Acta Polytechnica CTU Proceedings **19**:7–13, 2018
doi:10.14311/APP.2018.19.0007

available online at http://ojs.cvut.cz/ojs/index.php/app

SCALE AND SERPENT TWO-GROUP CROSS-SECTION DATA GENERATION

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Abstract. In this work, VVER fuel assembly is calculated using two different codes - Serpent and SCALE. Multiplication factor and several two-group macroscopic parameters including scattering cross-section, fission cross-section, total cross-section and diffusion coefficient were studied. In addition to this, fuel isotopic composition dependency on burnup was calculated as a part of this study. Obtained data are compared and differences are discussed. Both codes provides similar results for all studied parameters.

Keywords: VVER, Serpent, VVANTAGE-6, fuel cycle, burnup, SCALE, Temelin nuclear power plant, depletion calculation, homogenized cross-sections.

1. Introduction

The crucial part of nuclear safety is based on results obtained by calculation. To ensure accurate results, codes are compared with experimental data (benchmarking) and also among each other [8], [6].

In this work, VVER fuel assembly depletion is calculated using two different codes - Monte-Carlo code Serpent and deterministic sequence TRITON from SCALE package. Multiplication factor and several two-group macroscopic parameters including scattering cross-section, fission cross-section, total cross-section and diffusion coefficient are calculated and compared. In addition to that, fuel isotopic composition dependency on burnup were calculated. All values are calculated during the fuel depletion in order to cover the whole fuel cycle, which means burnup up to 60.5 MWd/kg$_U$. In addition, several Serpent memory optimization settings and their impact on macroscopic data generation were tested.

The TRITON calculation sequence from the SCALE package [5] represents the traditional approach to fuel depletion calculations and few-group data generation. It is based on deterministic code NEWT producing data for the well–established ORIGEN depletion code.

Serpent code [9] was selected due to the fact that the code is designed directly for reactor core calculations combining Monte-Carlo based transport calculations and advanced CRAM fuel depletion method [10].

Serpent and SCALE codes allow homogenized few-group cross-sections and other nuclear constants describing fuel assembly behavior to be produced. These results can be later used in full-core calculations. Both codes use different approach to obtain homogenized cross-section and other nuclear data. Therefore, comparison provides valuable information about the methods used. SCALE code has a longer history in this field of application compared to Serpent code, thus SCALE code was selected as the reference code for this study.

Firstly, the model and the calculation itself is described, then results are presented and discussed.

2. Fuel assembly description

For this particular study, fuel assembly model was created based on VVANTAGE-6 fuel design [2] (see Figure 1). VVANTAGE-6 fuel was developed by Westinghouse company for VVER-1000 reactors. Therefore, it features hexagonal fuel lattice. This fuel type was used in the Temelin Nuclear Power Plant reactor for the first 10 years of operation. The fuel assembly without IFBA absorber was selected for this study. Assembly parameters are listed in the Table 1. All fuel pins are identical, with flat 3% enrichment. Temperatures used in this study are listed in the Table 2.

3. Calculation setup

Two dimensional models of the fuel assembly in Serpent code (version 2.1.27) and SCALE code (version 6.2.1) were created based on the VVANTAGE-6 design specified in Table 1. Specific power 35.54 W/g$_{HM}$ was used in both calculations. B1-leakage corrected critical spectrum was applied in both calculations as well. In Serpent calculation, B1 correction used 238 group energy structure (scale238 [5]). Fast group (group 1) was above 0.625 eV and thermal group (group 2) below that for both codes.

Serpent calculation were conducted with 10000 neutrons per cycle, 400 active cycles and 50 inactive cycles. Input cross-section data for Serpent calculations were obtained from ENDF/B-VII.1 library [7].

