M&C 2023 - The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering · Niagara Falls, Ontario, Canada · August 13 – 17, 2023

Critical Spectrum Burnup Calculations with Serpent Monte Carlo Code

V. Valtavirta[1], **Y. Bilodid**[2]

[1]VTT Technical Research Centre of Finland Ltd
P.O. Box 1000, 02044 VTT, Finland

[2]Helmholtz-Zentrum Dresden-Rossendorf
Bautzner Landstraße 400 01328 Dresden, Germany

Ville.Valtavirta@vtt.fi, Y.Bilodid@hzdr.de

ABSTRACT

The novel critical spectrum burnup capability in Serpent 2 is demonstrated with lattice burnup calculations of two assembly types from the Khmelnitsky 2 VVER-1000 benchmark. The effect of critical versus infinite spectrum on nuclide densities and system reactivity are evaluated. Results calculated with HELIOS serve as a comparison.

KEYWORDS: Lattice calculations, burnup, critical spectrum, fundamental mode, Serpent

1. INTRODUCTION

Two dimensional infinite lattice models for fuel assemblies are widely used for applications such as group constant generation and inventory calculations. This choice of geometry means that the modelled system is generally not critical. In operating reactors, local imbalances in neutron production and removal are compensated by the inflow of neutrons from surrounding assemblies or the outflow of neutrons to those assemblies.

The flux energy spectrum obtained naturally from the infinite lattice calculation (the infinite spectrum) differs from that in a critical system, which is reflected in the condensation process of few-group constants for nodal calculations or in the evaluation of one-group cross sections and fluxes for fuel depletion. The critical spectrum can be approximated by first evaluating multi-group data, then using that data to solve a buckling iteration to obtain an approximate critical spectrum and finally condensing the multi-group data to a few-group or one-group structure based on that spectrum to obtain *leakage corrected* data.

The Serpent Monte Carlo code [1] offers three deterministic multi-group buckling iterations, the B1, P1 and FM approaches, that can be used for the condensation of few-group data from intermediary multi-group data [2]. Recently, an approach was implemented for solving the FM buckling iteration with continuous energy Monte Carlo during the neutron transport process instead of as a deterministic multi-group solution in postprocessing [3]. This approach was showed to yield similar effects on homogenized few-group constants as the deterministic multi-group implementation in Serpent. The new approach offered two large benefits compared to the previous implementation:

1. The Fundamental Mode buckling iteration is solved using continuous energy Monte Carlo instead of a multi-group approach.
2. All results are inherently evaluated with the critical spectrum instead.

The second benefit is utilized in this work to demonstrate burnup calculations using the critical spectrum based on the Fundamental Mode buckling iteration. Serpent is used to deplete two fuel assembly types from the Khmelnitsky 2 benchmark [4] up to 60 MWd/kgU burnup with infinite and critical spectra. The resulting nuclide compositions, k_∞ and group constants are compared between the two calculations.

To provide reference data, the same lattices are also depleted with HELIOS [5], a deterministic multi-group code using infinite spectrum and B1 critical spectrum.

2. MONTE CARLO CRITICAL SPECTRUM SOLUTION IN SERPENT

The fundamental mode (FM) leakage correction is a buckling iteration approach for applying a spectrum correction to generated group constants. In the deterministic multi-group approach, the critical spectrum is iterated using pre-generated infinite-spectrum multi-group constants. The FM method is based on solving a single group of equations, one for each micro-group g:

$$\Sigma_{t,g}\phi_g + D_g B^2 \phi_g = \chi_g + \sum_{g'} \Sigma^0_{s,g'\to g}\phi_g \tag{1}$$

Here $\Sigma_{t,g}$, D_g, χ_g and $\Sigma^0_{s,g'\to g}$ are multi-group constants evaluated from an infinite lattice transport calculation. The flux is normalized to unity removal and the buckling B^2 is iterated to yield a critical system. In essence, the term $D_g B^2 \phi_g$ corresponds to a neutron removal term if B^2 is positive and to a neutron production term if B^2 is negative.

