

Calculations of a burnup credit benchmark #ISTC 2670 VVER PIE

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Summary		
<p>A simplified benchmark based on #2670 ISTC PIE has been calculated. The benchmark describes the irradiation history of eight samples cut out of four fuel pins of a VVER-440 fuel assembly irradiated to the average burnup of 38.5 MWd/kgU. The purpose of the work was to validate Serpent's burnup calculation methods for burnup credit applications and to repeat earlier calculations of the same benchmark because of an error in the fuel definition.</p> <p>Nuclide concentrations [kg/U_{init}] for nuclides recommended in actinide and fission product burnup credit evaluation were calculated and compared to measurement values. The calculations were performed using three different cross section libraries ENDF/B-VII.1, JEFF-3.2 and JENDL-4.0. The different libraries yielded rather consistent results except for Ag-109 with JEFF-3.2 for which the results differed 10 % from the results with the other libraries. The calculations corresponded rather well to the measurement results for U-238, U-236, most plutonium isotopes and Am-241. Large differences (> 100 %) were observed in Ag-109, Eu-151, Eu-153 and Gd-155. For the other nuclides, differences were mostly of the order of 1-10 %, but larger differences were observed in some nuclides like U-234, Np-237, Pu-238 and samarium isotopes. Some of the differences can be explained by measurement uncertainty. Some differences may also arise from the way the sample specific power values have been determined in the benchmark specifications.</p> <p>Some sensitivity calculations were also performed using different burnup related modelling options and algorithms. Differences to reference calculations were rather small. The use of substep method and TTA method had a notable effect of approximately 1-2 % to the nuclide concentrations. Spatial discretization had a small effect of 0,5 - 1,5 % for some actinides and Gd-155.</p>		
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1. Introduction

One of the most important matters to consider in the safe and secure handling, transport and storage of nuclear fuel outside a nuclear reactor is criticality safety. The objectives of criticality safety are to prevent a self-sustained nuclear chain reaction and to minimize the consequences of this if it were to occur. The subcriticality of a system containing fissile material such as nuclear fuel can be ensured by controlling one or several parameters such as e.g. mass, concentration and density of fissile material. [1]

Nuclear fuel outside the reactor is generally most critical when it is fresh. In spent fuel, some or most of the fissile nuclides have been depleted and burnup credit can be utilized. This means that the decreased reactivity of the burned fuel is taken into account in the criticality safety analysis of the fuel. Computational determination of burnup credit requires the validation of the methods used to calculate nuclide concentrations and the multiplication factor by comparison to measurement data. Measurement data can be used to calculate isotope correction factors (ICF) for the nuclides used in the criticality calculations [2]. The correction factors can then be applied to determine conservative estimates for the calculated nuclide concentrations.

In this work, nuclide concentrations have been calculated in a benchmark involving eight samples cut out of four fuel pins of one irradiated VVER-440 fuel assembly [3]. All calculations were performed with the multi-purpose Monte Carlo particle transport code Serpent, developed at VTT [4]. The work is based on an earlier work in SAFIR/KATVE project calculating the same benchmark exercise [5]. The purpose of this work was to further validate Serpent's depletion calculation methods and to test the sensitivity of the results to some burnup related options and algorithms. One purpose was also to repeat the earlier calculations since during the course of this work it was discovered that oxygen had been accidentally omitted from the fuel definition of the earlier work. Also, some Serpent related problems were encountered and solved during the work.

The report is divided in sections beginning with a brief description of the calculated benchmark in section 2. In section 3 this is followed by the presentation of the Serpent model and the introduction of the various cases calculated during the work. Results are presented in section 4 and finally some conclusions and summary are given in section 5.

2. Benchmark description

The benchmark is described in detail in the earlier VTT report [5]. Only the key information is repeated in this chapter.

The benchmark is based on the #2670 ISTC project providing VVER-440 PIE data for eight samples cut out of four fuel pins of the Novovoronezh NPP fuel assembly No. D26135 with average burnup of 38.5 MWd/kgU. The examined fuel assembly was irradiated in the reactor in four cycles for 1109 effective full power days (efpd). The assembly with pin numbers is presented in Figure 1 [6]. The samples were cut out of the fuel pins 65, 67, 68 and 69 marked with red colour in the figure. The central tube is presented with light blue colour.

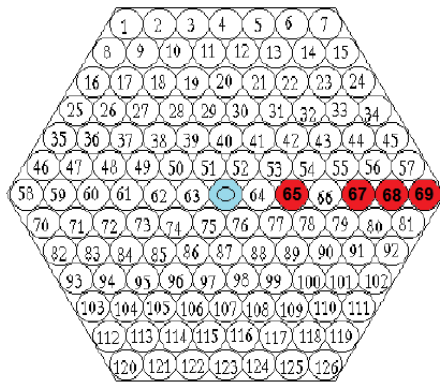


Figure 1. The measured fuel assembly. The measured samples were cut out of the fuel pins marked with red.

The positions of the 10 mm samples cut out of the fuel pins are presented in Figure 2 [3]. Three samples were cut out of pins 65 and 69 at three axial positions and one sample from the middle position was cut out of pins 67 and 68. The samples are identified with sample numbers presented in the figure.

