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Hybrid stochastic-deterministic method of generating one-group cross sections for transient analysis applied to Sodium Fast Reactor

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Abstract

The paper presents a hybrid stochastic-deterministic method in which one-group cross sections are 1) generated with a Monte Carlo code for selected core states using the whole-core model and 2) adjusted for diffusion solution applying a sampling technique to improve the agreement between the prediction of static parameters by the Monte Carlo and nodal diffusion codes. The hybrid method was applied for an analysis of the Superphenix Sodium Fast Reactor core [1] using Serpent 2 as a continuous energy Monte Carlo code [2] and the PARCS (Purdue Advanced Reactor Core Simulator) reactor kinetics code [3] as a nodal diffusion solver. Assuming correspondence between two models, the universes of the Serpent 2 whole-core model are defined to represent the nodes of the PARCS whole-core model. Universe-wise one-group cross sections and fluxes and k-effective value were generated for selected core states using Serpent 2. The cross sections were then used in a series of PARCS simulations involving a correction sampling technique, an iterative procedure, in which one-group transport cross sections are randomly variated assuming uniform distribution in a specified range in order to find a PARCS solution for k-effective and 3D flux distribution as close to the Serpent 2 results as possible. To obtain a more global picture about the capability of the hybrid method and its convergence, three core configurations have been simulated, namely, the reference critical core, a Doppler reactivity effect case with increased temperatures of fissile and fertile materials, and a sodium density reactivity effect with reduced sodium density. For all core configurations, a good agreement has been achieved between the PARCS and Serpent 2 predictions of the static parameters (k-effective within 10 pcm and flux within 2%), providing a potential for fast-running and acceptably accurate transient core simulations.

KEYWORDS: Serpent, PARCS, Superphenix, Sampling method

Introduction

Due to the continuous increase in computational power, Monte Carlo methods are progressively more frequently used for various calculations in the nuclear field. On the one hand, one of the most important advantages of these methods is that any arbitrary geometry can be reproduced together with a continuous neutron energy treatment allowing a simulation with high level of fidelity. On the other hand, the greatest disadvantage of the Monte Carlo methods is the required computational time in order to achieve results with high level of statistics which is the main limitation on such applications as transient simulations. The current paper has the main purpose to offer a solution to this situation and introduce a hybrid method by combining the accuracy of the Monte Carlo simulations with the computational speed of the deterministic methods. In addition to the combination of the methods, a new technique was used to adjust the transport cross sections utilized for the simulations. This new technique is called the Sampling method and its main function is to increase the accuracy of the results. By using the above mentioned procedure, good agreement was achieved between the reference Monte Carlo results and the mentioned hybrid method. Consequently, improved transient simulations can be achieved which is still not practicable today by using Monte Carlo codes due to its computational time requirement.

For the stochastic part of the proposed method, the Serpent 2 Monte Carlo code was used which is a continuous energy Monte Carlo code developed at the VTT Technical Research Center of Finland [2]. As Monte Carlo codes are based on stochastic methods, probabilities (cross sections) are used to simulate the different neutron interactions and through the tracking of these interactions the solution is obtained for the neutron transport equation.

Serpent was chosen to be the reference Monte Carlo calculation tool considering different factors. First, this code has been used in multiple studies for cross section generation, *e.g.* [4, 5, 6], which is a very important feature for the currently described work, not to mention the fact that the code is openly

and freely available. The next reason for selecting Serpent as the stochastic computation tool is the high performance which comes mainly from two applied methods. 1) Woodcock delta tracking [2] is used in Serpent in contrast to the more general ray tracing technique which allows a decrease in computation time by avoiding the recalculation of the neutron mean free path every time a neutron crosses a material region. 2) The second feature is the use of the unionized energy grid [2] which provides an increase in performance by constructing it from the continuous energy cross sections. It is worth mentioning that, by using the unionized energy grid technique, although the calculation time is decreased, the required memory is enlarged as part of the process which can be an issue for calculations which already have a high memory demands, such as burnup simulations.

Method description

As the described method is a hybrid technique, it can be divided into two separate parts, stochastic and deterministic. The stochastic part, which is represented by Serpent 2, is used to obtain the one energy group homogenized cross section data which is later used in the deterministic calculation. The deterministic solution is attained through the PARCS nodal diffusion solver [3]. This spatial nodal diffusion solver is coupled to an in-house script [7] called Sampling method, which is utilized to adjust the raw cross section output from the Serpent calculation. This cross section adjustment can be done based on the assumption that Serpent does not calculate totally accurately the transport cross section data [4][8].