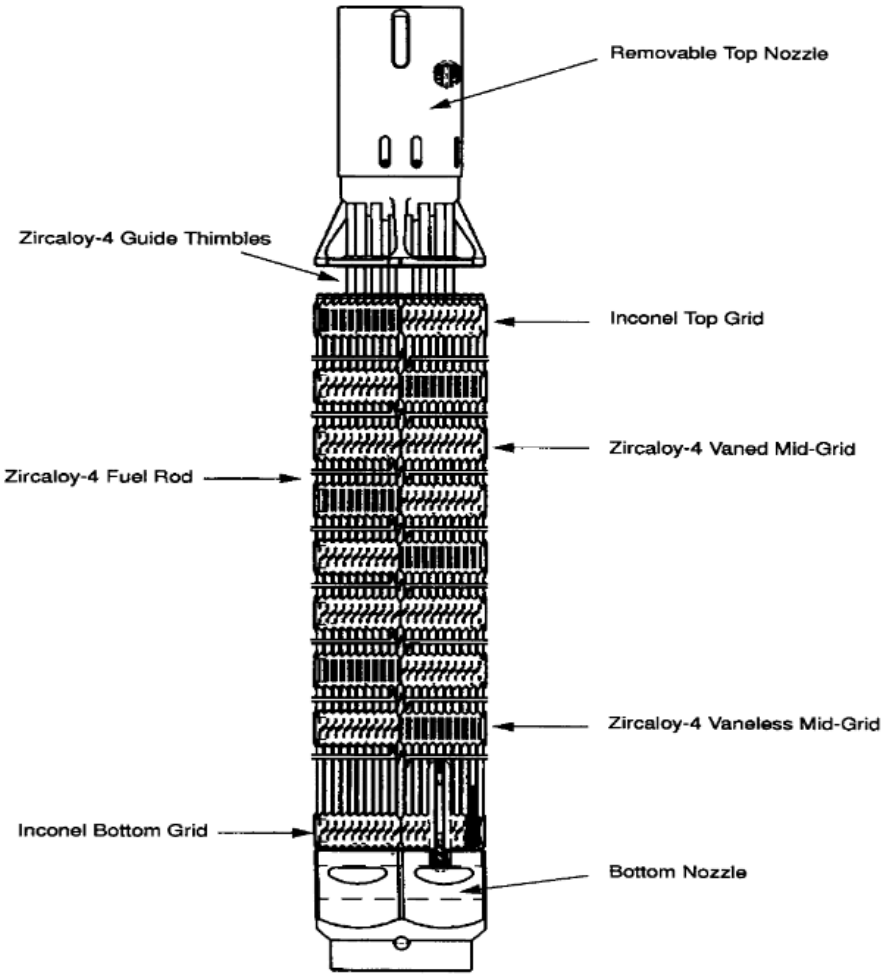


Figure 1. VVANTAGE-6 fuel assembly [11].

Parameter	VVANTAGE 6
Pin cladding outer diameter [mm]	9.144
Pin cladding inner diameter [mm]	8.001
Pin cladding thickness [mm]	0.5715
Pin cladding material	Zr-4 (303)
Fuel pellet outer diameter [mm]	7.844
Number of fuel pins in FA	312
Pin pitch [mm]	12.75
Number of instrumentation tubes	1
Tube material	Zr-4 (303)
Inner tube diameter [mm]	12.6
Outer tube diameter[mm]	11.0
Tube thickness [mm]	0.8
Number of guide tubes	18
Tube material	Zr-4 (303)
Outer tube diameter over the absorber area [mm]	12.6
Inner tube diameter over the absorber area [mm]	11.0
Tube thickness over the absorber area [mm]	0.8
Outer tube diameter in the absorber area [mm]	10.41
Inner tube diameter in the absorber area [mm]	8.6
Tube thickness in the absorber area [mm]	0.905
Total assembly weight [kg]	766
UO_2 density [g/cm^3]	10.412
Zr-4 density [g/cm^3]	6.53

Table 1. Fuel assembly parameter summary [3].

Fuel temperature	1005 K
Soluble boron concentration	525 ppm (3 g/kg)
Coolant density	0.7169 g/cm^3
Coolant temperature	578 K

TABLE 2. Calculation parameters.

SCALE code used the default detailed ENDF/B-VII.1 252 group library. Reflective boundary conditions resulted in infinite lattice calculation for both codes.

