Budapest University of Technology and Economics
Institute of Nuclear Techniques

Development of a finite-element-based reactor physics code system for the solution of the simplified P_3 approximation to the neutron transport equation

Ph.D. thesis booklet

Boglárka Babcsány

Supervisors: Dr. Dániel Péter Kis and Dr. Sándor Fehér

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Background

For safe, reliable and economical reactor operation, accurate simulation of the reactor physical behavior of the reactor core is of utmost importance. One of the main tasks of reactor core analysis is determining core criticality and power distribution, which provides the basis for power profile, power peaking factor and therefore thermal limit calculations; it is the starting point of fuel loading optimization, while calculation of the effective multiplication factor for different operational states is needed for reactivity coefficients estimation in order to account for different temperature, power and resonance feedbacks. Today, the most widely applied deterministic neutron transport approximation for nuclear reactor core analysis, monitoring and design is the neutron diffusion theory. However, the accuracy of diffusion theory is limited in the case of irregular geometries, strongly heterogeneous material configurations, particularly in regions where steep spatial flux gradients are present, hence near absorber rods or assemblies and in the vicinity of the core boundary and reflectors. Advanced nuclear reactors and fuel assembly designs are becoming increasingly complex regarding both their geometry and material composition which pose challenges to diffusion-based reactor core analysis and more and more entails the need for the industrial application of higher-order transport approximations.

In Hungary, the Paks Nuclear Power Plant has also based both its off- and online core monitoring and analysis system on a diffusion code called C-PORCA, which solves the three-dimensional two-group diffusion equations based on parameterized group constants generated by the HELIOS lattice physics code [1]. The Reactor Physics Department of the Paks NPP in close cooperation with the Institute of Nuclear Techniques of the Budapest University of Technology and Economics decided to investigate the possible extension of C-PORCA with a higher-order transport solver. The initiative was also motivated by the new nuclear power plant project featuring two VVER-1200 reactors with more complex reactor cores in terms of neutronics. The multigroup simplified spherical harmonics (SP_N) theory [2–4], which is based on the expansion of the angular dependence of the angular neutron flux in a finite series of spherical harmonics functions was a self-evident choice, as the governing equations form a system of diffusion-like, second-order elliptic partial differential equations, hence the further development of the efficiently parallelized and fast diffusion solver algorithm applied within the Paks NPP was relatively straightforward.

Objectives

Although the SP_N theory has quite an extensive literature and a broad range of applications [5], there were several areas that needed further research and development before the theory could have been applied in the C-PORCA code system. Most existing SP_N codes have been developed as an integrated extension of a diffusion solver that can be effectively realised from a numerical and programming perspective by taking the so-called within-group form of the SP_N equations by assuming only isotropic scattering between different energy groups and neglecting anisotropic group-to-group scattering [6–8]. Besides, in order to maintain the same group constant input structure as in the diffusion module, as well as to spare the regeneration of parameterized group constants for SP_N calculations necessitating higher-order anisotropic within- and group-to-group scattering terms, the higher-order scattering group constants are usually considered to be zero [9]. Using these simplifications that are again, traditionally motivated by numerical and programming considerations, one obtains a further simplified SP_N theory, with a potential of not always being able to yield more accurate results compared to fine-tuned diffusion calculations as opposed to theoretical expectation.

The main focus of my research was to analyze the applicability of a higher-order transport approximation, the SP_3 theory for industrial applications, and develop finite element based solution of the SP_3 equations that can be efficiently used in VVER reactors. Aiming to provide a more accurate tool for future core analysis than the state of the art, fine-tuned diffusion approximation, I did not introduce any simplifications, and developed semi-analytical and numerical solution methods and implemented algorithms for the solution of the full anisotropic scattering form of the SP_3 equations. I conducted my research in close cooperation with the Reactor Physics Department of the Paks Nuclear Power Plant with the aim of extending their diffusion-based reactor physics code system C-PORCA with an SP_3 module to further increase its accuracy with only a limited increase in computational resources. The SP_3 module of C-PORCA – after comprehensive verification and validation – will be applied by the Paks Nuclear Power Plant for core loading pattern evaluations.

Methods

Numerical solution methods necessitate reliable reference results for verification purposes. In contrast with the diffusion theory, which has extensive analytical and numerical verification resources due to the well-known analytical solutions and mathematical benchmark calculations with available reference results, the availability of such references for the verification of numerical SP_3 solution methods are limited, and there is a complete lack of reference results with the possible inclusion of third-order scattering anisotropy. In the first part of my thesis, I presented

semi-analytical solutions of the one-group homogeneous SP_3 equations with up to third-order scattering anisotropy, which I derived in order to fill this gap in SP_3 verification problems. Supporting the applicability of the developed mathematical verification benchmark, I also showed that with the provided semi-analytical solution method Capilla's isotropic test problem [10] can also be reproduced.

