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INFLUENCE OF NUCLEAR DATA EVALUATIONS ON FULL SCALE REACTOR CORE CALCULATIONS

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ABSTRACT

Nuclear data are mainly validated by the re-calculation of critical experiments. Since most of these systems are of compact size and room temperature, they are not necessarily representative for power reactors in operating conditions. In this paper, results of Monte Carlo calculations for large UO_2/MOX PWR and VVER reactor core configurations obtained with different nuclear data evaluations based on JEFF, ENDF/B, and JENDL are presented. The agreement between the resulting multiplication factors is reasonable, but it is found that the influence of the choice of the nuclear data basis on the radial power distributions can be significant, leading to differences of more than 10 % in the fuel assembly power for the most unfavourable case. Influences of this type can normally not be observed in calculations for compact critical assemblies.

Key Words: Nuclear data, Monte Carlo, critical benchmarks, core calculations

1. INTRODUCTION

Evaluated nuclear data are continuously improved. During the last years, the European library was updated from JEF-2.2 to JEFF-3.1 [1], the American library from ENDF/B-VI to ENDF/B-VII [2], and the Japanese library from JENDL-3.2 to JENDL-3.3/AC-2008 [3], with the aim to increase the agreement of calculated and measured results for integral systems. Along with this, growing attention is paid to uncertainty and sensitivity studies concerning the nuclear data evaluations, accompanied by improvements in the covariance data files describing the uncertainties of nuclear cross section data, and the calculation methods using these covariance data.

For the validation of the nuclear data libraries, a large number of integral experiments with all kinds of fissile and moderator materials and a large range of spectral conditions are used. A collection of descriptions of such experiments is found in the “International Handbook of Evaluated Criticality Safety Benchmark Experiments” [4]. The vast majority of these validation calculations refers to multiplication factors, although other measured quantities like fission rate distributions and reactivity coefficients are increasingly considered; corresponding experiments are described in the “International Handbook of Evaluated Reactor Physics Benchmark Experiments” [5]. Almost all of the systems considered are compact assemblies, mainly at room temperature. Likewise, uncertainty and sensitivity investigations based on covariance data, as performed, e.g., with the TSUNAMI code package [6], primarily consider the multiplication factors of critical assemblies. Such compact critical systems at low temperatures are not necessarily representative for power reactors at operating conditions.

In this paper, we investigate the differences in the multiplication factors and power distributions of problems representative for large reactor cores arising from the use of different evaluated nuclear data libraries. For this purpose, the MCNP-5 [7] code is used since the Monte Carlo method with continuous energy data currently provides the highest level of accuracy for neutron transport calculations, without significant restrictions in the geometrical modelling, and without preceding spectral calculations for cross section preparation. Therefore it is best suited to disclose nuclear data influences. Calculations with various nuclear data evaluations are performed for two full core benchmark arrangements recently dealt with in the framework of OECD/NEA international calculation benchmarks, namely the steady states of the “PWR MOX/UO_2 Core Transient Benchmark” [8] and the “VVER-1000 MOX Core Computational Benchmark” [9].

2. DESCRIPTION OF THE FULL CORE BENCHMARKS

Both the PWR MOX/UO_2 Core Transient Benchmark and the VVER-1000 MOX Core Computational Benchmark specifications describe mixed MOX/UO_2 cores with a MOX loading of approximately 30 %. The Westinghouse type PWR core consists of 193 fuel assemblies with 17x17 pin cells, and the VVER core of 163 hexagonal fuel assemblies with 331 pin cells, with various UO_2 and MOX fuel types at several burn-up states up to 40 GWd/t HM. The fresh fuel assemblies contain burnable absorbers.

	1	2	3	4	5	6	7	8
A	U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	U 4.5% (CR-SD) 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5
B	U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5
C	U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.3% 35.0
D	U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0
E	U 4.5% (CR-SD) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5	
F	M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5	
G	U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SA) 17.5	U 4.5% 32.5	fuel type burn-up	
H	U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0				

Figure 1. Core layout of the PWR MOX/UO_2 Core Transient Benchmark.