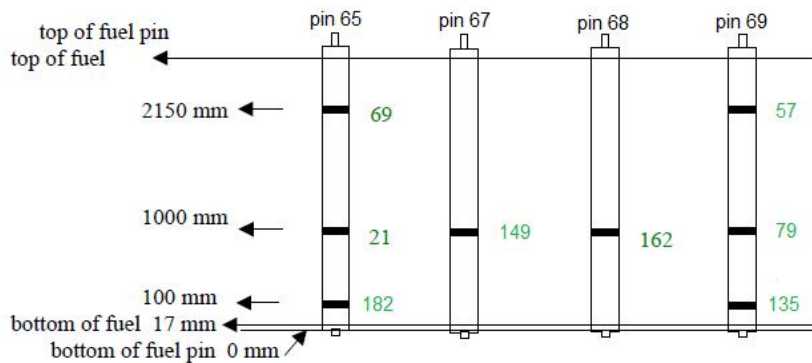


Figure 2. Sample positions in the fuel pins with sample numbers.

The geometry and material data are provided in detail in reference [3]. The irradiation history data is provided separately for each sample [3]. The four irradiation cycles (15, 16, 17 and 18) are divided in four phases, except for cycle 17 which only has two phases. Power at sample position and fuel, moderator and cladding temperature are specified separately for each phase and each sample. Boron concentration is adjusted for each phase but remains the same for all samples.

The sample specific parameters in the benchmark specifications such as linear power and different temperature values at sample position have been calculated based on the irradiation history data and fuel assembly design characteristics [3].

3. Models and methods

3.1 Serpent model

All calculations were performed with the multi-purpose Monte Carlo transport code Serpent, developed at VTT [4]. Version 2.1.31 was used for the final results but versions 2.1.30 and 2.1.29 were also tried during the work.

Each sample was modelled as one fuel pin in a two dimensional infinite lattice with reflective boundary conditions. An example of a modelled assembly is presented in Figure 3 for sample 149. The sample was cut out of fuel pin 67 and is marked with red colour in the figure.

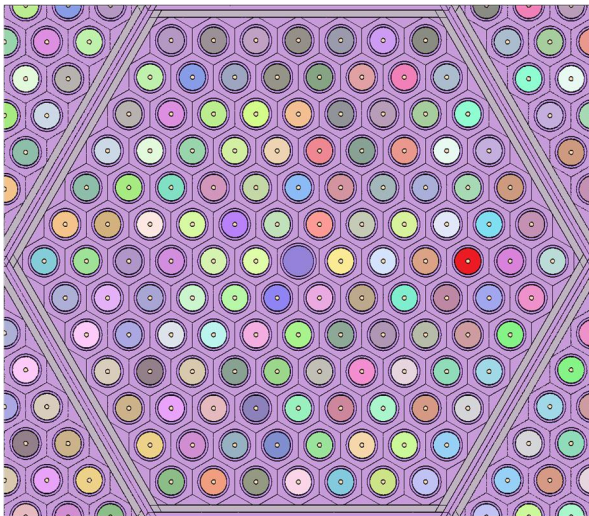


Figure 3. Modelled assembly for sample 149. The sample is presented with red colour.

In the calculations, power was normalized to the power produced by the sample under examination. Moderator density was not provided in the benchmark specifications, but it was calculated for each phase and each sample from the information provided on moderator temperature and pressure. CRAM method (Chebyshev Rational Approximation Method) was applied as the burnup calculation mode [7,8]. Burnup step length began with 2, 3 and 5 efpd and was increased to 10 for the remaining calculation. According to Serpent, this corresponds to roughly 0,5 MWd/kgU or 0,4 MWd/kgU towards the end of the calculation.

Each fuel pin was modelled as one burnup zone. The fuel material for the sample under examination was defined separately as one burnup zone. In some calculations the burnup zone division for the examined sample was refined using Serpent's automated depletion zone division.

Fourteen different input files were written for each sample to account for the changes in irradiation history during each cycle and phase. The scripts and data files written for input creation in the previous work [5] were utilized also in this work.

3.2 Calculation cases

The same benchmark exercise was calculated in the earlier work in order to compare measured nuclide concentrations to those calculated with Serpent [5]. The original purpose of the present work was to refine the earlier calculations and to test the sensitivity of the results to various options related to burnup algorithms and options calculating just one or a few samples. However, it was discovered that there was an error in the earlier calculations. In the

Serpent model, oxygen had been accidentally omitted from the fuel composition. Therefore, it was decided to repeat the earlier calculations for all samples with corrected fuel composition. Nuclide concentrations were calculated for all measured samples using three different cross section libraries ENDF/B-VII.1, JEFF-3.2, and JENDL-4.0.

Additionally calculations were performed for samples 149, 57, 79 and 182 using different burnup related modelling options and algorithms using the ENDF/B-VII.1 cross section libraries. The additional calculations are presented in Table I. The highlighted calculations were repeated for all samples 149, 57, 79 and 182 and the rest were done only for sample 149. Sample 149 was chosen because the average burnup of its fuel pin, 37,6 MWd/kgU, is close to the average burnup of the whole assembly 38,5 MWd/kgU and its location is quite well in the middle of the central tube and the assembly corner. The other samples were chosen in order to see if the sample location and burnup has any effect when determining whether the calculations would benefit from spatial discretization (burnup zone division).

