Verification of the SP3 Solver in FENNECS with C5G7 Test Cases using HELIOS Cross Sections

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Abstract:

Due to the worldwide growing interest in Small Modular Reactors (SMRs) and Micro Modular Reactors (MMRs), the development of tools for their safety assessment is of particular interest. These reactors have compact and complex geometries with strong neutron flux gradients. One possibility could be to use Monte Carlo methods, which require an enormous resources demand especially for transients, on the contrary to most deterministic codes. For this reason, the Finite ElemeNt NeutroniCS (FENNECS) deterministic code is particularly suited due to its geometric flexibility. FENNECS provides a solver based on the diffusion approximation of the transport equation. However, this approximation may not hold for small and heterogeneous configurations. To overcome the limitations of diffusion theory, an option are deterministic transport codes, but they also may be computationally expensive. An adequate possible solution is the third order Simplified Spherical Harmonics (SP_3) approximation of the transport equation.

A short summary of the theoretical derivation of the SP_3 in the finite elements formalism and its implementation into FENNECS will be given. To carry out validation and verification, the C5G7 benchmark is taken as example. Macroscopic pin cell homogenized cross sections and pin power distributions were generated with HELIOS-1.12 for the UO_2 and MOX assemblies. These cross sections were verified with the transport code TORT-TD and used to simulate the same geometries with the diffusion as well as with the SP_3 solver of FENNECS. Pin power distributions and multiplication factors obtained by the SP_3 solver satisfactorily agree with the respective HELIOS results.

1 INTRODUCTION

The increasing interest in small modular reactors (SMRs) and micro modular reactors (MMRs) requires adequate tools for their safety assessment, either Monte Carlo or deterministic. The first category offers a high geometrical flexibility, which is necessary to model the complex geometries of SMRs and MMRs. However, their biggest disadvantages are not sufficient maturity for transient applications and a large requirement of computational resources, especially for transients, making them not suited for routine applications. On the contrary, deterministic codes do not suffer from this limitation, allowing them to perform transient calculations more efficiently [1–3].

Neutronic codes can be also categorized depending on the physical and mathematical model behind them. Here, one possibility is to use codes relying on transport theory: the transport equation accurately describes the angular neutron flux in a medium, taking into account neutron sinks and sources. However, this is formulated with seven independent variables (five for the space-angular dependency, one for energy and one for time). Therefore, to solve it, a considerable amount of resources is required. A solution to this problem is to apply approximations to the transport equation [4–7].

The most common approximation of the transport equation is diffusion theory, which consists in assuming isotropic scattering, only low neutron absorption compared to scattering, and low variation of the neutron flux in space. The first assumption holds only for heavy nuclei.

The second one is not fulfilled by fuel and control materials. Finally, the last consideration can be applied only to large (with respect to the mean free path) and homogenous media. Even in this case, this assumption holds only a few mean free paths away from the medium boundary. Thus, diffusion theory may not be suited to model the compact and inhomogeneous cores of SMRs and MMRs [8–10].

Therefore, an adequate approximation of the transport equation must be found to perform the safety assessment of these systems. A possible candidate for this task is the third order Simplified Spherical Harmonics approximation, or SP_3, which is more accurate than diffusion theory. This approximation consists in expanding the angular dependency of the transport equation with Legendre polynomials, even for three-dimensional models, without the necessity to replace them with spherical harmonics [4,11,12].

For this reason, the Finite ElemeNt NEutroniCS (FENNECS) code, described in section 2, was extended by a steady state SP_3 solver and the mathematical model behind it is briefly described in section 3. Within the validation process, the UO_2 and MOX fuel assemblies specified by the C5G7 benchmark were used. As explained in section 4, the single fuel assemblies were modelled with HELIOS-1.12 to generate reference eigenvalues and pin power distributions and the pin cell-homogenized cross sections libraries, which were validated with the transport code TORT-TD [13]. Finally, with the obtained libraries, the UO_2 and MOX fuel assemblies were modelled with FENNECS.