Serpent allows automatic division of fuel pins into radial regions for more realistic depletion calculations. All fuel pins were divided into 5 radial regions and each region was burned separately in this study. In addition, there were unique materials for all fuel pins in the fuel assembly, thus their material compositions were treated separately.

SCALE calculation used 60° symmetry to limit the number of depleted materials. Fuel pins in symmetrical positions were considered as identical material. No radial regions in fuel pins were defined as there is no burnable absorber.

SCALE and Serpent calculation used 51 burn steps with final burnup at 60.5 MWd/kg$_U$[1]. Seven steps were between 0 MWd/kg$_U$ to 1, followed by 44 steps with approximately 1.3 MWd/kg$_U$ distance.

Additional 231 isotopes were added in SCALE burnup calculation using addnux=3 parameter. Serpent used the default isotope inventory setting.

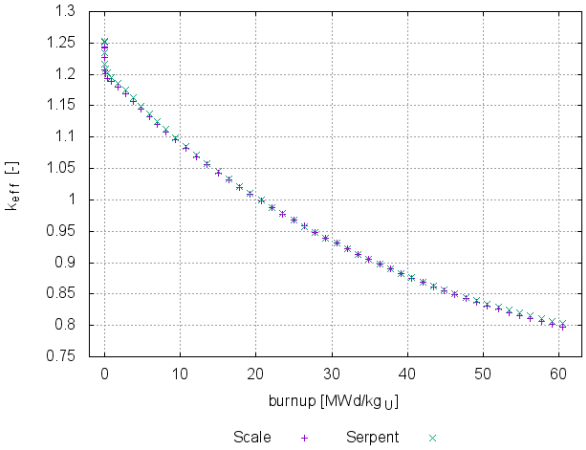
4. RESULTS

The following parameters were studied: multiplication factor, scattering cross-section (from first group to the second one). In addition to these, fission cross-section, total cross-section and diffusion coefficient, all for two groups. All these parameters were studied for different Serpent memory optimization setup. Nominal optimization (number 4) was used to produce results which are compared with SCALE values.

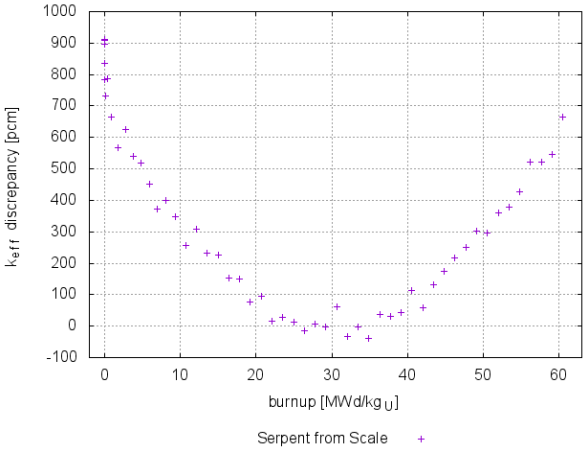
4.1. MULTIPLICATION FACTOR

Multiplication factor results are plotted in Figure 2a. In order to better show the differences, absolute differences between SCALE and Serpent results were calculated and plotted in Figure 2b (SCALE is the reference one). Statistical uncertainty in Serpent results is only 22 pcm. Uncertainty introduced by nuclear data may reach several hundreds of pcm. However, Serpent and SCALE calculation used nuclear data from an identical library (ENDF/B-VII.1). SCALE calculation used preprocessed data in 252 group library, Serpent used continuous version. Serpent values are higher compared to SCALE results for BOC and EOC. Values around 30 MWd/kg$_U$ are similar for both codes. Initial multiplication factors differ more than 900 pcm from SCALE results. Difference change to 0 pcm reached around 30 MWd/kg$_U$. EOC difference reached almost 600 pcm.

[1]60 MWd/kg$_U$ is considered as maximal burnup value for currently fuel used.



(A).



(B).

