

Macroscopic Data Generation for Full-Core VVER Reactor Calculations by Serpent

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Abstract - This contribution summarizes experience gathered at Department of reactor physics and fuel cycle support of UJV Rez with macroscopic data generation for full-core calculation by Monte-Carlo code Serpent. The full-core analyses are conducted by ANDREA nodal code. Serpent provides in this regard an alternative to HELIOS lattice code. Monte-Carlo codes generally allow a great level of detail of the problem geometry and continuous nuclear data, but on the other hand, there are limitations coming from running times. The current methodology of these calculations is explained together with direct comparison of data generated by HELIOS and Serpent and resulting full-core calculations using these macroscopic data.

I. INTRODUCTION

Department of reactor physics and fuel cycle support of UJV Rez is developing a full-core reactor nodal code ANDREA for fuel cycle and safety analyses of primarily VVER pressurized-water reactors [1]. Macroscopic data for the ANDREA code are by default generated by HELIOS lattice code [2]. The methodology of this process is very elaborated. In order to follow the current trends in nuclear data development, other options for these macroscopic data generation are pursued, including utilization of stochastic code Serpent.

Serpent is Monte-Carlo reactor physics code that is focused on detailed assembly-level fuel depletion calculations and spatial homogenization, and group constant generation [3]. The method of solution ensures realistic simulation of physical phenomena that combined with continuous energy nuclear data results in little or no approximations during calculations. Monte-Carlo method is straightforward and it is less demanding for correct application in reactor physics calculations compared to deterministic codes.

The process of nuclear macroscopic data generation by the Serpent code will be explained and compared to the deterministic code HELIOS. The resulting data will be compared first directly and they will be also used for full-core calculations of VVER reactor cycles. Libraries presented in this study were generated using HELIOS version 2.1.1 and Serpent version 2.1.26. Calculations with HELIOS were conducted with the default ENDF/B-VII.0 library [4] with 49 neutron energy groups. Serpent calculations utilized data from the latest ENDF/B-VII.1 library [5].

II. VVER REACTORS IN CZECH REPUBLIC

There are six VVER reactors in the Czech Republic in two locations: Dukovany and Temelin. The Dukovany site consists of four VVER-440 units and the Temelin site has two VVER-1000 units.

Both reactor types are pressurized-water reactors with hexagonal fuel assemblies (FA) in a triangular fuel lattice. The main parameters of these Czech units are compared in Table I.

This study requires generation of macroscopic data for many types of fuel assemblies. They will be summarized in the following sections.

Parameter	VVER-440	VVER-1000
Electric power	510 MW	1055 MW
Number of FA	349	163
Number of fuel pins in FA	126	312
Fuel specific power	36.85 W/g _{HM}	39.69 W/g _{HM}
Water inlet/outlet temp.	267/297 °C	290/320 °C

TABLE I. Main parameters of Czech VVER-440 and VVER-1000 reactors.

1. VVER-440 Fuel Assemblies

The VVER-440 units in Dukovany site have been operated for 30 years. During this time, nine generations of FA were loaded in the core. The early types had maximum enrichment 3.6 % and no enrichment profiling or burnable absorbers. The current design has improved material specifications and its enrichment profiling was optimized with prospects of further improvements [6]. The FA schematic drawing is in Fig. 1. It features three enrichment levels, burnable absorber (B1) in form of Gd₂O₃, and central instrumental tube (CT).

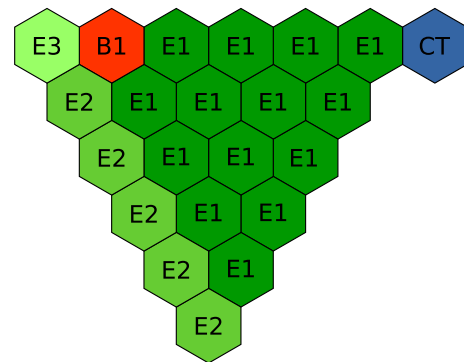


Fig. 1. Current VVER-440 fuel assembly design

2. VVER-1000 Fuel Assemblies

The Czech VVER-1000 units were originally operated with Westinghouse VVANTAGE-6 fuel assemblies. These were replaced by TVSA-T fuel from TVEL Company. Both types are in detail documented in report [7]. This study will deal with this latter fuel design. A typical FA schematic drawing is shown in Fig. 2. There are usually two or three enrichment levels, Gd₂O₃ burnable absorber (B1), central (CT), and guide tubes (GT).

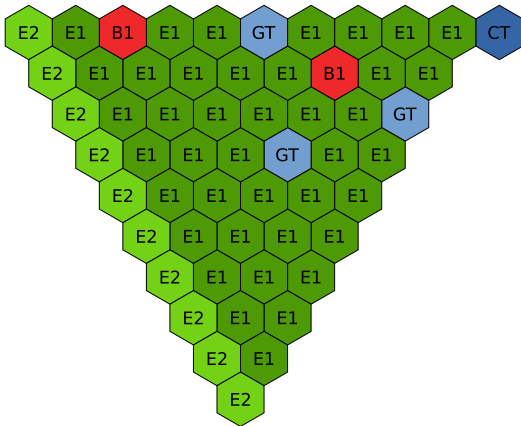


Fig. 2. Current VVER-1000 fuel assembly design

III. ANDREA MACROSCOPIC DATA GENERATION

Generation of application macroscopic data for the ANDREA code is controlled by QUADRIGA framework [8]. There are currently three supported microcodes for this purpose: HELIOS, Serpent, and SCALE. With the exception of fuel temperature profile, all fuel data are common for these codes, although individual input sets and processing procedures are implemented to reflect differences among the codes. The described procedures are used for the HELIOS codes. Procedures for the Serpent code are explained later.