2 FENNECS

The code FENNECS was recently developed at Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH. Initially, it was a three dimensional few-group diffusion code capable to model steady state as well as transient core configurations. FENNECS relies on the continuous Galerkin weighted residual approach using upright triangular finite elements with linear basis functions as spatial elements. To run the calculations, cross-section libraries in NEMTAB format must be provided. Furthermore, the main advantage of the FENNECS code is its high geometrical flexibility, which is an essential requirement to model complex and irregular system, like most of the SMRs and MMRs [14,15].

3 MATHEMATICAL MODEL BEHIND THE SP_3 SOLVER OF FENNECS

The steady state SP_3 approximation is derived from the Spherical Harmonics approximation of third order (P_3), which consists in expanding the angular terms of the steady state one dimensional transport equation with Legendre polynomials up to the third order. The transition to the SP_3 approximation is performed by moving to 3D solely by replacing the double derivative with the Laplacian operator and without the necessity to replace the Legendre polynomials with spherical harmonics [10,16–18].

As mentioned in section 2, FENNECS relies on the Galerkin finite element approach. Therefore, the steady state SP_3 equations must be casted into the Galerkin formalism, as it is explained in [19].

4 C5G7 TEST CASES

The geometry specifications of the C5G7 fuel assemblies were taken from [20]. The geometry of the C5G7 benchmark consists of a minicore made of four fuel assemblies in total, where two of them are made of UO_2 and the remaining two of MOX.

In this work, single-assembly models of the two types of fuel assemblies were considered using reflective boundary conditions. The calculations were performed firstly with HELIOS-1.12, using the collision probabilities solver, from which the reference values for the effective multiplication factors and for the pin power distribution, together with the pin cell-wise homogenized macroscopic cross-section libraries were obtained. The libraries were validated with the deterministic transport code TORT-TD. Then, using the validated cross sections,

calculations with the diffusion as well as with the SP_3 solver of FENNECS using various mesh refinements (4 and 16 radial elements per pin cell) were performed. Finally, the multiplication factors as well as the normalized power distributions calculated by FENNECS were compared with the HELIOS reference calculations results. In particular, in the case of the multiplication factors, the analysis was performed calculating the reactivity deviation from the refence, and for the normalized power distributions the root mean square (RMS) as well as the maximum and minimum value of the deviation for each pin was considered.

4.1 UO_2 fuel assembly

The multiplication factor calculated by HELIOS for the UO_2 fuel assembly, illustrated in Figure 1, is 1.32705 and this value is used as refence. As it can be observed in Table 1 and Table 2, for both FENNECS solvers, the discrepancies in the effective multiplication factors, as well as in the RMS and the maximum error of the power distribution, decrease with increasing number of radial elements per pin cell.

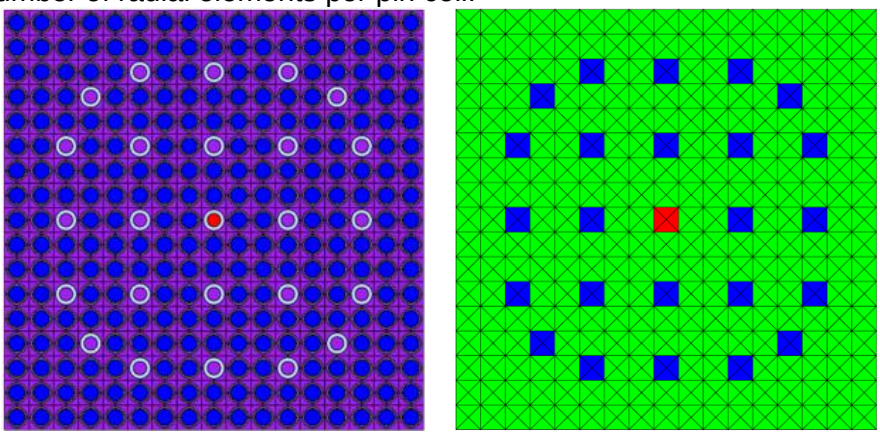

Figure 1: UO_2 fuel assembly (left) and its FENNECS model (right) of the C5G7 minicore with a mesh using 4 radial elements per pin cell. In the FENNECS model, the green cells contain UO_2 fuel pins. The blue cells contain the guide tubes and the central red cell is the fission chamber.

