Challenge of PWR new core design simulation: a focus on uncertainties due to nuclear data and reflector modelling

Y. Perin, A. Aures*, V. Salino***

*GRS mbH – Boltzmannstrasse 14 – 85748 Garching bei München – Germany
**IRSN – 31, avenue de la Division Leclerc – 92260 Fontenay-aux-Roses – France

Abstract:
This paper presents a new topic of collaboration between GRS and IRSN on reactor core calculation uncertainties. Two types of uncertainties affecting the predictions of power distribution in the core of a nuclear reactor are discussed: the uncertainties of basic nuclear data and those due to modelling approximations in reflector modelling. Overall, the results obtained at GRS and at IRSN are in good agreement. Furthermore, the paper raises new topics of interest which will be jointly studied.

1 INTRODUCTION

The core power distribution plays a key role for the determination of several critical safety parameters, such as the maximum fuel and cladding temperature or the minimum DNBR[1]. The uncertainties on power distribution are usually evaluated by means of comparison to core flux measurements. This solution is of course not available for new core design,. In the same time, those cores are challenging for the modelling due to innovations.
Monte Carlo codes, such as KENO, can solve the neutron transport equation without any approximations in the geometry or the material composition. This is why Monte-Carlo calculations can be used as numerical reference for the core power distribution.
The studied case is a part of the OECD/NEA UAM Benchmark, which defines so-called GEN-III case, with two core loadings: an UOX core and a partially MOX-loaded core, both surrounded with a massive steel reflector. In this study, IRSN and GRS decided to jointly assess the ability of their simulation codes' chains to predict core power distributions on thoses configurations.

2 ON APPROACHES OF MULTI-SCALE PROBLEMS IN REACTOR PHYSICS

The standard process for neutronic core simulation relies on a 3 levels multiscale approach. At the microscopic scale (first level), each neutron-nuclide interaction property is taken into account. They are treated and used in so-called lattice codes (second level) modelling the fuel assembly in 2D. The result of this step is a set of macroscopic cross sections which describes the properties of homogeneous meshes at the assembly scale. Finally those macroscopic cross-sections are used at the core scale in diffusion codes which compute the 3D core power distribution (third level).
Microscopic nuclear cross-sections are the basis of any reactor core simulation. They are measured in nuclear experiments and are closely evaluated before being released in standard nuclear data libraries. Different standard libraries exist and they can have a significative effect on the simulated core power distribution. Two of them: ENDF/B and JEFF are compared in Section 5.1. Any measurement has an uncertainty. The SCALE system provides a set of covariance matrices which contains an estimation of the uncertainties and

[1]Departure from Nucleate Boiling Ratio.

correlations in the basic nuclear data. These covariances come from a variety of sources, including ENDF/B-VI and VII, JENDL3.1 libraries. In Section 5.1, those nuclear data uncertainties are directly propagated through the whole calculation chain with the GRS code package XSUSA.
The second level is the assembly scale. In lattice codes, each fuel assembly type is modeled pin-by-pin. The lattice code performs a 2D multigroup transport calculation and generates macroscopic cross-section of the fuel assembly taking into account all the different materials (including fuel and moderator). This process is called homogenization. Depending on the modelling and on the numerical method, significative differences can appear in the resulting macroscopic cross-sections, and thus, in the core power distribution. A comparison of the power distribution computed with different macroscopic cross-sections is presented in Section 5.2.
At the core scale (third level), two kinds of source of uncertainties are investigated. The first one is the numerical method used to solve the diffusion equation in 3D. A comparison of the power distribution computed with different methods in both institutes is presented in Section 5.3. For that comparison, different codes using the same inputs are used. These inputs include : the geometry, the boundary conditions, and the macroscopics cross sections.
Concerning boundary conditions, the second source of uncertainties investigated is the reflector cross sections. Those reflector cross sections act as boundary conditions around the core in a deterministic diffusion calculation. They have therefore an influence on the radial power distribution. Regarding this specific point, the stainless steel reflector, also called heavy reflector, is challenging. The conventional method used in Section 5.2 to 5.3 consists in a flux-volume homogenization of the 1-D geometry representative of the reflector region, as it will be discussed in Section 5.4.
However, if the reflector cross sections are adjusted to fit the nominal power distribution, questions can be raised on the accuracy of power distribution computed with the same reflector cross sections in disturbed conditions such as accidental states. To study this issue, a new reference Monte Carlo calculation has been performed taking into account an hypothetic assymetric fuel temperature distribution. A comparison with the deterministic solution is discussed in Section 5.5.

3 PRESENTATION OF THE SIMULATION TOOLS

3.1 Monte Carlo Reference Code

A Monte Carlo calculation called hereafter “reference” performed with SCALE 6.0/KENO V.a multigroup is used in order to judge the quality of the deterministic results.
The reference calculations for both the UOX core and the MOX core are performed with the CSAS5 sequence of the SCALE6.0 code system [1]. First, this sequence undertakes the cross-section processing in the resolved and the unresolved resonance range to obtain a problem-dependent multigroup cross-section library. Afterwards, the transport calculation is performed with the three-dimensional (3-D) Monte Carlo code KENO V.a.

3.2 Lattice codes

In this study, the applied lattice codes for cross-section generation are the DRAGON code for IRSN and the NEWT code from SCALE 6.0 for GRS. First, the ENDF/B-VII.0 basic nuclear data library is used in both SCALE 6.0 and DRAGON. A second set of cross sections is generated with DRAGON using the JEFF basic nuclear data library. Comparison of the results obtained with those libraries demonstrates the influence of the basic nuclear data library.
NEWT is a two-dimensional (2-D) neutron transport code. It solves the multigroup transport equation using the discrete-ordinates (S_N) method. NEWT is used to prepare the 2-group collapsed weighted cross-sections for the core simulators QUABOX/CUBBOX and PARCS.

DRAGON [2] is an open source 3-D neutron transport code. The main existing methods are available in DRAGON to solve the multigroup transport equation (P_{ij}, S_N, MoC). In our case, we have used a combination of P_{ij} and MoC methods with a two-level lattice calculation, which is generally considered as a state-of-the-art calculation scheme. It is possible to use any ENDF-formatted nuclear data, such as ENDF/B from US or JEFF from Europe. Self-shielding and resonance effects are taken into account through state-of-the-art methods ; we selected a physical subgroup method also available in HELIOS or WIMS-7, combined with the 281 groups SHEM energy mesh.

3.3 Core Simulators

The diffusion codes are QUABOX/CUBBOX (in-house code) for GRS and DONJON (open source code) for IRSN. Both GRS and IRSN also applied the PARCS code which is available in the two organizations.
QUABOX/CUBBOX solves the space-time neutron diffusion equations using a flux expansion method. The spatial approximation of the neutron flux is done by a local polynomial expansion.This expansion can be done be either 2nd, 3rd or 4th order polynomials and also cubic splines. For this study, 4^{th} order polynomial is used.
In PARCS, different spatial approximations for the flux are available: the Finite Difference Method (FDM), the Analytic Nodal Method (ANM), the Nodal Expansion Method (NEM) and finally the hybrid ANM-NEM method which is the standard option. The hybrid method is used for this study.
Finally, a quadratic finite elements method is used in DONJON, although finite differences methods are also available.