In either case, the calculations are conducted in 2D geometry representing axially infinite slice through the 3D geometry. A single fuel assembly with black boundary condition would have too low multiplication factor for practical depletion calculations, thus infinite lattice of identical fuel assemblies is modeled. This configuration is achieved by either periodic or reflecting boundary conditions.

The data generation begins with depletion calculation with nominal fuel and moderator parameters. The depletion period covers the typical operation time of the fuel assembly. Initial steps are shorter in order to ensure linear interpolation of calculated quantities even for the beginning of fuel depletion, where the system is approaching equilibrium concentration xenon and other important neutron poisons. Fuel assembly symmetry is exploited in order to limit calculation times.

It is required to prepare following macroscopic data:

- fission, absorption, scattering cross-sections, and diffusion coefficient with critical spectrum correction,
- fission spectrum, neutron and energy production.

Apart from the above list, multiple microscopic data are calculated. These cover number densities and microscopic absorption (and possibly fission) cross-sections for boron, gadolinium, uranium, plutonium nuclides, and neutron poisons.

The above listed microscopic and macroscopic data are generated also for set of branch-off states that must cover usual and expected deviations of operational parameters from their nominal values. For example, it is common that FAs are depleted in a reactor core at various specific power levels depending on their position. This effect is accounted for by branch-off calculations where FA specific power is either reduced to one-half or doubled. The three resulting values are inputs for parametrization process that leads to development of a formula that represents important fuel characteristics for the whole interval of powers or fuel temperatures.

The nominal moderator temperature is changed plus/minus 10 °C. Corresponding density changes are also respected.

Reactor power control is realized in VVER-1000 reactors by absorbing clusters inserted into guide tubes of fuel assemblies at certain positions in the reactor core. The main absorbing material is B₄C. Absorbing rod tip is made from dysprosium oxide. There are dedicated branch-off calculations for evaluating influence of these materials.

Completely different system or reactivity control is realized in VVER-440 reactors. There are absorbing elements connected with a fuel assembly. It means that when absorbing part is inserted in the reactor core, fuel part is simultaneously removed. Effectiveness of such a system in reactivity control is great. This system is called CFA - Control Fuel Assembly. Full-core calculations require also data for these CFA. They are generated by separate calculations mixing absorbing elements with surrounding fuel assemblies. Data for the fuel part is identical to a regular FA. Data for the absorbing part are currently only generated in HELIOS and they are used even in calculations where other data were generated by Serpent.

There is an ongoing effort at the Department of reactor physics and fuel cycle support of UJV Rez to conduct the macroscopic data generation calculations in 3D using the Serpent code. It would also solve issues with modeling of axial structures by 2D codes like HELIOS. The CFA is a typical example, where creative approach is necessary for generation of all necessary data.

It was already mentioned that the default HELIOS calculations are taking into account radial distribution of fuel temperatures in five radial zones. This temperature model is either precalculated by FEMAXI or TRANSURANUS code, or it can be on-line calculated by TRANSURANUS based on the actual material and geometry specification of the fuel assemblies.

1. Procedures for Serpent Microcode

For a certain fuel assembly type, number of calculations for such a set of macroscopic data can due to multiple depletion steps and branch-off calculations easily reach to hundreds. It is of a primary interest to keep calculation times for the Serpent code as low as possible, but still preserving correct-

ness of the calculations. Despite this effort, it requires days to prepare a typical set of macroscopic data by Serpent compared to hours in HELIOS. The applied model simplifications and procedures will be explained. Only fuel assembly data are generated by Serpent at this moment.

Although the whole FA is always modeled in Serpent, depletion is calculated only in one third or one sixth of the fuel pins. Fuel assembly symmetry is utilized to reduce number of unique materials.

Fuel homogenization is defined for the whole fuel assembly in model and assembly discontinuity factors are calculated at the boundaries of the model.

Current Serpent calculations work with alternative temperature model. It is part of the QUADRIGA framework and it is derived from the default HELIOS model. Temperatures are not changed during the course of fuel depletion in Serpent, thus the whole temperature model contains only one average temperature for all burnup levels. E.g. a HELIOS calculation is conducted with individual fuel pin temperatures depending on the burnup level in the range from about 850 °C to more than 900 °C. In Serpent for the same case all depletion steps are done with identical temperature 868 °C.

Once fuel pins are defined, an internal Serpent code ability is used to adjust available microscopic data to the desired temperature. The closest lower temperature cross-section data are selected and adjusted to the new temperature. This temperature remains for the whole depletion, and it only changes in branch-off calculations. Currently the older tmp method implemented in Serpent is used as the more recent tms method requires more computer resources. The tmp method works correctly in our case, because it is possible to use relatively fine mesh of fuel temperatures with 10 °C step for the calculations.