The FM leakage correction approach is used e.g. in the CASMO-4 [6] and LANCER02 [7] lattice physics codes.

The Monte Carlo solution to this set of equations in Serpent is based on representing the buckling term $D_g B^2 \phi_g$ as an additional reaction mode in the neutron transport resulting in either the loss of the neutron ($B^2 > 0$) or the production of an additional neutron at the same energy ($B^2 < 0$) with the macroscopic cross section of

$$\Sigma_{L,g} = D_g |B^2|. \tag{2}$$

The energy dependent diffusion coefficient needed to evaluate $\Sigma_{L,g}$ is based on a Cumulative Migration Method [8] estimate, collected during the transport solution itself.

3. DEMONSTRATION

This capability was demonstrated in lattice burnup calculations to allow for the evaluation of the critical spectrum effect in Serpent simulations. The same problem was also solved with the HELIOS lattice code which utilized the B1 critical spectrum iteration. Due to the different critical spectrum iteration methods and the different neutron transport solutions a perfect match between the two codes is not expected, but the reference solution should provide a baseline to compare against.

3.1. Specifications

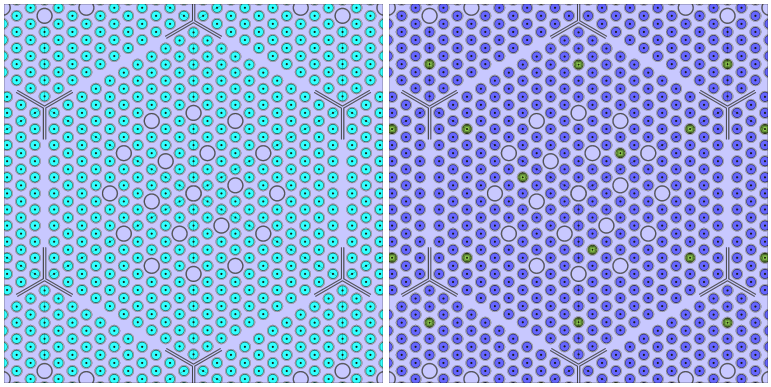

Figure 1: Lattice geometries of the 22AU (left) and 30AV5 (right) fuel assemblies used for the demonstration.

Two assembly types from the Khmelnitsky 2 VVER-1000 full core depletion benchmark were chosen for the demonstration:

1. 22AU, which is unprofiled and consists simply of 312 fuel rods of 2.2 wt.% enrichment.
2. 30AV5, which contains 303 fuel rods of 3.0 wt.% enrichment and 9 fuel rods of 2.4 wt.% enrichment and 5.0 wt.% of gadolinia.

The lattice geometry of the two assemblies is shown in the Serpent geometry plots presented in Figure 1. The material compositions and the assembly geometry are based on Ref. [9] except for a reduction in the central tube inner and outer radius in order to fit it in the hexagonal lattice cell. The inner radius was reduced from 0.55 cm to 0.523 cm and the outer radius from 0.65 cm to 0.635 cm.

The calculation was conducted at the state point defined for Task 1 (lattice depletion) of the benchmark in Ref. [10]:

- Fuel temperature of 1005 K.
- Moderator temperature of 578 K.
- Boron concentration of 525 ppm.
- Power density of 42.5 W/gU.

The burnup points used for determining the depletion steps and comparing the results are (in MWd/kgU): 0, 0.1, 0.3, 0.6, 1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 24, 27, 30, 33, 36, 39, 42, 45, 48, 51, 54, 57, 60.

3.2. Calculation Setup

The Serpent calculation was divided into two parts:

1. The burnup calculation using the critical spectrum iteration, which produced nuclide compositions for each of the burnup points.
2. Restart calculations utilizing those burnup points to evaluate k_∞ and group constants without using the critical spectrum iteration.

The Serpent burnup calculation applied the predictor-corrector method with 10 substeps using linear extrapolation on predictor and linear interpolation on corrector. Serpent used 10^5 neutrons per cycle, 500 active cycles, 50 inactive cycles for the first transport solution and 25 for the later ones. Resonance upscattering treatment was utilized in the calculation based on the Doppler broadening rejection correction method implemented in Serpent and the unresolved resonance range probability table sampling was turned on.

