

Application of SPH Method for Sodium Fast Reactor Analysis

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Abstract - In this study, the capability of the DYN3D-Serpent codes system to simulate highly heterogeneous sodium-cooled fast systems was investigated. The BFS-73-1 critical assembly was chosen for the investigation. Initially, a 3D full model of the BFS-73-1 critical assembly was simulated using the Serpent Monte-Carlo (MC) code, and the basic neutronic characteristics were evaluated and compared against experimental values. This part meant as a first step towards the use of the Serpent MC code as a tool for preparation of homogenized group constants, and as a reference solution for code-to-code comparison with the DYN3D code. At the second part of the investigation, the BFS-73-1 critical assembly was modeled using the DYN3D code with few-group cross-sections generated by the Serpent MC code. It was suggested that for highly heterogeneous systems, such as the BFS experiments, the Superhomogenization (SPH) method should be applied to correct the few-group cross-sections of the different regions of the system. The SPH method is described and demonstrated for the BFS-73-1 critical assembly. It is shown that the application of the SPH method improves the accuracy of the DYN3D nodal diffusion solution, and therefore, it can be considered as a promising candidate of homogenization method for pin-by-pin calculations of sodium-cooled fast systems.

I. INTRODUCTION

The feasibility of using the Serpent Monte-Carlo (MC) code (1) as a tool for preparation of few-group homogenized cross-sections for nodal diffusion analyses of sodium-cooled fast reactor (SFR) cores was demonstrated in several studies (2, 3, 4). In these studies, a few-group cross-sections generation methodology was developed for the analysis of conventional SFR core configurations. The few-group cross-sections generated using the Serpent code were employed by the DYN3D nodal diffusion code (5), and the results were verified against a full core Serpent MC solution. The studies presented a good agreement between the DYN3D and the Serpent solutions, and therefore, it can be concluded that the DYN3D-Serpent codes system can be used for the analysis and further design development of SFR cores.

In this study, the possibility of using the DYN3D-Serpent codes system for more complex, highly heterogeneous sodium-cooled fast systems is investigated. For that purpose, the BFS-73-1 critical assembly (6) was selected and analyzed. The BFS-73-1 was constructed at the BFS-1 critical experiment facility located at the Russian Institute of Physics and Power Engineering (IPPE). The BFS-73-1 assembly has a substantial heterogeneous configuration, in both the axial and radial directions. Therefore, the generation of accurate few-group cross-sections for such an assembly is quite a challenge due to the strong spectral interaction between the different regions of the assembly. Applying the direct few-group cross-sections generation methodology as proposed in (2, 3, 4) for the DYN3D nodal diffusion analysis of the BFS-73-1 assembly will result in some deviations in the results, especially in the power distribution. A more accurate DYN3D nodal

diffusion solution for such a highly heterogeneous system, however, can be achieved by applying the Superhomogenization (SPH) method to correct the few-group cross-sections of the different regions of the system. The SPH method is an equivalence procedure proposed by Kavenoky (7), and later extended by Hebert (8). In this method, the regions-average reaction rate obtained from the heterogeneous calculation is preserved by multiplying a correction factor (SPH factor) to the regions-average few-group cross-sections. The SPH method is typically used to produce few-group cross-sections for pin-by-pin whole LWR cores analyses (9, 10). In this study, the SPH method was applied for the analysis of the fast, highly heterogeneous BFS-73-1 critical assembly.

The paper is organized as follows. Section II gives a brief description of the experimental configurations of the BFS-73-1 critical assembly. In Section III, the results of the Serpent analysis are presented and compared against the experimental values. Section IV describes the generation methodology of the few-group cross-sections and SPH factors, and presents the results of the DYN3D calculations with and without the SPH correction in comparison with the full assembly Serpent MC solution. Finally, the summary and the main conclusions are given in Section V.

II. DESCRIPTION OF THE BFS-73-1 CRITICAL ASSEMBLY

The BFS-73-1 critical assembly (6) was constructed at the BFS-1 facility to investigate the basic neutronics characteristics of a sodium-cooled fast reactor with metal uranium fuel. The assembly is constructed from a set of vertical stainless steel (SS) tubes with an outer diameter of 5.0 cm, 0.1 cm wall thickness, and length of 195.996 cm.