3.4 The XSUSA code package for uncertainty analysis

The XSUSA code package [3] propagates nuclear-data uncertainties to uncertainties of integral quantities such as the multiplication factor and local quantities such as the power distribution. This method performs spectral calculations in BONAMI and CENTRM using the ENDF/B-VII nuclear data in the SCALE 238-group structure to obtain a problem-dependent cross-section library condensed into 44 energy groups. The application of SCALE 44-group covariance library allows then the generation of *N* problem-dependent multigroup cross-section libraries. With each library a transport calculation can be performed by NEWT to determine *N* perturbed, homogenized few-group cross-section libraries.
Subsequently, these *N* perturbed few-group libraries serve as a basis for core simulators such as QUABOX/CUBBOX. Finally, statistical analysis can be done on the results of all *N* core simulations.

4 CORE MODELS DESCRIPTION

4.1 Description of the cores

The following sections give descriptions of the so-called GEN-III core loadings used for this study. The specifications are taken from Exercise I-3 of the OECD/NEA Uncertainty Analysis in Modelling (UAM) benchmark [4].
The UOX core is built with four types of fuel assemblies distinguished by different enrichment values in terms of ^{235}U and by the use of Gd_2O_3 as a burnable neutron absorber.
The MOX core is set up with three different types fuel assemblies. Two of them are UOX assemblies with and without Gadolinium rods which are also found in the UOX core. The MOX fuel assembly consists of three different fuel rods with different Pu enrichment.
No burnup is considered and the thermal-hydraulic conditions are homogeneous in the core. They are representative of a hot full power state: moderator density is 702 kg/m³, fuel

temperature is 900 K. Moreover a boron concentration of 1300 ppm representative of a beginning of cycle is considered.

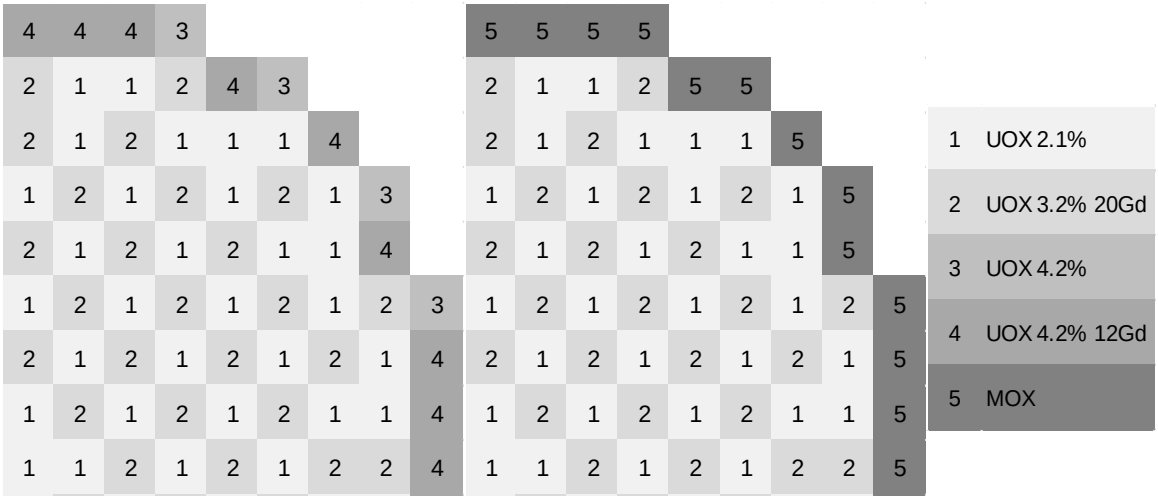

Figure 1 - Quarter core representation of the configurations of the two investigated GEN-III PWR cores: UOX core (left), MOX core (right)

4.2 KENO models

The UOX and the MOX core are built as 3-D models, however, no axial subdivision is applied to the fuel region. Both cores are surrounded radially by homogeneous assemblies containing stainless steel as a reflector material. Beyond them, borated water is present. Additionally, axial reflectors are modelled at the bottom and at the top of the fuel assemblies. Similar to the dimensions of the fuel assemblies, the axial reflectors are represented by assemblies that are filled with clads. These clads are surrounded by borated water, and at the bottom reflector they contain a zircaloy tube and helium, whereas the clads at the top reflector are filled with a diluted stainless steel composition to represent springs.
At both models, the fuel assemblies were placed in quarter symmetry.
The boundary conditions beyond the radially arranged borated water and beyond the axial reflectors are modelled as vacuum. The temperatures of the fuel and the structure materials are set according to the Hot Full Power condition specified in the benchmark.
To obtain Monte Carlo converged results, 20200 generations each with 50000 neutron histories were simulated. The first 200 generations were skipped with regard to source convergence. Moreover, the SCALE 238-multigroup ENDF/B-VII.0 library serves as a nuclear data library.
For the subsequent analysis of the power distribution, the fission rates of ^{235}U, ^{238}U were recorded in the UOX model and of ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am in the MOX model.

5 RESULTS OF THE UNCERTAINTY ANALYSIS

5.1 Uncertainty due to nuclear data

5.1.1 Effect of three nuclear data evaluations

DRAGON has the noticeable capability to be fed with any nuclear data, as long as it is properly formatted as defined by the international ENDF format. As an introduction to the sensitivity of nuclear data source, we compared the power distributions of the UOX core obtained with different nuclear data evaluations:

- the American nuclear data evaluation, ENDF/B-VII.0,
- the European nuclear data evaluation, JEFF-3.1.1,
- the older European nuclear data evaluation, JEF-2.2.

The calculation scheme described in Section 3.2 has been used in DRAGON to produce cross sections for DONJON, for the three cases.
The comparison of the radial power distributions (see Fig. 2) shows the following results:

- between ENDF/B-VII.0 and JEFF-3.1.1, the maximum deviation on core power distribution is 3%,
- between ENDF/B-VII.0 and JEF-2.2, the maximum deviation goes up to 8%.

The first result can be explained by the fact that ENDF/B-VII.0 and JEFF-3.1.1 exchanged data on both ways. For example, a lot of isotopes' evaluations are actually exactly the same in both evaluations.
The second result shows the continuous development of the basic nuclear data and underlines the convergence of the different evaluations shown in the first result. In the rest of the study, only ENDF/B-VII.0 is used.
Those discrepancies are only a starting point. As we will see in the next section, the discrepancies are smaller than the global uncertainties due to nuclear data that we can estimate using sensitivities and covariance matrix methods. Indeed, the interest of covariance matrices is to take into account the state-of-the-art uncertainties on nuclear data, including those coming from experiments used for nuclear data measurement. This is the best way to evaluate properly the uncertainties due to nuclear data.