Currently all branch-off calculations in Serpent are done off-line from the main depletion branch. Serpent is capable to print material compositions for all fuel depletion states. These composition are loaded into subsequent branch-off calculations, where desired changes to the fuel or moderator parameters are realized by prepared processing program.

All calculations are conducted with 20000 neutrons per cycle, 300 active cycles and 20 inactive cycles. These settings are sufficient for both VVER-440 and VVER-1000 fuel assemblies and all desired characteristics. The only exception is data for TVSA-T fuel blankets. These data are calculated with reduced specific power. It means that branch-off calculations lead to only to small changes to fuel blanket temperature and their effect on the resulting fuel characteristics could be hidden in calculation statistics. Number of neutrons per cycle is increased to 50000 and number of active cycles to 500 for these cases.

Macroscopic data are prepared for critical spectrum. This can be switched on in Serpent by setting the fundamental mode. In this mode Serpent collapses calculated multigroup data into few-group (commonly two-group) structure. The multigroup structure is part of input specifications. It is generally recommended to use at least 70 energy groups. On the other hand, high number of energy groups can lead to wrong answers if the characteristics are not calculated in each energy group with sufficient reliability due to low number of neutrons or cycles in the calculation. This is not this case, thus built-in WIMS

172 energy group structure is used in these fundamental mode calculations.

There is currently limitation to this fundamental mode in Serpent. Fuel depletion is still done in the infinite spectrum and only the output macroscopic data are adjusted to the critical spectrum.

One of the last options that needs to be commented in order make this list complete is Serpent memory optimization mode. Serpent can run in multiple modes with substantially different memory requirements. This type of calculation allows optimization mode 4 that offers the best performance at the expense of system memory allocation. It was found that the most complex calculations at this 2D level requires approximately 20 GB RAM.

Specific issue with Serpent calculations is correct determination of microscopic data. If specified naturally to be averaged across the whole FA model, it is weighted by the total model neutron spectrum, but it should be weighted only by spectrum of those materials containing the respective nuclide. It was found that this is the most important for gadolinium isotopes, where the self-shielding effect can easily reduce the calculated microscopic absorption cross-section to one third of the system-wide values. This is at this point solved by the Serpent calculations postprocessing, where different parts of the output file are read based on the specific situation.

2. Testing of Serpent Calculation Model

The initial Serpent model for preparation of macroscopic data was prepared in 2013. It was subjected to extensive testing. There are multiple settings that can influence calculation correctness and offer space for calculation time optimization.

It was believed in the beginning that due to the fact that only homogenized fuel assembly characteristics are required, grouping of fuel pins based on their enrichment level and presence of burnable absorber is sufficient. It was later discovered that such a model poorly predicts power distribution in a the fuel assembly. In order to remedy this situation, all fuel pins are modeled individually. It means that they have their own data for depletion calculation. Further power distribution improvement was achieved by implementing radial division of fuel pins with Gd₂O₃ burnable absorber into five zones. Still no temperature radial profile in these pins is used.

One of the features that makes Serpent faster compared to other Monte-Carlo codes is that unresolved resonances are not by default integrated in the calculation. It was found that switching the unresolved resonance sampling on makes the calculations about three times longer while bringing no statistically significant change in the two-group macroscopic characteristics.

IV. COMPARING DIRECTLY MACROSCOPIC DATA

Comparison of results of deterministic and stochastic data generation processes can be based directly on the calculated characteristics. Sample results for fast and thermal diffusion coefficient during fuel depletion are plotted in Fig. 3 and Fig. 4, respectively. These calculations were conducted for recent VVER-440 reactor fuel with gadolinium burnable absorber.

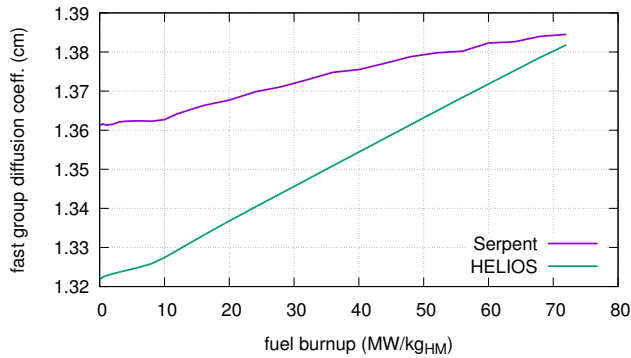


Fig. 3. Fast group diffusion coefficient comparison for VVER-440 reactor FA

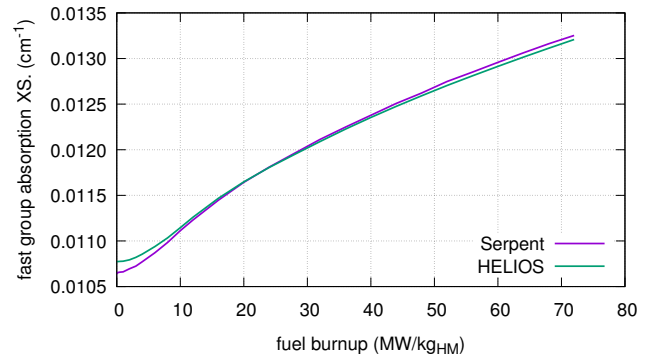


Fig. 5. Fast group macroscopic absorption cross-section comparison for VVER-440 reactor FA

