M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

Uncertainty Analysis for VVER-1000 Core Simulations with MCNP/ATHLET

Wolfgang Bernnat, Nicole Guilliard, Janis Lapins

Institute for Nuclear Technology and Energy Systems, Universität Stuttgart, Pfaffenwaldring 31, 70550 Stuttgart, Germany
wolfgang.bernnat@ike.uni-stuttgart.de, nicole.guilliard@ike.uni-stuttgart.de, janis.lapins@ike.uni-stuttgart.de

Alexander Aures, Friederike Bostelmann, Jérémy Bousquet, Kiril Velkov, Winfried Zwermann

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Boltzmannstraße 14, 85748 Garching, Germany
Alexander.Aures@grs.de, Friederike.Bostelmann@grs.de, Jeremy.Bousquet@grs.de, Kiril.Velkov@grs.de, Winfried.Zwermann@grs.de

Abstract – *Based on a coupling scheme between the Monte Carlo neutron transport code MCNP6 and the thermo-hydraulics code ATHLET, developed earlier, steady-state calculations for the full-power state of a VVER-1000 reactor core specified within an OECD/NEA benchmark were performed. This was done with the multi-group option of MCNP6, with self-shielded cross sections for all materials generated beforehand with the SCALE 6.1.2 code system, thus enabling uncertainty and sensitivity analyses with respect to the underlying nuclear data using the XSUSA package. Nuclear data and covariance data are taken from SCALE 6.1.2. Analyses were also performed with stand-alone MCNP6 calculations, yielding results for radial power distribution not much different from results obtained with continuous-energy data in the framework of the benchmark, confirming the high quality of the multi-group approach. Uncertainties in the radial power distribution are significant, with values of up to 9% for the relative standard deviation in the core center. The obtained uncertainties in the radial power distribution from the coupled MCNP6/ATHLET simulation are very similar to those from the stand-alone MCNP6 calculation, meaning that the thermo-hydraulic feedback does not significantly change the uncertainties. Sensitivity analyses show that the main contributions to the uncertainties in the radial power distribution are due to uncertainties in the average number on neutrons per fission of ^{239}Pu.*

I. INTRODUCTION

For many decades, nodal diffusion-based codes, either with an intrinsic modelling of thermo-hydraulic processes, or with an external coupling to a thermo-hydraulics (TH) code, have successfully served for simulating the steady-state and transient behavior of (mainly light water) reactor cores. However, these methods introduce a number of approximations, mainly the description of the neutron transport by diffusion theory, possibly with corrections to account for transport effects, a coarse representation of the energy dependence with a small number of energy groups, and a coarse representation in space, with nodes typically of the linear size of fuel assembly widths. By the nodal approach, local effects on the fuel pin level cannot be directly captured in the core simulation, but rather have to be described approximately by pin power reconstruction methods from the nodal full-core solution and the pin-wise fluxes in the individual fuel assemblies pre-calculated by a lattice code.

To avoid the approximations mentioned above, one can perform the core simulation directly with the Monte Carlo (MC) method with a high resolution of the energy and spatial dependence of cross sections and fluxes. In recent years, it has become possible by the increasing computer power to perform MC full-core simulations with a sufficiently high number of neutron histories to obtain a local resolution of the pin power distribution with statistical uncertainties on the percent level [1]. Such MC calculations for the neutron transport can also be coupled to a TH code, which again will significantly increase the computational effort. For steady-state simulations, this has been realized by coupling MCNP6 [2] with the system code ATHLET [3]; a description can be found in [4].

In stand-alone MC full-core simulations of large reactor cores with constant TH parameters, it has turned out, e.g. in the framework of the UAM-LWR workshop [5], that uncertainties in the underlying nuclear data may cause a substantial uncertainty in the output quantities, in particular in the radial power distribution. Therefore, it is advisable to evaluate uncertainties also for coupled MC/TH calculations. In the present contribution, an approach is being presented to perform such uncertainty analyses for coupled MCNP6/ATHLET full-core simulations. To this end, the sampling-based uncertainty analysis package XSUSA [6] is used. As application case for evaluating nuclear data uncertainties for a light water reactor core calculation, a core from the OECD/NEA VVER-1000 MOX Core Computational Benchmark has been chosen [7].