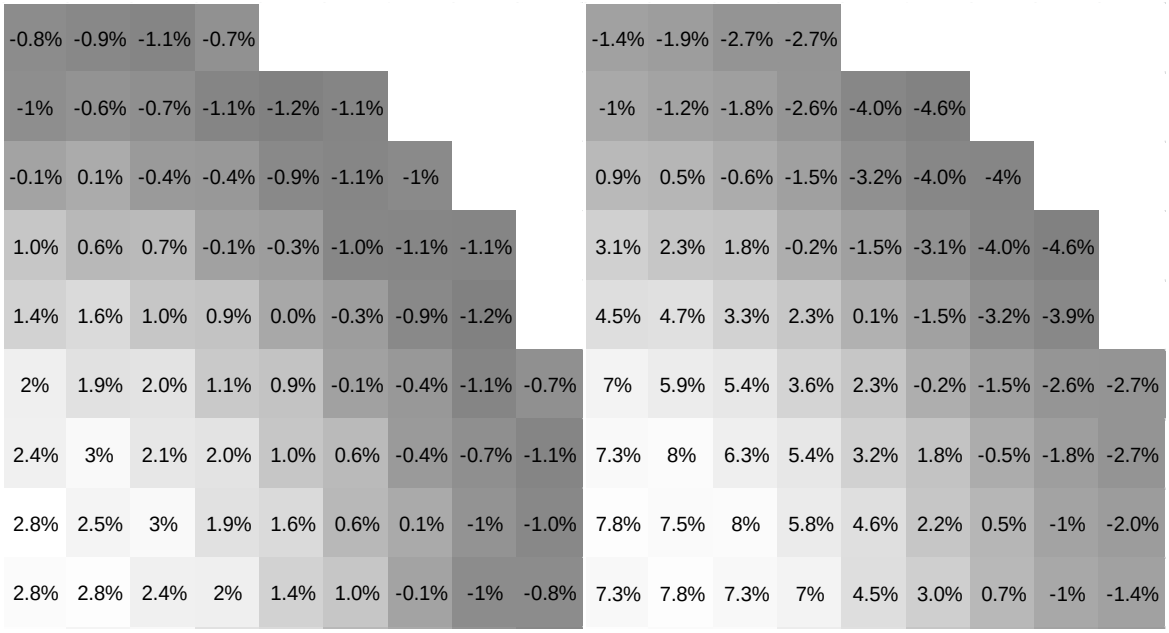

Figure 2 - Relative standard deviations for the power distribution in the UOX core obtained with different nuclear data libraries – ENDF/B-VII.0 vs JEFF 3.1 (left) and ENDF/B-VII.0 vs JEF 2.2 (right). Results obtained with DRAGON and DONJON.

5.1.2 Propagation of uncertainties due to nuclear data

The following results have already been presented in details in Ref. [5].
Applying the method described in Section 3.4 with N = 300, as sample size, we generated 300 sets of complete 2-group macroscopic cross-section libraries. These few-group libraries serve as input for QUABOX/CUBBOX which calculates the power distribution for each individual run.
The distribution of the uncertainty (relative standard deviations) shows a similar behaviour in both UOX and MOX cores. The uncertainty is distributed in rings where the maximum is reached in the center of the core and the minimum in halfway between the center and the outer boundaries of the core (see Fig. 3). The magnitude of the uncertainty is significantly higher in the MOX core. While the maximum uncertainty reaches 13% at the center of the MOX core (see Fig. 3 – right side), it is only 5.3% in the UOX core (see Fig. 3 – left side). This is due to the larger uncertainty on the Plutonium than the on Uranium isotopes.
The uncertainties calculated with XSUSA/KENO (not represented here) are in excellent agreement, thus showing that the nuclear data uncertainty quantification is independent from whether the method used is Monte-Carlo or deterministic.

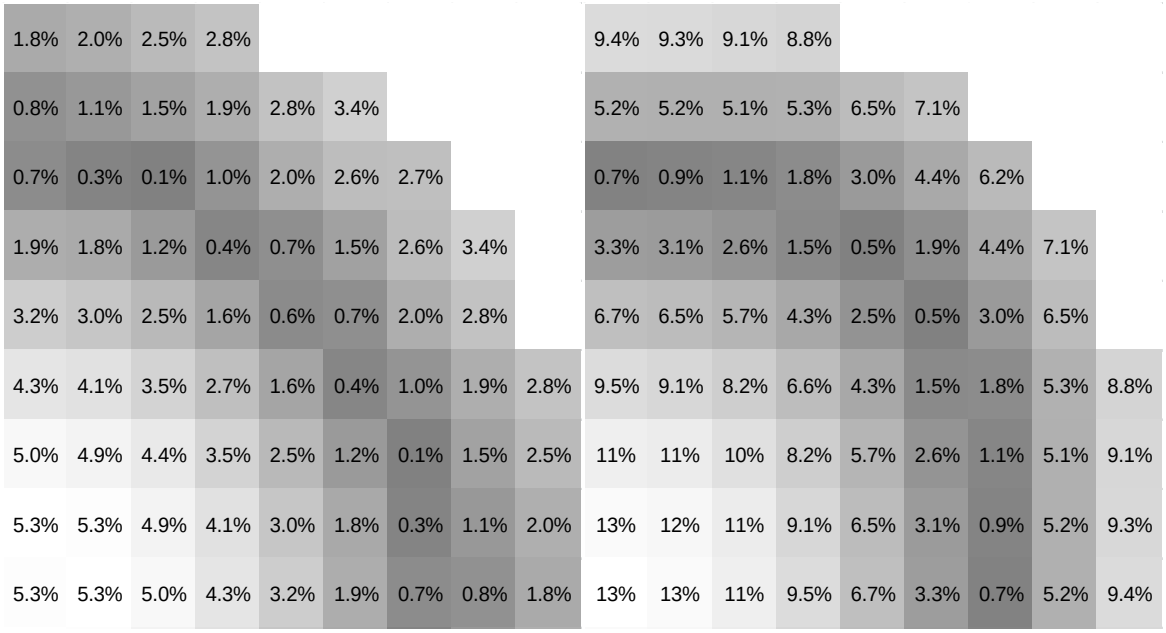

Figure 3 - Relative standard deviations for the power distribution of the UOX core (left) and of the MOX core (right) obtained by XSUSA, NEWT and QUABOX/CUBBOX.

5.2 Effect of different assembly calculation schemes

In this section, the power distributions issued from the same nuclear data (ENDF/B-VII.0) but using different assembly calculation scheme are compared.
In particular, the NEWT code is used and the produced cross sections are introduced in DONJON. The result is compared to a classical DRAGON-DONJON result.