The tubes are arranged in a hexagonal lattice with a pitch of 5.1 cm. The spaces between the tubes are filled with cylindrical SS dowels with an outer diameter of 0.8 cm.

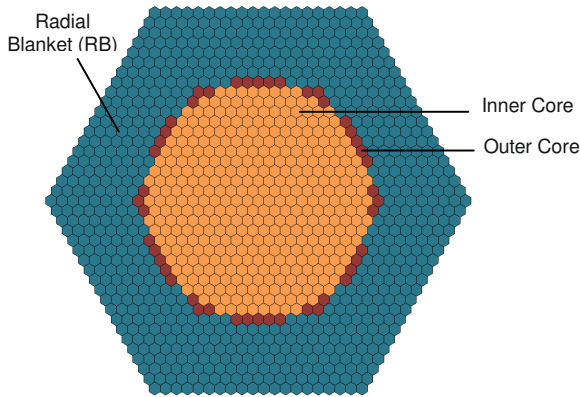


Fig. 1. Radial layout of the BFS-73-1 critical assembly

A schematic view of the BFS-73-1 critical assembly configuration is shown in Fig. 1. The assembly is composed of three types of tubes: inner core tube, outer core tube, and radial blanket tube. Each tube is filled with pellets of fissile or structural materials in a repeated cell arrangement. The pellets diameters are in the range of 4.6–4.7 cm and approximately 10 mm high, depending on the pellet material. Each of the pellets is bare or closed in SS or Aluminum can. The inner and outer core tube can be axially divided into three regions: lower blanket, core, and upper blanket. Both, the lower the upper blankets, consist of 50 depleted UO_2 pellets. The core region contains sixteen core cells. Each of the core cells consists of two uranium metal pellets of 36% enrichment, one depleted uranium metal pellet, and four sodium pellets. The difference between the inner and outer core tube is in the exact enrichment of the uranium metal pellet. The uranium metal pellet in the inner and outer core tube has an enrichment of 36.41% and 36.45%, respectively. Each of the radial blanket tubes, surrounding the core, contains 201 depleted UO_2 pellets.

III. SERPENT MC CALCULATIONS

In the first stage of the study, the BFS-73-1 critical assembly was modeled and analyzed using the Serpent Monte-Carlo (MC) code. This stage is an important part of the study. It is meant as a first step towards the use of the Serpent MC code as a tool for preparation of homogenized group constants, and as a reference solution for code-to-code comparison with the DYN3D code.

The Monte-Carlo is the best-suited method for the simulations of highly heterogeneous systems such as the BFS experiments. The BFS-73-1 critical assembly was modeled in detail, without using any approximations. Each single pellet and its can, the BFS tubes, and the SS dowels in the inter-tube spaces were modeled separately. The

simulations were performed using 550 skipped cycles, 2000 active cycles, and 800,000 neutron histories per cycle. All the calculations were performed using ENDF/B-VII.0 nuclear data files at room temperature. The effective multiplication factors (k_{eff}) and the fission rate distributions of several isotopes were evaluated and compared against available experimental data.

Table I. k_{eff} : experimental results vs. Serpent calculations.

Experimental (E)	Serpent calculation (C)	C/E
1.00080 ± 0.00290	0.99629 ± 0.00002	0.9955

The calculated and measured k_{eff} values of the BFS-73-1 critical assemblies are presented and compared in Table I. As can be noted, the calculations using the ENDF/B-VII.0 library underestimate the k_{eff} by about 0.45%. The k_{eff} , as well as other integral parameters, is very sensitive to the nuclear data files been used. The demonstration of the impact of different up-to-date and modified data files on the k_{eff} of the BFS-73-1 critical assembly can be found in (11).