Table I. Additional calculations for samples 149, 57, 79 and 182. Highlighted calculations were done for all afore mentioned samples and the rest were done only for sample 149.

Calculation	Explanation
reference	Normal calculation without modifications in the burnup options
repetition	The reference calculation was repeated for five times in order to find out the statistical accuracy of the calculations
densBUsteps	Reduced burnup step length
pcc LE/LI	3/5 substeps in predictor/corrector, LE/LI time integration method
pcc LE/QI	3/5 substeps in predictor/corrector LE/QI time integration method
pcc LE/QI 10	10/10 substeps in predictor/corrector LE/QI time integration method
tta	Burnup calculation mode TTA (Transmutation Trajectory Analysis) [9]
div10	Sample burnup zone divided in 10 equal size rings
div10rad	Sample burnup zone divided in 10 equal size rings and 8 sectors

Reduced burnup step length calculations (densBUsteps) applied a burnup step of 1 efpd up to 20 efpd. Then a step length of 2 efpd was applied up to 400 efpd. After that the step length was 5 efpd. These correspond to roughly 0.05, 0.1 and 0.2 MWd/kgU.

The substep method developed for burnup calculations in Serpent [10] was also tested in the calculations named "pcc ...". The purpose of substeps is to reduce discretization errors arising from the need to use constant reaction rates in the depletion calculations. This is achieved by dividing the depletion step in substeps and solving depletion separately for each of them. Two time integration methods were applied i) linear extrapolation in predictor and linear interpolation in corrector step (LE/LI) or ii) linear extrapolation in predictor and quadratic interpolation in corrector (LI/QI). Both methods were applied using 3 substeps in predictor and 5 substeps in corrector. These methods and numbers were chosen based on the findings in references [10,11] where the substep method was introduced and different time integration methods were compared. A calculation was also run using 10 substeps in both predictor and corrector with LE/QI method in order to see if the increased substep numbers would make any difference.

The calculations were originally started with Serpent version 2.1.30 which is the currently distributed most recent version of Serpent. However, the calculations yielded suspiciously large differences when compared to the measurement results. The problem was finally tracked to Serpent's restart file procedure. Restart files were needed since the calculation of every sample had to be divided in 14 consecutive calculations in order to change several parameters such as e.g. boron concentration during the calculation. The problem was fixed in Serpent version 2.1.31 which is currently under development. Before the problem with the restart files was discovered some sensitivity calculations were performed for sample 149 to see how much small errors in some input parameters would affect the results. In these calculations mainly the effect on U-238 concentration was studied since it should be the easiest nuclide to model.

Some calculations were also performed with Serpent version 2.1.29 that had been used in the previous calculations [5]. These calculations agreed with the ones performed with the fixed Serpent version 2.1.31. It was concluded that the restart file problem concerned only Serpent version 2.1.30.

4. Results

The measured and calculated burnups [MWd/kgU] for each sample are presented in Table II. In the table, "Measured" stands for the measured concentration of fission products that has been converted into MWd/kgU. "S calc" stands for Serpent calculation results and "Rus calc" presents burnups calculated in Russia based on the sample specific linear power values calculated for the benchmark exercise and used in the Serpent calculations. In this way, the values directly comparable to each other are "Rus calc" and "S calc", but the measured values are provided as an indication of the comparability of the measurement results to the calculated ones.

Table II. Measured and calculated sample burnups in MWd/kgU. "Rus calc" stands for burnup calculated in Russia according to the linear power specifications given in the benchmark. "S calc" stands for Serpent calculations at VTT.

	182	21	69	149	162	135	79	57
Measured	22.18	40.48	30.46	40.94	43.22	29.04	45.25	35.32
Rus calc	25.86	44.08	32.09	45.80	46.23	30.65	50.20	36.99
S calc	25.82	44.04	32.04	45.72	47.58	30.60	50.11	36.91

The Serpent results presented in Table II were calculated using ENDF/B-VII.1 cross section libraries but the results with the other libraries, JEFF-3.2 and JENDL-4.0, agreed with the ENDF/B-VII.1 calculations within 0.007 % for all samples. The difference between Serpent calculated and measured burnup values are between 4.5 % and 16.4 %. The differences for some samples are somewhat large but when comparing to the burnup results calculated in Russia from the sample specific linear power values given for the benchmark, the differences remain below 0.21 % for all but sample 162 for which the difference is 2.9 %.

Figure 4 presents the effective multiplication factors, k_{eff} , for all samples. The k_{eff} values are strongly critical in the beginning of the calculation for all samples. The multiplication factors decrease clearly below unity well before the end of the calculation for all but samples 182 and 135 that are the two least burned samples. Sample 182 is presented with bright green colour in the figure and its curve follows closely the curve of sample 135 which makes it difficult to distinguish in the figure. It can be seen that the k_{eff} values agree rather well with the calculated

and measured burnup values in the sense that the four highest burnup samples undergo the strongest reduction in the multiplication factor whereas the k_{eff} values of the middle burned samples 69 and 57 stay between the highest burned samples and the lowest burned, 182 and 135.