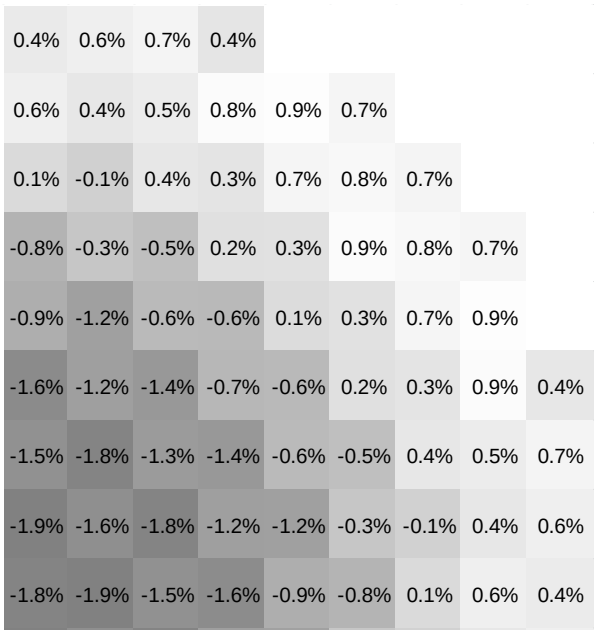

Figure 4 - Relative differences of the UOX core power distributions between NEWT+DONJON and DRAGON+DONJON (using ENDF/B-VII.0 standard library). Quarter symmetry is displayed.

As it can be observed on Fig. 4, the maximum discrepancy is 2%, where we could meet up to 8% for discrepancies due to nuclear data. This result shows that nuclear data prevails over assembly calculation scheme concerning power distributions. Other parameters, such as pin-by-pin power, are known to be more sensitive to assembly calculation scheme.
In all the following sections, DONJON will always be fed with cross sections issued from DRAGON, while QUABOX/CUBBOX will always use cross sections from NEWT.

5.3 Effect of different core simulators

In this section, we compared the various deterministic calculations between them.

5.3.1 UOX Core Results

When using the cross sections calculated by NEWT, the maximum deviation between PARCS and QUABBOX/CUBBOX is 3% when PARCS is used with it's ANM solver (see Fig. 5 – left side). When using NEM solver of PARCS, the maximum deviation drops to 1%. More specifically, it can be seen that QUABOX/CUBBOX slightly underpredicts the power in the assemblies with burnable absorber rods, whereas PARCS slightly overpredicts the power in the pure UOX assemblies. The relative difference between the QUABOX/CUBBOX and the PARCS radial power reveals a gradient from the edge toward the center of the core.
On the other side, when using the cross sections calculated by DRAGON, the maximum deviation between PARCS with it's NEM solver and DONJON is 1.5% (see Fig. 5 – right side).
We can see that the effect of the core simulator is indeed very small, as long as diffusion equation is used in all cases, with the same cross sections.

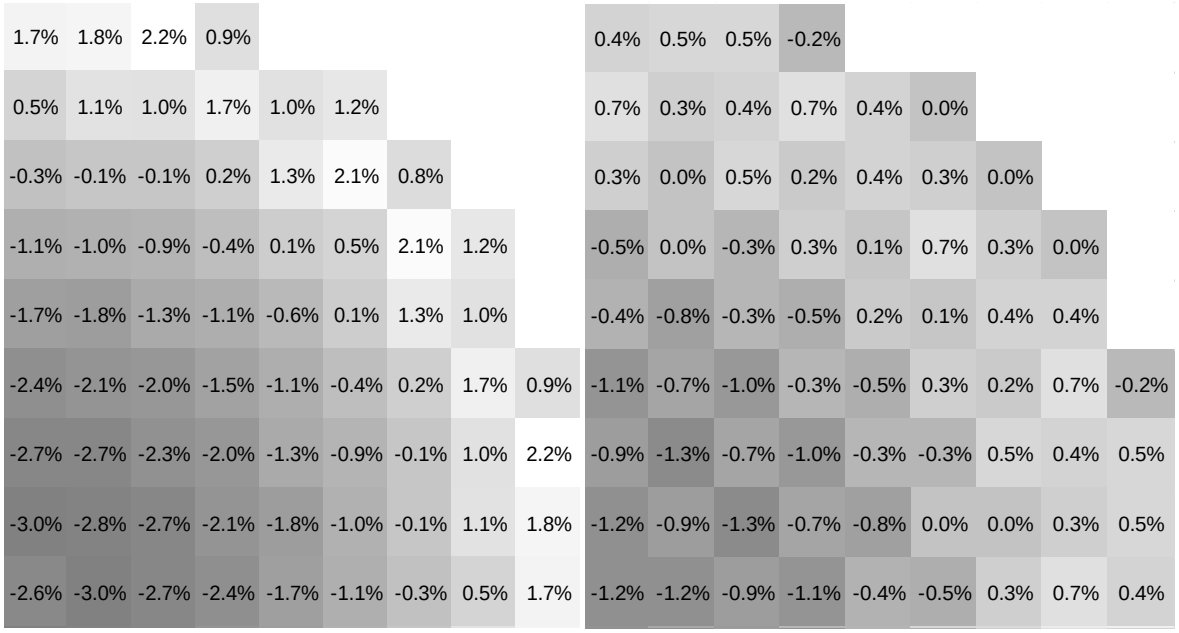

Figure 5 - Power distribution in the UOX core: relative differences between the QUABOX/CUBBOX and PARCS results both using a cross-section library generated with NEWT (left) and DONJON and PARCS results both using a cross-section library generated with DRAGON (right). Quarter symmetry is displayed.

In order to compare the deterministic calculations which use different cross sections, we must use a common reference to judge the various results. The reference used is the KENO Monte-Carlo calculation (see Fig. 6 – left side), which avoids the main approximations of deterministic calculations[2], as seen in Section 3.1.
As we can see in Fig. 6 (right side), a very good agreement is reached between KENO and QUABBOX/CUBBOX, with a maximum deviation of 3%. The same figure is obtained when comparing PARCS with NEWT cross sections and KENO (see Fig. 7 – left side).
However, the maximum deviation between DRAGON-DONJON and KENO results is larger (up to 7.8%, see Fig. 7 – right side). This result will be explained in Section 5.4.

[2] Except for the multigroup approximation.

