlab/S3kPlot
addpath /home/prog/dvlp/CMSCODES/CMSlab/cmsview
addpath /home/prog/dvlp/CMSCODES/CMSlab/CmsTools
addpath /home/prog/dvlp/CMSCODES/CMSlab/CmsPlot
addpath /home/prog/dvlp/CMSCODES/CMSlab/cmscore
addpath /home/prog/dvlp/CMSCODES/CMSlab/CmsRead

cmsinfo=read_cms('simout_50T_16-20.cms');
mat=[]; %skapa en tom matris som senare fylls i m.h.a for-loopen nedan:

%% 1.2 Metod för att hänvisa av antalet utvärderingar av respektive cykel
utbsteg= read_cms_scalar(cmsinfo, 'CYCLE EXPOSURE (GWD/MT)');
%all utvärderingssteg
utbsteg=utbsteg';

%tempo=[]; % temporär vektor
n=0; % ----
cykellang= []; %vektorn kommer senare att innehålla antalet steg i varje cykel

% hitta slutpunkter i varje cykel och spara dess värde i vektorn tempo.
for r=1:max(size(utbsteg)-1)
    while (utbsteg(r+1)<utbsteg(r))
        if (utbsteg(r+1)<utbsteg(r))
            r;
            n=n+1;
            tempo(1,n)=r;
            break
        end
    end
end
tempo2 = max(size(tempo));

end

tempo(tempo2+1) = max(size(utbsteg));

tempo;

% kopiera element från vektorn, rakna ut steglangd och spara längden av
% cyklar i vekorn cykellangd.
cykellangd(1) = tempo(1);
for i = 2:max(size(tempo))
cykellangd(i) = (tempo(i) - tempo(i-1));
end
tempo;

cykellangd; % [11 11 5 7 15]
tempo2 = [0];
tempo2 = [tempo2 tempo];
cykelnamn = [18 19 20 21 22];

% 1.3 Håller rätt förde för nedanstående parametrar vid rätt nod, rätt position, rätt cykel och rätt utbrytningsteg. Under
processförloppet sparas värdena i matrisen 'mat' som senare
finjusteras i matrisen 'Resultat'

positioner = [12 95 111 59 79];
% for x = 1:length(cykellangd)
%     position = positioner(x)
% for x = 1:(length(tempo2)-1)
pos = positioner(x);
%         end
% for i = (tempo2(x)+1):tempo2(x+1)
%     mat(k+1,i) = den3{i}(nod,position); % utbrytningsteg i
%     end
% kronologisk ordning. nod = nod + position. position kolumnnummer. Datat
% för det aktuella knippet, dvs 50T, finns i kolumnnummer 12.

[k, l] = size(mat);
% rpf3 = read_cms_dist(cmsinfo,'3RPF');
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    mat(k+1,i)=rpf3{i}(nod,position);
  end
end

[k,l]=size(mat);
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    mat(k+1,i)=exp3{i}(nod,position);
  end
end

[k,l]=size(mat);
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    mat(k+1,i)=tfu3{i}(nod,position);
  end
end

[k,l]=size(mat);
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    mat(k+1,i)=flx31{i}(nod,position);
  end
end

[k,l]=size(mat);
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    flx32{i}(nod,position);
    if flx32{i}(nod,position) >= 10;
      flx32{i}(nod,position)/10;
    elseif flx32{i}(nod,position)<1;
      flx32{i}(nod,position)*10;
    end

    mat(k+1,i)=ans;
  end
end

[k,l]=size(mat);
for x = 1:(length(tempo2)-1)
position = positioner(x);
  for i=(tempo2(x)+1):tempo2(x+1)

    mat(k+1,i)=tem{i};
  end
end

[k,l]=size(mat);
for x = 1:length(tempo2)-1
    position = positioner(x);
    for i=(tempo2(x)+1):tempo2(x+1)
        mat(k+1,i)=usteg(i);
    end
end

[k,l]=size(mat);
for x = 1:length(tempo2)-1
    position = positioner(x);
    for i=(tempo2(x)+1):tempo2(x+1)
        mat(k+1,i)=pow3(i);
    end
end

Resultat=[];
Resultat(:,1)=mat(8,:);
Resultat(:,2)=mat(7,:);
Resultat(:,3)=mat(3,:);
Resultat(:,4)=mat(2,:);
Resultat(:,5)=mat(1,:);
Resultat(:,6)=mat(4,:).*10^14;
Resultat(:,7)=mat(5,:).*10^13;