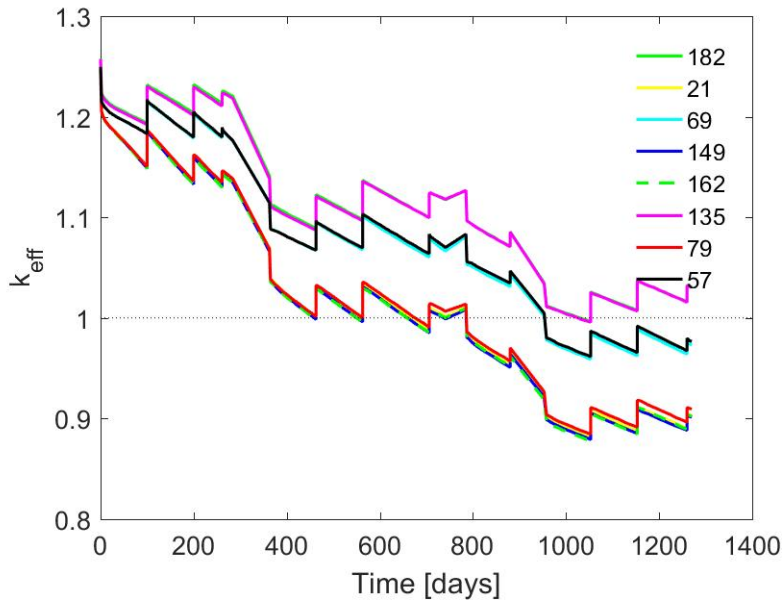


Figure 4. Effective multiplication factors for all examined samples.

Table III-Table VIII present the ratio of calculated masses to the measured masses (C/E) for selected nuclides. Nuclide selection is based on the ISG-8R3 [12] recommended nuclides for actinide and fission product burnup credit evaluation. The tables do not include the recommended nuclide Rh-103 because no measurement data was provided for that nuclide in the benchmark specifications [3].

The ratio of calculated to measured nuclide masses for some of the nuclides such as especially U-238 but also U-236, plutonium isotopes apart from Pu-238, Am-241 and some fission products are very close to unity. On the other hand deviation from unity is very large for some nuclides and samples such as Ag-109, Eu-151, Eu-153, Gd-155 and Np-237. Some of the deviations are explained by rather large measurement uncertainties. For nuclides Mo-95, Tc-99, Ru-101, Sm-151, U-234, Np-237, Pu-238, Am-241 and Am-243 all or most of the differences are smaller than the measurement uncertainty. Also, it must be kept in mind that the sample specific benchmark specifications such as linear power at the sample position are a result of calculations based on the actual operating history. The sample burnups based on these calculations (“Rus calc” in Table II) deviate from the measured burnup values. This indicates that the actual power at sample position may not have been exactly what has been specified in the benchmark specification and therefore the calculated nuclide concentrations might also somewhat differ from the measured values.

Table III. Calculated masses of uranium isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
U-234								
ENDF	1.659	0.870	1.165	0.850	0.826	0.883	1.600	1.802
JEFF	1.667	0.876	1.171	0.852	0.829	0.886	1.610	1.807
JENDL	1.683	0.892	1.188	0.870	0.849	0.897	1.645	1.839

U-235								
ENDF	0.913	0.947	1.012	0.926	0.914	0.888	1.129	0.953
JEFF	0.913	0.946	1.010	0.925	0.912	0.888	1.127	0.952
JENDL	0.915	0.952	1.014	0.930	0.919	0.891	1.137	0.957
U-236								
ENDF	1.148	1.081	1.087	1.071	1.062	1.133	1.081	1.101
JEFF	1.143	1.074	1.082	1.063	1.055	1.129	1.074	1.096
JENDL	1.140	1.073	1.080	1.063	1.054	1.127	1.074	1.095
U-238								
ENDF	0.997	0.997	0.998	0.995	0.995	0.999	0.994	0.998
JEFF	0.997	0.997	0.998	0.995	0.995	0.999	0.994	0.998
JENDL	0.997	0.997	0.998	0.995	0.996	0.999	0.994	0.999

Table IV. Calculated masses of plutonium isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
Pu-238								
ENDF	1.612	1.543	1.407	1.720	1.457	1.655	1.282	1.446
JEFF	1.600	1.490	1.384	1.651	1.384	1.634	1.206	1.406
JENDL	1.650	1.580	1.438	1.758	1.486	1.699	1.308	1.477
Pu-239								
ENDF	1.039	1.008	1.025	1.039	1.040	1.058	1.057	0.992
JEFF	1.038	1.010	1.025	1.042	1.044	1.058	1.059	0.995
JENDL	1.040	1.010	1.027	1.041	1.042	1.059	1.058	0.994
Pu-240								
ENDF	1.062	0.994	1.016	1.012	0.995	1.023	0.952	1.000
JEFF	1.067	1.002	1.023	1.022	1.004	1.029	0.963	1.006
JENDL	1.054	0.986	1.011	1.009	0.991	1.018	0.946	0.994
Pu-241								
ENDF	1.083	0.969	0.984	0.989	0.968	0.993	1.003	0.966
JEFF	1.076	0.963	0.975	0.983	0.963	0.985	0.996	0.960
JENDL	1.078	0.966	0.977	0.981	0.962	0.985	0.998	0.962
Pu-242								
ENDF	1.209	1.018	0.967	1.034	1.004	1.109	1.093	1.023
JEFF	1.199	1.011	0.959	1.026	0.995	1.102	1.087	1.016
JENDL	1.201	1.010	0.959	1.026	0.994	1.101	1.085	1.013