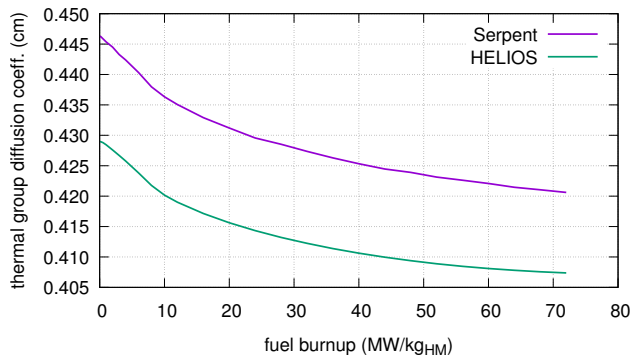


Fig. 4. Thermal group diffusion coefficient comparison for VVER-440 reactor FA

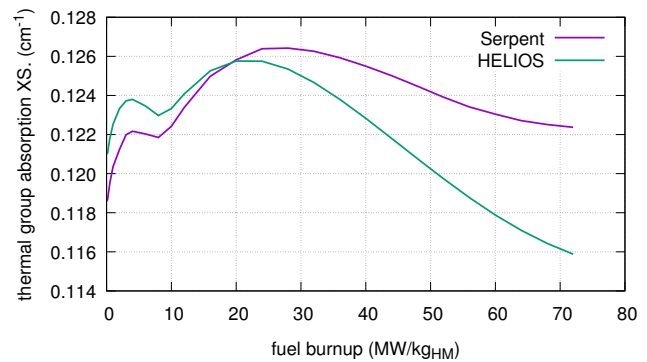


Fig. 6. Thermal group macroscopic absorption cross-section comparison for VVER-440 reactor FA

Diffusion coefficient is the principal macroscopic characteristic of a fuel assembly. It directly influences neutron migration, thus its effect can be on multiple levels.

It can be seen from the presented plots in Fig. 3 and Fig. 4 that the Serpent code calculations lead to a little higher value diffusion coefficient for both thermal and fast neutron group. The observed difference is getting progressively lower in the fast group and goes from about 3 % to less than 1 %.

The observed difference between Serpent and HELIOS calculations of the diffusion coefficient remains relatively constant for thermal neutron group. The result from Serpent is higher by about 3 to 4 % than results from the HELIOS calculations.

Next two plots in Fig. 5 and Fig. 6 show comparison of calculated macroscopic absorption cross-sections for fast and thermal neutron groups.

There is a great agreement between the two microcodes for the fast neutrons. Differences remain below 1 % for the whole depletion interval. More complex dependence can be seen for the thermal neutron group. The Serpent calculated value is initially below the HELIOS result. At about 20 MWd/kg_{HM} burnup level Serpent determined value is getting above HELIOS. The maximum difference is reaching 6 %.

Before full-core results are presented, two mode micro-

scopic characteristics are presented. It is number density (ND) of ²³⁹Pu and ¹⁵⁷Gd. It is interesting to see also these values as both microcodes differ also in fuel depletion methodology and nuclear data.

The first plot in Fig. 7 confirms that both microcodes follow the same trend in ²³⁹Pu production from the initially uranium fuel. Its number density is gradually increasing and gets saturated at burnup level about 40 MWd/kg_{HM}. Afterwards, a slow decline can be observed.

Differences between both microcodes are plotted in Fig. 8. The curve shows relative number density difference of the Serpent result from the HELIOS result. Although the differences remain low, it is easy to see that ²³⁹Pu is produced faster in the Serpent calculation. The explanation can be found in higher absorption cross-section of ²³⁸U for the fast neutron group in the Serpent calculation.

Modern nuclear fuel for PWR usually contain some sort of burnable absorber material. The compared fuel assemblies are using Gd₂O₃. It was found and it is shown primarily in Fig. 10 that use of the Serpent microcode leads to faster calculated gadolinium depletion in the fuel.

The other plot of ¹⁵⁷Gd number density in Fig. 9 clearly demonstrates that the observed different rate of gadolinium depletion is important only for burnup levels below 10 MWd/kg_{HM}.