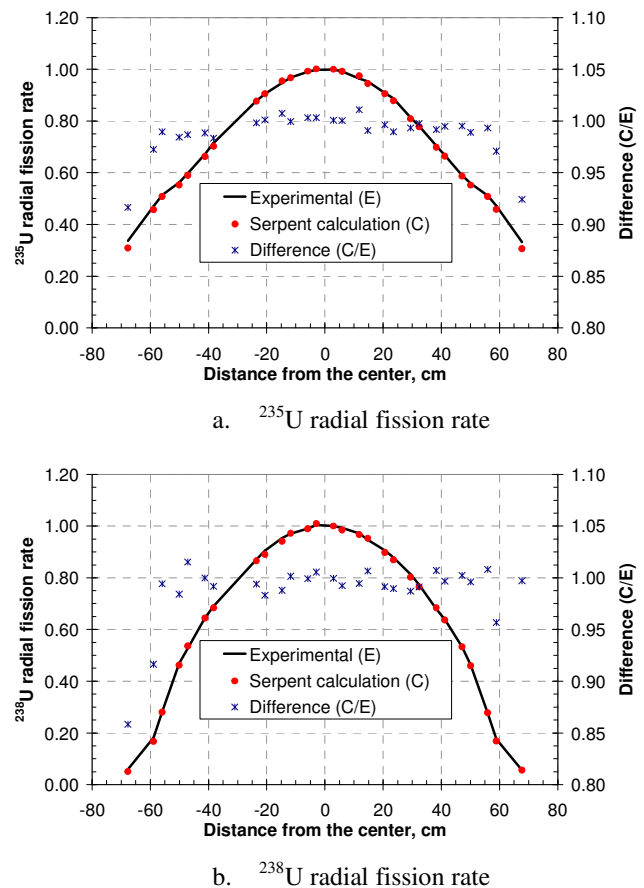


Fig. 2. Radial fission rate distribution: experimental results vs. Serpent calculations.

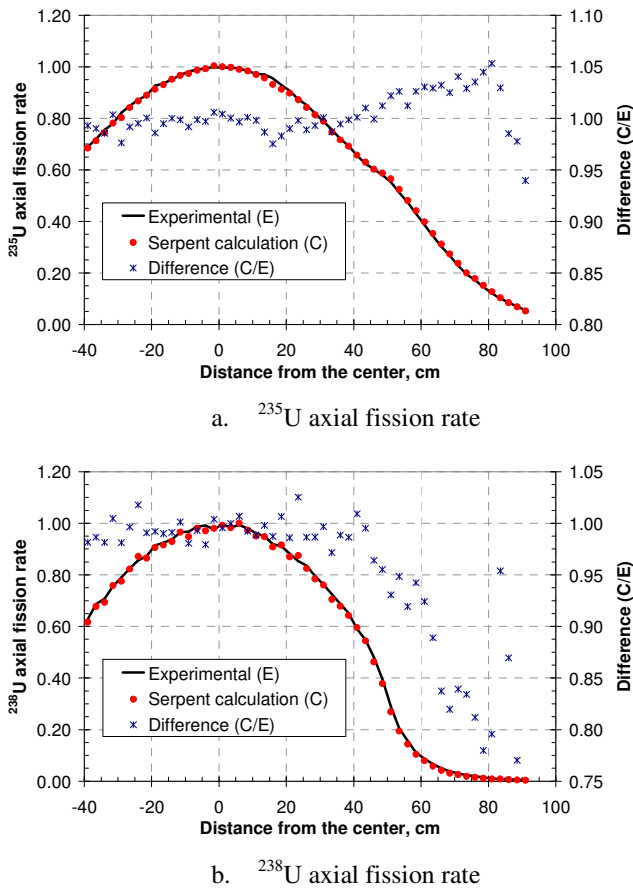


Fig. 3. Axial fission rate distribution: experimental results vs. Serpent calculations.

The fission rate distributions provide essential information for the estimation of power distribution in the core. The fission rate distributions were measured by small size fission chambers placed in the inter-tube spaces throughout the assembly. The measurement values at each position were normalized to the measured one at the center. For comparison purposes, the calculated values presented here were normalized in the same way, i.e. to calculated value at the center.