% Beräkning av PDE, dvs omvandla effekten i MW till effektdensitet i KWL
konstant=1e6/(365.76*157*21.5*21.5);
for i=1:length(POW_sim3)
    DPE(i)=POW_sim3(i).*RPD_sim3(i).*konstant;
end
DPE=DPE';
bor=[];

fid=fopen('exp.txt','r');
expfil = textscan(fid,'%s','delimiter','\n');
expfil = expfil{1};
fclose(fid);

for kk=1:length(cykelnamn)
    reply= expfil{kk};
    [A B C]=importdata(reply,'');

    j=1;
    [w,q]=size(A.textdata);
    for i=4:w

        utbranning(j,kk)=str2num(A.textdata{i,1});
        j=j+1;
    end

% utbranning=utbranning';
utbranning;
j=1;

[w,q]=size(A.data);
for i=1:w

    bor(j,kk)=A.data(i,3);
    j=j+1;
end
bor;

end
bor;
utbranning=utbranning./1000;

[w,q]=size(bor);
borz={};
utbranningz={};
bestfit={};
for i=1:q
    borz{i}=strcat('bor_', num2str(cykelnamn(i)));
    utbranningz{i}=strcat('utb_', num2str(cykelnamn(i)));
    bestfit{i}=strcat('utb_', num2str(cykelnamn(i)));
end

for i=1:q

    testa=isnan(bor(1,i));
    if testa ==1
        borz{i}=bor(2:end,i) ;
    end

end
```matlab
utbranningz{i}=utbranning(2:end,i);

elseif testa==0
    borz{i}=bor(:,i);
    utbranningz{i}=utbranning(:,i);
end
end

borz2={};
utbranningz2={};
for i=1:q
    for j=1:length(borz{i})
        if (borz{i}(j)>0)
            borz2{i}(j)=borz{i}(j);
            utbranningz2{i}(j)=utbranningz{i}(j);
        else
            break
        end
    end
end
for i=1:q
    bestfit{i}=polyfit(utbranningz2{i}(:),borz2{i}(:),1);
end

borreg1=[];
boreg3=[];
boreggg=[];
for x = 1:(length(tempo2)-1)
    boreg1=polyval(bestfit{x},utbsteg);
    boreggg=[boreggg boreg1];
    for i=(tempo2(x)+1):tempo2(x+1)
        boreg3=[boreg3; boreggg(i,x)];
    end
end
end
test=[];
boreg=[];
for i=1:length(boreg3)
    if (boreg3(i)>1)
        boreg(i)=boreg3(i);
    else
        boreg(i)=0;
    end
end
```
% resss=[utbsteg borreg];

disp (' [usteg] [TMOD] [3EXP] [3RPD] [3DEN] [3TFU] [3FLUX 1] [3FLUX 2] [BOR]
')
format short g
Resultat2=[Resultat borreg']

disp (' [usteg] [TMO] [3EXP] [3RPD] [3DEN] [3TFU] [3FLUX 1] [3FLUX 2] [BOR]
')

%% 3.1 Hvårjar sista steget i förloppet som först skapar en exempel.txt fil med en viss rutvald struktur.
%% Filen fylls sedan på med nedanstående specifika parametrar.
reply=input('Vill du fortsätta med laborationen? [Y/N] ', 's');

if reply=='Y'
  fid=fopen('50TRGU1-3.templ','r');
  TOCASMO = textscan(fid, '%s', 'delimiter', '
', 'whitespace', '');//
  TOCASMO = TOCASMO{1};
  fclose(fid);

  fid=fopen('exempel.inp','w');
  for i=1:106
    fprintf(fid, '%s
', TOCASMO{i});
  end

  cyklar= [1 tempo2(2:length(tempo2))+1];
  J=[];
  for kk=1:length(cyklar)-1
    for jj=cyklar(kk):cyklar(kk+1)
      J(jj)= cykelnamn(kk);
    end
  end

  TFU_sim3(:)=TFU_sim3+50

  for i=1:max(size(DEN_sim3))
    fprintf(fid, '*TTL * NOD=%s RRGU1 cy %1.0f
', num2str(nod), J(i));
    fprintf(fid, 'PDE %0.2f ' 'KWL' 
',DPE(i));
    fprintf(fid, 'COO %0.2f ' 
',DEN_sim3(i));
    fprintf(fid, 'TMO %0.2f ' 
',TMO_sim3(i));
    fprintf(fid, 'TFU %0.2f ' 
', TFU_sim3(i));
    fprintf(fid, 'BOR %0.2f ' 
',borreg(i));
    fprintf(fid, 'DEP %0.2f ' 
',DEP_sim3(i));
    fprintf(fid, 'STA
');
  end
end

% fprintf(fid,'********** The burnup has been corrected for by assuming correct Nd-isotopes concentrations and U-235 abundance\n');
% fprintf(fid,'DEP -65.8\n');
% fprintf(fid,'STA\n');

fprintf(fid,'END\n');
fclose(fid);

type exempel.inp
else
    break
end
end