II. THE VVER-1000 MODEL

The original benchmark as specified in [7] describes a two-dimensional arrangement. It is a mixed UO_2/MOX core

with fuel assemblies at various burn-up states, represented by corresponding isotopic compositions given in the benchmark specification. One peculiarity of the arrangement is that the MOX fuel contains plutonium with a high amount of ^{239}Pu and ^{241}Pu.

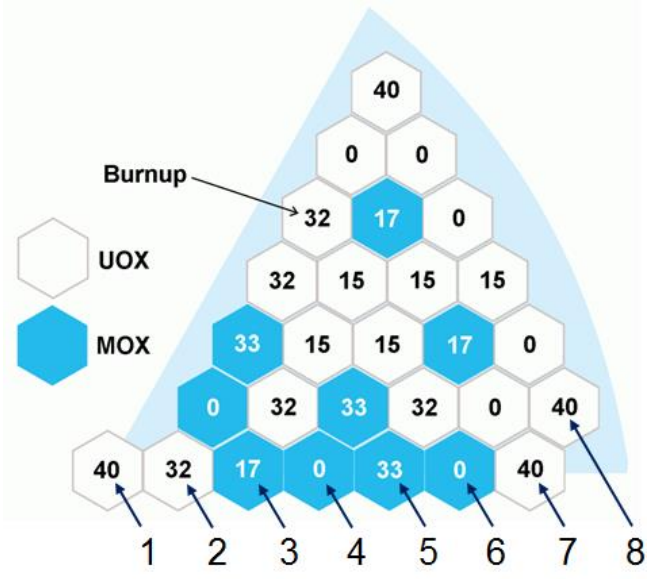

Fig. 1. Horizontal cut of the VVER-1000 MOX core in 1/6 core representation.

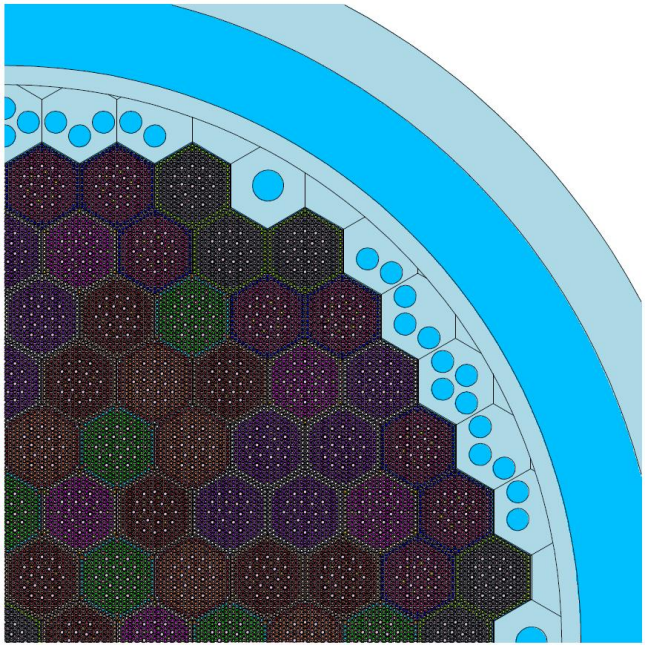

Fig. 2. Horizontal cut of the VVER-1000 MOX core model in detail.

A horizontal cut is sketched in Fig. 1, where the positions of UO_2 and MOX fuel assemblies are indicated as well as the individual burn-up levels in units of GW-days per metric ton of initial heavy metal. Figure 2 illustrates the detailed spatial resolution of the calculation model described below. For the present analysis, the benchmark model has been expanded in axial direction to allow for a TH parameter distribution representing the full-power state. Also, a lower and an upper plenum were added for an approximate modelling of a real reactor core. The isotopic compositions in the individual fuel assemblies are taken from the specification, without an axial burn-up distribution, because it is outside the scope of the paper to perform cycle burn-up calculations.

III. CALCULATION METHODS

This section briefly describes the calculation methods used for performing coupled full-core simulations accompanied by sampling-based uncertainty and sensitivity analyses with respect to the basic nuclear data.

