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Utilization of VTT's Monte Carlo Code Serpent2 in Validation of Lattice Physics Methods at Westinghouse

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ABSTRACT

A lattice physics code is a vital tool, forming a base of reactor core analysis. It enables the numeric properties of the fuel assembly to be calculated and generates a proper set of data to be used by a 3-D full core simulator. The code's methodology of solving the neutron transport equation has to be validated to make sure it provides a reliable output. This paper shows the feasibility of using a reference Monte Carlo simulation to aid the validation of the deterministic lattice physics methods. A comparison of results between code Serpent 2 and HELIOS 1.8 is presented for a representative BWR fuel assembly. The comparison highlights certain issues intrinsic to the deterministic methods implemented in HELIOS. Selected aspects of creating a reference Monte Carlo solution are explored as well.

1 INTRODUCTION

A full-core analysis is usually a task of 3-D nodal simulators, due to their versatility and speed of calculations. However, all material's cross sections and other neutronic parameters, used by the nodal code are generated by a lattice physics code.

Thus, it is of crucial importance that methods implemented in a given lattice physics code yield correct results. One of the ways of validating the code is to compare its results with a reference numerical solution. This paper summarizes the efforts in creating the stochastic reference calculation using the Monte Carlo code Serpent developed at VTT Technical Research Centre of Finland [1].

The benchmarked deterministic code is HELIOS version 1.8. It implements a very similar method of solving the neutron transport equation (Current Coupling Collision Probability method) as the new lattice physics code currently under development at Westinghouse Sweden [2]. Thus, any issues with the method found should be addressed with the new code.

2 MODEL

The geometry chosen for this benchmark calculation is the SVEA-96 Optima 3 BWR fuel assembly with significant burnable absorber (gadolinium) loading. Details of the geometry created in both codes were taken from [3]. The geometry representation in Serpent is shown in Figure 1. The equivalent model was also made in HELIOS. The water cross in the middle (coloured with yellow) and the external bypass (coloured in orange) is denser than the boiling water inside the fuel box, which is one of the challenging aspects of the heterogeneous nature of the BWR fuel lattices.

Fuel pin types with respective ^{235}U enrichment and burnable absorber content are listed in Table 1 and follow the colour code used in Figure 1.

In each code, the basic depletion will be performed at 60% of the coolant void and until the average assembly depletion reaches 80 MWd/kgU. The selected branch cases will be then calculated in both HELIOS and Serpent. Branch cases presented in this paper are coolant density branches (coolant void momentaneous changing from 0% to 99%).

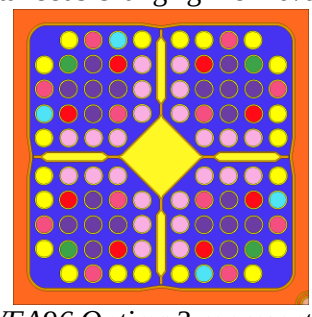

Figure 1: *SVEA96 Optima 3 representation in Serpent.*

Table 1: *Fuel pin types*

# of fuel pins	U-enrichment	Gd-content
20	3.2	0
8	3.4	0
4	4	0
20	4.2	0
24	4.5	0
4	3.4	4.0
8	4.5	4.5

3 THE REFERENCE MONTE CARLO SOLUTION

3.1 General considerations

Although Monte Carlo Codes offer the advantage of explicitly mimicking the physical interactions between neutrons and matter with very little approximations, they have their own issues which need to be considered if one desires to obtain a reliable reference solution. Generally recognized three main issues that need to be dealt with when solving the neutron transport equation with stochastic methods are [4]:

a) Convergence of the power iteration method
b) Bias in results of the multiplication factor and reaction rate distributions
c) Bias in uncertainties for k and reaction rate distributions

The problem of convergence (a) was shown to be effectively dealt with by discarding appropriate amount of initial cycles[1] [5]. For this model the number of 200 initial cycles is discarded for conservatism.

The bias in the Monte Carlo tallies comes from the normalization of the number of neutrons between the cycles and has been shown [6] to be inversely proportional to the number of neutrons used per cycle, M:

$$\Delta k \propto \frac{1}{M} \qquad (1)$$

The neutron population size is also a concern from the point of view of error propagation from the transport solution into the depletion calculations. However, as long as the standard deviation is kept relatively low, the error propagation is negligible [7][8]. The neutron population was chosen such that the standard deviation reported by Serpent for k_∞ was mostly below 10 pcm. In this case 40 million neutron histories are used for each neutron transport calculation.

3.2 Spatial discretization of burnable absorber bearing pins

Due to a fact that fuel depletion is to be taken into considerations, a proper discretization of the gadolinium bearing pins is called for. ^{155}Gd and ^{157}Gd are strong neutron absorbers and introduce a strong self-shielding in the model. Thus, coarse division of these fuel pins might lead to erroneous rates of the burnable absorber.