For both core designs, the fresh MOX fuel contains a high percentage of ^{239}Pu in the isotopic composition. The nuclide densities of all fuel materials in each burn-up state are given in the specifications.

The core layouts are sketched in Figures 1 and 2. MOX fuel assemblies are displayed in grey. The detailed descriptions of the arrangements are given in refs. [8] and [9]. For stationary calculations, it is sufficient to represent the core in 2-D geometry with 90° rotational symmetry for the square lattice, and 60° rotational symmetry for the hexagonal lattice.

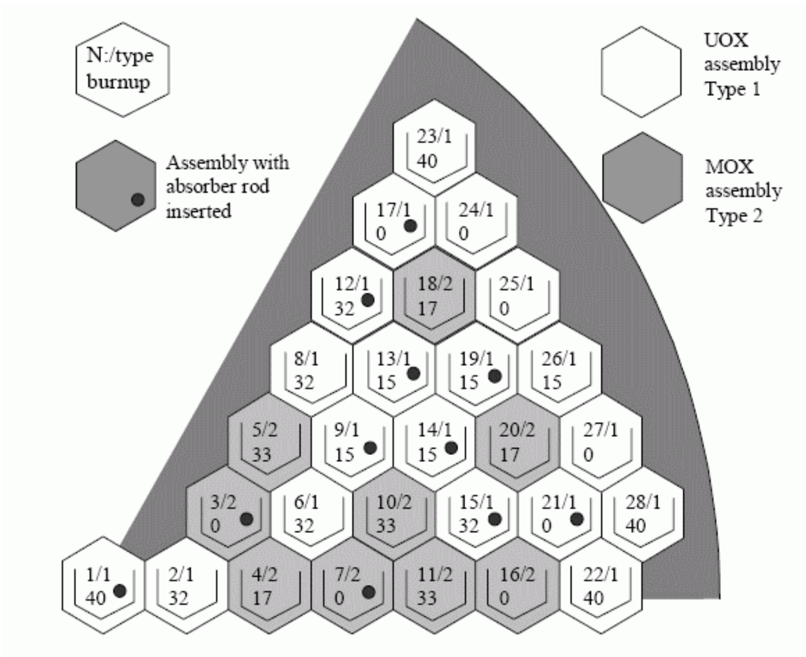

Figure 2. Core layout of the VVER-1000 MOX Core Computational Benchmark.

3. NUCLEAR DATA USED

With the aim to cover the influence of a broad spectrum of modern evaluated nuclear data libraries, JEF/JEFF, ENDF/B and JENDL data were used for the investigations. The comparison comprises JEF-2.2 and JEFF-3.1, ENDF/B-VII.0, JENDL-3.2 and JENDL3.3/AC-2008. The JEFF-3.1 and JENDL-3.2 data are available from the NEA data bank as packages NEA 1768 ZZ-MCJEFF3.1NEA and NEA-1424 ZZ-FSXJ32, respectively. The JEF-2.2, ENDF/B-VII.0, and JENDL-3.3/AC-2008 data were processed by IKE Stuttgart. The JEF-2.2 data are extensively validated and used in production calculations, see, e.g., [10]. For the ENDF/B-VII.0 and JENDL-3.3/AC-2008 data, only hydrogen, oxygen, and the actinides were processed; in the corresponding calculations, JEFF-3.1 data were used for the remaining structure material, absorber, and fission product nuclides. Therefore, “JENDL-3.3/AC-2008” is to be understood as JENDL-3.3 for hydrogen and oxygen, and JENDL/AC-2008 for the actinides.