The first step to use the hybrid method is to run the Monte Carlo code to obtain the reference multiplication factor, one-group flux distribution and the one-group cross-section data which is going to be used as input for the deterministic solver. As a second step, the deterministic solver is run with the cross sections generated by Serpent previously. Following this, the multiplication factors and the one-group flux values in the different regions are compared between the Serpent and PARCS results. This comparison is done using Eqs. 1.1 – 1.4:

$$\Delta\phi_i = \left|\phi_i^P - \phi_i^S\right| \tag{1.1}$$

$$\mu = \frac{1}{N}\sum_{i=1}^{N}\Delta\phi_i \tag{1.2}$$

$$\sigma_1 = \sqrt{\frac{1}{N(N-1)}\sum_{i=1}^{N}(\Delta\phi_i - \mu)^2} \tag{1.3}$$

$$\sigma_2 = \left|k_{eff}^P - k_{eff}^S\right| \tag{1.4}$$

where ϕ_i^P and ϕ_i^S represent the flux values in region *i*, *i.e.* PARCS node and Serpent universe, respectively; *N* is the number of the regions, whereas, k_{eff}^P and k_{eff}^S are the resultant multiplication factors predicted by PARCS and Serpent, respectively.

This comparison is incorporated into the applied Sampling method. After the determination of the initial differences in flux and k-effective, multiple PARCS calculation iterations are run changing the transport cross sections from the previous iteration for each region using a uniform random distribution within a selected domain: maximum change between two iterations is 1.5% and maximum deviation from the original Serpent value is 50%. This domain was selected by a trial-and-error optimization of the calculational time and reached accuracy. When the obtained σ_1 and σ_2 values are both smaller than in the preceding iteration, the vector of the transport cross sections is stored and the search continues for better accuracy. When the required accuracy is reached, the script is terminated, while the resultant final transport cross section data are stored as the best estimate for characterization of this core state and can be used further in transient analysis.

Description of reference SFR core

The model which was used for the Serpent simulation was based on the Superphenix benchmark calculation presented in [1]. Compared to the reference model, few modifications have been introduced, affecting mostly the number of universes present in the model. The mentioned modifications were done to obtain region wise cross sections for all the individual subassemblies present in the model. Each of the subassemblies is then further divided into several axial layers, which are shown in Fig.1. for the Serpent model. The indicated dimensions represent the subassembly partition heights at hot zero power conditions corresponding to 673K sodium inlet temperature.

The current research was completed on three different core configurations (Reference, Doppler, Sodium density) to obtain results related to different reactivity feedback effects describing some important separate effects occurring during a transient event. Two specific feedback effects were considered as part of the study, namely, the Doppler effect and the effect of sodium density change. 1) The Doppler feedback effect is introduced by the temperature change of the fuel material, mainly, the U-238. The increase of temperature in the material will increase the thermal motion of the target atoms, increasing the parasitic absorption of the neutrons, causing a negative reactivity effect. This feedback works in the same way as it is for a conventional Light-water reactor. 2) The density change of the sodium has a peculiar and, in case of sodium boiling, an important feedback effect. As the density of the sodium decreases, its moderation effect declines resulting in a harder neutron spectrum which translates into a positive reactivity effect on the core. In the same time, the density decrease will result in an increase of leakage out of the system introducing a negative reactivity effect. The overall feedback effect depends on the spatial position inside the core, meaning close to the central region the spectrum hardening dominates, whereas at the periphery the leakage is the main contributor.
As for the first case, in relation to the Doppler effect, the temperature of the fertile and fissile material was increased by from 600K to 1500K. To investigate the effect of the sodium density change, the nominal density corresponding to sodium temperature of 673K was decreased to the sodium density corresponding to the sodium temperature of 1073K in the fertile and fissile core regions for all subassemblies in the axial regions of the fissile height and above.