Table V. Calculated masses of neptunium and americium isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
Np-237								
ENDF	0.544	0.491	0.494	0.487	0.485	0.552	0.467	0.497
JEFF	0.554	0.500	0.504	0.496	0.492	0.561	0.473	0.505
JENDL	0.543	0.487	0.493	0.483	0.482	0.553	0.463	0.496
Am-241								
ENDF	1.114	1.079	1.025	1.000	1.019	1.062	1.011	1.049
JEFF	1.098	1.063	1.006	0.984	1.004	1.044	0.995	1.033
JENDL	1.109	1.076	1.017	0.991	1.014	1.054	1.007	1.044

Am-243								
ENDF	1.279	1.106	0.989	1.032	1.022	1.214	0.926	0.993
JEFF	1.310	1.152	1.024	1.071	1.064	1.242	0.959	1.030
JENDL	1.275	1.103	0.980	1.020	1.022	1.202	0.918	0.994

Table VI. Calculated masses of selected fission product isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
Mo-95								
ENDF	1.160	1.054	1.026	1.078	1.071	1.045	1.076	1.081
JEFF	1.164	1.058	1.030	1.082	1.076	1.050	1.082	1.086
JENDL	1.158	1.053	1.024	1.076	1.070	1.044	1.075	1.079
Tc-99								
ENDF	1.159	1.060	1.029	1.096	1.088	1.038	1.115	1.072
JEFF	1.158	1.059	1.028	1.094	1.086	1.037	1.113	1.070
JENDL	1.156	1.058	1.027	1.093	1.085	1.035	1.111	1.069
Ru-101								
ENDF	1.142	1.042	1.026	1.070	1.059	1.024	1.075	1.052
JEFF	1.153	1.054	1.036	1.083	1.071	1.034	1.088	1.063
JENDL	1.145	1.048	1.030	1.076	1.065	1.027	1.081	1.056
Ag-109								
ENDF	1.678	2.053	1.739	2.149	2.202	1.661	2.547	1.864
JEFF	1.853	2.269	1.920	2.369	2.430	1.837	2.817	2.065
JENDL	1.680	2.055	1.742	2.152	2.204	1.661	2.547	1.866
Cs-133								
ENDF	1.085	1.084	0.997	1.050	1.043	0.998	1.096	1.003
JEFF	1.066	1.065	0.979	1.030	1.024	0.981	1.076	0.986
JENDL	1.073	1.067	0.984	1.033	1.026	0.987	1.077	0.990

Table VII. Calculated masses of selected Nd, Eu and Gd isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
Nd-143								
ENDF	1.157	1.032	1.045	1.033	1.020	1.015	1.011	1.030
JEFF	1.152	1.023	1.039	1.023	1.008	1.009	0.998	1.022
JENDL	1.156	1.032	1.044	1.033	1.020	1.015	1.011	1.030
Nd-145								
ENDF	1.095	0.950	0.955	0.964	0.969	0.971	0.960	0.964
JEFF	1.100	0.953	0.959	0.967	0.972	0.975	0.963	0.968
JENDL	1.090	0.945	0.951	0.958	0.962	0.966	0.952	0.958
Eu-151								
ENDF	0.798	6.486	2.107	1.949	3.728	2.249	7.737	2.960
JEFF	0.810	6.579	2.137	1.983	3.792	2.282	7.878	3.004
JENDL	0.790	6.379	2.080	1.921	3.686	2.229	7.634	2.922
Eu-153								
ENDF	4.091	6.993	4.878	7.512	8.131	4.424	11.611	5.841
JEFF	4.128	7.196	4.960	7.736	8.411	4.490	12.024	5.970
JENDL	4.152	7.153	4.968	7.712	8.371	4.506	11.960	5.965

Gd-155								
ENDF	5.847	7.528	6.365	7.525	7.764	5.875	8.291	6.738
JEFF	5.669	7.307	6.176	7.332	7.548	5.647	8.075	6.568
JENDL	5.738	7.374	6.243	7.406	7.643	5.710	8.135	6.626

Table VIII. Calculated masses of samarium isotopes relative to the measured ones C/E.

Sample	182	21	69	149	162	135	79	57
Sm-147								
ENDF	0.932	1.065	0.995	1.008	1.052	1.034	1.097	1.054
JEFF	0.942	1.084	1.008	1.024	1.070	1.044	1.116	1.068
JENDL	0.935	1.075	1.001	1.017	1.062	1.039	1.111	1.063
Sm-149								
ENDF	1.009	1.222	1.286	1.129	1.121	0.979	1.166	1.233
JEFF	0.961	1.178	1.234	1.098	1.093	0.938	1.134	1.192
JENDL	0.998	1.206	1.270	1.121	1.112	0.970	1.154	1.220
Sm-150								
ENDF	1.029	1.142	1.068	1.095	1.111	1.053	1.137	1.086
JEFF	1.021	1.138	1.062	1.090	1.106	1.045	1.132	1.079
JENDL	1.029	1.144	1.067	1.096	1.114	1.053	1.140	1.086
Sm-151								
ENDF	0.994	1.227	1.166	1.100	1.121	0.932	1.132	1.058
JEFF	1.008	1.244	1.182	1.119	1.140	0.944	1.152	1.073
JENDL	0.968	1.188	1.133	1.068	1.091	0.909	1.100	1.028