There are two phenomena to consider when trying to properly capture the depletion of a heavily self-shielding nuclide in the numerical model.

First is the so-called 'onion-skin' effect, presented in Figure 2. Gadolinium will firstly deplete at the pin's rim, allowing more neutrons to reach deeper inside of the fuel pin. Therefore, a proper number of radial rings is required.

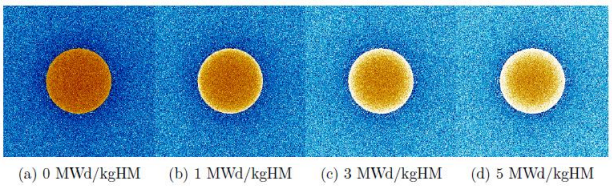

Figure 2: *Visualization of the 'onion-skin' effect. Shades of red correspond to the relative fission power (scale ranges from white: largest fission power, to black: no fissions).*

The other phenomena to consider is the very heterogeneous neutron flux in the model due to non-zero coolant void and non-boiling moderator in the bypass regions. Figure 3 shows the neutron flux magnitude along the model's diagonal computed using Serpent. The dips in the flux are where the burnable absorber pins are located. This shows the importance of finer azimuthal division of the gadolinium bearing pins.

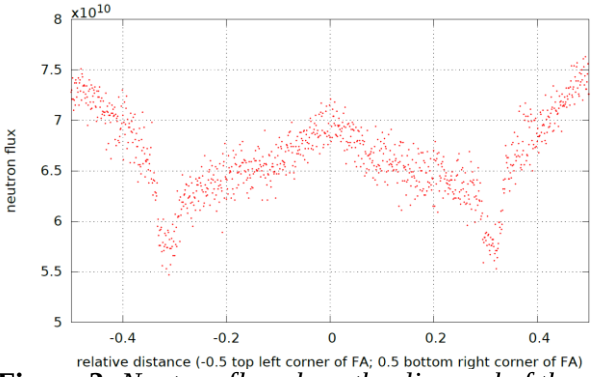

Figure 3*: Neutron flux along the diagonal of the considered fuel assembly.*

The number of radial rings and azimuthal sectors in the aforementioned pins is steadily increased until the largest relative difference in ^{155}Gd and ^{157}Gd number densities between two consecutive cases is below 1%. The final pin's spatial discretization is: 20 radial rings and 8 azimuthal divisions. Therefore, it results in each Gd pin to be divided into 160 zones of equal volume.

[1] Monte Carlo calculation is divided into so-called cycles. During each cycle a selected number of neutron histories are simulated. The number of neutrons (or neutron weights) is normalized between the cycles.

4 RESULTS AND DISCUSSION

The results are presented in 3 distinct parts. First the fresh fuel conditions are discussed followed by the depletion and then branch cases.

4.1 Fresh fuel conditions

Table 2 presents a comparison of the infinite multiplication factor (k_∞) calculated by HELIOS and Serpent for fresh fuel conditions (no burnup) and different coolant voids.

Table 2*: Differences for the fresh fuel.*

Coolant void	k_∞ HELIOS	k_∞ Serpent	difference [pcm]
0%	1.02490	1.02750	-260
30%	1.01285	1.01471	-186
60%	0.99682	0.99825	-143
90%	0.97827	0.97816	11
99%	0.97311	0.97217	94

The obtained differences exhibit a very strong dependence on the coolant void fraction. Pearson *r*-correlation coefficient between the coolant void and inter-code discrepancies in k_∞ is 0.96, which suggest a strong positive correlation. The bias associated with the coolant void content was observed and reported in other instances of deterministic codes, which (as HELIOS) rely on the Current Coupling Collision Probability (CCCP) method to solve the neutron transport problem [9].

It is speculated that the assumptions of spatially flat and isotropic source and isotropic scattering with outflow transport approximation might be the largest factors contributing to the observed bias. The anisotropic scattering becomes more important the larger the coolant void in the model is.

Nevertheless, discrepancies in k_∞ predicted by HELIOS and Serpent are judged to be acceptable. Smaller differences should not be expected since both codes use cross section libraries derived from different releases of the United States Evaluated Nuclear Data File (ENDF/B). ENDF/B-VI is used with HELIOS and ENDF/B-VII in case of Serpent.

4.2 Depletion Calculation Results

Figure 4 shows evolution of differences in k_∞ between the codes as the burnup progresses.

In the beginning, the discrepancy increases, to reach its peak at around 7 MWd/kgU. Its trend reverses thereafter. Burnup of ^{155}Gd and ^{157}Gd, which are very strong neutron absorbers, is slower in HELIOS than it is in Seprent (see Figure 5).