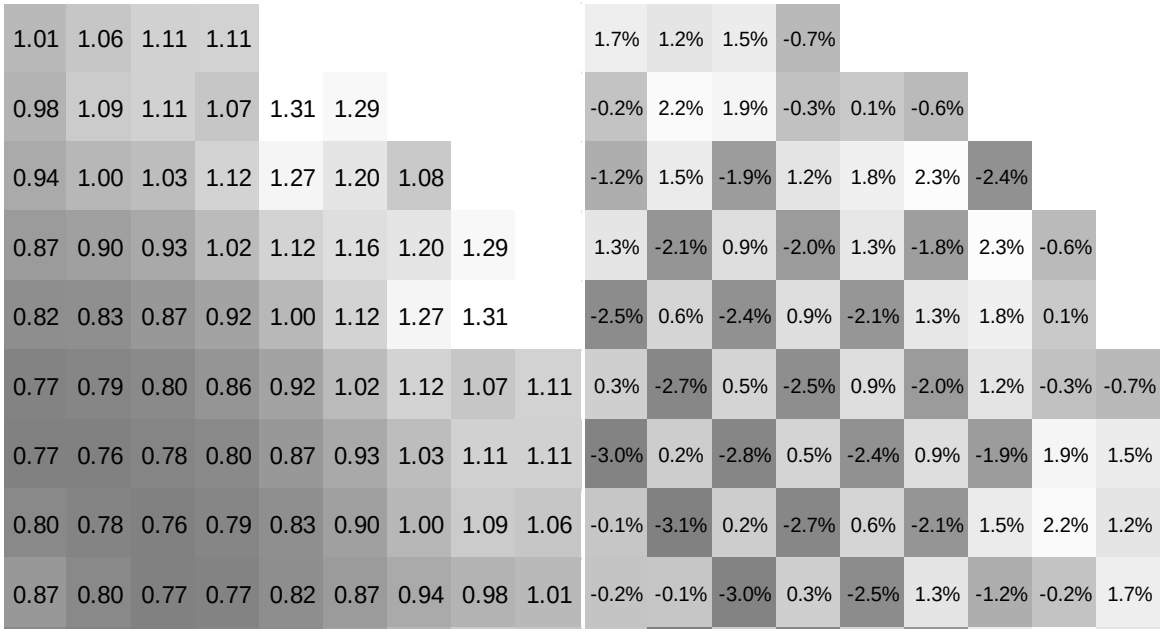

Figure 6 - Power distribution in the UOX core: KENO V.a results (left) and relative differences between KENO V.a and QUABOX/CUBBOX results (right). Quarter symmetry is displayed.

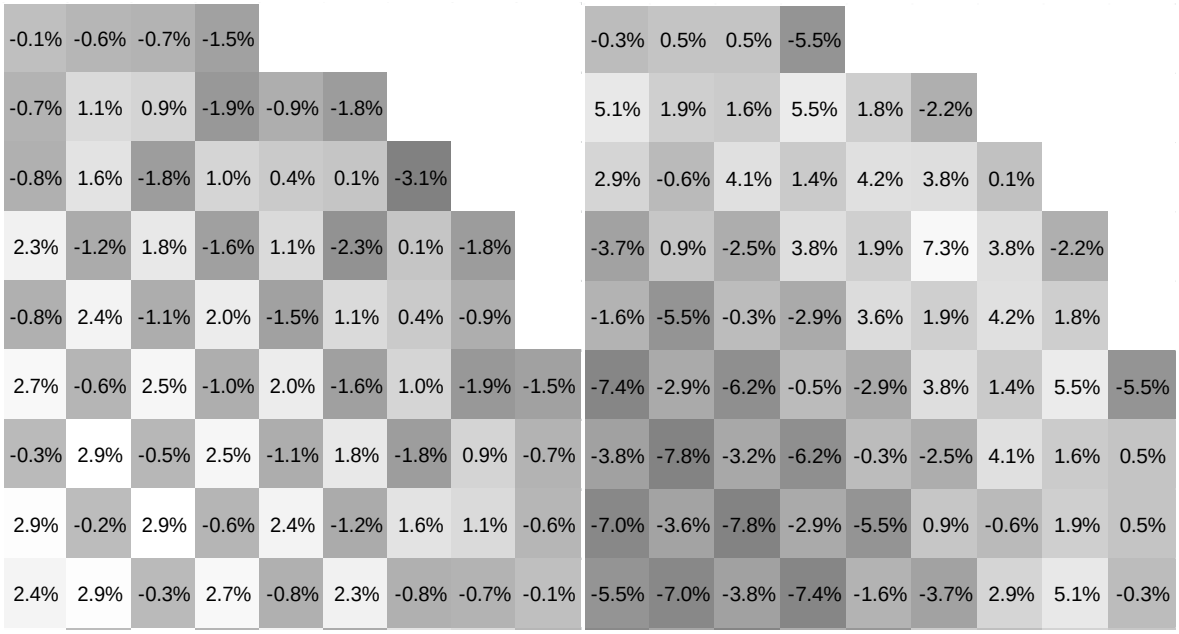

Figure 7 - Power distribution in the UOX core: relative differences between the PARCS – cross-section library generated with NEWT – and KENO V.a results (left) and between DONJON – cross-sections generated with DRAGON – and KENO V.a (right). Quarter symmetry is displayed.

5.3.2 MOX Core Results

Figure 8 (left side) shows the radial core power distribution obtained from the KENO reference calculation. The relative difference with the QUABOX/CUBBOX (Figure 8 – right side) and with the PARCS (Figure 9 – left side) solutions shows a rather good agreement between the stochastic and the deterministic codes. The maximum deviations for the partially MOX loaded core are slighty larger than for the UOX core, which can be explained by the strong flux spectrum heterogeneity, caused by the presence of Plutonium. The relative difference between the QUABOX/CUBBOX and the PARCS radial power distributions is presented in Figure 9 (right side). Except for a few assemblies next to the reflector, the same gradient as in the UOX core is observed. Since the two codes are using the same cross-

section libraries and the same boundary conditions, the differences only comes from the different numerical methods.
In conclusion, we observed that switching from one simulator code to another yields only a couple of percents of differences in the power distribution.