The comparisons of the calculated and measured ^{235}U and ^{238}U fission rate distributions in the radial direction are given in Fig. 2. It can be noted that the calculated fission rate distribution, of both of the isotopes, agrees well with the measured values. The calculations slightly underestimate the ^{235}U fission rate distribution by about 0.3% in the core region, i.e. up to about 55 cm from the center, and 3.2% in the blanket region on the average, respectively. The calculation of the ^{238}U fission rate distribution also shows underestimation of about 0.3% in the core region on the average, but a little larger underestimation of about 3.6% in the blanket region. The calculated ^{235}U and ^{238}U fission rate distributions in the axial

direction are compared with measured data in Fig. 3. As can be noted, in the core region, the relative difference is less than 1.5% on the average for both of the isotopes. However, the relative difference tends to increase as the measurement point gets far off the core center, especially in the blanket region. The average relative difference in the blanket region is about 3.1% and 14.2% for the ^{235}U and ^{238}U fission rate distributions, respectively. It should be noted that the ^{235}U and ^{238}U fission rate distributions were measured with an accuracy of about 1.5-2% and 2-3% in the core region, respectively. In the blanket region, they were measured with an accuracy of about 3-4% and 5-7%, respectively. Considering these uncertainties in the measurements, it can be concluded that the calculated ^{235}U and ^{238}U fission rate distribution, in both of the directions, agrees reasonably well with the measured values.

In general, the results presented above show a good prediction capability of the Serpent neutronic calculations. This fact indicates that the Serpent MC code can be used for the preparation of homogenized group constants for SFR cores, and as a reference solution for code-to-code verification with the DYN3D code.

IV. DYN3D CALCULATIONS

In the second stage of the study, the BFS-73-1 critical assembly was modeled and analyzed using the DYN3D nodal diffusion code. The assembly was analyzed on two levels: three-dimensional (3D) single fuel rod level, and a 3D full assembly level. The DYN3D calculations were performed using the Serpent few-group cross-sections with and without the SPH correction, to demonstrate the impact of the SPH correction on the accuracy of the results. The following sub-sections describe the generation procedure of the few-group cross-sections and SPH factors, and present the results of DYN3D analysis in comparison with the reference Serpent MC solutions.

1. Generation of Few-Group Cross-Sections and SPH Factors

The few-group cross-sections for the fuel rod and full assembly analysis were generated using the Serpent MC code. The Serpent simulations were performed using 550 skipped cycles, 2000 active cycles, and 800,000 neutron histories per cycle. All the calculations were performed using ENDF/B-VII.0 nuclear data files at room temperature. The few-group energy structure, which was selected for the preparation of the few-group cross-sections, is a 24-group subset of the 33-group energy structure of the ERANOS code (12), which was developed and validated for analysis of SFR cores. The 24-group energy structure is given in Table II. The selection procedure of this energy structure can be found in detail in (2, 3). It should be noted that the 24-group diffusion coefficients were generated by flux weighting of 240-group inverse of transport cross-section.

Table II. 24-group energy structure

Group number	Upper energy limit, MeV	Group number	Upper energy limit, MeV
1	2.0000E+01	13	4.0868E-02
2	1.0000E+01	14	2.4788E-02
3	6.0653E+00	15	1.5034E-02
4	3.6788E+00	16	9.1188E-03
5	2.2313E+00	17	5.5309E-03
6	1.3534E+00	18	3.3546E-03
7	8.2085E-01	19	2.0347E-03
8	4.9787E-01	20	1.2341E-03
9	3.0197E-01	21	7.4852E-04
10	1.8316E-01	22	4.5400E-04
11	1.1109E-01	23	3.1203E-04
12	6.7379E-02	24	1.4894E-04

In the first level analysis, the fuel rod was divided into 26 axial regions: 5 regions of lower blanket (each contains 10 depleted UO₂ pellets), 16 regions of core components (as the number of core cell), and 5 regions of upper blanket (each contains 10 depleted UO₂ pellets). The few-group cross-sections for each of the axial regions were generated using a 3D detail single fuel rod model with reflective radial and black axial boundary conditions.

In the full assembly analysis, each of the rods was divided into 10 axial nodes. To account for the strong spectral transition between the core and blanket regions, the few-group cross-sections were generated using the 3D core-blanket model depicted in Fig. 4. The few-group cross-sections were homogenized over each ring of rods of the same type.