1. Steady-State MCNP6/ATHLET Core Simulations

The calculations with MCNP6 for the neutron transport and ATHLET for the thermo-hydraulics are performed with an iterative coupling scheme. A first MC calculation is performed with a guess for the TH parameters. The power distribution resulting from this calculation then is passed to the TH code, which subsequently calculates the corresponding set of TH parameters for the axial sections of the TH channels. Here, one TH channel per fuel assembly is chosen, without cross flow between the sub-channels. This is no principal restriction; a sub-channel code could be used as well, however again with a drastic increase of the computation time. The TH parameters of this calculation are then used for the next MC calculation step. This procedure is continued until convergence is reached. The coupling to the thermo-hydraulics may require the application of a relaxation method to improve or achieve convergence.

For an efficient use of MCNP6 with a huge number of materials at different temperatures and densities, a modification to MCNP6 is used that allows the transfer of the distribution of these parameters via an interface file without the necessity of changing the user input [4]. Cross sections are available on a grid of the TH parameters; for values not directly lying on the grid points, linear combinations of the cross sections are used with appropriate weights. In contrast to most of the coupled MCNP6/ATHLET analyses performed so far, which used cross section data in continuous-energy representation, for the present study multi-group data suitable for MCNP6 have been generated in order to be able to perform the corresponding subsequent uncertainty analyses with XSUSA. The MCNP6 calculations were performed with 640 active cycles after 35 inactive cycles with 680,000 neutrons per generation. For a well converged MCNP6/ATHLET solution, about 6-8 iteration steps were required, leading to a total computing time per coupled simulation of approx. 6x60 - 8x60 min on a Cray XC40 cluster with Intel Xeon processors, each with 144 processors

per MCNP run. Using SPMD instructions always 25 parameter variations were processed at same time.

2. Multi-Group Cross Section Generation for MCNP6

The multi-group cross sections are provided in high spatial resolution, i.e. for all fuel pins with individual isotopic compositions on a grid of the TH parameters. These are the fuel temperature, for which the grid points are 575 K, 900 K, and 1300 K, and the moderator temperature with 560 K, 580 K, and 600 K. The resonance self-shielding calculation is done by the standard sequence T-XSEC (with BONAMI using Bondarenko factors in the unresolved resonance region and CENTRM/PMC solving the transport equation with continuous-energy cross sections in the resolved resonance region) from the SCALE 6.1.2 code system [8] using ENDF/B-VII.0 based cross section data. Due to the large number of individual cross section sets, and by a multiplication with the sample size (see the next subsection), a huge amount of cross section data has to be handled. To reduce this amount of data, the original master library with 238 energy groups has been pre-collapsed with a representative LWR spectrum to 44 energy groups. This finally yields macroscopic self-shielded cross section sets in AMPX format, which cannot directly be used with MCNP6. An additional processing step is required, namely the transformation of these AMPX libraries into MCNP TYPE1 multi-group format. This is accomplished by the CRSRD code [9] which is capable of making cross sections in various common formats available for MCNP multi-group calculations. These data would be sufficient for performing the MCNP6 transport calculations; however, for the coupling to a TH code, the spatially resolved power distribution is required, usually evaluated in MCNP by specifying a so-called F7 tally. For this, the pin-wise macroscopic cross sections have to contain $\kappa \sigma_f$, the fission cross section times the energy per fission. In order to provide the macroscopic cross sections for the individual fuel materials, extra pin-cell calculations were performed with the S_N code NEWT from the SCALE 6.1.2 system before transforming the AMPX libraries to MCNP TYPE1 multi-group format. The file size for the cross sections of all materials in an individual TH state is approx. 13 – 15 MB; with nine combinations of TH parameters and a sample size of 1000 (see below), the total amount of cross section data is approx. 130 GB.

3. Uncertainty Analyses

With the set of MCNP TYPE1-formatted cross sections, everything is in place to run a full nominal steady-state core simulation with MCNP6/ATHLET. For performing uncertainty analyses, a sampling-based procedure is applied: variations of the microscopic cross sections are generated with XSUSA on the basis of the corresponding uncertainty data available in so-called covariance matrices. A set of covariance data in multi-group representation (the same 44-group structure to which the cross sections were collapsed) is included in the SCALE 6.1.2 system and has been used for the present study. After the variation of the shielded cross sections in AMPX format, and again generating (varied) MCNP TYPE1-formatted data, a number of coupled MCNP6/ATHLET calculations corresponding to the sample size can be performed; in the present study, a sample size of 1000 has been chosen to be able to determine the main contributors to the uncertainties via a sensitivity analysis in spite of the high CPU time demand.