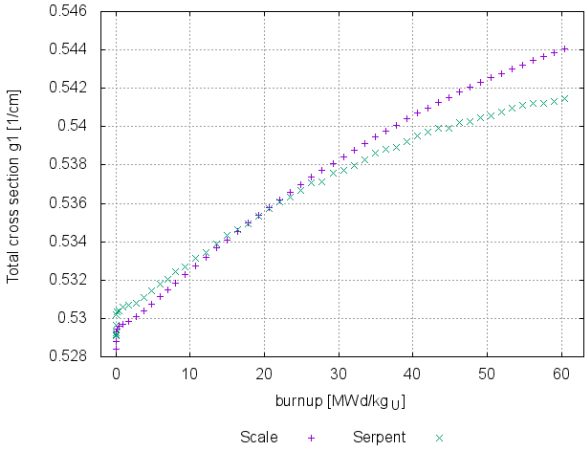
FIGURE 2. Multiplication factor from SCALE and Serpent calculation (a) and SCALE difference from Serpent results (b).

4.2. TOTAL CROSS-SECTION

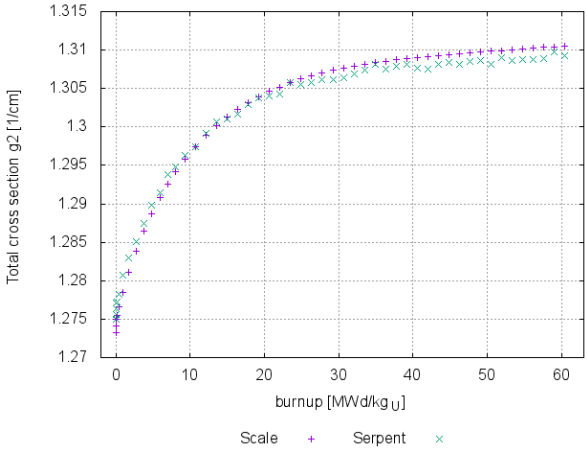
Total cross-sections for both codes are in good agreement. Values are plotted in Figure 3a for the fast group and in Figure 3b for the thermal group. The Serpent code initially calculates the total cross-section by about 0.4 % greater than SCALE. The value gradually increase during the course of fuel depletion. At burnup level about 20 MWd/kg$_U$ the SCALE value gets greater and the final difference is 0.4 %. Results for the thermal group results are almost identical. Except for the initial limited period, the differences are limited to 0.1 %. Serpent value relative uncertainty is only 0.015% for thermal group and 0.014% for fast group.

4.3. DIFFUSION COEFFICIENT

The diffusion coefficient is an important macroscopic parameter. Diffusion coefficient was calculated for both groups. The coefficient values are plotted in

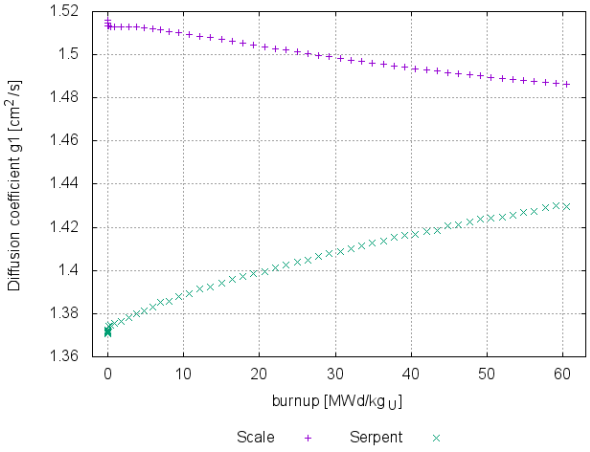


(A).

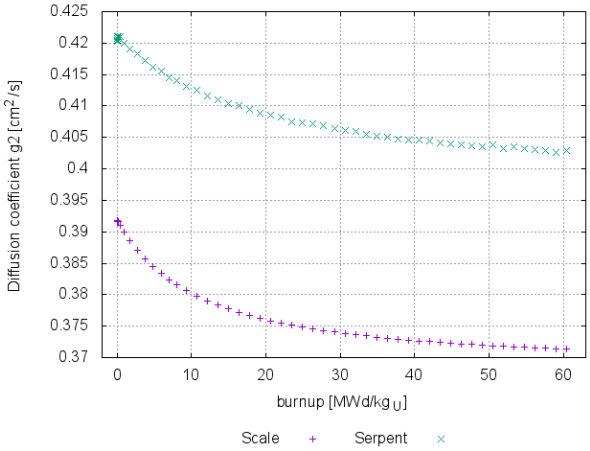


(B).