In the second part of the thesis, I presented the continuous Galerkin finite element solution of the multigroup SP_3 equations with full scattering anisotropy, which I developed with the aim of being able to examine arbitrary and irregular core configurations, as well as being able to provide high-fidelity reference results for mathematical code verification purposes. I implemented the solution algorithm in my code SPNDYN, and verified it against the one-group semi-analytical solutions that I provided including third-order scattering anisotropy for homogeneous one-dimensional slab, cylindrical and spherical reactor models. I extended the scope of existing mathematical SP_3 benchmarks by providing high-fidelity reference results with detailed SP_3 power distributions for the two- and three-dimensional VVER-440 Seidel [11] and the three-dimensional VVER-1000 Schulz benchmarks [12]. By similarly extending Makai's four-group VVER-1000 benchmark [13], I also provided reference SP_3 solutions for future four-group SP_3 code verification purposes.

With the continuous Galerkin finite element solver as part of the SPNDYN code system, I participated in a code-to-code and code-to-measurement benchmark on the BME Training Reactor. Besides showing that the SPNDYN diffusion results are in good agreement with the available reference PARCS [14] diffusion results, I was able to show that using SPNDYN with diffusion coefficients in SP_3 mode, i.e. by assuming linearly anisotropic scattering, the accuracy of SP_3 calculations are in line with that of the diffusion results, while running SPNDYN in SP_3 mode with full anisotropic scattering, the accuracy of the obtained SP_3 results are close to that of the S_{10} PARTISN calculations [15] concluding that the SP_3 theory, if full anisotropic scattering is considered, has a higher transport correction potential. Regarding the comparison with measurements, the agreement was generally good, however, both the PARTISN and SPNDYN SP_3 calculations with full anisotropic scattering significantly overestimated the excess reactivity of the core, which is a consequence of a revisited conclusion regarding the inconsistent weighting of the higher-order anisotropic scattering matrices by Serpent 2 [16] of which the distortive effect becomes significant in the case of high leakage (small-sized), strongly heterogeneous and fast reactors [17].

Although the continuous Galerkin finite element SP_3 module of the SPNDYN code can be applied for arbitrary geometry, and it has a potential for multi-physics R&D&I applications, due to the necessity of radially and axially similarly fine meshing, it is not optimal for industrial application. The C-PORCA diffusion code of the Paks NPP uses a hybrid finite element algorithm, that applies radially finite element, axially analytical solution coupled through the radial and axial leakages as Lagrange multipliers. This method allows – by making use of the axially smoother flux

distribution – the application of much finer mesh in the radial direction than in the axial direction leading to a more efficient solution of the diffusion equations. In the second part of my dissertation, I focused on deriving the hybrid finite element solution of the SP_3 equations, which I also implemented as a separate module in the SPNDYN code, and integrated it into the C-PORCA code system (CPL-SP3). I also provided and implemented a method for the inclusion of assembly-wise surface discontinuity factors in the hybrid finite element solution algorithm. I tested the hybrid finite element SP_3 solver on various test problems, and showed that in the axially analytical solution at least second-order source fitting needs to be applied, while at least second-order finite elements are necessary in the radial direction.

Finally, I modeled VVER-440 and VVER-1000 two-dimensional "full-core" benchmarks [18, 19] in Serpent 2 with the dual purpose of group constant and assembly-wise surface discontinuity factor generation, as well as providing reference transport solutions, and showed that the hybrid finite element SP_3 solver using discontinuity factors provides more accurate results than the diffusion approximation with discontinuity factors. I also showed that taking into account higher-order scattering anisotropy until the second-order can further improve the accuracy, in the case of the presented VVER problems, however, the effect of including third-order compared to second-order anisotropic scattering is insignificant.

New scientific results

The main results of my research can be summarized in the following statements.

1. I provided semi-analytical solutions to the one-group SP_3 equations in homogeneous slab, cylindrical and spherical geometries taking into account up to third-order scattering anisotropy, thereby extending existing SP_3 benchmark problems with up to third-order scattering anisotropy, as well as two- and three-dimensional test cases. I have demonstrated the applicability of the semi-analytical benchmark solutions in the verification of two different numerical SP_3 solvers, as well as in the reproduction of Capilla's isotropic P_3 test problem. [P1]

2. I derived the continuous Galerkin finite element solution of the SP_3 equations by taking into account full anisotropic scattering, arbitrary number of neutron energy groups and one- to three-dimensional reactor geometry. I implemented the corresponding finite element solution algorithm, which can handle unstructured meshes, in the SPNDYN code and verified the solution algorithm using semi-analytical SP_3 solutions and numerical benchmarks. I provided high-fidelity finite element SP_3 solutions for VVER benchmark problems for nodal code verification purposes. [P3], [P7], [P8]

3. I performed SP_3 calculations for the BME Training Reactor with the purpose of code-to-code comparison and code-to-measurement validation of the continuous Galerkin finite element module of SPNDYN. By comparing calculated excess reactivitity, control rod worths and assembly worths with measured values, as well as with available PARCS and PARTISN reference diffusion and S_{10} results, I showed that the accuracy of the SP_3 solution with linearly anisotropic scattering in a small-sized thermal reactor such as the BME Training Reactor is comparable to diffusion, while with full anisotropic scattering it is close to the S_{10} solution. [P4]