4. RESULTS OF THE FULL CORE CALCULATIONS

The cores were modelled according to the specifications [8] and [9] concerning geometry and nuclide concentrations. Although some details relevant for real reactor calculations, like thermal expansion of the geometry, were neglected in the specification, this should not influence comparisons between calculation results obtained from different nuclear data. For the VVER benchmark, the specified fuel nuclide compositions are restricted to oxygen, actinides, and some fission products. For the PWR benchmark, the lists of nuclides for the depleted fuel assembly states given in the specification is rather bulky such that for the calculations, likewise only oxygen, actinides, and some fission products were considered. The absorption of the neglected fission products was approximately taken into account by increasing the numbers of the considered fission products correspondingly. For the comparisons of results obtained with different nuclear data, the hot zero power uncontrolled state was chosen for the PWR ("ARO" in ref. [8]), and the hot zero power controlled state for the VVER ("S6" in [9]), because for these states, the differences in the calculated power distributions turned out to be highest. Although a completely controlled core with a multiplication factor higher 1.0, as it is the case for the VVER state, is not typical for a reactor in operation, it has some relevance , e.g., for accident situations in case of a boron dilution transient.

Table I. Multiplication factors obtained from MCNP with JEFF, ENDF/B and JENDL data for steady states of the PWR MOX/UO_2 Core Transient Benchmark and the VVER-1000 MOX Core Benchmark.

	PWR, hot zero power, uncontrolled	VVER, hot zero power, controlled, boron-free
JEF-2.2	1.06065	1.04740
JEFF-3.1	1.05795	1.04633
ENDF/B-VII.0	1.05935	1.04705
JENDL-3.2	1.06261	1.05011
JENDL-3.3/AC-2008	1.06096	1.04970
Spread	0.00466	0.00378

In Table I, multiplication factors calculated with MCNP using JEFF, ENDF/B, and JENDL nuclear data are given for the two benchmark arrangements. The calculations were performed with 500 or 1,000 millions of active neutron histories, with 100 or 200 million histories skipped, leading to statistical uncertainties in k_{eff} of 0.00002 - 0.00003 on the 1σ level. The differences between the minima and maxima of the calculated values are approximately 400 - 500 pcm; this seems reasonable regarding the number of different nuclear data evaluations used. As expected, the JEFF-3.1 and ENDF/B-VII.0 results are in very good agreement. JENDL-3.2 clearly yields the highest values in both cases; the multiplication factors obtained with the newer evaluations JEFF-3.1 and JENDL-3.3/AC-2008 are smaller than those with the older data JEF-2.2 and JENDL-3.2, respectively. When using JENDL-3.3 also for the actinides, the resulting multiplication factors were lower than with the AC-2008 file, namely 1.05856 and 1.04674 for the PWR and VVER case, respectively. The values from JEFF-3.1 and ENDF/B-VII.0 are surprisingly low in comparison with JEF-2.2; this is different from most observations based on calculations for cold critical LWR type fuel lattice assemblies, thereby indicating a dependence on the size and the temperature of the systems under consideration.