Fig. 4. 3D super-cell model for the full assembly cross-section generation

As mentioned above, to further account for the strong spectral interaction between the different regions of the rod/assembly configuration, the SPH method was applied to correct the flux volume weighted few-group cross-sections of each of the regions. The SPH factors were obtained iteratively using the Serpent and DYN3D codes as follows:

- The 3D rod/assembly model is calculated using the DYN3D code with the few-group cross-sections generated by Serpent, and an average homogeneous flux ($\phi_{r,g}^{\text{hom}}$) is obtained for each region r and energy group g .
- The SPH factor μ for each region r and energy group g is then calculated by:

$$\mu_{r,g} = \frac{\bar{\phi}_{r,g}^{\text{het}}}{\phi_{r,g}^{\text{hom, norm}}} \quad (1)$$

where $\bar{\phi}_{r,g}^{\text{het}}$ is the average heterogeneous flux in region r and energy group g obtained from the Serpent detailed calculations, and $\phi_{r,g}^{\text{hom, norm}}$ is the normalized average homogeneous flux in region r and energy group g .

The normalization of the average homogeneous flux obtained from the DYN3D solution is given by:

$$\phi_{r,g}^{\text{hom, norm}} = \phi_{r,g}^{\text{hom}} \frac{\sum_r V_r \bar{\phi}_{r,g}^{\text{het}}}{\sum_r V_r \phi_{r,g}^{\text{hom}}} \quad (2)$$

where V_r is the volume of region r .

- The obtained SPH factors are used to correct the few-group cross-sections of each region r and energy group g as follows:

$$\tilde{\Sigma}_{r,g} = \mu_{r,g} \Sigma_{r,g} \quad (3)$$

- The 3D rod/assembly model is calculated again using the DYN3D code with the corrected few-group cross-sections. Then, the obtained average homogeneous fluxes are used to calculate a new set of SPH factors. The iterative process continues for n iterations, and finished if the convergence criterion

$$\max_{r,g} \frac{|\mu_{r,g}^n - \mu_{r,g}^{n-1}|}{\mu_{r,g}^n} < \epsilon \quad (4)$$

is satisfied with the recommended value of 10^{-5} .

2. Fuel Rod Level Analysis

Each of the BFS-73-1 fuel rod types was analyzed with the DYN3D code using the Serpent few-group cross-sections with and without the SPH correction. The SPH factors were evaluated iteratively, as described above, for a fuel rod model divided into 26 axial regions.

The k-inf obtained from the DYN3D and Serpent calculations for the different fuel rod is presented and compared in Table III. As can be noted, the DYN3D without the SPH correction overestimates the k-inf, for both of the fuel rod types, by 99 pcm. However, the difference reduces to about 35 pcm, when the SPH-corrected few-group cross-sections are used.

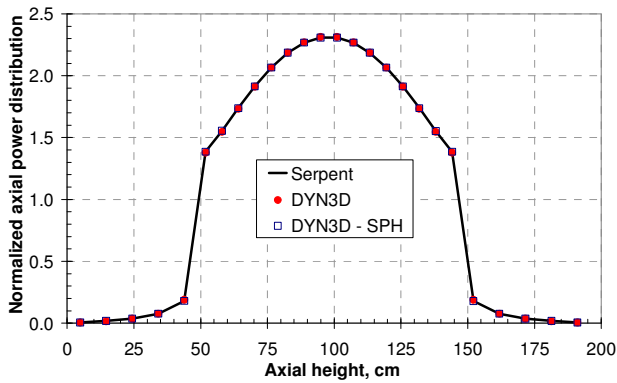
A comparison of the central core fuel rod normalized axial power distribution between the Serpent and DYN3D codes is shown in Fig. 5. The normalized axial power distribution predicted by DYN3D without the SPH correction presents relatively large deviation from reference Serpent solution. In the fuel region (between 50 and 100 cm), the average/maximum differences are about

0.21/0.48%. The relative difference tends to increase as the calculated point gets far off the fuel rod center, especially in the blanket regions. The average/maximum differences in the blanket region are about 5.38/9.05%. The use of the SPH correction shows a significant improvement in the prediction accuracy. In this case, the average/maximum differences in the fuel region are only about 0.02/0.05%. The average/maximum differences in the blanket region are remarkably reduced to about 0.19/0.52%.