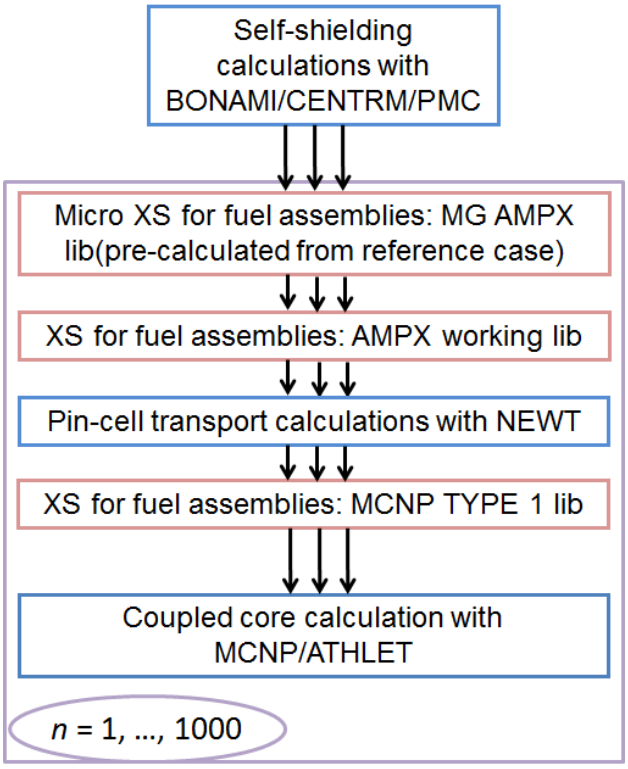

Fig. 3. Flow diagram of the calculation chain.

A flow diagram of the calculation chain including the variations is given in Fig. 3. Here, the multiple arrows indicate that the calculations have to be performed for a variety of fuel assemblies on a grid of TH parameters, and *n* denotes the elements of the sample. Finally, output uncertainties corresponding to the input nuclear data uncertainties can be evaluated by determining mean values and standard deviations from the set of simulation results for quantities of interest, such as assembly powers.

With XSUSA, the variations are applied to the shielded cross sections; this means that it is assumed that the cross section variations are propagated unchanged through the resonance self-shielding calculation, and thus implicit effects are currently not considered. However, a method for taking the change of the cross section variation in the self-shielding calculation into account by means of perturbation theory is under investigation [10].

4. Sensitivity Analyses

By sensitivity analyses, it is possible to determine the contributors (certain reaction cross sections of certain isotopes) to the output uncertainty [6]. To do so, a group sensitivity analysis is well suited, viewing individual reactions of individual isotopes as groups. This is performed by determining the squared multiple correlation coefficient R^2 as uncertainty importance indicator, giving the relative amount of output uncertainty coming from the uncertainty of the respective isotope and reaction.

IV. RESULTS

This section summarizes the main results of the nominal MCNP6/ATHLET simulation of the VVER-1000 core, along with the corresponding uncertainties originating from he uncertainties in the basic nuclear data, and a sensitivity analysis to determine the main contributors to the result uncertainties.

1. Nominal Values

In addition to the coupled MCNP6/ATHLET calculations, stand-alone two-dimensional MCNP6 calculations were performed at a constant TH condition representative for the full-power state, as given in [7]. The resulting radial power distribution, normalized to the number of fuel assemblies, is displayed in Fig. 4.