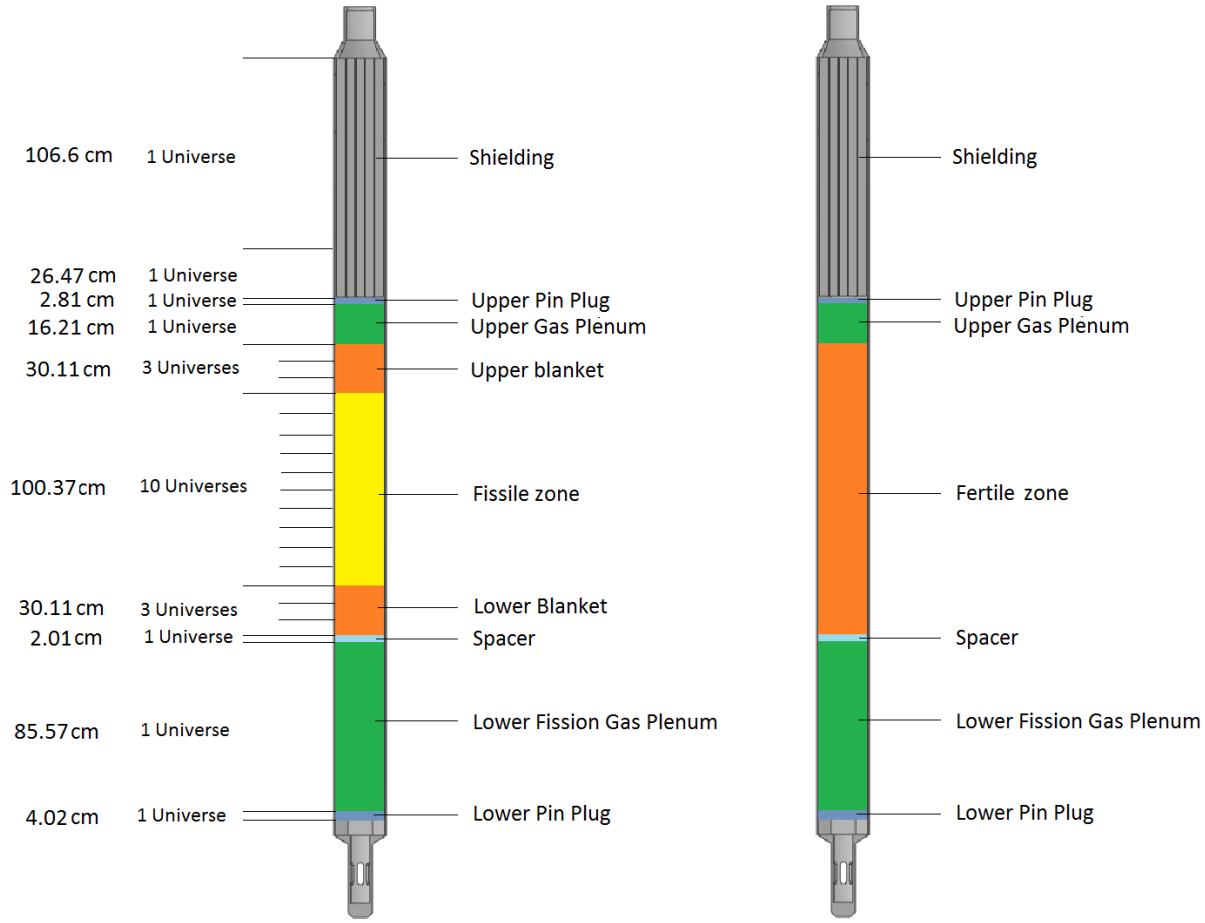

Fig.1. Subassembly axial structure of the fissile core (left) and the breeder region (right)

PARCS model description

The PARCS model of the Superphenix core follows the Serpent model except some minor simplifications. In the Serpent model, a very detailed axial structure is presented with some adjacent layers being highly different in thickness, such as Spacer and Lower Blanket. In general, for nodal diffusion codes, the usage of significantly different node thicknesses is detrimental as it can prohibit the convergence of a solution. To avoid this problem, the geometry of the reactor core has been slightly simplified for PARCS, meaning a subassembly division in 40 axial layers having a similar, thickness (~10 cm) throughout the whole subassembly neglecting few thin layers, such as the Pin Plugs and the Spacer. Radially, the pitch of the subassemblies is kept the same 18.02 cm as was for the Serpent model.

In regard to the cross section input for the PARCS model, 307 subassemblies with corresponding axial subdivision have been simulated with one-group homogenized cross sections individually. The number of subassemblies corresponds to the third of the whole core which simplification can be justified as the core has 120º symmetry.