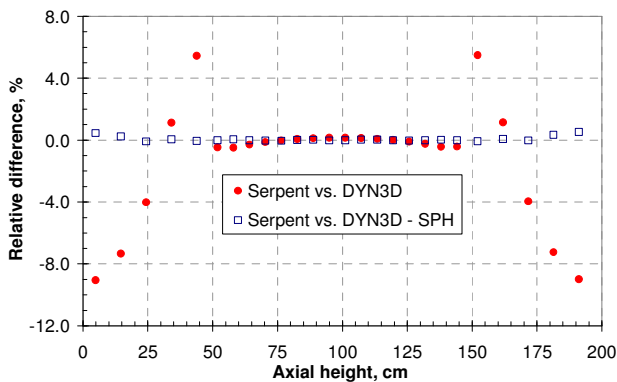
Table III. k-inf of different fuel rod: Serpent vs. DYN3D calculations.

Fuel rod	Serpent k-inf ^a	Difference, pcm	
		Serpent vs. DYN3D	Serpent vs. DYN3D-SPH
Central core	1.254810	99	35
Outer core	1.258420	99	36

^a σ_{k-inf} is 0.000013.



a. Normalized axial power distribution



b. Relative difference

Fig. 5. Axial power distribution for the central core fuel rod: Serpent vs. DYN3D calculations.

The SPH factor values which were used to correct the few-group cross-sections of the central core fuel rod are shown in Fig. 6. As can be noted, the SPH factors are higher

in the thermal energy group. This can be explained by the large statistical uncertainties in the neutron flux of that group. However, it should be mentioned that setting the SPH factors of the thermal energy group to unity does not affect the accuracy of the results.

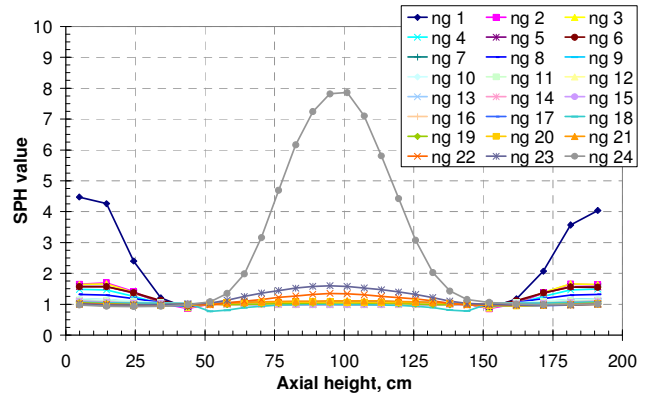


Fig. 6. SPH factor values for the central core fuel rod

3. Full Assembly Level Analysis

A 3D full BFS-73-1 assembly model was calculated using the Serpent and the DYN3D codes. The k-eff and the radial power distribution obtained from the Serpent calculations were used as a reference solution for code-to-code comparison with the DYN3D code. The full assembly normalized radial power distribution calculated with the Serpent code is shown in Fig. 7.

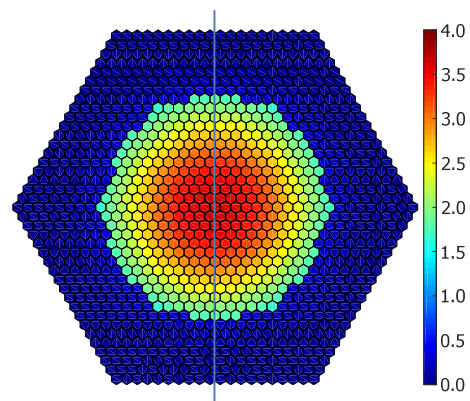


Fig. 7. BFS-73-1 radial power distribution: Serpent reference solution

In the DYN3D analysis, each of the fuel rod of the BFS-73-1 assembly model was divided into 10 axial nodes. The analysis was performed using the Serpent few-group cross-sections with and without the SPH correction. The SPH factors were evaluated iteratively using the Serpent and DYN3D codes for a full assembly model. The SPH factors were calculated for each of the assembly rods (i.e. pin-by-pin SPH factors). In this case, denoted as case A, a pin-wise