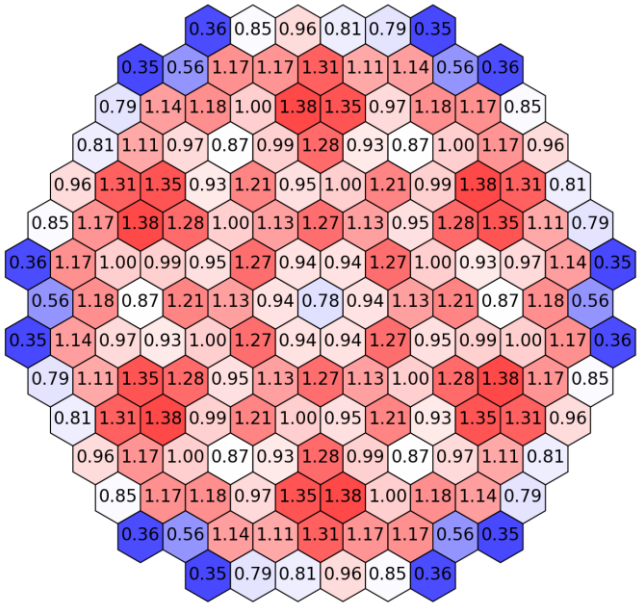

Fig. 4. Radial power distribution from the stand-alone MCNP6 simulation of the VVER-1000 core.

Here, and for the following results, the symmetry feature of the VVER-1000 core has been made use of, i.e. the fact that the geometry is invariant with respect to a rotation by 60° around the z axis. Therefore, the individual values for the fuel assembly powers, which do not exactly possess this symmetry due to the statistical nature of the solution, have been averaged over the six equivalent positions. The somewhat unusual distribution with its maximum values at positions far from the core center is due to the very heterogeneous arrangement of the fuel assemblies (Fig. 1). It is observed that the radial power distribution is in very good agreement with solutions of stand-alone two-dimensional Monte Carlo calculations with continuous-energy data performed earlier in the framework of the benchmark [7], confirming the suitability of the multi-group cross sections for the core simulations.

In Fig. 5, the nominal result for the axially integrated radial power distribution, again normalized to the number of fuel assemblies, is displayed. The power distribution from the coupled MCNP6/ATHLET calculation is in good qualitative agreement with the solution of the stand-alone two-dimensional Monte Carlo calculations (Fig 4).

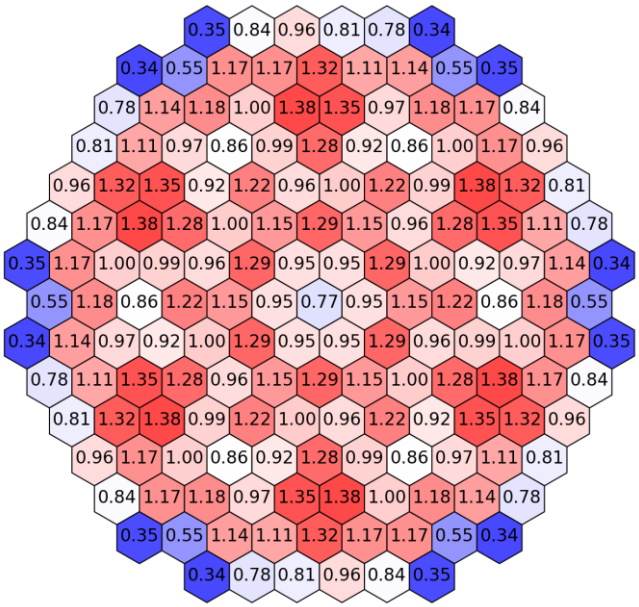

Fig. 5. Axially integrated radial power distribution from the MCNP6/ATHLET simulation of the VVER-1000 core.

2. Uncertainties

In Fig. 6, relative uncertainties of the radial power distribution from the stand-alone two-dimensional MCNP6 calculation are displayed. In particular in the central part of the core, the relative uncertainties can reach substantial values of up to approx. 9% on the 1σ level. This is much higher than the statistical uncertainties from the Monte Carlo method which are on the 1% level.

Correspondingly, in Fig. 7, relative uncertainties of the axially integrated radial power distribution from the coupled MCNP6/ATHLET calculation are shown. It can be seen that the uncertainties in the coupled calculation are very similar

to the uncertainties in the stand-alone calculation; this means that in the case under consideration, the TH feedback does not significantly influence the uncertainties in the power distribution due to a relatively weak variation of the TH parameters over the core.