3.3. Results

The scalar flux spectrum in the fresh 22AU assembly type is shown in Figure 2 tallied from the infinite and critical spectrum calculations. The infinite multiplication factor of the assembly is 1.15810 ± 0.00008. The k-eigenvalue iteration of the infinite spectrum calculation scales the fission neutron production with the inverse of this k_∞ reducing the amount of produced fission neutrons. In the critical spectrum calculation, the critical buckling is iterated to a positive value ($B^2 \approx 2.17 \times 10^{-3}$), which means that the reaction mode corresponding to Eqn. 2 results in the loss of neutrons. This may not be immediately evident from the plot of the two flux spectra, after all, the critical spectrum is mostly larger in magnitude than the infinite spectrum. As the interaction cross section (Eqn. 2) is proportional to the diffusion coefficient and the diffusion coefficients in LWR systems generally increase with increasing energy, the interaction cross section is at its largest at high energies and most of the neutrons are lost there. At thermal energies, the infinite spectrum and critical spectrum match well due to the normalization of flux to the fixed power level in a thermal system. Since the power normalization makes the spectra match well at thermal energies and additional neutrons are lost in the critical spectrum calculation compared to the infinite spectrum, the critical spectrum needs to be higher than the infinite spectrum at high energies.

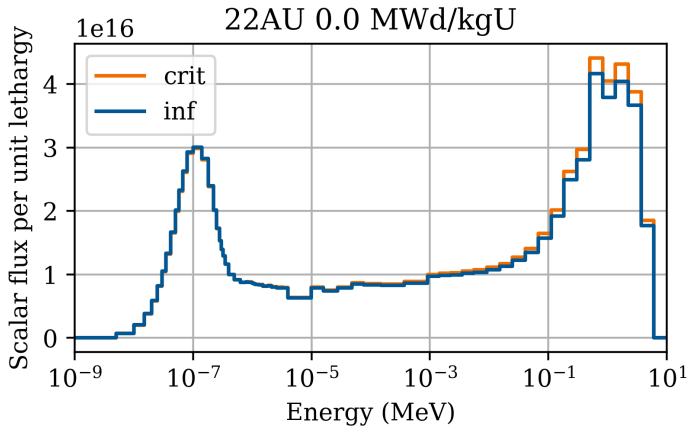

Figure 2: Comparison of the infinite and critical (FM) flux spectra for the fresh 22AU assembly.

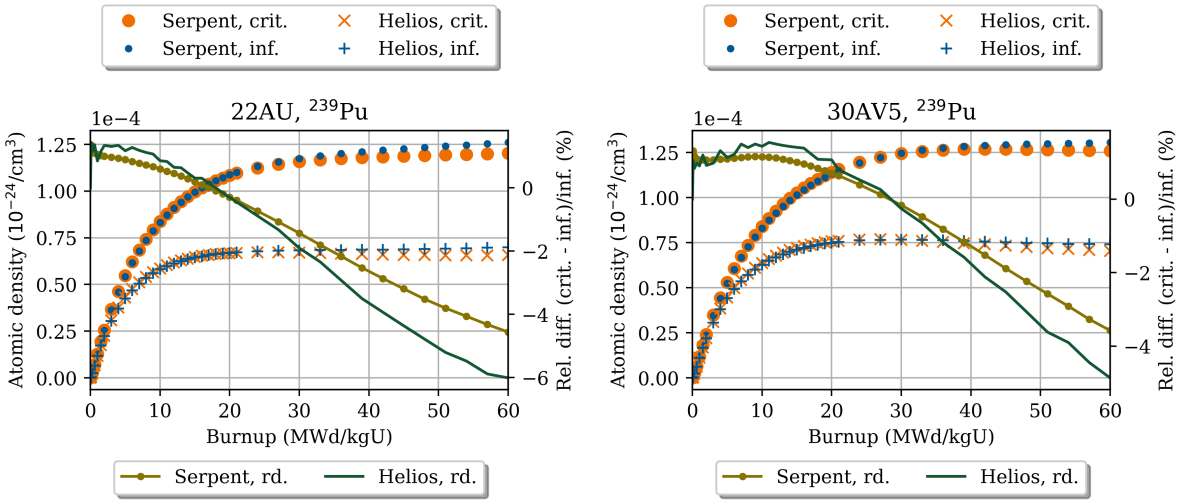

Figure 3: Effect of critical spectrum burnup calculation on the accumulation of ^{239}Pu in assembly types 22AU (left) and 30AV5 (right).