Figure 3. Total cross-section dependency on burnup for fast group (a) and for thermal group (b).



(A).



(B).

Figure 4. Diffusion coefficient dependency on burnup for fast group (a) and for thermal group (b).

Figures 4a and 4b. Fast group coefficient obtained by SCALE calculation is higher compared to Serpent results. Thermal group results are opposite, Serpent values are higher compared to SCALE results. Difference for fast group starts approximately at 10% at BOC, slowly decreasing and reaching only 3% at EOC. Slow group values differs by −7% at BOC, drop to −8.6% where it remains till the end. The difference observed in both groups is probably rooted in code structure (stochastic vs deterministic) and in nuclear data difference.

Serpent value relative uncertainty is only 0.025% for thermal group and 0.021% for fast group.

4.4. Fission cross-section

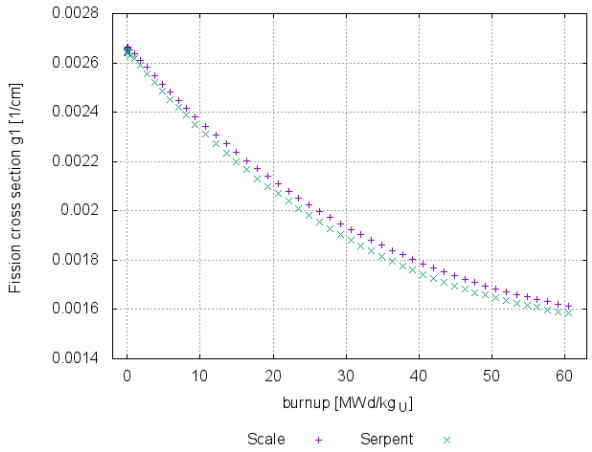
Fission cross-sections for two energy groups are plotted in Figures 5a and 5b. Discrepancies from Serpent results are plotted in Figures 6a (fast group) and 6b (thermal group). Fission cross-section for thermal group behaves similarly to the multiplication factor. SCALE cross-section increases in the first part of fuel cycle, which probably results in decrease of k_{eff} difference. Maximum is observed similar to minimum of k_{eff} difference around 30 MWd/kg$_U$. Serpent value relative uncertainty is only 0.038% for thermal group and 0.053% for fast group.

4.5. Scattering cross-sections

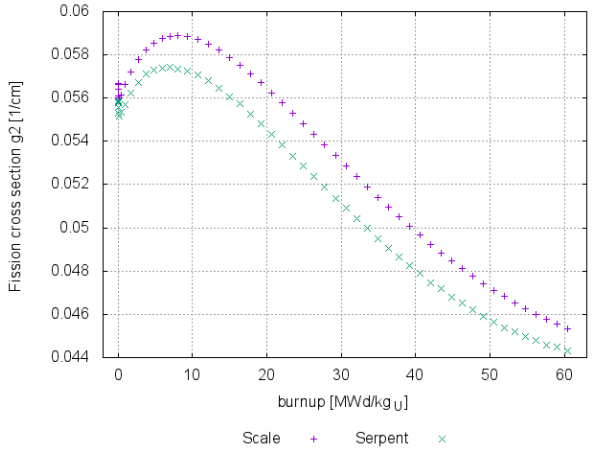
Scattering cross-section from fast group to thermal group is plotted in Figure 7. Both results have similar behavior. Serpent values differ from 0.7% to 1% in discrepancy. Serpent value relative uncertainty is only 0.014%.