4. I developed a novel hybrid finite element solution method of the SP_3 equations with full anisotropic scattering, which I implemented in SPNDYN and in the C-PORCA reactor physics code system. I showed in various test problems that using second-order triangular Lagrange elements in the radial direction and quadratic polynomial source fitting in the axial direction with node height less than 10 cm can provide sufficient accuracy for the hybrid finite element SP_3 method in VVER core calculations, which is hence proven to be in line with the diffusion approximation. [P2], [P5], [P6]

5. I developed a method for the application of flux moment discontinuities in the hybrid finite element solution of the SP_3 equations, implemented the obtained partial current-like moment discontinuity equations, and verified the suggested method using VVER-440 and VVER-1000 reactor benchmarks. I concluded that in the case of macro calculations of VVER reactors with discontinuity factors, second-order anisotropic scattering in SP_3 calculations results in improved accuracy, however, taking into account third-order scattering anisotropy does not bring noticeable further improvement. [P2], [P5], [P9]

List of Publications

Related journal articles

[P1] B. Babcsány, D. P. Kis, "Semi-analytical methods for SP_3 equations solver verification including third-order scattering anisotropy," *Annals of Nuclear Energy*, vol. 148, 107671, 2020.

[P2] B. Babcsány, I. Pós, D. P. Kis, "Hybrid finite-element-based numerical solution of the multi-group SP_3 equations and its application on hexagonal reactor problems," *Annals of Nuclear Energy*, vol. 155, 108148, 2021.

[P3] B. Babcsány, T. Bartók, D. P. Kis, "Finite element solution of the time-dependent SP_3 equations using an implicit integration scheme," *Kerntechnik*, vol. 85(4), pp. 292-300, 2020.

[P4] A. Sz. Ványi, B. Babcsány, Z. I. Böröczki, A. Horváth, M. Hursin, M. Szieberth, Sz. Czifrus, "Steady-state neutronic measurements and comprehensive numerical analysis for the BME Training Reactor," *Annals of Nuclear Energy*, vol. 155, 108144, 2021.

[P5] B. Babcsány, I. Pós, D. P. Kis, "Hybrid finite-element-based numerical solution of the SP_3 equations – Part II. SP_3 solution of two- and three-dimensional VVER reactor problems," *Annals of Nuclear Energy* (under review)

Related conference proceedings and presentations

[P6] B. Babcsány, S. Fehér, I. Pós and T. Parkó, "Hybrid finite element solution of the simplified P_3 equations," *Presentation at and in proceedings of the twenty-fifth Symposium of Atomic Energy Research; Balatongyörök, Hungary; 13-16 October 2015*, pp. 535–558, 2015.

[P7] B. Babcsány, S. Fehér, "Finite-element-based SP_3-solver development," *Presentation at the Atomic Energy Research Working Group C & G Meeting; Balatongyörök, Hungary; 25-26 May 2017*, 2017.

[P8] B. Babcsány, T. Bartók, D. P. Kis, "Finite element solution of the time-dependent SP_3 equations using an implicit integration scheme," *Presentation at and in proceedings of the twenty-ninth Symposium of Atomic Energy Research; Energoland, Mochovce NPP, Slovakia; 14-18 October 2019*, pp. 331-346, 2019.

[P9] B. Babcsány, I. Pós, "SP_3 solution of the full-core VVER-440 RK3+ and VVER-1000 benchmarks using Serpent group constants and discontinuity factors," *Presentation at the Atomic Energy Research Working Group A & B Meeting; Online; 15 June 2021*, 2021.

Related technical reports

[P10] S. Fehér, B. Babcsány, "Further development of the HELIOS – C-PORCA code system with a module capable of the reactor physical characterization of irregular geometric configurations, Part III. Testing and verification of the developed SP_3 method," Technical Report, BME-NTI-706/2014 (in Hungarian), Budapest University of Technology and Economics, 2014.

[P11] B. Babcsány, S. Fehér, "Improving the accuracy of the SP_3 method integrated into the C-PORCA program by taking into account anisotropic neutron scattering," Technical Report, BME-NTI-826/2017 (in Hungarian), Budapest University of Technology and Economics, 2017.

[P12] B. Babcsány, M. G. Halász, "Analyzing the possibilities for increasing the accuracy of the SP_3 method integrated into the C-PORCA program," Technical Report, BME-NTI-864/2018 (in Hungarian), Budapest University of Technology and Economics, 2018.

[P13] B. Babcsány, "Two-dimensional modeling of the VVER-440 core with the application of the SP_3 method," Technical Report, BME-NTI-908/2019 (in Hungarian), Budapest University of Technology and Economics, 2019.

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[19] V. Krýsl, P. Mikoláš, D. Sprinzl, and J. Švarný, "Proposal of Full-Core VVER-1000 calculation benchmark," in *26th Symposium of AER on VVER Reactor Physics and Reactor Safety*, (Helsinki, Finland), 10-14 October 2016.

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