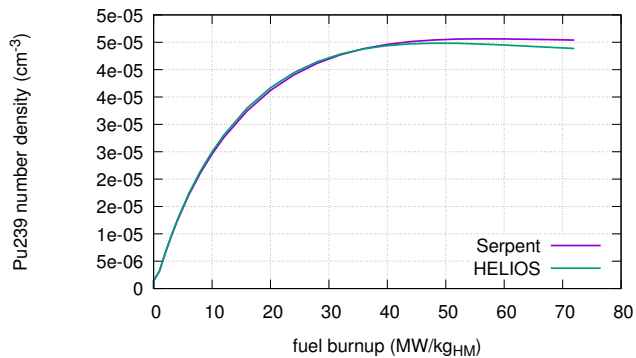


Fig. 7. Number density of ^{239}Pu calculated by Serpent and HELIOS during fuel depletion

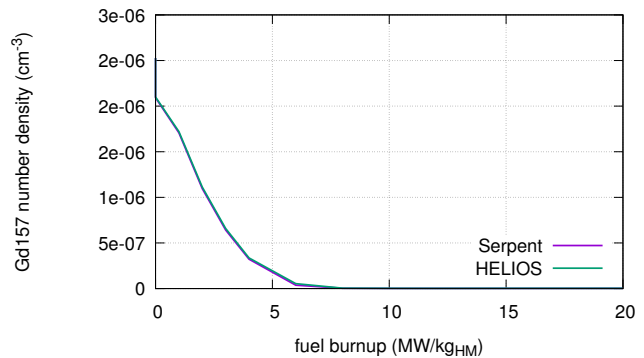


Fig. 9. Number density of ^{157}Gd calculated by Serpent and HELIOS during fuel depletion

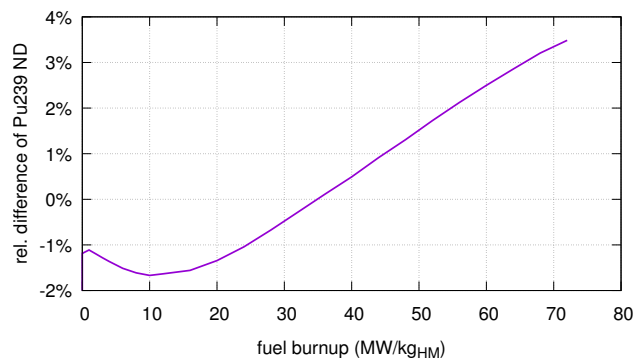


Fig. 8. Relative difference of ^{239}Pu number density calculation by Serpent from HELIOS during fuel depletion

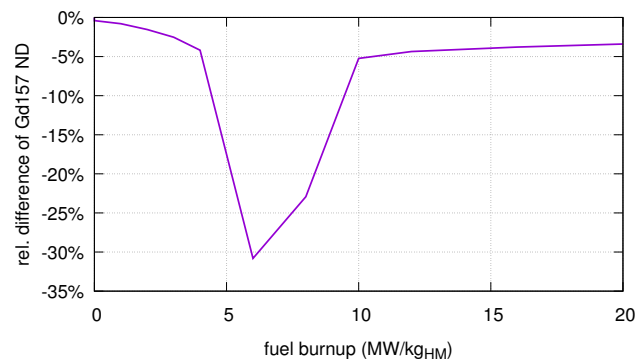


Fig. 10. Relative difference of ^{157}Gd number density calculation by Serpent from HELIOS results during fuel depletion

V. COMPARING FULL-CORE CALCULATIONS

The next step from the macroscopic data generation is their application for full-core calculations. Some important outputs from the ANDREA code calculations can be found in the following plots. The Serpent libraries were prepared for ANDREA version 2.1.7. The library generation procedure is currently being adopted to new library format in ANDREA 2.3. Majority of results presented in this chapter were calculated for VVER-440 Dukovany reactors by ANDREA version 2.1.7 with either Serpent or HELIOS data. At the end of this chapter there are result for the first TVSA-T fuel loadings in VVER-1000 reactor Temelin and these data are compared with current stable ANDREA release 2.2.2.

There are four units in the Dukovany site. The presented results are for unit 3 for seven cycles in which identical FA type was loaded in the reactor. Fuel cycle lengths reflect the real cycle lengths, but the depletion was calculated for nominal power and without CFA movements. This facilitates comparison of results.

1. Full-Core Results for Boric Acid Concentration

The most important operational parameter for fuel cycle length is boric acid concentration expressed in grams per kg

of moderator. Long-term compensation of excess reactivity is achieved by boric acid dissolved in moderator. Reactor must be shutdown when zero boric acid concentration is reached with all other absorbing elements removed from the core. Plot in Fig. 11 shows typical time evolution of boric acid concentration in two selected cycles.

It can be seen from plot in Fig. 11 that boric acid concentration is generally higher when macroscopic data generated by Serpent are used. It was confirmed for all analysed cycles. Absolute differences between calculated boric acid concentrations with Serpent data and HELIOS data are plotted in Fig. 12.

