

Impact of the Various Nuclear Data Libraries on the NPP Krško Spent Fuel Characterization

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ABSTRACT

Since the neutron nuclear data profoundly influence predictions of the nuclear systems behaviour, it is prudent to evaluate their impact on the spent fuel isotopic composition and consequently their impact on the most important spent fuel observables such as decay heat, activity, neutron multiplication factor, and neutron and photon source term. In this paper ENDF/B-VII.0, ENDF/B-VII.1, ENDF/B-VIII.0 and JEFF-3.3 libraries are considered. A typical NPP Krško fuel assembly is analysed with the Monte Carlo code Serpent 2. Burnup of up to 60 GWd/tU and cooling times up to 100 years are considered in the analysis. Comparison of results showed noticeable differences, which should be considered in the library selection and in the uncertainty evaluation of the spent fuel characteristics determination.

1 INTRODUCTION

Spent fuel characterization is an important parameter for many nuclear facilities, such as: fuel storage pools in nuclear power plants, spent fuel transportation systems, interim storage facilities, reprocessing plants and final disposal sites. The depletion Monte Carlo code Serpent 2 [1] developed by the VTT Finland has a function of calculating many variables that are related to the nuclide inventories at different burnup and cooling steps. These integral observables are activity, decay heat, neutron and photon emission rate. Serpent 2 code has been widely used in various fields for the calculation of irradiated nuclear fuel since the code is relatively fast and widely used. To obtain accurate calculation results, it is also important to use relevant crosssection libraries. In this paper a few selected cross section libraries, together with fission yield and decay data, are evaluated, since our previous work indicated considerable differences in fuel isotopic composition during the fuel burnout [2].

2 TEST CASE MODEL OF THE BENCHMARK

A 2D model representing PWR 16×16 pin-array configuration of the UO₂ fuel with periodic boundary conditions, as it is in the Krško NPP core, is presented in Figure 1. For the presented burnup calculations, the limit in the burnup value is 60 MWd/tU. Fuel rods are divided in 10 concentric rings in burnup calculations with the following operational conditions:

- Power density: 39.8050E-03 kW/g.
- Coolant density: 0.70871 g/cm³ with constant boron concentration 1000 ppm.
- Fuel density: 10.24341 g/cm³ and fuel enrichment: 4.95% U-235.
- Fuel temperature: 900 K, cladding temperature: 620 K and water temperature 580.46 K.



Figure 1: Layout of the PWR assembly with fuel cells and empty water cells

All burnup calculations were performed using Serpent 2 code, version 2.1.32, with 30000 neutrons in 1000 active neutron cycles at each time step were used. Depletion history was defined using the following depletion time intervals (day step): 3.7684, 12.5612, 25.1225, 50.2449, 75.3674, 100.4899, 125.6124, 188.4185, 251.2247, 314.0309, 376.8371, 439.6433, 502.4494, 565.2556, 628.0618, 690.8680, 753.6742, 879.2865, 1004.8989, 1130.5112, 1256.1236, 1381.7360, 1507.3483 and cooldown was defined using the following cooling time intervals (day step): 1, 9, 20, 70, 265.25, 182.625, 547.875, 730.5, 913.125, 913.125, 1826.25, 1826.25, 3652.5, 7305, 9131.25 and 9131.25. Burnup calculations were performed using CRAM method [3] and time integration method LE [4], which considers the linear extrapolation for predictor using 10 substeps.

3 NUCLEAR DATA LIBRARIES

In this section nuclear data libraries used in this paper are presented. Nuclear data activities are related to measurements, evaluations and applications. A nuclear data library is the final product once the evaluations are performed. In this paper four libraries are used: ENDF/B-VII.0 [5], ENDF/B-VII.1 [6], ENDF/B-VIII.0 [7] and JEFF-3.3 [8]. The list of isotopes and reactions taken into account during our simulation may vary from one library to another. In this paper only the summary data (data from Serpent 2 .out file) are presented for each of the libraries. These data are presented in Table 1.