Table IX presents results of calculations of sample 149 applying different burnup related modelling options. The “Ref” column gives the nuclide concentration in kg/tU_{initial} for the reference calculations. The reference calculation is an average of five independent calculations using the default modelling options explained in section 3.1. The rest of the columns present the differences to the reference calculations in %. “Meas” refers to measurement results. Column “stat err” gives the largest difference of the five independent calculations to the reference calculation. Its purpose is to help to understand which differences are related to modelling options and which are only statistical uncertainty. Column “tta” means calculations using Transmutation Trajectory Analysis as the burnup mode [9]. “densBUsteps” refers to calculations with shorter burnup steps. The “pcc” columns refer to calculations applying the substep method with 3/5 or 10/10 substeps as explained in section 3.2. “leli” refers to linear extrapolation/interpolation in predictor/corrector and “leqi” refers to linear extrapolation/quadratic interpolation in predictor/corrector.

Table IX. Results of calculations of sample 149 with different burnup related modelling options. “Ref” presents the nuclide concentrations [kg/tU_{initial}] and the other columns present differences to the reference calculation (ref) in %.

Nuclide	Ref [kg/tU _{init}]	Meas [%]	stat err [%]	tta [%]	dens BUsteps [%]	pcc leqi [%]	pcc leli [%]	pcc leqi10 [%]
Mo-95	1.00	-7.22	-0.02	0.44	0.00	0.44	0.44	0.45
Tc-99	1.05	-8.75	0.02	-0.22	0.01	-0.20	-0.20	-0.21
Ru-101	1.06	-6.52	0.01	1.18	0.01	1.20	1.19	1.20
Ag-109	0.116	-53.45	-0.22	10.03	0.10	10.39	10.36	10.36
Cs-133	1.486	-4.71	-0.04	-1.81	0.02	-1.84	-1.82	-1.86
Nd-143	1.001	-3.21	-0.02	-1.01	0.01	-0.96	-0.98	-0.98
Nd-145	0.879	3.70	0.04	0.31	0.00	0.34	0.32	0.34

Sm-147	0.300	-0.71	-0.08	1.53	0.00	1.79	1.63	1.61
Sm-149	0.00361	-11.51	-0.45	-2.80	0.14	-3.00	-3.01	-3.07
Sm-150	0.4035	-8.64	0.02	-0.36	0.01	-0.42	-0.39	-0.38
Sm-151	0.0123	-9.18	0.11	1.52	0.04	1.71	1.72	1.50
Sm-152	0.129	-3.52	0.36	2.30	-0.02	2.39	2.39	2.19
Eu-151	0.001252	-48.73	0.11	1.59	0.05	1.77	1.78	1.56
Eu-153	0.1608	-86.69	0.11	2.94	-0.01	3.00	2.87	3.10
Gd-155	0.0105	-86.70	-0.11	-2.29	0.02	-2.41	-2.19	-2.04
U-234	0.161	17.74	-0.25	0.27	0.05	0.27	0.35	0.39
U-235	6.47	8.04	-0.06	-0.25	0.07	-0.09	-0.17	-0.13
U-236	5.66	-6.60	-0.02	-0.71	-0.02	-0.65	-0.74	-0.72
U-238	927.17	0.5203	0.0009	0.0042	0.0012	0.0024	0.0016	0.0037
Np-237	0.71	105.46	0.08	2.04	-0.04	1.68	1.97	2.02
Pu-238	0.355	-41.93	-0.13	-4.10	-0.02	-4.31	-4.04	-4.33
Pu-239	6.491	-3.78	-0.05	0.11	0.10	0.17	0.32	0.04
Pu-240	2.90	-1.17	0.11	0.88	-0.05	1.10	1.16	1.08
Pu-241	0.977	1.17	-0.08	-0.64	0.10	-0.82	-0.70	-0.77
Pu-242	0.86	-3.34	-0.11	-0.67	0.16	-0.73	-0.74	-0.93
Am-241	0.855	0.07	-0.07	-1.60	0.10	-1.76	-1.65	-1.71
Am-243	0.20	-2.70	0.38	3.85	-0.23	4.00	3.64	4.83
Burnup	45.723	-10.461	0.002	0.001	0.002	0.002	0.001	0.002

Most differences to the reference calculation are rather marginal compared to the differences to the measurement results. Shorter burnup step length doesn't seem to effect the results practically in any way. On the other hand, substep method seems to have some effect, although rather small, to the calculation results. The effect might be larger if the modelled nuclides included short lived isotopes since the substep method is more effective for short lived nuclides. Both time integration methods LE/LI and LE/QI give the same results. Increasing the number of substeps from 3/5 ("pcc leqi" and "pcc leli") to 10/10 ("pcc leqi10") doesn't seem to have any effect and 3/5 seem to be sufficient numbers for the substeps. Interestingly the same effect as applying the substep method seems to be achieved using the TTA burnup mode.

Table X presents results calculated for different samples using burnup zone division into 10 equal area rings ("div10") and further into 8 radial sectors ("div10rad"). Column "stat err" is the same as in Table IX. It represents the largest statistical differences encountered in the repetition calculations of sample 149. The rest of the columns refer to differences compared to the reference calculation of the sample in question.