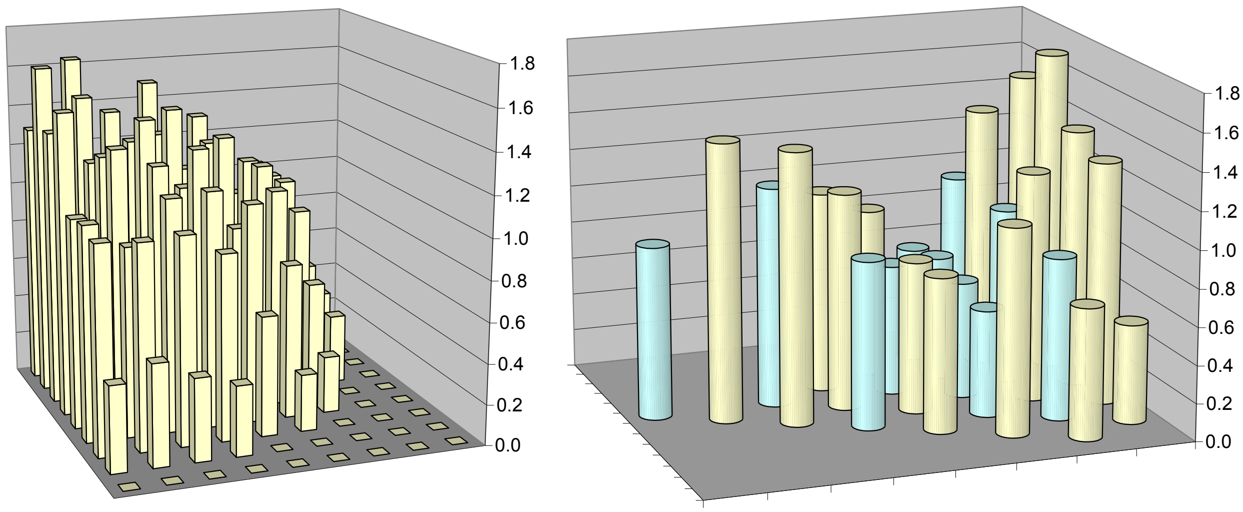

Figure 3. Power distributions for one quarter of the uncontrolled state of the PWR core (left) and one sixth of the controlled state of the VVER core (right), calculated with JEFF-3.1 data. The distributions are normalized to the number of fuel assemblies. The core centre is on the left. Values for the controlled VVER fuel assemblies are marked in blue.

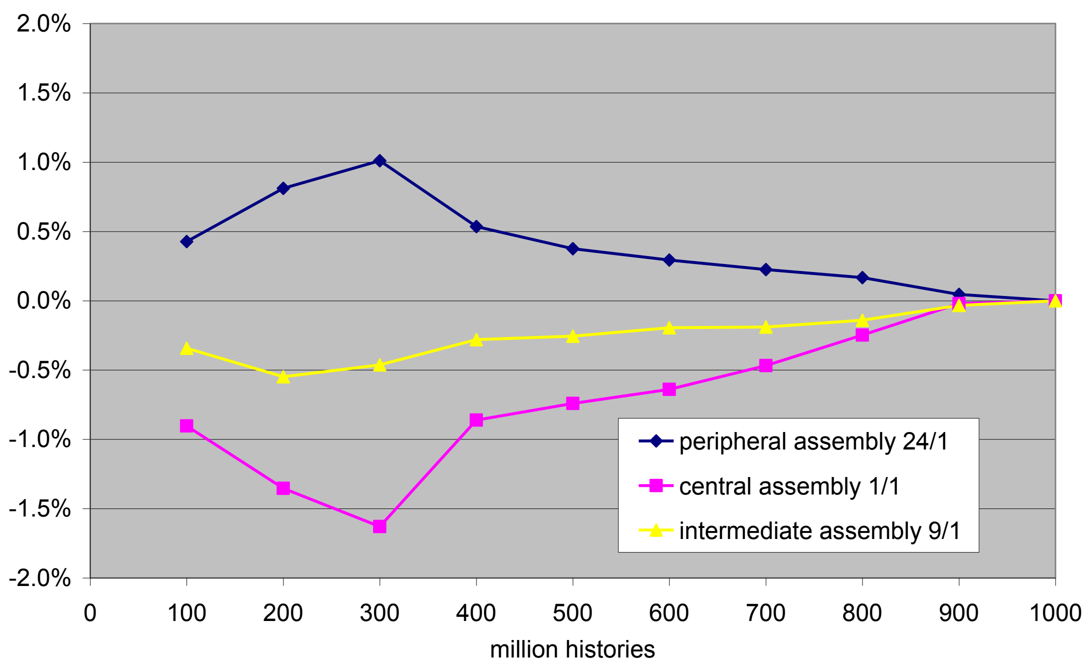

Figure 4. Relative difference of the power of three VVER-1000 fuel assemblies from the final value after 1,000 million histories, as a function of neutron histories, obtained with JEFF-3.1 data.