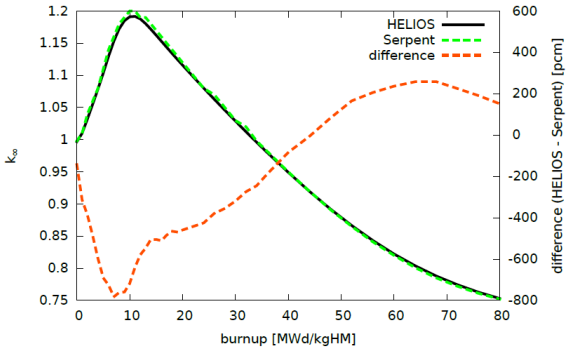

Figure 4: *Comparison of k_∞ evolution with burnup in HELIOS and Serpent.*

The large difference in k_∞ vanishes as discrepancies in the gadolinium content become less and less pronounced. There could be several reasons for the deterministic code to under-estimate the burnable absorber depletion rate. One of them could be discrepancies in the basic nuclear data used by both codes. The other could be non-equivalent meshing (i.e., spatial discretization) of gadolinium bearing pins.

The trend occurring thereafter seems to be driven by the different plutonium build up in both codes, (presented in Figure 6). However, due to the fact that both codes use different variants of the predictor corrector method to couple the transport and depletion calculations and fundamentally different approaches to dealing with Bateman equations, it is very hard to pinpoint exact reasons for the trends observed during depletion.

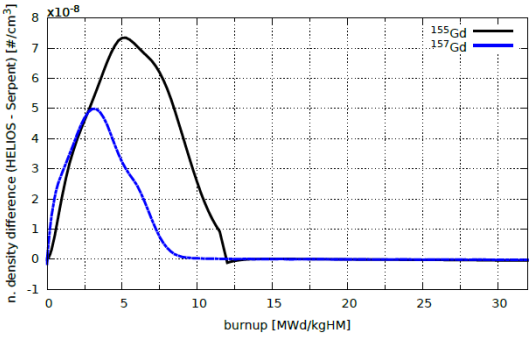

Figure 5: *Difference in gadolinium number densities.*

5 BRANCHES

The k_∞ differences in the coolant density branches are presented in Figure 7.

The trend with burnup is the same as the one already shown in Figure 4. It is worth pointing out that the coolant void bias observed in the fresh fuel conditions is consistently present during burnup as well.

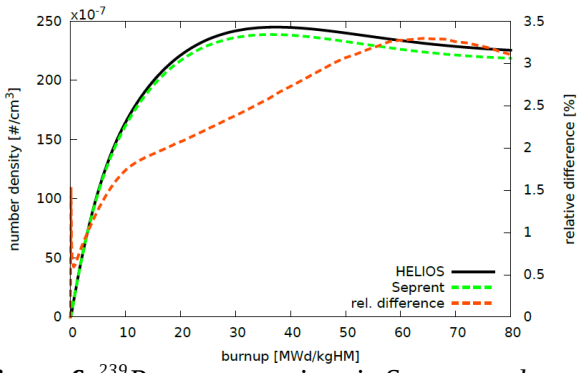

Figure 6: *^{239}Pu concentrations in Serpent and HELIOS.*

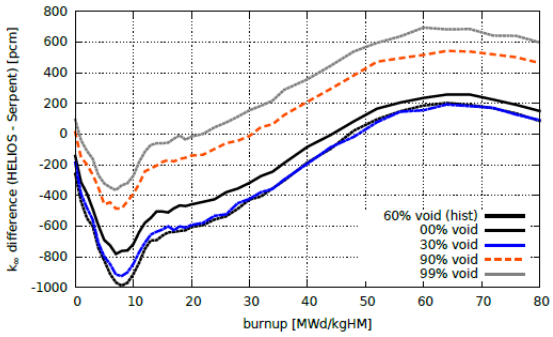

Figure 7: *Coolant density branch k_∞ differences.*

The use of Serpent allowed for an automatic calculation of the branch cases following the basic depletion calculations without a need for development of external wrapper scripts.

6 CONCLUSIONS

The work conducted showed the feasibility of using the Monte Carlo codes for validation of the methods used in the deterministic lattice codes.

The built-in capabilities of Serpent allowed for a relatively quick setup and execution of the detailed depletion calculation with an automatic restart feature for consecutive branch cases.

Even though the use of different ENDF/B releases in the compared codes somewhat contaminated the results, it was possible to highlight several important issues, such as: the coolant void bias (in the results calculated by HELIOS), the importance of running thorough sensitivity studies to come up with proper spatial discretization of the fuel pins, a need for improved way to account for increasing importance of anisotropic scattering at high coolant void content.

These findings will be considered in the development and consecutive validation of the new lattice physics code developed at Westinghouse Sweden (PHOENIX5 [2]), which will also employ the CCCP method of solving the neutron transport problem.

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