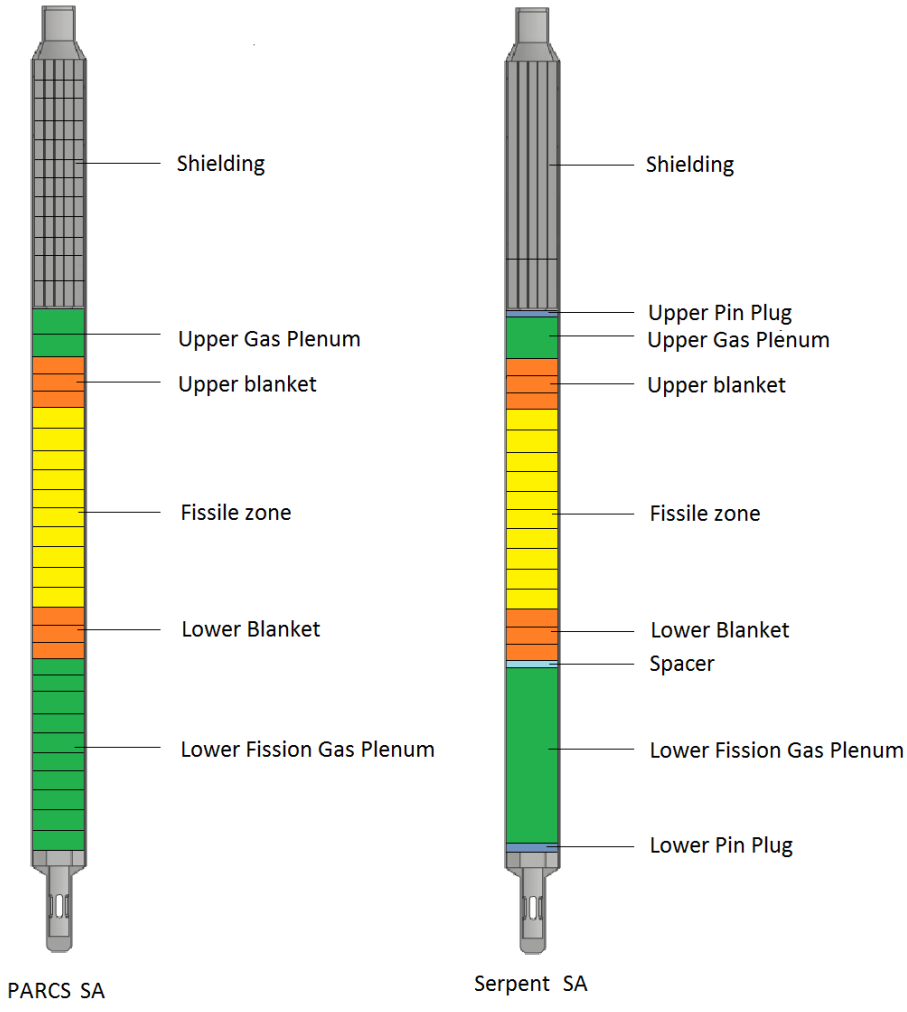

Fig.2. Comparison of subassembly axial division between the PARCS nodes and the Serpent universes for a fissile subassembly

Results

The simulation results regarding the multiplication factors are summarized in Table 1. Four different cases are presented in the table. The first case is the reference critical state without the usage of the Sampling cross section correction methodology and the following three cases are the three core configurations calculated with the Sampling method to measure the reactivity effect.

Core configuration	k_{eff} value		Δk_{eff}, pcm
	Serpent (std=1.6pcm)	PARCS	
Reference critical, without cross section correction method	0.99895	1.00312	417
Reference critical	0.99895	0.99889	6
Doppler effect	0.98862	0.98857	5
Sodium density effect	0.99969	0.99970	1

Table 1. Comparison of multiplication factors for PARCS and Serpent

The presented k-effective values clearly show the effectiveness of the presented transport cross section correction methodology. For the critical state when the Sampling method is not used, the difference in k-effective is 417 pcm, whereas when the method is applied it goes down to 1-7 pcm.