The difference in the flux spectrum affects the depletion calculation, resulting in various differences in the depleted nuclide composition. As an example, the evolution of the fuel average ^{239}Pu content in the two assembly types is shown in Figure 3. Both assembly types have a $k_\infty > 1$ at low burnups leading to the critical spectrum being harder than the infinite spectrum. This leads to more ^{239}Pu being accumulated in the critical spectrum burnup calculation at low burnups. At high burnups, both assembly types have a $k_\infty < 1$, leading to the critical spectrum being softer than the infinite spectrum and a reduction in the production of ^{239}Pu. The absolute concentrations of ^{239}Pu do not match well between Serpent and HELIOS, but the critical spectrum effect on the concentration, evaluated as the relative difference between the critical spectrum concentration and the infinite spectrum one, follows a similar trend with both codes. The agreement in the nuclide concentration of ^{241}Pu is much better as is shown in Figure 4.

The differences in nuclide compositions then affect the reactivity of the assembly. Evaluating the k_∞ with the depleted fuel compositions from different burnups shows differences in k_∞ up to 1600 pcm in the 22AU assembly type and up to 1100 pcm in the 30AV5 assembly type, as shown in Figure 5. The spectral effect

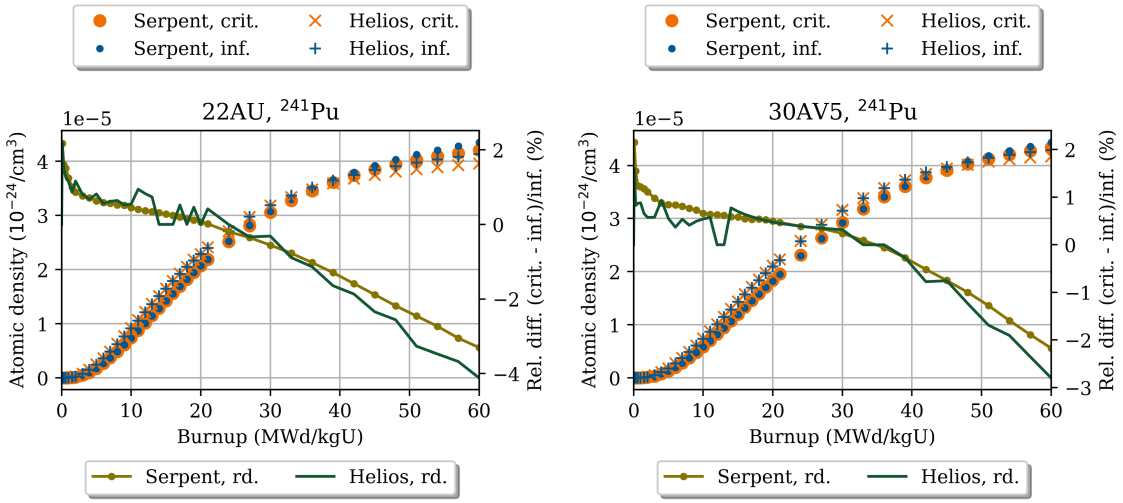

Figure 4: Effect of critical spectrum burnup calculation on the accumulation of ^{241}Pu in assembly types 22AU (left) and 30AV5 (right).