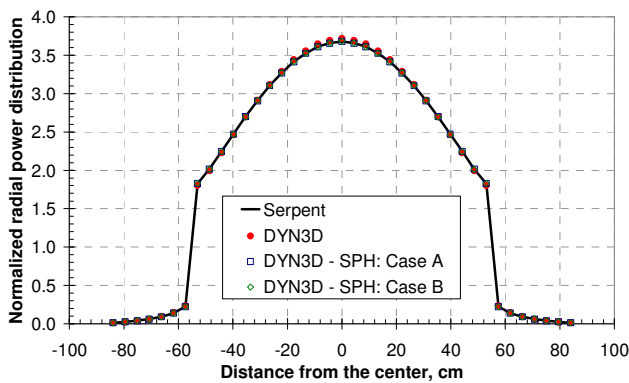
DYN3D assembly calculation is performed, and therefore, a large amount of data is required. For that reason, a second case was studied. In the second case, denoted as case B, the SPH factors were calculated only for each pin-material type, i.e. for each ring of rods of the same type.

The k-inf obtained from the DYN3D and Serpent calculations is presented and compared in Table IV. As can be noted, the DYN3D without the SPH correction considerably overestimates the k-eff by about 304 pcm. When the SPH-corrected few-group cross-sections are used, the difference reduces to about 72 and 69 pcm for case A and Case B, respectively.

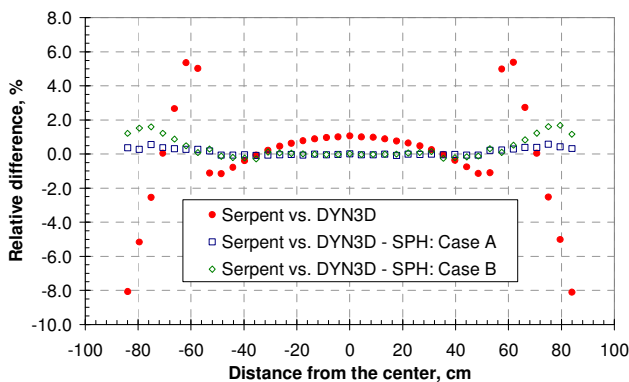
Table IV. Assembly k-eff: Serpent vs. DYN3D calculations.

Serpent k-eff ^a	Difference, pcm		
	Serpent vs. DYN3D	Serpent vs. DYN3D-SPH	
		Case A	Case B
0.99629	304	-72	-69

^a $\sigma_{k\text{-eff}}$ is 0.00002.



a. Normalized radial power distribution



b. Relative difference

Fig. 8. Radial power distribution of the BFS-73-1 assembly: Serpent vs. DYN3D calculations.

The advantage of using the SPH method for the analysis of a fast, highly heterogeneous system is clearly seen from results of the normalized power description. A comparison of the assembly normalized radial power distribution between the Serpent and DYN3D codes is given Fig. 8. The comparison was performed for the main diagonal along the marked line in Fig. 8. As can be noted from, without the SPH correction, the deviation of the DYN3D solution from the reference Serpent solution is quite large. In the fuel region (between -53 and 53 cm), the average/maximum differences are about 0.72/1.14%. The average/maximum differences in the blanket region are about 4.12/8.11%. As for the single fuel rod problem, the use of the SPH correction for the full assembly calculation shows a significant improvement in the prediction accuracy. The average/maximum differences in the fuel region, obtained for case A, are only about 0.05/0.22%. While for case B, the average/maximum differences in the fuel region are about 0.11/0.31%. In the blanket region the average/maximum differences are about 0.36/0.58% and 1.01/1.68% for case A and case B, respectively. It should be noted that the results obtained from case A are slightly more accurate than that obtained from case B. In general, it can be concluded that the SPH method can noticeably improve the accuracy of nodal diffusion codes applied for fast, highly heterogeneous system analysis.