As the Sampling method is used through many iterations (10000 in this specific work) the evaluation of the multiplication factor is plotted in Fig.3. The mentioned figure shows the changes in the k-effective value after every successful iteration when the transport cross section is adjusted. The plot shows that, after around 70 successful cycles, the k-effective value is converged to the value of the reference Serpent case in a predefined error (7 pcm). As the k-effective value has converged, successful iterations do not cease which shows that difference in flux must be kept on decreasing as that is the second argument which is tested in the script for a successful iteration to happen.

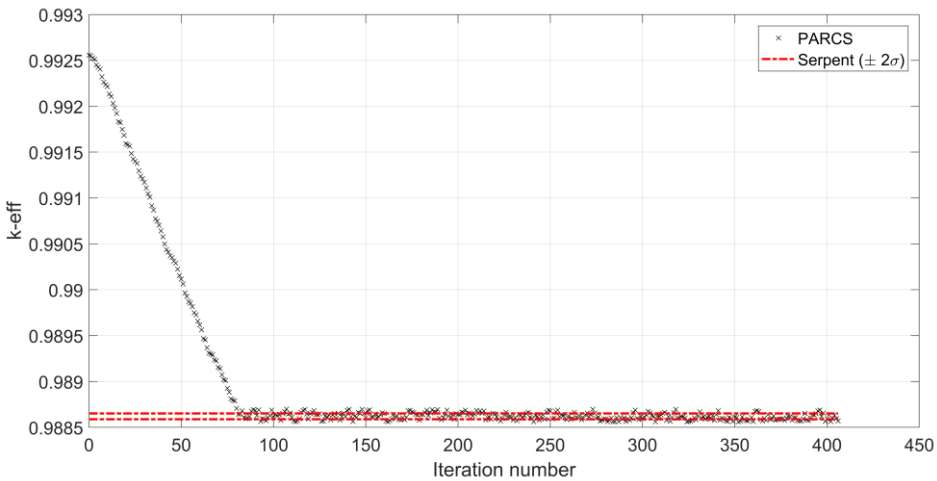

Fig.3. Multiplication factor convergence to the reference Serpent value by using the Sampling method

The core power map for the critical case is presented in Fig.4. From the power map, it can be read that the maximum power subassemblies are close to the middle of the reactor core, peaking at around 10 MW. As the breeder region is approached, the power slowly decreases to 4–5 MW at the periphery. In the breeder region, there is a sharp drop in power down to around 0.01–0.3 MW.

To obtain a better picture of the reactor core related to the effect of the Sampling method, a comparison of power map between the Serpent and PARCS simulations is shown for the Doppler case in Fig.5. In this figure, a power peaking factor has been utilized to scale the plotted error according to the power output of the individual subassemblies. In this sense, where the power output of the subassembly is above the average power output, the error is emphasized, whereas for the low power subassemblies, the error is diminished. Considering this, it can be read from the plot that the maximum subassembly wise power difference between the two calculation methods is around 2% which happens to be close to the periphery between the fissile and breeder core regions. In contrast, in the breeder region, very low error can be seen, between 0 and 0.01%. This low error is due to the fact that the average power output from these subassemblies are very low compared to the fissile region and, through the utilization of the power peaking factor, the error is scaled down corresponding to the importance of the subassembly.

For comparison to the previously presented results when the Sampling method has been utilized, the same power difference is plotted in Fig.6. as previously but this time without the use of the Sampling correction technique. The difference in the presented error is clearly visible, having a peak value of around 7.5% not to mention the fact that, this time, the highest error is around the middle of the reactor core where the highest power output subassemblies are located. In addition to this, at the periphery of the fissile region, the error is again higher than it was for the case with Sampling, close to 7%. To continue with, in the breeder region of the core, there is no significant difference between the plotted error compared to the same region in Fig.5.