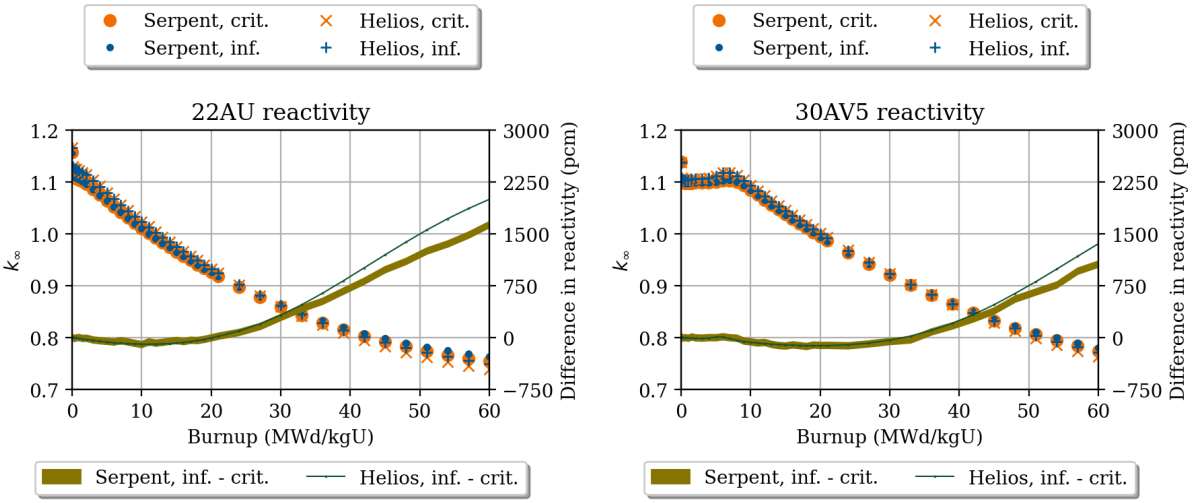

Figure 5: Effect of critical spectrum burnup calculation on the infinite lattice reactivity of the assembly in assembly types 22AU (left) and 30AV5 (right).

on reactivity is evaluated in a very similar manner by Serpent and HELIOS up to a certain burnup (around 33 MWd/kgU for 22AU and around 45 MWd/kgU for 30AV5). At larger burnups HELIOS predicts a larger effect than Serpent, which may be due to the FM and B1 methods leading to different critical spectra. The burnups at which the two solutions start to differ from each other correspond to a k_∞ between 0.80 – 0.85.

The differences in nuclide compositions are also reflected in any few group constants generated based on the compositions. This is shown in Figure 6, into which the ratio of several two-group constants based on the critical spectrum and the infinite spectrum compositions are plotted.

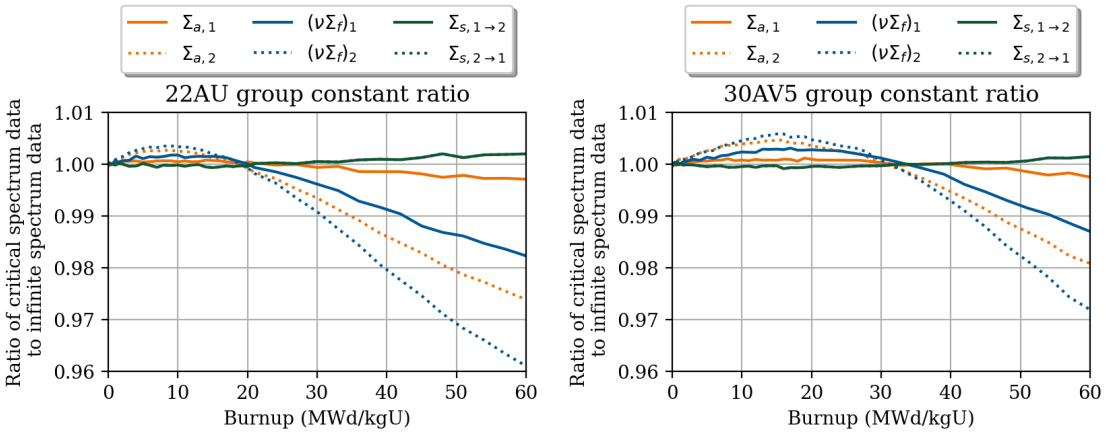

Figure 6: Effect of critical spectrum burnup calculation on the infinite spectrum group constants in assembly types 22AU (left) and 30AV5 (right).