Table X. Differences of four samples applying burnup zone division to reference calculations. Columns "div10" and "div10rad" refer to burnup zone division into 10 equal size rings and 10 equal size rings plus eight sectors, respectively.

Nuclide	stat err [%]	182	div10	149	79	57			
		div10 [%]	rad [%]	div10 [%]	div10rad [%]	div10 [%]	div10rad [%]	div10 [%]	div10rad [%]
Mo-95	-0.02	-0.02	-0.02	-0.01	-0.01	-0.02	-0.01	-0.01	0.00
Tc-99	0.02	-0.02	-0.01	-0.01	0.00	-0.02	-0.02	0.00	0.00
Ru-101	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.01	0.02
Ag-109	-0.22	0.25	0.23	0.07	0.00	0.03	-0.18	0.19	0.16
Cs-133	-0.04	-0.02	-0.01	0.01	-0.01	-0.01	0.01	0.03	-0.01
Nd-143	-0.02	-0.02	-0.02	-0.04	-0.06	-0.03	-0.07	-0.03	-0.05
Nd-145	0.04	0.00	0.01	-0.01	-0.01	-0.03	-0.02	-0.03	-0.02
Sm-147	-0.08	0.02	-0.05	-0.13	-0.02	-0.10	-0.09	0.04	0.02
Sm-149	-0.45	0.15	0.19	-0.19	0.07	0.16	-0.03	-0.49	-0.33

Sm-150	0.02	-0.03	-0.02	-0.02	-0.06	-0.07	-0.08	-0.07	-0.06
Sm-151	0.11	-0.23	-0.16	0.01	-0.06	0.01	-0.08	-0.20	-0.14
Sm-152	0.36	-0.09	0.25	-0.17	0.10	-0.03	-0.02	0.01	0.22
Eu-151	0.11	-0.24	-0.16	0.00	-0.07	0.01	-0.08	-0.20	-0.14
Eu-153	0.11	0.25	-0.03	0.28	0.21	0.20	0.12	0.22	0.04
Gd-155	-0.11	0.08	0.27	0.07	-0.13	0.44	0.42	0.81	0.42
U-234	-0.25	0.11	0.12	-0.05	0.09	-0.02	-0.14	0.19	0.06
U-235	-0.06	0.08	0.08	0.22	0.20	0.38	0.35	0.20	0.20
U-236	-0.02	-0.05	-0.07	-0.03	0.01	0.04	0.04	-0.04	-0.04
U-238	0.001	0.004	0.004	0.007	0.006	0.007	0.009	0.005	0.006
Np-237	0.08	-0.08	0.00	-0.22	-0.57	-0.39	-0.43	-0.29	-0.33
Pu-238	-0.13	-0.03	-0.07	-0.09	-0.21	-0.38	-0.54	-0.17	-0.27
Pu-239	-0.05	-0.68	-0.72	-0.75	-0.69	-0.92	-1.00	-0.60	-0.81
Pu-240	0.11	-0.64	-0.84	-0.89	-0.81	-1.10	-1.33	-1.20	-1.22
Pu-241	-0.08	0.30	0.47	-0.30	-0.43	-0.41	-0.44	-0.01	0.00
Pu-242	-0.11	1.08	1.26	0.55	0.40	0.73	0.90	1.03	0.99
Am-241	-0.07	0.29	0.46	-0.32	-0.44	-0.42	-0.45	0.00	-0.01
Am-243	0.38	1.64	1.76	1.31	1.74	0.72	0.68	1.25	1.74
Burnup	-0.002	-0.001	-0.001	0.001	0.001	0.001	-0.001	0.002	0.002

According to Table X, burnup zone division doesn't seem to have any significant effect on the calculated concentration of fission products except perhaps for Gd-155 in samples 79 and 57. However, there seems to be some small effect on some actinides such as U-235, Pu-239, Pu-240, Pu-241, Am-241 and Am-243. These differences are highlighted in the table. Division into 10 equal area rings versus division to the same rings and 8 radial sectors doesn't produce any clear differences. Therefore, at least for these samples, radial sector division seems redundant. Overall, the different samples benefit relatively similarly from the burnup zone division. Sample 79 might benefit slightly more than the other samples. Sample 79 was cut out of the middle of a fuel pin located in the corner of the assembly. Closer proximity to the central tube (sample 182) doesn't seem to increase the differences in results calculated using burnup zone division relative to the other samples.

Table XI lists the sensitivity calculations performed for sample 149 with Serpent version 2.1.30. Boron concentration is given in the benchmark specification as $\text{g}(\text{H}_3\text{BO}_3)/\text{kg}(\text{H}_2\text{O})$. In the default calculation, boron concentration in water is calculated by determining the mass fraction of boron m_B in the water containing boric acid. Then, the mass fraction of water is calculated by $1 - m_B$. This way of calculation contains a small approximation since it doesn't take into account the mass fraction of the rest of the boric acid but adds it to the mass of water. However, in the Serpent model only water and boron are given in the definition of borated water. In the calculation named "boron" in Table XI boron concentration has been defined exactly without this approximation. This slightly increases the boron content versus the default calculation.