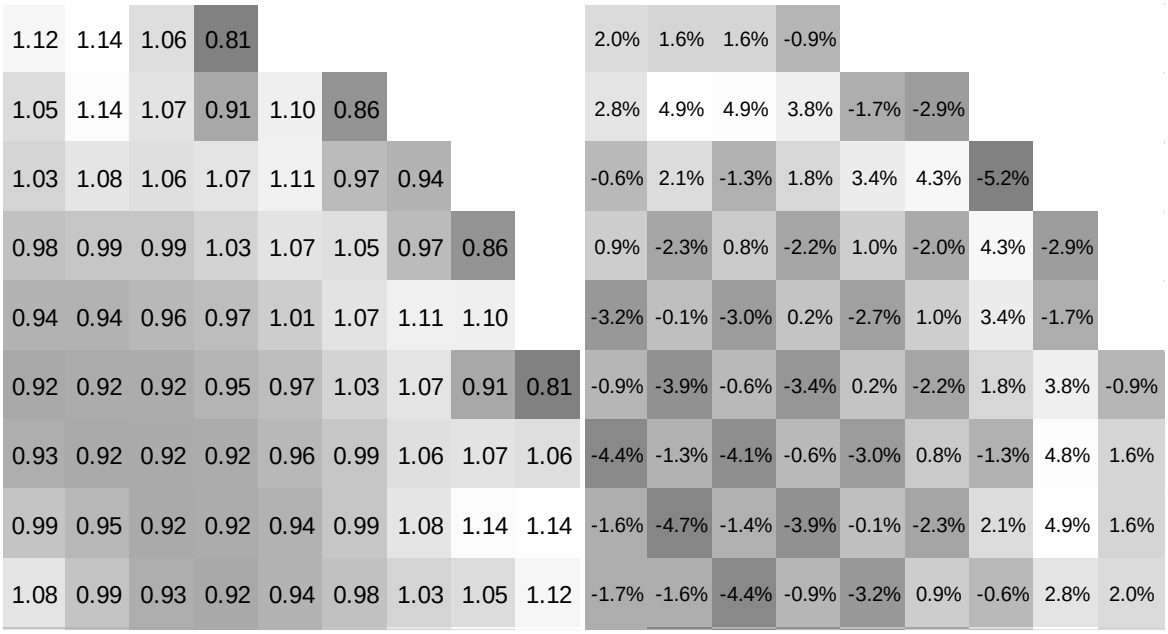

Figure 8 - Power distribution in the MOX core: KENO V.a results (left) and relative differences between KENO V.a and QUABOX/CUBBOX results (right). Quarter symmetry is displayed.

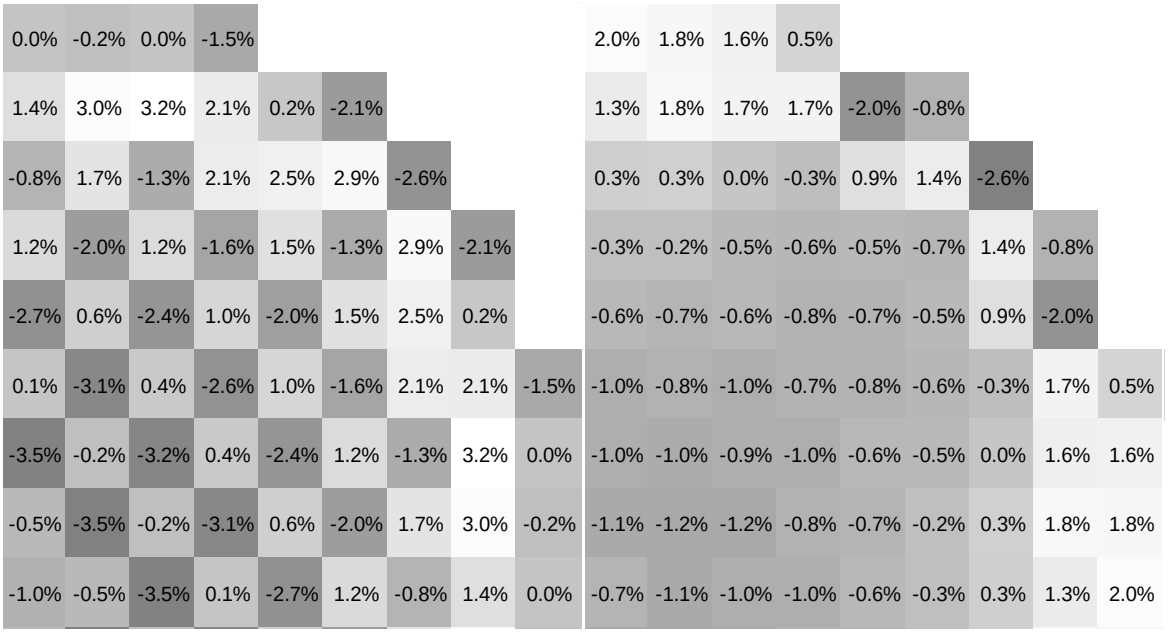

Figure 9 - Power distribution in the MOX core: relative differences between PARCS and KENO V.a results (left); PARCS and QUABOX/CUBBOX results (right) for the MOX core. Quarter symmetry is displayed.

5.4 Reflector Modelling

Beside macroscopic cross sections, other sensitive inputs of core models are the reflector cross sections. Those reflector cross sections act as boundary conditions around the core in a deterministic diffusion calculation. This is why they have an influence on radial power distribution.
For this paper, we used a conventional method. A 1-D geometry representative of the reflector region is computed with a transport code, NEWT. The steel reflector region is homogenized to obtain the reflector cross sections. Then, an iterative process is used in order to adjust those cross sections. Various modifications of the geometry and to the obtained cross sections are made to find a power distribution with QUABOX/CUBBOX which is very similar to the one obtained with KENO. This widely used "minimization" procedure done on the reflector cross sections leads to small discrepancies between the reference calculation and the deterministic calculation.
In our case, this procedure has been performed using ENDF/B-VII.0 with NEWT and QUABOX/CUBBOX. As it is very sensitive, any significant change can lead to a greater deviation. For instance, this is the main reason for the larger discrepancy between DRAGON-DONJON and KENO. Indeed reflector cross sections used have been optimized through QUABOX/CUBBOX and KENO comparisons. A future work is foreseen in IRSN to perform a similar minimization using JEFF-3.1.1 with DRAGON and DONJON.

5.5 Preliminary investigation on abnormal state

Uncertainty evaluation is usually performed on a core placed in its normal state which is the case for all the work presented from Section 5.1 to Section 5.4.
Nevertheless, as far as safety is concerned, the question of uncertainties evaluation in abnormal state is raised. Especially, the minimization-fitting process used to find the reflector cross sections (done in normal state) may lead to an increase of the uncertainty when the core is placed in an abnormal state. Using the reflector cross sections from normal state into an abnormal state is an extrapolation made for accidental state.
This approach is tested thereafter. The selected "abnormal" state has been chosen in order to allow an easy modelling in a Monte-Carlo calculation. This hypothetic case differs from the reference "normal operating" case, by dropping from 900K to 600K the fuel temperature in one quarter of the core (see Fig. 10).

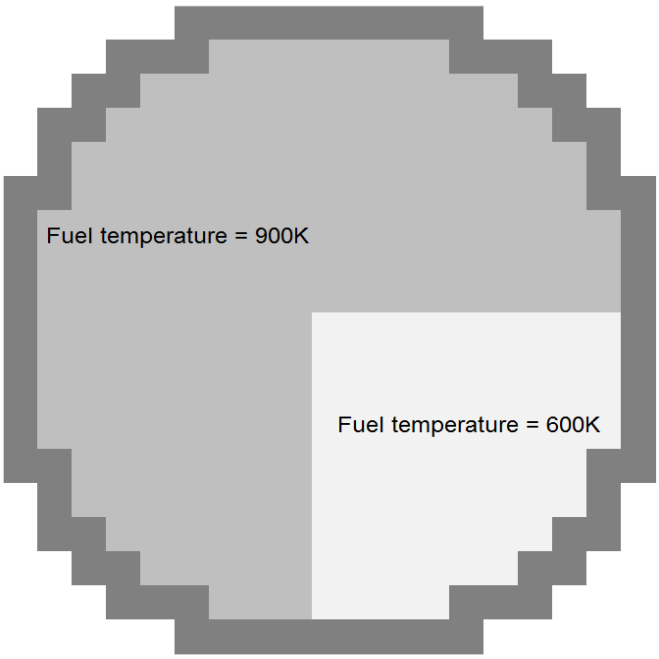

Figure 10 - Core fuel temperature distribution for a hypothetical perturbed asymmetric case

Deterministic calculations have been performed using the tools presented previously. Reflector cross sections used are also the one described in Section 5.4 . In order to quantify the discrepancy, a new KENO Monte-Carlo reference calculation of this abnormal state (see Fig. 11) has been computed.