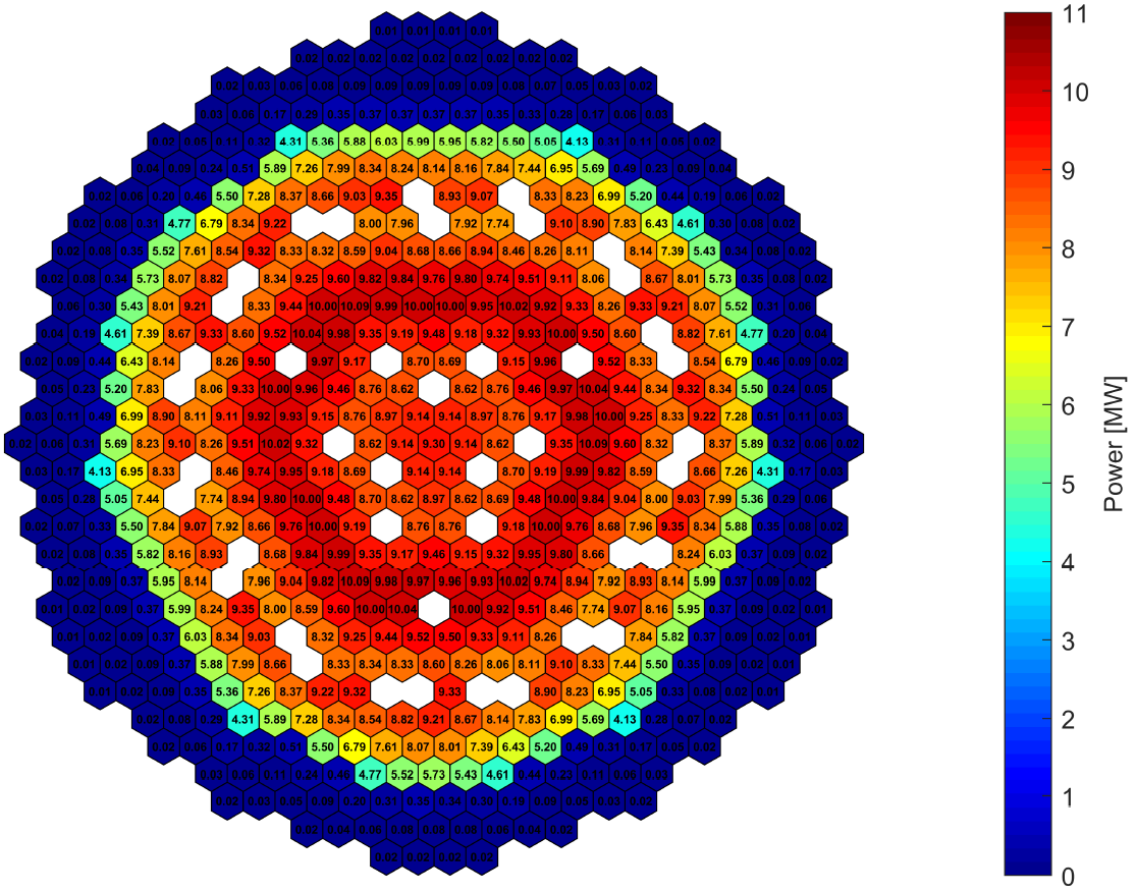

Fig.4. Core power map calculated by Serpent for the critical core configuration

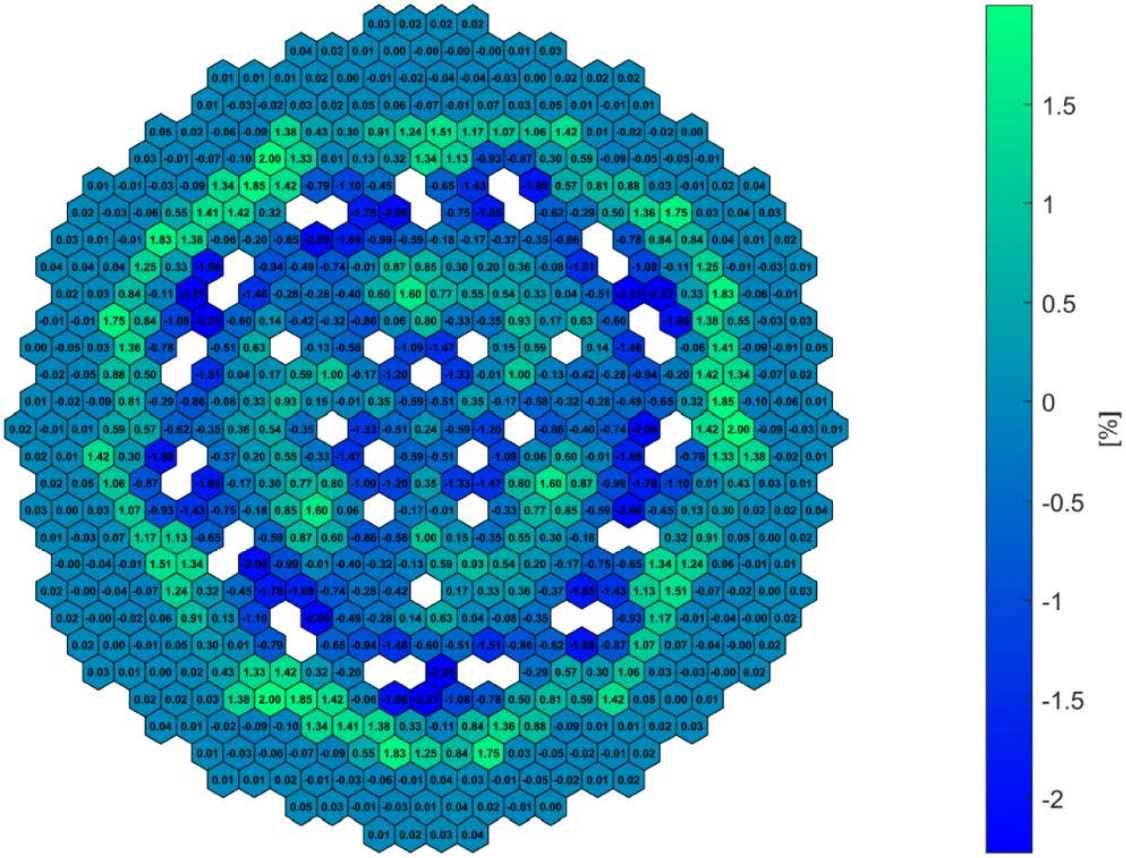

Fig.5. Relative power difference between the reference Serpent calculation and the PARCS