In the calculation "fueldens", the fuel density was 10.6 g/cm^3 which is an average value for fuel pellet density given in reference [6]. The default value 10.0037 g/cm^3 is given in the benchmark specifications [3].

Table XI. Sensitivity calculations performed for sample 149 with Serpent version 2.1.30.

Calculation	Explanation
U235H	U-235 fission heating value set to 200 MeV (default is 202.27 MeV)
boron	Boron concentration defined exactly (default contains a small approximation)

powdens	Power defined as power density instead of power (linear power)
Salfa	Thermal scattering data for hydrogen interpolated between two library values (default extrapolates to one given library value)
fueldens	Fuel density 10.6 g/cm ³ (default is 10.0037)
waterdens	Water density 0.759, 0.764, or 0.769 in all phases (in default calculations the density varies between these values during different phases of irradiation cycles)

No significant differences were found in the calculated U-238 concentration between the sensitivity calculations and the reference calculation applying default parameter values except for “fueldens” where the fuel density had been changed. For that calculation U-238 concentration differed 0.26 % from the reference calculation and the concentration of U-235 differed 16 %. Differences for the other nuclides were mainly between 1 - 8 %. Changing U-235 fission heating value had a small effect of the order of 1 % for other nuclides but U-238. For U-235 the difference to reference calculation was 2.3 %. No significant differences were observed in the other sensitivity calculations. The accurate definition of boron concentration had no effect at all. It can be concluded that the approximation in the definition of boron concentration is valid.

The version 2.1.30 contained a bug related to the treatment of restart files. However, based on several repetition calculations the error is expected to behave similarly in all calculations. Therefore, the main findings of these sensitivity calculations can be expected to be valid also for the corrected Serpent version.

5. Conclusions and summary

A simplified benchmark defining the irradiation history of eight samples cut out of four fuel pins of a VVER-440 fuel assembly has been calculated [3]. The purpose was to continue the validation of Serpent’s depletion calculation methods and to test the sensitivity of the results to some burnup related algorithms and modelling options. One purpose was also to repeat earlier calculations [5] because oxygen had been accidentally omitted from the fuel definition.

Nuclide inventory has been calculated with Serpent version 2.1.31 using three different cross section libraries ENDF/B-VII.1, JEFF-3.2. and JENDL-4.0. The reference calculations to which all other calculations were compared were done with the ENDF/B-VII.1 libraries. The nuclide selection was based on Interim Staff Guidance 8 revision 3 [12]. Correction factors defining the ratio of calculated nuclide concentrations to measured ones was calculated for all samples. The different libraries yielded consistent results for U-238 but there were some differences for other nuclides. The calculated actinide concentrations differed mostly less than 1 % between the libraries. The largest differences in the JEFF-3.2 calculated actinide concentrations compared to the ENDF/B-VII.1 were 0.7 - 5.9 % in Pu-238 depending on the sample and 2.3 - 4.2% in Am-243. The largest differences in actinides with JENDL-4.0 libraries were 1.4 - 2.8 % in U-234 and Pu-238. For the fission products the differences between ENDF/B-VII.1 and the other two libraries were mostly of the order of 1 or 2 % or less for JENDL-4.0. A clear exception was Ag-109 where the differences for JEFF-3.2 were approximately 10 % for all samples. However, for JENDL-4.0 the differences in Ag-109 concentrations were negligible.

The calculated correction factors are close to unity for U-238, U-236, plutonium isotopes apart from Pu-238, Am-241 and some of the fission products. The difference between calculated and measured nuclide concentrations for U-238 is between 0.1 - 0.6 % depending on the

sample. For other nuclides the differences are larger but remain mostly between 1 - 10 %. For some nuclides, the differences are explained by rather large measurement uncertainties for all or most of the samples. The largest differences that cannot be explained by measurement uncertainty are observed in nuclides Ag-109, Eu-151, Eu-153 and Gd-155 where the differences are between 66 - 680 %. The concentration of these nuclides is also rather low which can make them more difficult to model. In case of Ag-109, the different libraries also yielded clearly different results but this cannot alone explain the differences.

One explanation for differences between measured and calculated nuclide concentrations could be found in the values given for linear power at the sample positions in the benchmark definition. Linear power at sample positions given in the benchmark have been calculated based on the actual irradiation history and the fuel assembly design characteristics. Sample burnup values determined in these calculations differ from the measured burnup values, but agree well with the values calculated by Serpent. This might indicate that the linear powers given in the benchmark definition might not be exactly correct. That would naturally cause discrepancies between calculated and measured nuclide concentrations.

Some samples were calculated also using different burnup related modelling options and algorithms. The largest differences to reference calculations were observed when using the substep method or TTA method [9] as the burnup algorithm instead of CRAM method [7,8]. However, these differences were rather small, mostly of the order of 1 - 2 %.

Differences to the earlier calculations [5], where oxygen had been omitted from the fuel material definition, can be seen most clearly by examining the multiplication factors. In the earlier calculations, the multiplication factors are clearly larger for all examined samples and decrease below unity only for the most burned samples. In the new calculations the multiplication factors remain above unity throughout the irradiation history only for the two samples with lowest burnup.

One way to improve the calculated results relative to the measurements would be to use the measured burnup values of the samples in the depletion calculations. In this case however, one would have to find a way to estimate the values of the other parameters such as linear power and temperature values at sample position.

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