2. Full-Core Results for Axial Offset

Axial offset gives relative difference in % between power of the upper and lower part of reactor core according to the following equation:

$$AO = \frac{P_t - P_b}{P_t + P_b} \times 100 \quad (1)$$

Axial offset is one of the limited values during reactor operation. There are natural reasons for negative axial offset like partially inserted absorbing elements from the top of the core. The axial offset is changing during fuel cycle due to

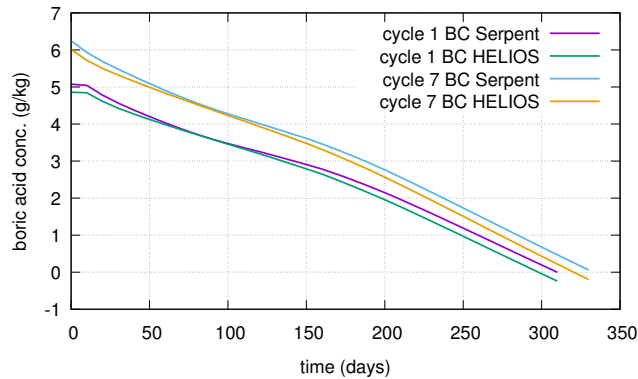


Fig. 11. Boric acid concentration during selected Dukovany fuel cycles

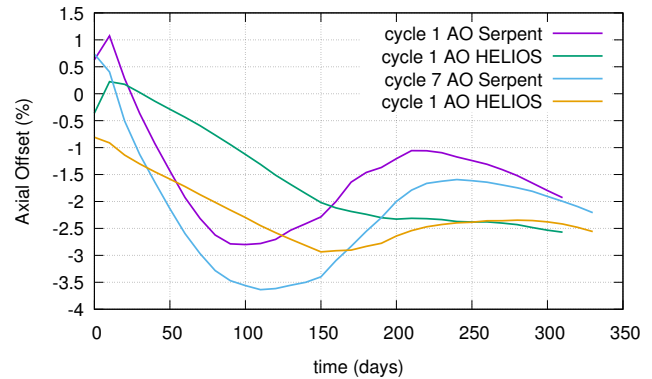


Fig. 13. Axial offset during selected Dukovany fuel cycles

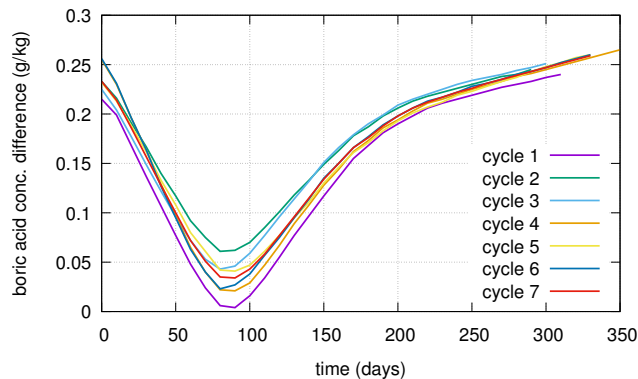


Fig. 12. Boric acid concentration difference during selected Dukovany fuel cycles

fuel depletion. Axial offset is also frequently used to measure xenon axial oscillations.

Axial offset was calculated by both sets of macroscopic data for two fuel cycles. Results are in plot in Fig. 13. It can be seen that results greatly depend on the set of macroscopic data. Changes of axial offset during fuel cycle are more profound with Serpent data.

3. Full-Core Results for Maximum Relative Assembly Power

Parameter FHA is used to quantify maximum relative assembly power in the reactor core during a fuel cycle. Use of different macroscopic data influences also this important safety parameter. Plot in Fig. 14 shows example time dependence of this characteristic for the compared sets of macroscopic data. There is only limited influence on FHA and there is no observable trend in the results for either macroscopic data.

The next plot in Fig. 15 shows relative differences between results obtained with Serpent and HELIOS data during the fuel cycles. The difference is limited to 1 % for majority of the states.

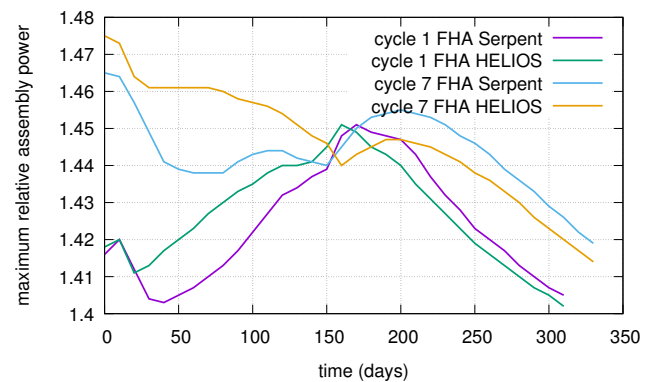


Fig. 14. Maximum relative assembly powers during selected Dukovany fuel cycles

4. Full-Core Results for Xenon Concentration and Effective Fraction of Delayed Neutrons

It is possible to find multiple other characteristics important for various aspects of reactor operation. It was decided to present two more that depend more profoundly on macroscopic data preparation: xenon concentration during fuel cycle and effective fraction of delayed neutrons.

Isotope ^{135}Xe is the single most important nuclide in the core from the reactivity perspective. Its equilibrium concentration is function of multiple variables: xenon yield from fission, its absorption cross-section and decay constant, reactor power and number of fissions. Despite this complex dependence, plot in Fig. 16 confirms that there is maximum 1 % difference for the alternative sets of macroscopic data and it remains relatively constant during the cycle.

When reactor kinetics or dynamics is in question, effective fraction of delayed neutrons is of essential importance. Serpent calculates their characteristics by adjoint Meulekamp method. Effective fraction of delayed neutrons is rather integral characteristic depending on several calculation components. Apart from the microcode itself responsible for data collapsing and critical spectrum calculation, effective fraction of delayed neutrons depends greatly on fuel material composition and input microscopic data.