solution utilizing the Sampling method (Doppler case)

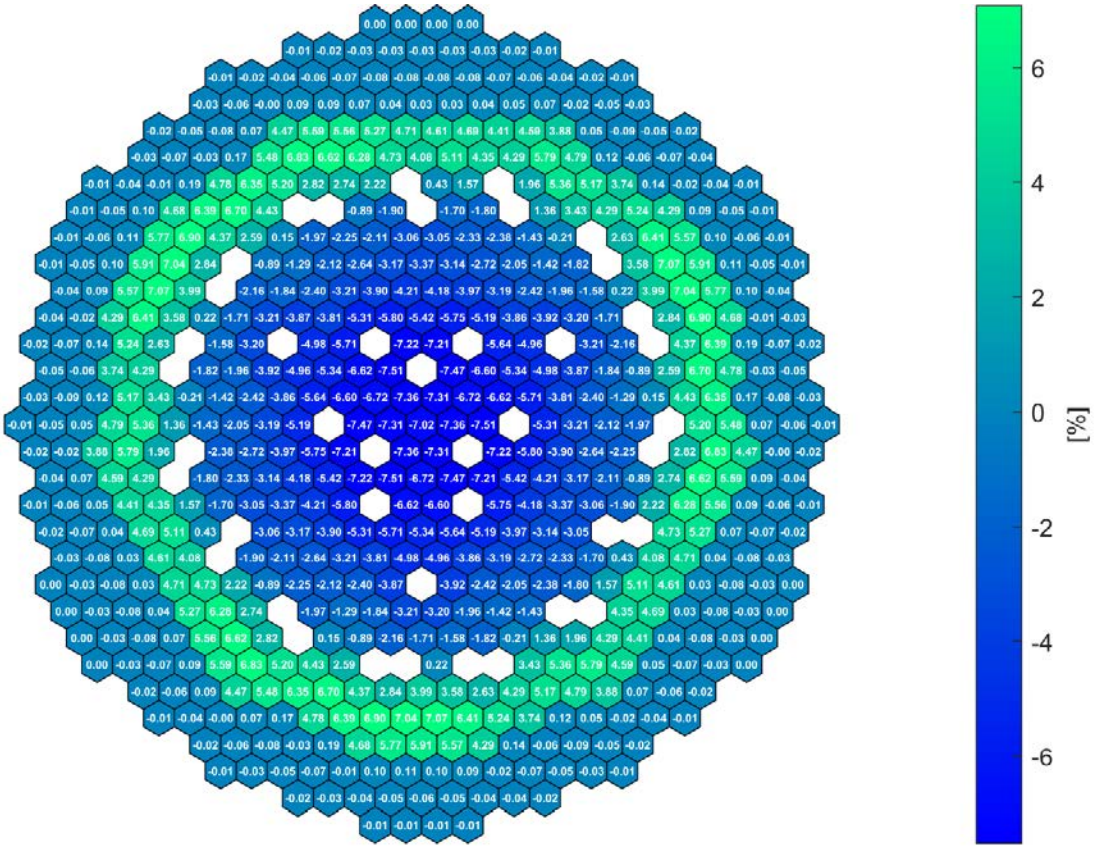

Fig.6. Relative power difference between the reference Serpent calculation and the PARCS solution without utilizing the Sampling method (Doppler case)