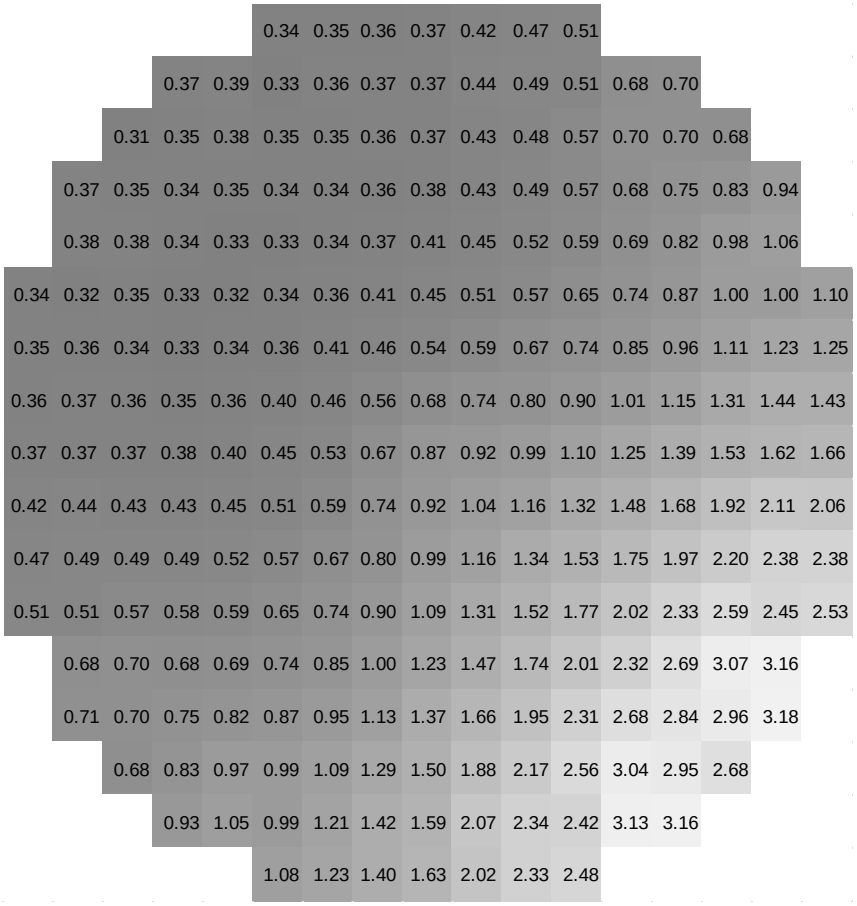

Figure 11 - KENO V.a power distribution of the pertured UOX core

The increases of deviation between the results from KENO and the one from the deterministic codes are the following:
We observe a slight – but existing – increase of deviation between the results from KENO and the one from the deterministic codes. The following raises of deviation, compared to the ones showed in Section 5.3, are observed:

- 1% raise when considering QUABOX/CUBBOX (see Fig. 12),
- 2% raise when considering PARCS (see Fig. 13),
- 1% raise when considering DONJON (see Fig. 14).

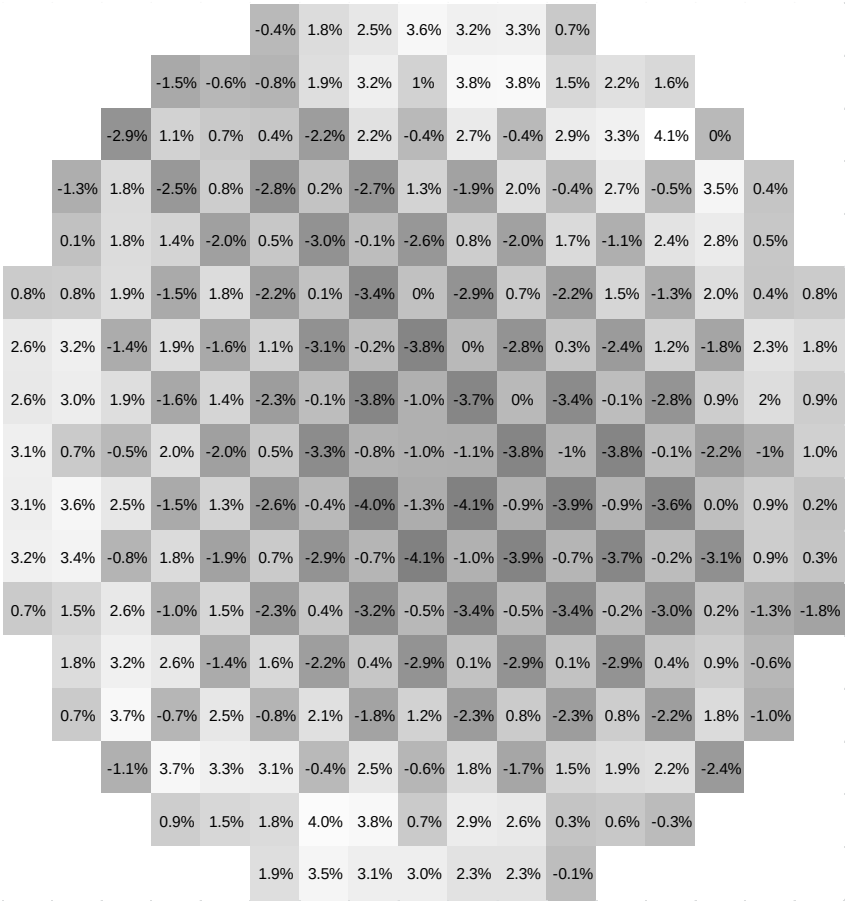

Figure 12 - Power distribution of the perturbed UOX core: relative differences between QUABOX/CUBBOX and KENO V.a