In Figure 3, the normalized assembly power distributions for both core arrangements calculated with JEFF-3.1 nuclear data are plotted. A high degree of non-uniformity of the power distributions is observed due to the heterogeneity of the core loadings, and in the VVER-1000 case in particular due to the controlled fuel assemblies.

The numbers of active neutron histories in the MCNP full core calculations were chosen sufficiently large to make sure that the observed effects in the power distributions are not caused by statistical uncertainties or source convergence issues. To be specific, the largest relative statistical uncertainties as given by MCNP (in the central fuel assemblies) are 0.0005 - 0.0007, again on the 1σ level. Inspecting the calculated assembly powers in dependence on the number of neutron generations, one recognizes that the fluctuations may be substantially larger than the statistical uncertainties. Concerning this slow convergence, the behaviour of the VVER-1000 arrangement is particularly unpleasant in some cases. In Figure 4, the dependence of the calculated assembly power on the number of neutron histories is displayed for selected fuel assemblies of the VVER core. Three fuel assemblies are chosen, the central one, one located on the core periphery, and one located in-between, denoted as 1/1, 24/1, and 9/1 in Figure 2. The quantities plotted are the relative deviations from the values determined with the final number of 1,000 million histories with the JEFF-3.1 data. In this case, 20,000 active cycles were run with 50,000 neutrons per cycle; 2,000 cycles were skipped. It is recognized that after a number of 500 million histories, which in most criticality calculations would be considered more than sufficient, the deviations of the central and peripheral assembly powers from their final values are still in the order of 0.5 - 1.0 %. As deviations are decreasing when approaching the final number of 1,000 million histories, it is reasonable to consider the relative uncertainty of the final distribution to be not larger than 1 %.

Substantial differences are observed for the radial power distributions calculated with different nuclear data libraries. For the uncontrolled state of the PWR benchmark, a tilt in the ratio of the distributions obtained with the different nuclear data libraries from the core centre to the periphery is found, with a maximum value of approximately 5 %. In Figure 5 (top left), the differences in the assembly powers between results obtained with JEF-2.2 and JEFF-3.1 are displayed, as a typical example of the influence of nuclear data of different generations. The JEFF-3.1 result is taken as reference, i.e. the quantities displayed in the figure are power(JEF-2.2)/power(JEFF-3.1)-1.

When comparing the results obtained with all nuclear data evaluations used, there are larger differences to JEFF-3.1 with the older evaluations JEF-2.2 and JENDL-3.2 as compared to the most recent evaluations ENDF/B-VII.0 and JENDL-3.3/AC-2008. When using JENDL-3.3 instead of AC-2008 for the actinides, the resulting power distribution is practically identical to that obtained with AC-2008, with relative differences of 0.5 % or below. One reason is the fact that in the newer data, significant changes were made in the ^{235}U capture and fission data; e.g., the ^{235}U capture resonance integral was increased by 5 – 6 % as compared to the older evaluations (approximately 140 barn vs. 132 barn). Looking at Figure 1, one recognizes that in the PWR core the MOX fuel assemblies tend to be located closer to the periphery of the PWR core, leading to a slight shift of the ^{235}U distribution to the core centre. However, there is also some smaller influence from the ^{239}Pu and ^{238}U data.