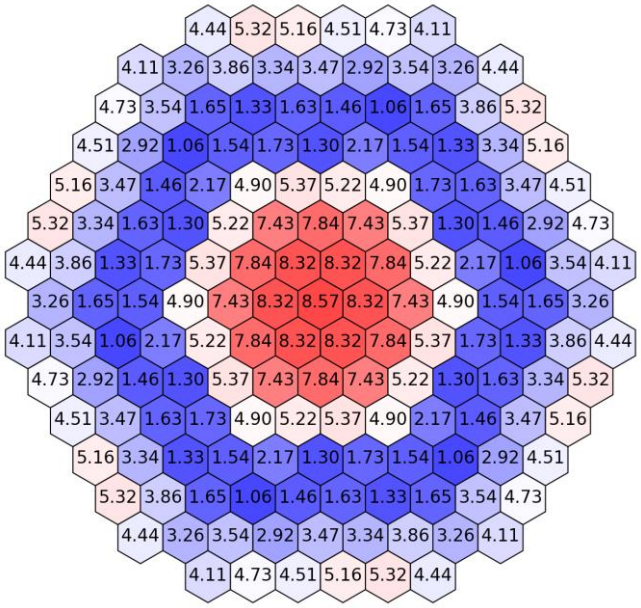

Fig. 6. 1σ uncertainties (%) of the radial power distribution from the stand-alone MCNP6 simulation of the VVER-1000 core.

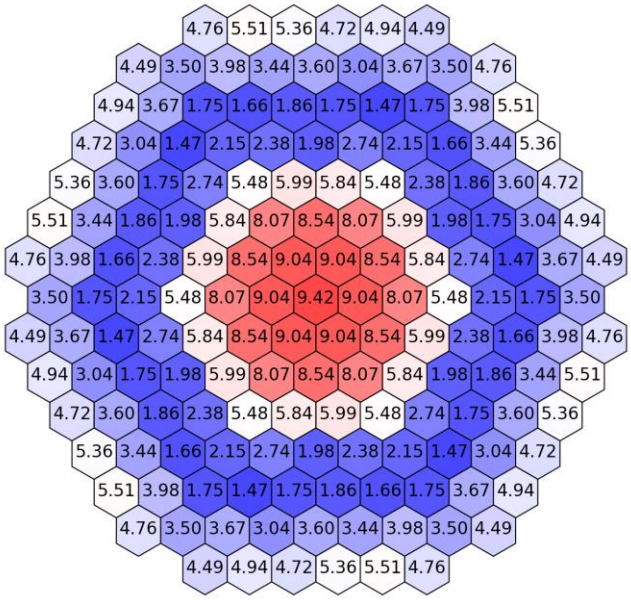

Fig. 7. 1σ uncertainties (%) of the axially integrated radial power distribution from the MCNP6/ATHLET simulation of the VVER-1000 core.

In Fig. 8, the axial power distributions in four selected fuel assemblies are shown together with their relative 1σ uncertainties (%) for each axial section. The selected assemblies are placed along the central horizontal traverse (see Fig.1). The power distributions are the assembly average of 1000 cross section variations. The uncertainties show a uniform behavior over the core height and reflect the values for the uncertainties in the radial power distribution, Fig. 7. The small deviations of the axial power values and their uncertainties from mirror symmetry with respect to the core mid-plane again confirm the relatively weak influence of the TH feedback.

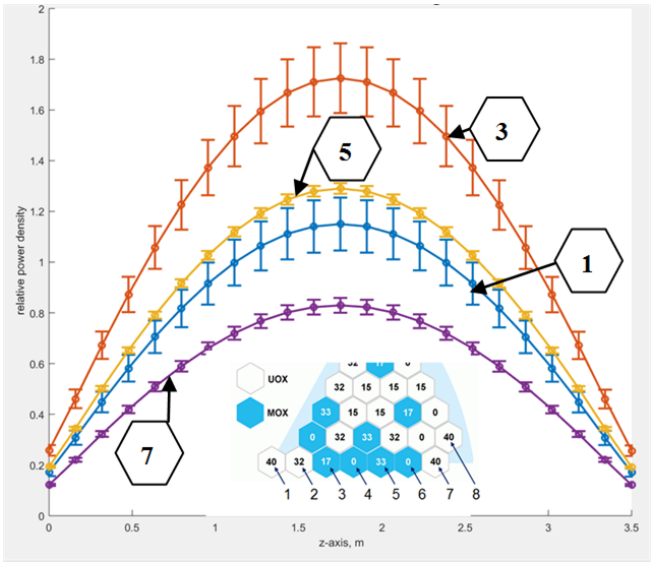

Fig. 8. Axial power distribution for four selected fuel assemblies with the corresponding 1σ uncertainties (%).