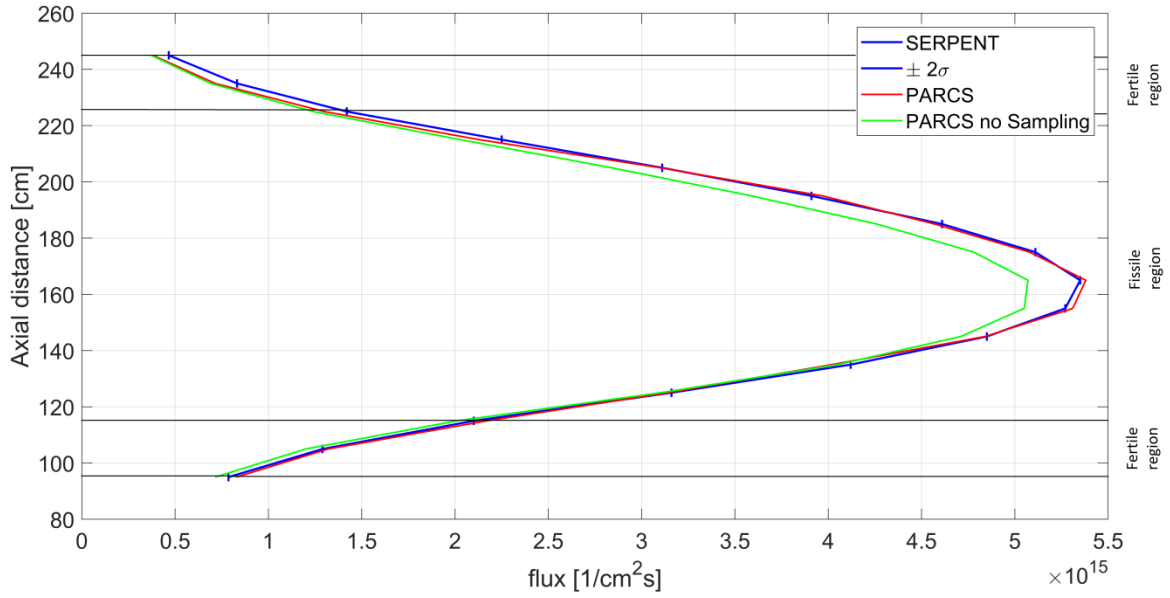

Fig.7. Axial flux profile comparison between the different simulation methods inside an inner fuel subassembly

A further parameter which can be compared is the flux profile inside the subassemblies. In Fig.7, the axial flux profile of a fuel subassembly is shown, portraying with red color the case when the Sampling method has been utilized, whereas the green line shows the flux profile in the same subassembly without using Sampling. In the figure, it is well visible how the correspondence is changing between the reference Serpent flux profile and the PARCS flux. In the fissile region when Sampling is used, the two lines go very well together whereas there is a big discrepancy in the highest flux regions when Sampling was not used. In the fertile region above the fissile zone, there is a bit of discrepancy between the fluxes for both cases which probably comes from the fact that some small simplifications have been applied on the geometry of the subassembly in these regions in particular.

Conclusions

Based on the Superphenix sodium fast reactor core benchmark analysis, reference Monte Carlo results have been compared to the PARCS diffusion solution coupled with the in-house Sampling transport cross section correction technique. One-group neutron cross sections have been attained through Serpent simulation which then was used for the PARCS model creating a hybrid calculation method. Three different core configurations comparison were performed between the two solution methods, examining both the k-effective and the flux values. More specifically, assessment was performed on perturbed reactor core states to quantify some of the main reactivity feedback effects, such as the Doppler effect and the sodium density effect. The analysis showed good agreement between the reference calculation and the proposed hybrid method, demonstrating the feasibility of the new method as a practical tool for transient analysis.

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