4. CONCLUSIONS

The capability of Serpent to deplete materials using a critical flux spectrum based on the Fundamental Mode (FM) buckling iteration was demonstrated with two VVER-1000 fuel assemblies. The differences between critical and infinite flux spectrum are reflected in depleted fuel compositions and thus any estimates based on those compositions, such as the calculated k_∞, the generated few-group constants for nodal codes, the estimates of decay heat production etc. Comparison against the spectral effect evaluated with HELIOS, using the B1 critical spectrum iteration shows a generally good agreement, although at high burnups the effects evaluated with Serpent and HELIOS start to differ.

The use of 2D infinite lattice geometry is a useful approximation, which does have its effects on the calculation results. While the FM based critical spectrum capability of Serpent is an approximation in itself, its results can be valuable in evaluating the spectrum related uncertainty in the results of lattice calculations.

ACKNOWLEDGEMENTS

This work has been funded from the LONKERO project under the Finnish National Research Programme on Nuclear Power Plant Safety, SAFIR2022.

This work has received funding from the DECAPOD project under the Finnish National Nuclear Safety and Waste Management Research Programme 2023-2028, SAFER2028.

REFERENCES

[1] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. "The Serpent Monte Carlo code: Status, development and applications in 2013." *Annals of Nuclear Energy*, **volume 82**, pp. 142 – 150 (2015). URL https://doi.org/10.1016/j.anucene.2014.08.024.

[2] J. Leppänen, M. Pusa, and E. Fridman. "Overview of methodology for spatial homogenization in the Serpent 2 Monte Carlo code." *Annals of Nuclear Energy*, **volume 96**, pp. 126 – 136 (2016). URL http://www.sciencedirect.com/science/article/pii/S0306454916303899.

[3] V. Valtavirta and J. Leppänen. "A novel Monte Carlo leakage correction for Serpent 2." In *proceedings of ANS M&C 2021*. Raleigh, North Carolina, USA (2021).

[4] T. Lötsch, V. Khalimonchuk, and A. Kuchin. "Proposal of a benchmark for core burnup calculations for a VVER-1000 reactor core." In *proceedings of the 19th AER Symposium on VVER Reactor Physics and Reactor Safety*. Varna, Bulgaria (2009).

[5] C. A. Wemple, H. N. M. Gheorghiu, R. J. J. Stamm'ler, and E. A. Villarino. "Recent advances in the HELIOS-2 lattice physics code." In *Proceedings of the International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource*. Interlaken, Switzerland (2008).

[6] D. Knott, B. H. Forssén, and M. Edenius. "CASMO-4, A Fuel Assembly Burnup Program, Methodology." Technical Report STUDSVIK/SOA-95/2, Studsvik of America, Inc. (1995).

[7] D. Knott and E. Wehlage. "Description of the LANCER02 Lattice Physics Codefor Single-Assembly and Multibundle Analysis." *Nucl Sci Eng*, **volume 155**, p. 331 (2007).

[8] Z. Liu, K. Smith, B. Forget, and J. Ortensi. "Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo." *Annals of Nuclear Energy*, **volume 112**, pp. 507 – 516 (2018). URL http://www.sciencedirect.com/science/article/pii/S0306454917303778.

[9] Y. Bilodid, E. Fridman, and T. Lötsch. "X2 VVER-1000 benchmark revision: Fresh HZP core state and the reference Monte Carlo solution." *Annals of Nuclear Energy*, **volume 144**, p. 107558 (2020). URL https://www.sciencedirect.com/science/article/pii/S0306454920302565.

[10] T. Lötsch, V. Khalimonchuk, and A. Kuchin. "Corrections and additions to the proposal of a benchmark for core burnup calculations for a VVER-1000 reactor." In *proceedings of the 20th AER Symposium on VVER Reactor Physics and Reactor Safety*. Helsinki, Finland (2010).