Result shown for one cycle in plot in Fig. 17 confirms

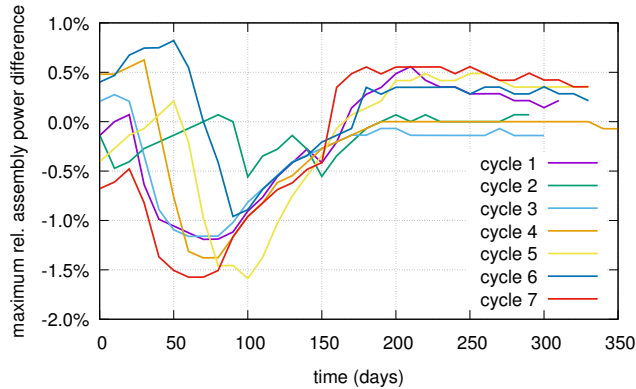


Fig. 15. Relative differences for FHA calculated with data from Serpent and HELIOS during selected Dukovany fuel cycles

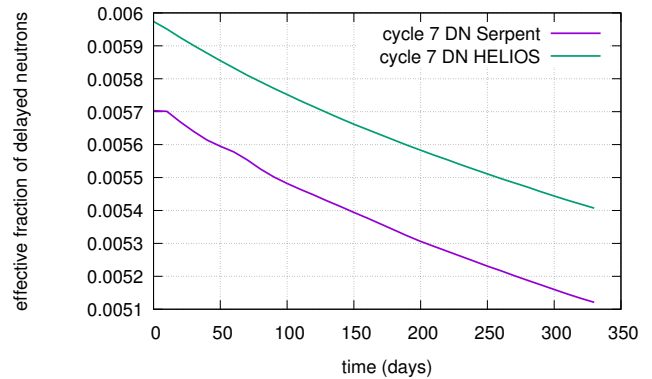


Fig. 17. Effective fraction of delayed neutrons in the Dukovany core during selected cycle

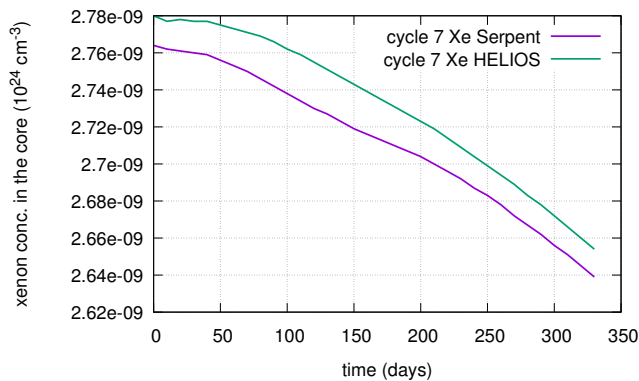


Fig. 16. Xenon concentration in the Dukovany core during selected cycle

that the value is decreasing during the cycle as a result of evolving fissile material composition towards higher fraction of plutonium. Yield of delayed neutrons from fission of ^{239}Pu is about three times lower than for ^{235}U . On the other hand, stable 5% difference for the two microcodes suggests that the primary source of this shift in yield of delayed neutrons lies in the provided nuclear data libraries.

5. Full-Core Results for First TVSA-T Cycles in Temelin NPP

The last set of data shown in this chapter is for VVER-1000 reactor unit 1 in Temelin NPP. This NPP switched from Westinghouse VVANTAGE-6 FA to TVEL TVSA-T fuel type. The presented plots in Fig. 18, Fig. 19, and Fig. 20. Were created by the QUADRIGA framework and it works with real operational data.

It is not possible to make detailed operational data public, but it is still possible to show the level of agreement between the reactor operation and calculation.

These first cycles with new fuel design are very demanding for macroscopic data. Calculation of the illustrated cycles required data for 12 different fuel types. Further data are required for reflectors, but these are currently not calculated by

Serpent and they are taken the same as for HELIOS.

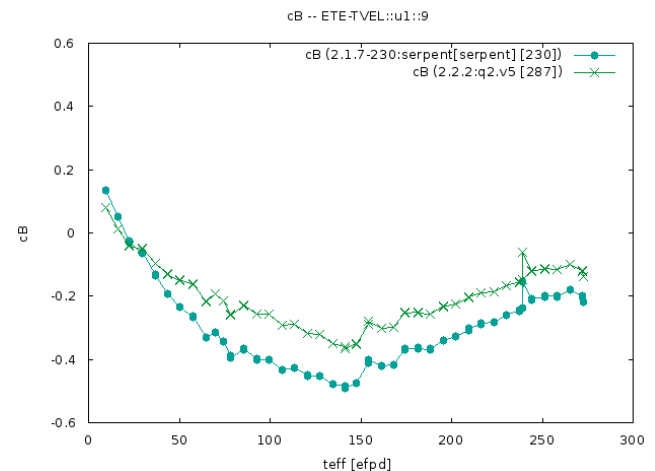


Fig. 18. Calculated boric acid difference from operational data for Temelin unit 1 cycle 9

The first compared cycle begins by overprediction of critical boric acid concentration using both sets of macroscopic data. Afterwards calculations generally predict lower boric acid concentration. It needs to be stressed that data calculated by HELIOS perform better, because calculations with data from Serpent are off by another 0.1 g/kg of H_3BO_3 .