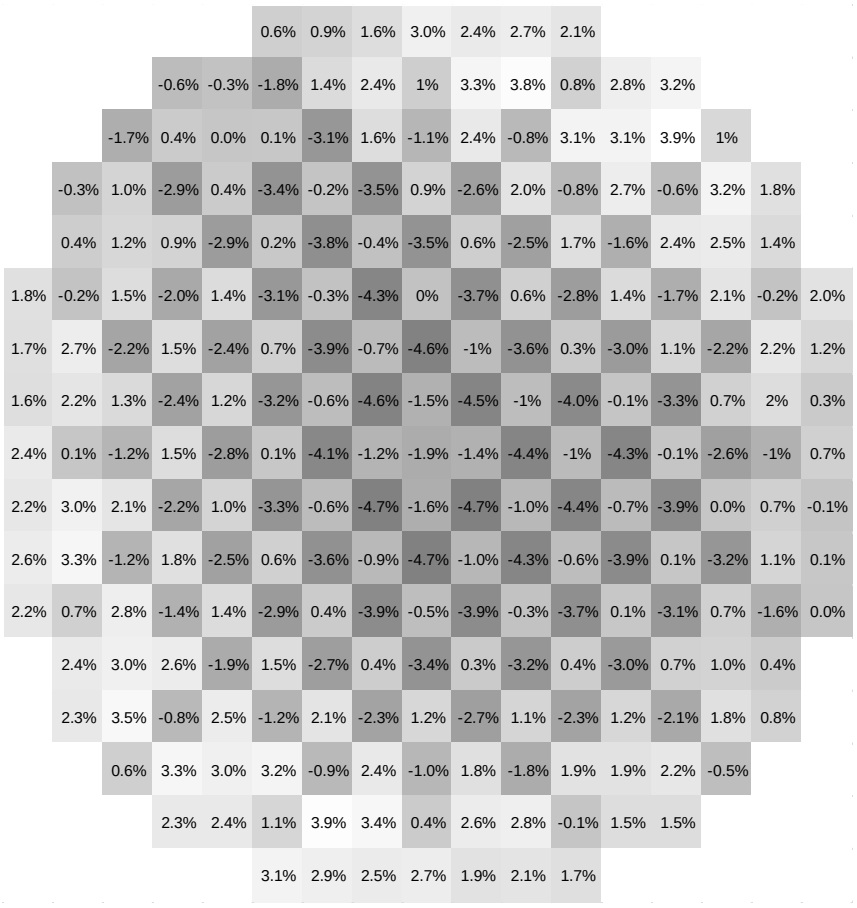

Figure 13 - Power distribution of the perturbed UOX core: relative differences between PARCS and KENO V.a

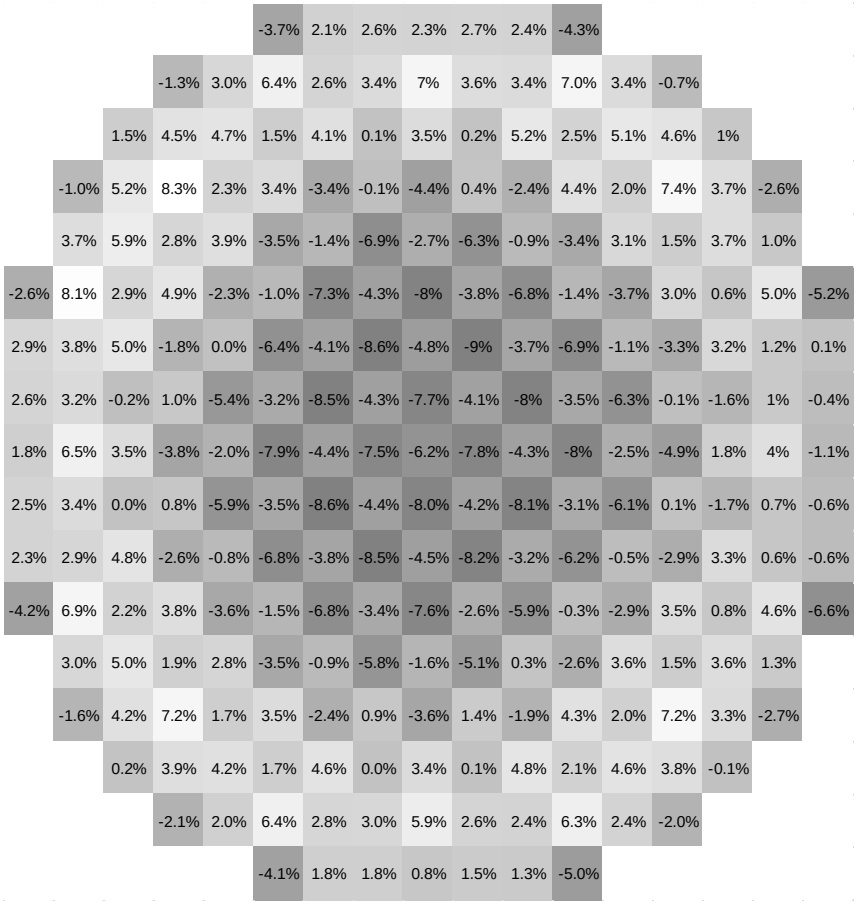

Figure 14 - Power distribution of the perturbed UOX core: relative differences between DONJON and KENO V.a

The order of magnitude of the increase of discrepancy on a very simple case on a UOX core is sufficient to trigger additionnal studies on states closer to more realistic accidental scenario.

6 CONCLUSIONS

The core power distribution plays a key role for the determination of several critical safety parameters. Different type of uncertainties affect the core power distribution.
Epistemic uncertainty due to basic nuclear data is one of the main important source of uncertainty. The precise quantification of these uncertainties should be performed with state-of-the-art method taking into account covariance matrices. This uncertainty also concerns the reference computation even if the reference is a Monte Carlo simulation. It is also important to note that nuclear data uncertainty more than doubles in presence of MOX assemblies.
The different numerical methods used in the core simulator also introduce discrepancies, which are usually small.
The stainless steel reflector is also a challenge for modelling. The reflector cross sections can be “tuned” to minimize the deviation with the reference as discussed in Section 5.4. Therefore, on going work investigates the consequences of this methodology on power distribution prediction accuracy in abnormal situations. In the simple example chosen here, the discrepancy increase was a couple of percents.
Quantification of uncertainties on core modelling is important for safety. This is why GRS and IRSN will continue joining their efforts on these topics.

ACKNOWLEDGEMENTS

This work was supported by the German Ministry of Economics and Technology. Valuable contributions by M. Klein are appreciated.

REFERENCES

[1] SCALE: A Comprehensive Modelling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee, June 2011. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785

[2] "*Towards DRAGON Version4*", A. Hébert, PHYSOR 2006 Conference, Vancouver, Canada.

[3] "*Influence of Nuclear Covariance Data on Reactor Core Calculations*", W. Zwermann, B. Krzykacz-Hausmann, L. Gallner, A. Pautz, WONDER 2009, Sep. 29 – Oct. 2, Cadarache (2009)

[4] Benchmark for Uncertainty Analysis in Modelling (UAM) for the Design, Operation and Safety Analasis of LWRs, Volume 1: Specification and Support Data for Neutronics Cases (Phase I), NEA/NSC/DOC(2013)7, K. Ivanovet al.

[5] "*Interaction of Loading Pattern and Nuclear Data Uncertainties in Reactor Core Calculations*", M. Klein, L. Gallner, B. Krzykacz-Hausmann, A. Pautz, K. Velkov, W. Zwermann, PHYSOR 2012, Knoxville, Tennessee, USA