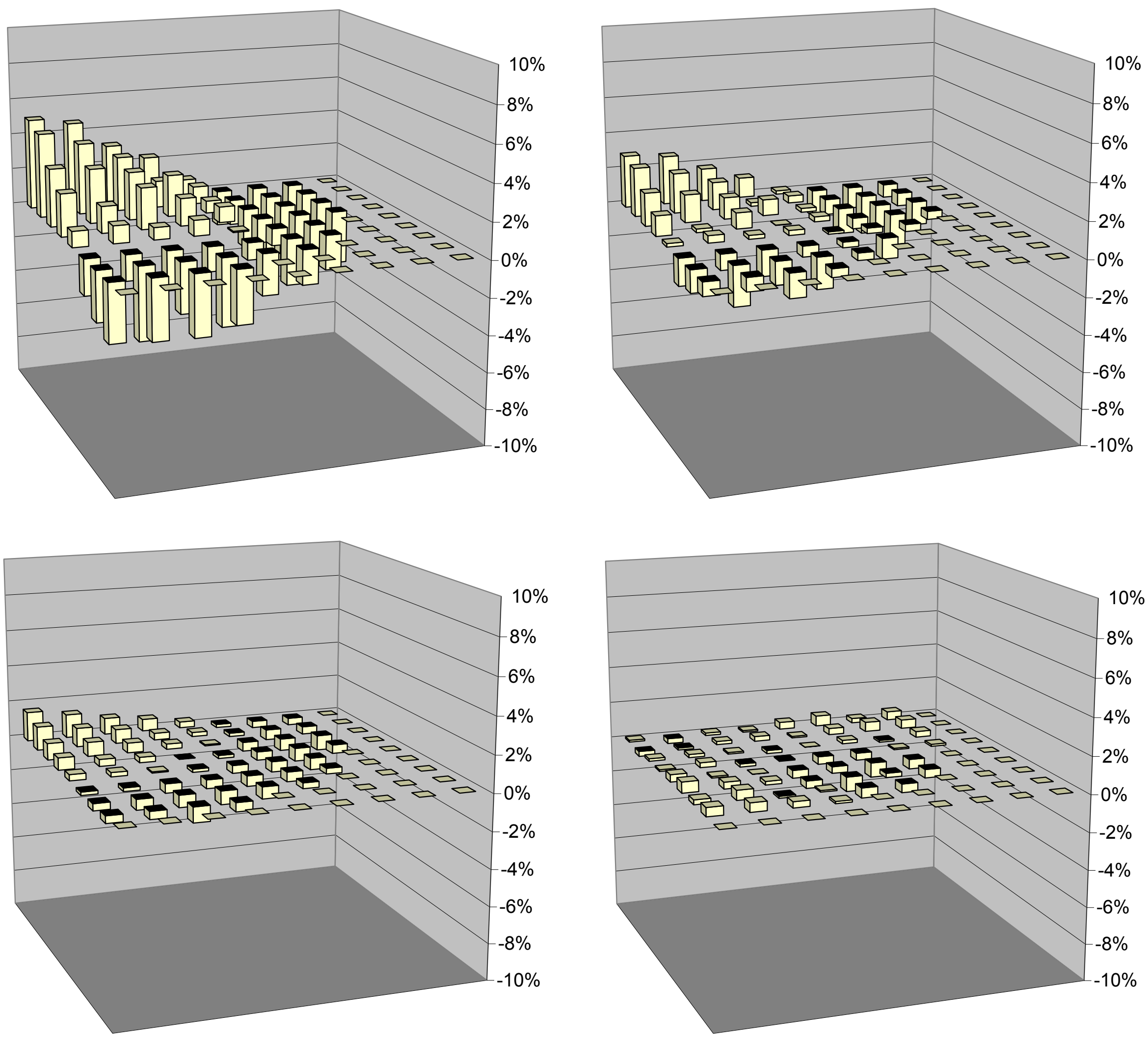

Figure 5. Relative difference of the radial assembly power distributions for the uncontrolled state of the PWR UO_2/MOX Core Benchmark, obtained with JEF-2.2 (top left), JENDL-3.2 (top right), ENDF/B-VII.0 (bottom left), and JENDL-3.3/AC-2008 (bottom right) as compared to results from JEFF-3.1 data.