4.6. Isotope concentrations

Number densities of dominant actinides ^{235}U, ^{238}U, and ^{239}Pu during fuel burnup were calculated to support understanding of fuel behavior. Results are printed in figures 8a, 8b and 8c (including difference from SCALE results). The observed isotopic changes are consistent but there are differences that can explain differences in the few-group cross-sections. It can be seen that Serpent calculates faster ^{235}U depletion than SCALE and also ^{239}Pu number density is lower for the majority of burnup levels. This con-

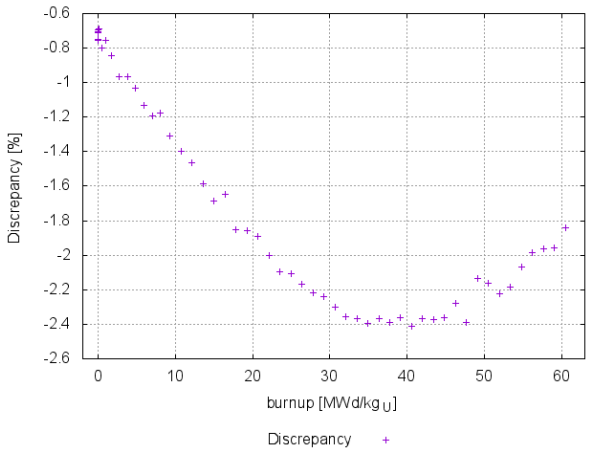


(A).

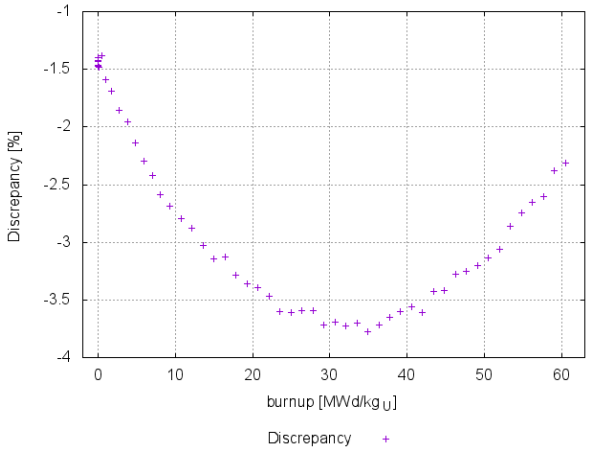


(B).

FIGURE 5. Fission cross-section dependency on burnup for fast group (a) and for thermal group (b).



(A).



(B).

FIGURE 6. SCALE fission cross-section discrepancy to Serpent values for fast group (a) and for thermal group (b).

tributes to different and total cross-sections calculated by these two codes.

4.7. Memory optimization option in Serpent code

Serpent 2 allows modify calculation in the RAM requirements using memory optimization. Default mode 4 is recommended for cross-section and other nuclear data generation and has the highest memory requirements. Modes 3, 2 and 1 have lower memory requirements and extend calculation duration. More differences are described in Serpent forum [1].

In order to compare memory optimization, multiplication factor and other nuclear data were calculated with different optimization. Results obtained are similar for all cases and the difference is under statistical uncertainty. The difference for multiplication factors are smaller than 70 pcm which within three standard deviations of the calculation.

5. Conclusion

Monte Carlo code Serpent and TRITON calculation sequence from the SCALE package were used to solve the identical task: calculations of multiplication factor and several two-group macroscopic parameters including scattering cross-section, fission cross-section, total cross-section and diffusion coefficient during depletion of a VVANTAGE-6 fuel assembly. In addition, fuel isotopic composition evolution of selected nuclides was determined. Both codes use different methods for solving this neutron transport and depletion coupled task. The results obtained were compared and differences were discussed for each studied parameter.

The multiplication factor obtained by both codes are compared in the Figure 2a and the differences are plotted in 2b. The initial multiplication factors determined by Serpent differs by more than 900 pcm from the SCALE code results, then it decreased to 0 pcm at around 30 MWd/kg$_U$, however the EOC difference reached almost 600 pcm.

Total cross-section for both codes is in a good agreement. Values are plotted in Figure 3a for the fast group and in Figure 3b for the thermal group. The relative difference is between ±0.4 %.