The other two compared cycles are quite similar to the first one. After brief initial period of the cycle where calculations predict higher boric acid concentration, the correct value is underestimated for the rest of the cycle. Data generated by HELIOS perform better with more consistent difference from the reference operational data.

VI. CONCLUSIONS

Dependable macroscopic data generation is essential for correct full-core calculations of power reactors. Methodology of these calculations using stochastic code Serpent is demonstrated for VVER reactors operated in Czech Republic. Full-core calculations of these reactors are conducted by the ANDREA nodal code. The well developed deterministic

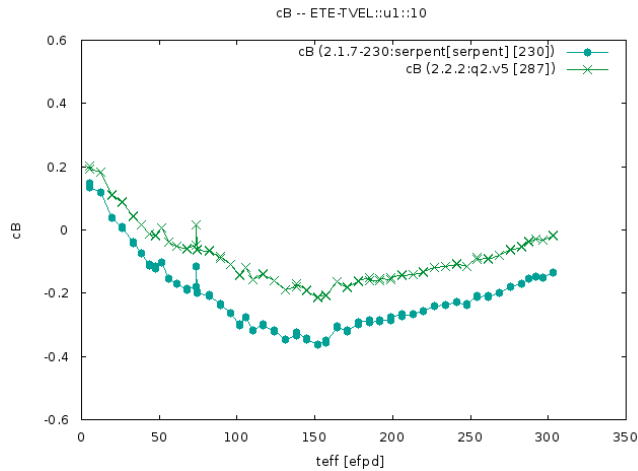


Fig. 19. Calculated boric acid difference from operational data for Temelin unit 1 cycle 10

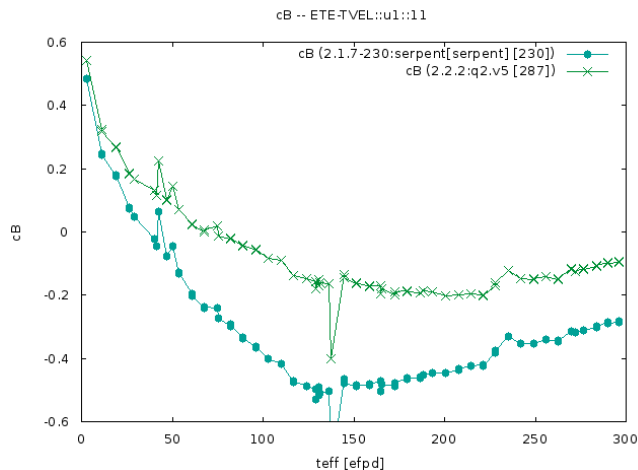


Fig. 20. Calculated boric acid difference from operational data for Temelin unit 1 cycle 11

HELIOS calculations are used for comparison.

After the reactors of interest are described, the main features of both microcodes are presented. In summary, HELIOS allows to reflect even radial profile of fuel temperatures and evolution of these temperatures during fuel burnup.

The first set of results was based on macroscopic data for diffusion coefficient and macroscopic absorption cross-section. It is supplemented by number densities of two of the most important nuclides: ^{239}Pu and ^{157}Gd . Serpent calculates higher plutonium content after about burnup level 30 MW/kg_{HM}. Also gadolinium isotopes are depleted faster in case of Serpent calculations. It is direct consequence of thermal absorption cross-section of the important gadolinium isotopes being greater by several percent for Serpent.

The comparison continued with fuel cycle characteristics calculated using both macroscopic data determined by either Serpent or HELIOS calculations. It was found that difference of calculated boric acid concentration is systematic among

multiple fuel cycles. The dependence of the difference for the first third of fuel cycles can be explained by different rate of gadolinium depletion. Difference in gadolinium depletion influences also axial offset.

Relatively small differences for the alternative Serpent set of data were found for assembly power peaking.

The last compared full-core characteristics were xenon concentration and effective fraction of delayed neutrons. Regardless of macroscopic data applied the time dependence during the fuel cycles are similar. Explanation for the observed differences was found in nuclear data.

The last part of the full-core results works with operational data from VVER-1000 reactor and they are presented as a deviation of calculations conducted with macroscopic data either from Serpent or HELIOS from the experimental data. It must be concluded that better agreement with operational data is achieved with HELIOS data. Still it can be seen that Serpent data are not far off the target.

The macroscopic data generation task is subject to permanent development at Department of reactor physics and fuel cycle support of UJV Rez. It was found advantageous to have multiple options for the macroscopic data calculations as it brings different views on the same issue. Macroscopic data generated by Serpent works well for the full-core VVER calculations. The next step in their utilization will be switch to automated burnup and branch-off sequence in Serpent. It is possible now as it includes microscopic data generation since the Serpent version 2.1.28. This will simplify the procedure and hopefully also accelerate it, which will open new space for improvements.

VII. ACKNOWLEDGMENTS

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