Even larger differences in the power distributions are observed for the controlled, boron-free state of the VVER-1000 MOX Core Benchmark; however, the centre to periphery tilt of the JEF-2.2 to JEFF-3.1 ratio is reversed as compared to the PWR case. This can be seen in Figure 6 (top left), where again the relative difference of the JEF-2.2 result as compared to the JEFF-3.1 result, i.e. power(JEF-2.2)/power(JEFF-3.1)-1, is displayed. A reason for this behaviour is that in the VVER core, the UO_2 assemblies are on the average located closer to the core periphery, see Figure 2. In the state with inserted absorber rods (fuel assemblies with a dot in Figure 2), most of the UO_2 assemblies located away from the core periphery are controlled, thus shifting the efficient ^{235}U distribution even closer to the periphery. For results obtained with ENDF/B-VII.0 data, there is again a very good agreement with the JEFF-3.1 results. However, the findings for the power distributions from calculations with the JENDL libraries are different from the PWR case: there are substantial differences between the JENDL-3.3/AC-2008 and JEFF-3.1 results of approximately 5 % in the core centre and for peripheral fuel assemblies. (Again, when using JENDL-3.3 instead of AC-2008 for the actinides, there are practically no differences in the power distributions). For JENDL-3.2, the differences to JEFF-3.1 are qualitatively similar as for JEF-2.2, but even larger in magnitude. When comparing the power distributions resulting from the older and newer data, JENDL-3.2 and JENDL-3.3/AC-2008, respectively, differences of more than 10 % in the core centre and periphery are obtained. This behaviour as well as the differences between the results obtained with JENDL-3.3/AC-2008 and JEFF-3.1 data can probably not be explained by the differences in the ^{235}U data alone. Obviously, there exist other differences in the old and new evaluations of the JENDL data, which become relevant for the VVER-1000 power distribution. This will be investigated by substituting single isotope data in the in individual calculations by the corresponding data of different evaluations.