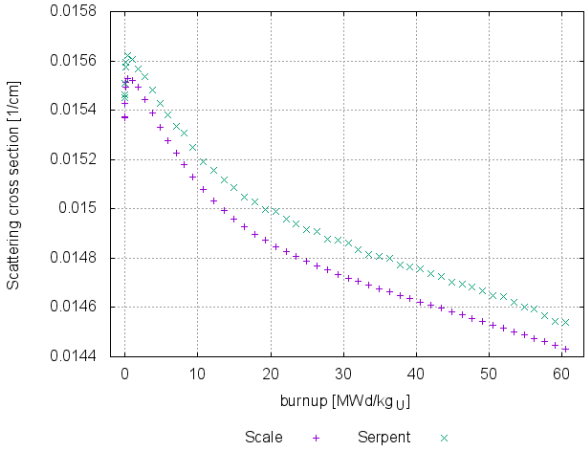


Figure 7. Scattering cross-section from fast group to thermal group, dependency on burnup.

The next studied parameter was the diffusion coefficient. Results for the fast group are shown in Figure 4a and for the thermal group in 4b. Higher differences can be seen for this parameter. They start for the fast group at approximately 10% for BOC, slowly decreasing and reaching only 3% at EOC. The thermal group values differs by −7 % at BOC, than dropping to −8.6 % where it remains till the end of fuel depletion.

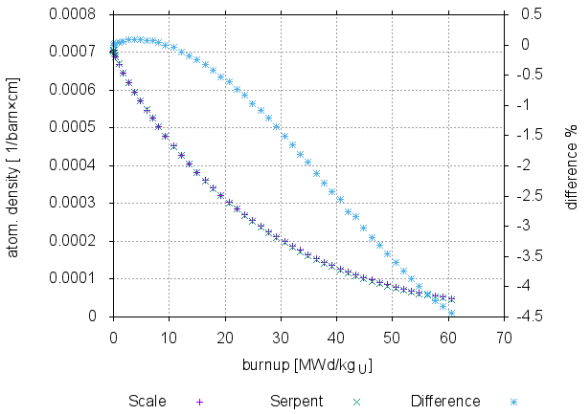
The fission cross-section results are plotted in Figure 5a for the fast group and in in Figure 5b for the thermal group. Differences between codes shown in Figures 6a and 6b have similar trends and Serpent results are consistently lower.

The last macroscopic parameter studied was the scattering cross-section. Obtained values are shown in Figure 7. Both codes determined similar burnup dependence with Serpent values being different from the SCALE results by 0.7% to 1%.

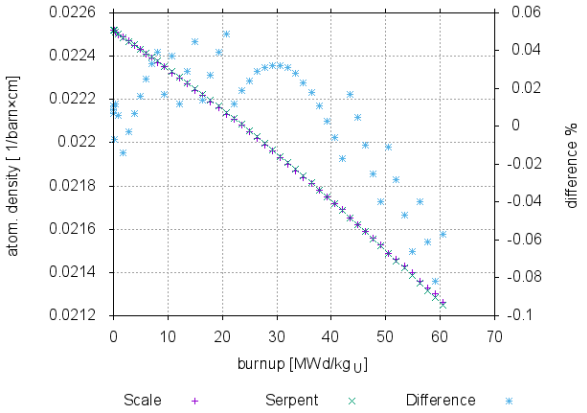
In addition to macroscopic cross-sections, several isotopic concentration were calculated and studied as well. Number densities of dominant actinides ^{235}U, ^{238}U, and ^{239}Pu during fuel burnup were calculated. Results (including Serpent differences from the SCALE results) can be seen in Figures 8a, 8b and 8c. Isotopic changes are mostly in agreement, however, Serpent calculates faster ^{235}U depletion than SCALE. Moreover, ^{239}Pu number density is lower for majority of burnup levels. This contributes to above observed differences of fission cross-section between these two codes.

The memory optimization option in Serpent code was studied as a part of this study. All four memory optimization were tested. Results for all cases were similar and therefore it can be stated that different memory optimization do not affect the results. Only the memory requirements and required computational time is affected.