3. Sensitivities

As detailed in Section III.3, main contributors to the uncertainties can be identified by evaluating the squared multiple correlation coefficient for individual groups of input parameters, each group consisting of an individual reaction of an individual isotope. Results for the stand-alone MCNP6 calculation are given in Table 1 for a row fuel assembly powers from the core center to the periphery, denoted by 1 – 8 in Fig. 1. The results for the coupled MCNP6/ATHLET simulation are very similar due to the relatively weak influence of the TH parameter distribution on the resulting uncertainties, cf. Figs. 6 and 7. The table displays the squared multiple correlation coefficients R^2 together with their 95% confidence intervals and 95% significance bounds. All the contributors shown are statistically significant on the 95% level; the number of contributors that can be identified strongly depends on the sample size. With the sample size of 1000 used for the analysis, it turned out that some 5 – 10 main contributors can be determined with statistical significance.

The isotope-reaction pairs are given in terms of their ZA-Identifiers and the reaction numbers in AMPX

nomenclature with 2 = elastic scattering cross section; 18 = fission cross section; 102 = n,γ capture cross section; 452 = average number of neutrons per fission; 1018 = fission spectrum. It can be seen that the uncertainties are dominated by ^{239}Pu, and specifically the average number of neutrons per fission. This is due to the very heterogeneous distribution of UO_2 and MOX fuel assemblies in the core, with high-quality Plutonium in the MOX assemblies, and the high values of the uncertainties of the average number of neutrons per fission in the SCALE 6.1.2 covariance data library.

Table I: Main contributors to the uncertainties of the normalized fuel assembly power distribution (selected assemblies).

Ass.	Isotope-Reaction	R^2	95% conf. interval	95% sign. bound
1	94239-0452	0.550	0.041	0.017
	94239-0018	0.137	0.038	0.060
	94239-0102	0.123	0.036	0.060
2	94239-0452	0.590	0.039	0.017
	94239-0018	0.140	0.038	0.060
	94239-0102	0.125	0.037	0.060
3	94239-0452	0.601	0.038	0.017
	94239-0018	0.156	0.039	0.060
	94239-0102	0.138	0.038	0.060
4	94239-0452	0.584	0.039	0.017
	94239-0018	0.169	0.040	0.060
	94239-0102	0.148	0.039	0.060
5	94239-0452	0.401	0.047	0.017
	92238-0002	0.176	0.041	0.045
	94239-0018	0.172	0.041	0.060
6	94239-0452	0.487	0.044	0.017
	92238-0002	0.159	0.040	0.045
	94239-1018	0.149	0.041	0.004
7	94239-0452	0.618	0.037	0.017
	94239-0018	0.147	0.039	0.060
	94239-0102	0.135	0.038	0.060
8	94239-0452	0.643	0.035	0.017
	94239-0018	0.152	0.039	0.060
	94239-0102	0.139	0.038	0.060

V. SUMMARY AND OUTLOOK

An approach for evaluating uncertainties of the results of coupled Monte Carlo/thermo-hydraulics full-core simulations originating from uncertainties in the basic nuclear data has been developed. This consists in a combination of MCNP6/ATHLET for the core simulations, with MCNP6 in multi-group mode, preparation of self-shielded cross sections with the SCALE code system, and the sampling-based XSUSA uncertainty analysis package. This approach has been applied to evaluating the power distribution of a VVER-1000 core at operating full-power condition in a full-scale calculation, along with the corresponding uncertainties and the main contributors to these uncertainties. Substantial uncertainties were found, similar to those from stand-alone Monte Carlo calculations for the VVER-1000 core in particular, and found earlier for LWR cores in general. For the case under consideration, the influence of the TH feedback is rather small; this will be different for a core with TH parameters strongly varying over the geometry, such as boiling water reactors. Since the underlying nuclear data are not the only sources of uncertainty, corresponding calculations considering all uncertain parameters (nuclear data, manufacturing data, TH data …) should be performed.