V. SUMMARY AND CONCLUSIONS

The feasibility of using the DYN3D-Serpent codes system for the analysis of highly heterogeneous sodium-cooled fast systems was examined. In the first part of the study, the BFS-73-1 critical assembly was modeled in details using the Serpent MC code, and the basic neutronic characteristics were evaluated and compared against experimental values. The calculated results agreed well with the measured values, and hence, it was concluded that the Serpent MC code can be used for the preparation of homogenized group constants for SFR cores, and as a reference solution for code-to-code verification with the DYN3D code. In the second part of the study, the Serpent MC code was used as a tool for homogenized group constants generation for the DYN3D steady-state calculations. The simulation of the BFS-73-1 critical assembly using the DYN3D code is quite a challenge due to the strong heterogeneity in the axial and radial directions. Therefore, the SPH method was applied to correct the few-group cross-sections of the different regions of the assembly. The DYN3D calculations were performed using the Serpent few-group cross-sections with and without the SPH correction, to demonstrate the impact of the SPH correction on the accuracy of the results. The results showed that the application of the SPH correction to the few-group cross-section leads to a better agreement in the assembly k-eff and radial power distribution. Hence, it can be concluded that SPH method can significantly improve the accuracy of

nodal diffusion codes applied for fast, highly heterogeneous system analysis.

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REFERENCES

1. J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, T. Kaltiainenaho, "The Serpent Monte Carlo code: Status, development and applications in 2013," *Ann. Nucl. Energy*, **82**, 142, (2015).
2. E. Fridman, E. Shwageraus, "Modeling of SFR cores with Serpent-DYN3D codes sequence," *Ann. Nucl. Energy*, **53**, 354, (2013).
3. R. Rachamin, C. Wemple, E. Fridman, "Neutronic analysis of SFR core with HELIOS-2, Serpent, and DYN3D codes," *Ann. Nucl. Energy*, **55**, 194, (2013).
4. E. Nikitin, E. Fridman, K. Mikityuk, "Solution of the OECD/NEA neutronic SFR benchmark with Serpent-DYN3D and Serpent-PARCS code systems," *Ann. Nucl. Energy*, **75**, 492, (2015).
5. U. Rohde, S. Kliem, U. Grundmann, S. Baier, Y. Bilodid, S. Duerigen, E. Fridman, A. Gommlich, A. Grahm, L. Holt, Y. Kozmenkov, S. Mittag: "The reactor dynamics code DYN3D – models, validation and applications", *Progress in Nucl. Energy*, **89**, 170 (2016).
6. G. Manturov et al., "BFS-73-1 assembly: experimental model of sodium-cooled fast reactor with core of metal uranium fuel of 18.5% enrichment and depleted uranium dioxide blanket," NEA/NSC/DOE, IRPHE Handbook, (2006).
7. A. Kavenoky, "The SPH homogenization method," *Proc. of specialists' meeting on homogenization methods in reactor physics*, Lugano, Switzerland, November 13-15, 1978, International Atomic Energy Agency (1978) (IAEA-TECDOC-231).
8. A. Hebert, "Consistent technique for the pin-by-pin homogenization of a pressurized water reactor assembly," *Nucl. Sci. Eng.*, **113**, 227, (1993).
9. U. Grundmann, S. Mittag, "Super-homogenisation factors in pinwise calculations by the reactor dynamics code DYN3D," *Ann. Nucl. Energy*, **38**, 2111, (2011).
10. T. Courau, M. Cometto, E. Girardi, N. Schwartz, "Elements of validation of pin-by-pin calculations with the future EDF calculation scheme based on APOLLO2 and COCAGNE codes," *Proc. ICAPP'08*, Anaheim, California, June 8-12, 2008, American Nuclear Society (2008).
11. R. Rachamin, S. Kliem, "Validation of the DYN3D-Serpent code system for SFR cores using selected BFS experiments. Part I: Serpent calculations," *Ann. Nucl. Energy*, **102**, 158, (2017).
12. J. M. Ruggieri et al., "ERANOS 2.1: International code system for GEN IV fast reactor analysis," *Proc. ICAPP'06*, Reno, Nevada, June 4-8, 2006, American Nuclear Society (2006).