Table 1: Multiplication factors calculated with the diffusion and SP_3 solvers of FENNECS with 4 and 16 radial elements per pin cell and the respective deviations from the HELIOS reference for the UO_2 fuel assembly.

Radial elements per pin cell	**Solver**	**k_{eff} from FENNECS**	**Deviation from HELIOS (pcm)**
4	Diffusion	1.32821	66
	SP3	1.32798	53
16	Diffusion	1.32779	42
	SP3	1.32752	27

Table 2: RMS (%), maximum and minimum value of the deviation of the normalized power distribution with respect to the HELIOS reference for the UO_2 fuel assembly.

Radial elements per pin cell	**Solver**	**RMS**	**Maximum error**	**Minimum error**
4	Diffusion	0.54%	1.43%	-0.06%
	SP_3	0.52%	1.48%	-0.17%
16	Diffusion	0.25%	0.68%	0.08%
	SP_3	0.23%	0.55%	0.00%

With both meshes, the FENNECS SP_3 solver delivers an effective multiplication factor closer to HELIOS and a smaller RMS of the power distribution, compared to the diffusion calculation: with 16 radial elements per pin, for the SP_3 solver the discrepancy in the multiplication factor is only 27 pcm and the RMS 0.23%, proving also the correct implementation of the methodology. However, it should be noted that the difference between the results of the two solvers is very small: for the k_{eff}, with 4 and 16 radial elements per pin, this is only 13 pcm and 15 pcm, respectively, and 0.02% for the RMS with mesh sizes. This can be explained by the very homogeneous composition of the UO_2 of fuel assembly.

4.2 MOX fuel assembly

For the MOX fuel assembly, depicted in Figure 2, the reference k_{eff} obtained with HELIOS is 1.17632. Here, an increase in the discrepancy between the multiplication factor calculated by the FENNECS diffusion solver and the reference can be observed after the mesh refinement, as shown in Table 3. In the case of the SP_3 solver, the increase in the number of radial elements per pin cell does not signifyingly affect the k_{eff}, whose discrepancy from the HELIOS reference is only 51 pcm for both meshes. On the contrary, for the normalized power distribution, a strong decrease of the pin power RMS, minimum and maximum error can be observed when decreasing the mesh size: with 16 radial elements per pin cell, the RMS and maximum error obtained with the SP_3 solver are only 0.46 % and 1.00 %, respectively, as it can be seen in Table 4. Therefore, for both assemblies, the very small errors observed FENNECS SP_3 results prove, besides its correct implementation, also that the accuracy of this methodology is very close to transport codes.