Library evaluation		JEFF		
Library release	VII.0	VII.1	VIII.0	3.3
Number of nuclides	1390	1424	1445	1779
Transport nuclides	324	333	416	478
Decay nuclides	1066	1091	1029	1301
Reaction channels	8842	9900	12369	21235
Special reactions	3813	4093	8809	4893
Transmutation reactions	2718	3161	3204	7256

Table 1: Summary of nuclide data for each of the libraries used with the Serpent 2 code

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Transmutation branch reactions	2148	2959	2549	7841
Decay reactions	1687	1887	1905	2061
Decay branch reactions	102	117	121	127
Lost transmutation paths	3522	3362	3427	26

4 RESULTS OF BURNUP CALCULATIONS

In this section the parameters important for handling, storage and disposal are analysed.

4.1 Multiplication factor analysis

The results of neutron multiplication factor (K_{inf}) calculations as function of the fuel burnup are presented in Figure 2. Our reference case for the burnup calculations was made with the Serpent 2 code using ENDF/B-VII.0 library. For each library the ΔK_{inf} (pcm) is defined as K_{inf} - K_{inf} (ENDF/B-VII.0). The differences in K_{inf} are < 200 pcm for the ENDF/B-VIII.0 library for burnups less than 50 MWd/kgU. On the other hand the differences with the results obtained with ENDF/B-VII.1 are larger (up to 700 pcm). At the start of the burnup the highest differences in K_{inf} are observed with JEFF-3.3 library, while the values of K_{inf} are overestimated for around 300 pcm for burnups around 20 MWd/kgU. After that ΔK_{inf} is decreased to almost zero at around 40 MWd/kgU and fall to -500 pcm at 60 MWd/kgU.



Figure 2: K_{inf} as a function of burnup obtained by different libraries (upper plot) and differences in K_{inf} (pcm) regarding the reference ENDF/B-VII.0 results (lower plot).

4.2 Decay heat and activity analysis

Decay heat and activity as a function of cooling time are shown in Figure 3. The total activity decreases from 2.5 10¹⁵ to 3.1 10¹² in 100 years, while the total decay heat decreases from maximum value of 200 W/kgU to almost zero. By comparing the values of different libraries with the reference values obtained form ENDF/B-VII.0 library, it can be seen that the highest differences are observed with JEFF 3.3 and ENDF/B-VII.1 libraries at the cooldown time of 30 days (0.082 years) and 100 years.

Results of most important nuclides that contribute to the total activity and total decay heat and the differences between various libraries are given in Figure 4 where the following normalization was used: *activity_i (library) – activity_i (reference)/ activity_total (reference). Activity_i (library)* is a nuclide activity for a given library (ENDF/B-VII.1, ENDF/B-VIII.0 or JEFF3.3), *activity_i (reference)* is a nuclide activity for an ENDF/B-VII.0 library and *activity_total (reference)* is a total activity for an ENDF/B-VII.0 library. Considering nuclide activities and the comparison between ENDF/B-VII.1 and ENDF/B-VII.0 it can be seen that in general the differences are below 1%. Most noticeable differences are for ⁸⁵Kr, ²³⁸Pu and ^{235m}U. Similar observations are observed comparing ENDF/B-VIII.0 and JEFF3.3 libraries.

The same normalization was used for a decay heat. It can be seen that the differences are larger, especially for ²³⁸Pu. The difference is around 2.5% for ENDF/B-VII.1 and ENDF/B-VIII.0 libraries and 3.5% for JEFF3.3 library.



Figure 3: Activity (left) and decay heat (right) as a function of cooling time obtained with different libraries. Absolute (upper part) and relative values compared to ENDF/B-VII.0 (lower part).

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Figure 4: Differences [%] in activities (LEFT) and decay heat (RIGHT) for most important nuclides between given libraries and reference library: ENDF/B-VII.1 (TOP), ENDF/B-VIII.0 (MIDDLE) and JEFF-3.3 (BOTTOM) at different cooling times (years).