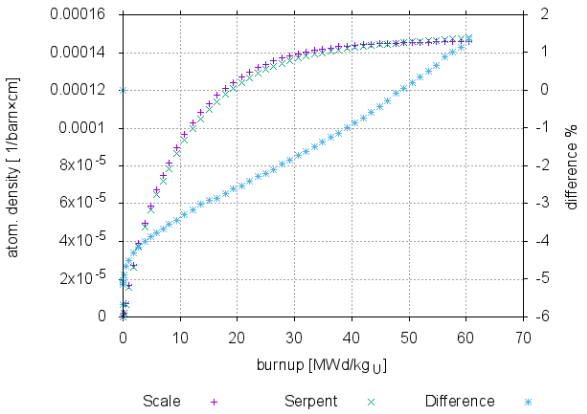
In summary, Serpent and SCALE code were compared for burnup calculation and macroscopic cross-section data generation for VVANTAGE-6 fuel assembly. Both codes provided mostly similar results. Some



(a).



(b).



(c).

Figure 8. Isotope concentration of (a) ^{235}U, (b) ^{238}U and (c) ^{239}Pu for both codes and difference between them.

differences were however observed in isotopic compositions. It is also reflected in the relevant macroscopic cross-sections.

Acknowledgements

The paper was supported by the project "Strengthening and development of research at Czech Technical Uni-

versity in Prague with the use of research infrastructure VR-1 Training Reactor for research activities" (reg. nr. CZ.02.1.010.00.016_0130001790) supported by Operational Programme Research, Development and Education co-financed from European Structural and Investment Funds and from state budget of the Czech Republic. Support from IAEA fellowship number C6/CZR/14007 was used in this work.

References

[1] Discussion forum for Serpent users [online]. 2007 [Accessed on 2017-04-15]. Available at: http://ttuki.vtt.fi/serpent/index.php

[2] J.R. Secker, R.W. Miller, L.T. Mayhue, R.N. Milanova: "Advanced Design and Operating Strategies to Enhance the Safety, Operability, and Efficiency of VVER-1000 Reactors." Nuclear Science and Engineering, 121 (1995) 142-145.

[3] O. Huml *Aplikace kódů MCNP/X pro výpočet vyhoření a jeho vlivu na neutronově fyzikální charakteristiky reaktorových systémů, Neutron physics and burnup calculation of nuclear reactor systems by MCNP/X code* . Prague, 2014. Disertation (Ph.D.). Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Nuclear Reactors (available in Czech only).

[4] O. Novák. *Study of VVER - 1000 Fuel Cycle Using NESTLE and ORIGEN Codes* . Prague, 2016. Diploma thesis (Ing.). Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Nuclear Reactors. Available at: https://www.academia.edu/32855663/Study_of_VVER_-1000_Fuel_Cycle_Using_NESTLE_and_ORIGEN_Codes

[5] B.T. Rearden and M.A. Jessee. *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2016). Available from Radiation Safety Information Computational Center as CCC-834.

[6] E. Fridman, J. Leppänen, "On the use of the Serpent Monte Carlo code for few-group cross section generation," Annals of Nuclear Energy, 2011, 38(6), 1399-1405. DOI: 10.1016/j.anucene.2011.01.032. ISSN 0306-4549.

[7] M.B. Chadwick, M. Herman, P. Oblozinsky, et al.: "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data." Nuclear Data Sheets, 2011, 112(12). DOI: 10.1016/j.nds.2011.11.002. 2887-2996.

[8] T. Lötsch, "Fuel assembly burnup calculations for VVER fuel assemblies with the MONTE CARLO code Serpent." Kerntechnik, 2014, 79(4), 295-302 [cit. 2017-02-16]. DOI: 10.3139/124.110455. ISSN 0932-3902.

[9] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, T. Kaltiaisenaho: "The Serpent Monte Carlo code: Status, development and applications in 2013," Ann. Nucl. Energy, 82 (2015) 142-150.

[10] J. Leppänen, A. Isotalo: "Burnup calculation methodology in the Serpent 2 Monte Carlo code." In proc. PHYSOR 2012, Knoxville, TN, Apr. 15-20, 2012.

[11] Mecir, V. "Temelin NPP fuel experience". 7 International conference on WWER fuel performance, modelling and experimental support, Bulgaria, 2008.