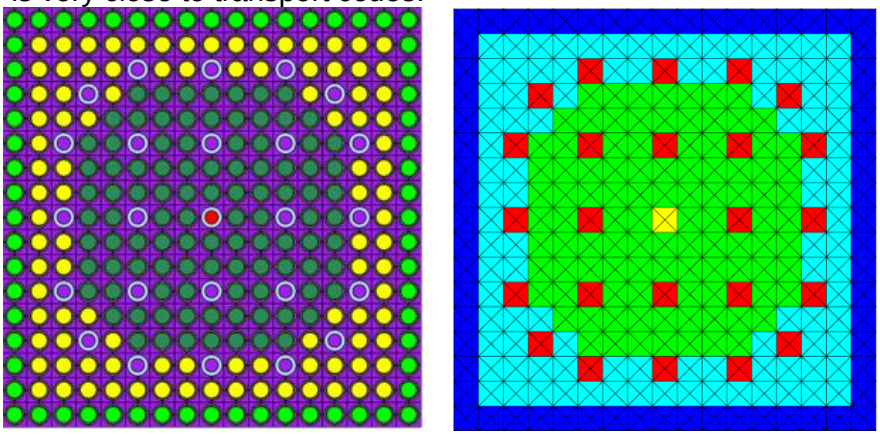

Figure 2: MOX fuel assembly (left) and its FENNECS model (right) of the C5G7 minicore with a mesh using 4 radial elements per pin cell. In the FENNECS model, the blue, light blue, and green cells contain fuel pins made of 4.3%, 7.0%, and 8.7% MOX, respectively. The red cells contain the guide tubes and the central yellow cell is the fission chamber.

Table 3: Multiplication factors calculated with the diffusion and SP_3 solvers of FENNECS with 4 and 16 radial elements per pin cell and the respective deviations from the HELIOS reference for the MOX fuel assembly.

Radial elements per pin cell	**Solver**	**k_{eff} from FENNECS**	**Deviation from HELIOS (pcm)**
4	Diffusion	1.17514	-85
	SP_3	1.17562	-51
16	Diffusion	1.17503	-93
	SP_3	1.17561	-51

Table 4: RMS (%) of the deviation of the normalized power distribution with respect to the HELIOS reference for the MOX fuel assembly.

Radial elements per pin cell	Solver	RMS	Maximum error	Minimum error
4	Diffusion	1.11%	1.95%	0.05%
	SP_3	0.88%	1.54%	0.05%
16	Diffusion	0.64%	1.44%	0.00%
	SP_3	0.46%	1.00%	-0.03%

Comparing the discrepancies in the multiplication factors as well as in the RMS of the normalized power distributions errors, it can be observed that the results from the SP_3 solver are closer to the HELIOS reference, compared to the ones calculated by diffusion theory. Compared to the UO_2 assembly, here the results from the FENNECS diffusion solver are more far away from the ones of the SP_3 solver as well as of HELIOS: for the multiplication factor and the RMS, the difference between the two FENNECS solvers ranges between 34 pcm and 42 pcm and between 0.18% and 0.23%, respectively, depending on the mesh. Furthermore, higher values for the deviation of the multiplication factor and the RMS are obtained, compared to the UO_2 fuel assembly: in particular, with the FENNECS diffusion solver and with 4 radial elements per pin, the RMS of the power distribution error is above 1%. These last two observations can be explained by the more heterogeneous composition of the MOX fuel assembly compared to the UO_2 assembly. Therefore, the limitations of the diffusion solver are emphasized and the higher accuracy of the SP_3 approximation, compared to diffusion theory, which was mentioned in section 1, is proven.

5 CONCLUSIONS

In this work, motivations for the importance of the development of an SP_3 solver in the FENNECS code were given. Furthermore, the theoretical derivation of the SP3 equation in the Galerkin formalism was briefly sketched.

Finally using the geometry of the C5G7 benchmark, single-assembly models of its UO_2 and MOX fuel assemblies were performed with HELIOS, which delivered the reference solutions and the cross sections that were used for the FENNECS calculations with the diffusion and SP_3 solver. Here, the multiplication factors and the normalized power distribution were analysed. For both quantities and both assemblies, the results of the SP_3 solver showed improvements against the diffusion approximation and a good agreement with the reference. In particular, in the case of the UO_2 fuel assembly, only small differences were observed between the results calculated with the diffusion and SP_3 solver, due to the homogenous configuration of this assembly. On the contrary, for the MOX assembly, the differences between the calculation results of these two solvers were larger, showing the expected benefit of the SP_3 approximation against diffusion theory in modelling heterogenous systems.

Therefore, the newly developed FENNECS SP_3 solver offers the possibility to model systems that could not be accurately modelled by the diffusion approximation, like SMRs and MMRs, with a precision that is very close to the one of a transport code. In the future, this research will be extended by modelling the whole C5G7 minicore, hence an even more realistic case.

6 ACKNOWLEDGMENTS

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