4.3 Neutron and photon emission rate

Spontaneous fission and (α, n) reactions are main source of neutron emission rate. Together with photon emission rate as a function of cooling are shown in Figure 5. It can be seen that the difference in neutron emission between EDNF/B libraries is within 1%, except at cooling times close to 100 years, where the differences can reach 3%. Results of JEFF 3.3 library are between 1% and 3% for first 10 years of cooling, and can reach 2% at cooling times 100 years. Diffences in photon emission are higher. At the beginning of the cooling, the diffences are between 5 and 8% for JEFF 3.3 and ENDF/B-VII.1 libraries, while in the period between 1 to 20 years, differences are within 1%. After that they increase to 4% at the end of the cooling time.



Figure 5: Neutron (left) and photon (right) emission rates as a function of cooling time. Absolute values (up) and values, relative to Serpent 2 ENDF/B-VII.0 values (lower).

In Figure 6 the contribution of the most important nuclides for various libraries are presented for neutron and photon emission rate. Considering neutron emission rate, the most relevant nuclide is ²⁴⁴Cm with its contribution > 90% for the cooling interval between 1 and 100 years. ²⁴⁶Cm and other Pu nuclides are also relevant for cooling times > 100 years. Regarding the differences between libraries, the difference in neutron emission for ²⁴⁴Cm is below 0.5% for ENDF/B-VII.1 library and around 1% for ENDF/B-VIII.0 library and around 1.5% for JEFF3.3 library. The difference in ²⁴⁶Cm for all three libraries is between 1.0%-1.5%. There is also a noticeable difference in ²³⁸U. Its contribution to total neutron emission rate is around 2% at larger cooling times. Large difference is due to much higher values of spontaneous fission (SF) rate calculations with the reference library where the difference in SF at cooling times 100 years is around two order of magnitude.

For photon emission rate the most relevant nuclide is 134 Cs for shorter cooling times (< 10 years), while for longer cooling times the contribution of 137m Ba is the most important. The differences for all libraries are around 1% for 134 Cs and below 1% for 137m Ba. Increased differences are observed for 241 Am, around 1% for ENDF/B libraries and around 4% for JEFF3.3 library. The difference for 238 Pu is around 0.5%–0.7% for all libraries but its contribution to the total photon emission rate is around 1% - 2% for cooling times > 50 years.



Figure 6: Differences [%] in neutron (LEFT) and photon (RIGHT) emission for most important nuclides between given libraries and the reference library: ENDF/B-VII.1 (TOP), ENDF/B-VIII.0 (MIDDLE) and JEFF-3.3 (BOTTOM) at different cooling times (years).

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5 CONCLUSION

The aim of this work was to provide a general overview of the impact of current nuclear data libraries on the calculation results by comparing K_{inf} for burned fuel and evaluating the contribution to total decay heat, activity, spontaneous fission and photon emission rate of the main nuclides. Based on our experience, the ENDF/B-VII.0 library was used as the reference case. Compared to the results obtained with other libraries, the difference for K_{inf} is within 700 pcm. The lowest deviation was observed with library ENDF/B-VII.0 library, while the highest deviation was obtained with library ENDF/B-VII.1.

Comparison of the total values of activity, decay heat, neutron emission rate and photon emission rate showed that the differences were generally in the range of a few percent, with the largest difference occurring in the case of JEFF3.3. In addition, for each observable, the contribution of the nuclides was evaluated, considering only the contribution of the most important nuclides. The results have shown that for most of the important nuclides the differences are 1% or less. There are some exceptions. In terms of decay heat, it was found that for large cooling times (~100 years), there is a difference of 2%-3% for ²³⁸Pu. Also, a difference of 1%-2% was observed in the neutron emission rate for ²⁴⁶Cm for longer cooling times, while a difference of about 1% was observed in the photon emission rate for ¹³⁴Cs, which is one of the main contributors to the photon emission rate.

Differences are large enough to be taken into consideration in the library selection process and in the uncertainty evaluation of the spent fuel characteristics determination.

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