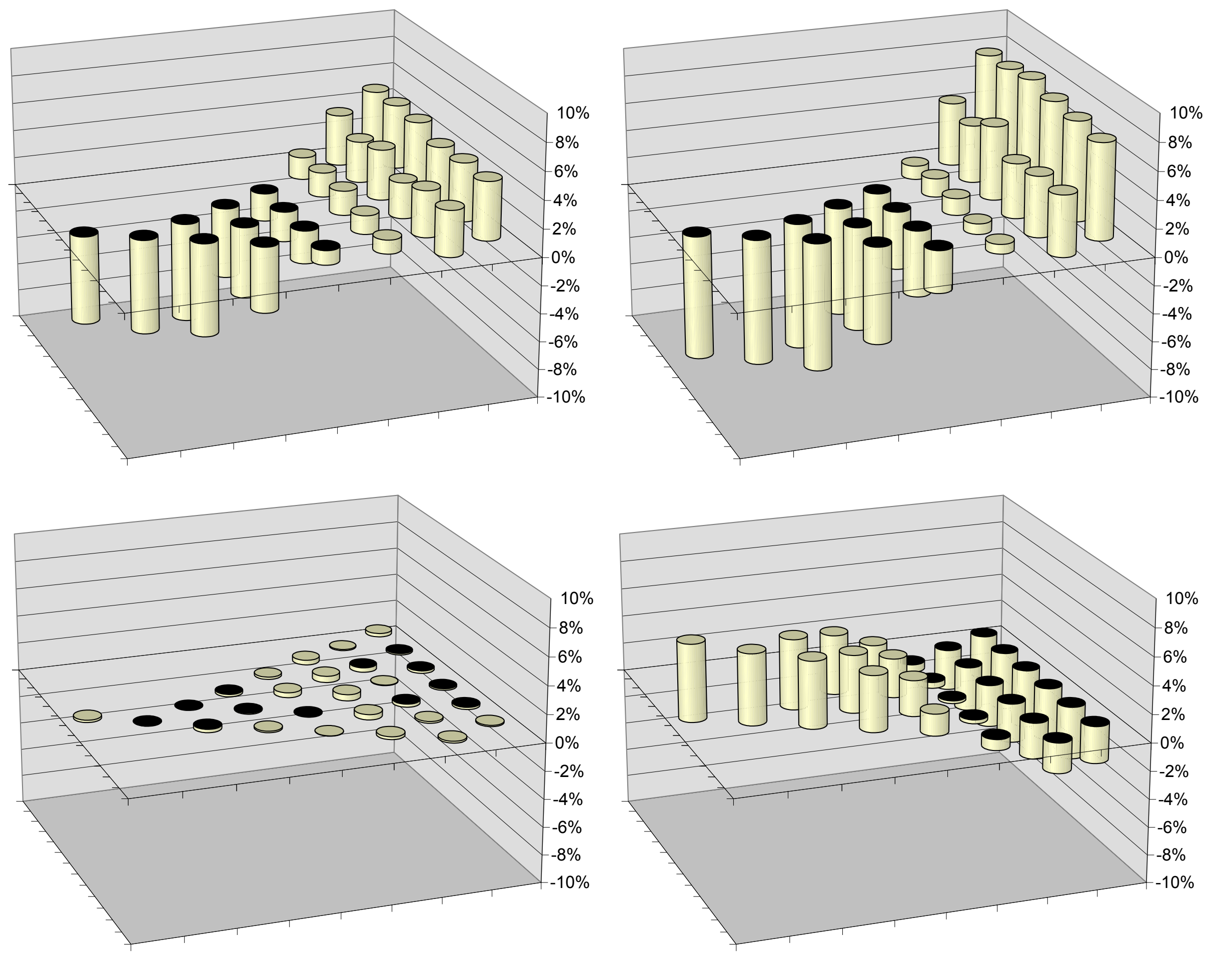

Figure 6. Relative difference of the radial assembly power distributions for the uncontrolled state of the VVER-1000 MOX Core Benchmark, obtained with JEF-2.2 (top left), JENDL-3.2 (top right), ENDF/B-VII.0 (bottom left), and JENDL-3.3/AC-2008 (bottom right) as compared to results from JEFF-3.1 data.

4. SUMMARY AND OUTLOOK

The Monte Carlo code MCNP-5 with continuous energy nuclear data based on JEF-2.2, JEFF-3.1, ENDF/B-VII.0, JENDL-3.2, and JENDL-3.3/AC-2008 was used for estimating the influence of differences in the evaluations on the multiplication factors and power distributions of large power reactors in operating conditions. The calculations were performed for two two-dimensional UO_2/MOX full core configurations used for calculation benchmarks performed under OECD/NEA auspices. Whereas the resulting multiplication factors were found to be in reasonable agreement (400 - 500 pcm differences), a significant effect was observed for the radial power distributions in certain cases. This effect seems to be specific for mixed cores with UO_2 and MOX with a high amount of fissile plutonium in the isotopic composition ("weapons-grade") and shows up due to the large size of the cores. The differences between the assembly powers obtained with the different evaluations reached 5 % for an uncontrolled, and more than 10 % for a controlled boron-free state. An important contribution to the discrepancies for these cases comes from differences in the ^{235}U cross sections in the different evaluations. Influences of this type can normally not be observed in calculations for compact critical assemblies, which primarily serve as the validation basis for nuclear data evaluations. For instance, practically no difference in the pin power distributions calculated with MCNP using JEF-2.2 and JEFF-3.1 data was observed for the mixed UO_2/MOX critical assemblies VENUS-7 [11]. This suggests that benchmark problems representative for large power reactor cores or even measurements from operation should be considered as much as possible by the nuclear data evaluation groups in the validation process of the libraries. Furthermore, it would be advantageous to have uncertainty and sensitivity analysis tools available to investigate the influence of nuclear data uncertainties on local quantities like power distributions.

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