Due to the high numerical effort for the coupled MC/TH simulations and a multiplication through the replication of these simulations for each varied set of nuclear data, it is highly desirable to significantly reduce the computation time, in particular to be able to evaluate the main contributors to the output uncertainty through sensitivity analyses by evaluating results from a sufficiently large sample size. Various ways are imaginable to reach this goal: by accelerating the convergence of each individual MC solution, e.g. by coarse mesh diffusion acceleration; by relaxing the requirement that in the MC/TH iteration process each MC solution converges individually, and instead aiming at a synchronous convergence of MC and TH; and by relaxing the requirement that each individual MC/TH solution converges for a given set of varied uncertain parameters, and instead trying to apply the "Fast GRS Method" [11] for evaluating uncertainties from MC runs with significantly reduced numbers of neutron histories, which so far has been successfully applied to stand-alone MC calculations and MC coupled with burn-up. Research in all of these directions is ongoing.

ACKNOWLEDGMENT

This work is supported by the German Federal Ministry for Economic Affairs and Energy.

REFERENCES

1. J.E. HOOGENBOOM, W.R. MARTIN, "The Monte Carlo Performance Benchmark Test – Aims, Specifications and First Results," *Proc. M&C 2011*, Rio de Janeiro, Brazil, May 8–12, 2011, (CD-ROM).
2. D.B. PELOWITZ (ed.), "MCNP6™ User's Manual Version 1.0," LA-CP-13-00634, Los Alamos National Laboratory (2013).
3. G. LERCHL, H. AUSTREGESILO, P. SCHÖFFEL, D. VON DER CRON, F. WEYERMANN, "ATHLET 3.1A

User's Manual," GRS-P-1/Vol. 1 Rev. 7, Gesellschaft für Anlagen- und Reaktorsicherheit, (2016).

4. W. BERNNAT, M. MATTES, N. GUILLIARD, J. LAPINS, W. ZWERMANN, I. PASICHNYK, K. VELKOV, "Monte Carlo Neutronics and Thermal Hydraulics Analysis of Reactor Cores with Multilevel Grids," *Proc. SNA+MC 2013*, Paris, France, Oct. 27–31, 2013, (CD-ROM).

5. M. AVRAMOVA, K. IVANOV, T. KOZLOWSKI, I. PASICHNYK, W. ZWERMANN, K. VELKOV, E. ROYER, A. YAMAJI, J. GULLIFORD, "Multi-Physics and Multi-Scale Benchmarking and Uncertainty Quantification within OECD/NEA Framework," *Ann. Nucl. Energy*, **84**, 178 (2015).

6. F. BOSTELMANN, W. ZWERMANN, B. KRZYKACZ-HAUSMANN, L. GALLNER, A. AURES, K. VELKOV, "Sampling-Based Nuclear Data Uncertainty Analysis in Criticality and Depletion Calculations," *Proc. ANS MC 2015*, Nashville, TN, USA, Apr. 19–23, 2015, (CD-ROM).

7. E. GOMIN, M. KALUGIN, D. OLEYNIK, "VVER-1000 MOX Core Computational Benchmark – Specification and Results," NEA/NSC/DOC(2005)17, OECD/NEA (2006).

8. "Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design," ORNL/TM-2005/39, Version 6.1 (2011).

9. J.C. WAGNER, E.L. REDMOND II, S.P. PALMTAG, J.S. HENDRICKS, "MCNP: Multigroup/Adjoint Capabilities," LA-12704, Los Alamos National Laboratory (1994).

10. F. BOSTELMANN, A. PAUTZ, W. ZWERMANN, "Treatment of Implicit Effects with XSUSA," submitted to *Proc. M&C 2017*, Jeju, Korea, Apr. 16–20, 2017.

11. D. ROCHMAN, W. ZWERMANN, S. VAN DER MARCK, A. KONING, H. SJÖSTRAND, P. HELGESSON, B. KRZYKACZ-HAUSMANN, "Efficient Use of Monte Carlo: Uncertainty Propagation," *Nucl. Sci. Eng.* **177**, 337 (2014).