New finite element neutron kinetics coupled code system FENNECS/ATHLET for safety assessment of (very) Small and Micro Reactors

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Abstract. Cores of (very) small and medium size reactor – (v)SMR – are often characterized by irregular geometries. Monte Carlo methods are not yet mature enough for transient applications. To perform coupled transient safety assessments of (v)SMRs, the Finite ElemeNt NEutroniCS (FENNECS) code is being developed at GRS. It solves the time-dependent and steady-state three-dimensional few-group diffusion equation in Galerkin finite element representation using upright triangular prisms with linear basis functions as spatial elements. FENNECS is also coupled with the GRS thermal-hydraulic system code ATHLET. For the special meshing, an external meshing tool is being developed as a Python software module. This paper considers the Heat Pipe Micro Reactor core. For the generation of cross sections to be used in FENNECS, Monte Carlo Serpent models are developed for two configurations: all absorber faces of control drums are turned out of the core (All Rods Out – ARO – configuration) and all absorber faces are turned in (All Rods In – ARI – configuration). The Serpent multiplication factors are in good agreement with the benchmark. In the FENNECS model, control drums are approximated by a 12-edges polygon or by a 24-edges polygon. The FENNECS multiplication factors agree well with Serpent reference results for both configurations. This demonstrates the applicability of FENNECS to (v)SMRs.

1. Introduction

In recent years, the interest in (very) small and medium size reactor concepts – (v)SMRs – has grown for specific purposes like energy delivery at remote locations or for space application. They are often characterized by irregular geometries. Though Monte Carlo methods are becoming more and more standard for steady state simulations, they are not yet mature enough for transient applications. To perform future coupled transient safety assessments of this kind of reactors and other innovative concepts, the Finite ElemeNt NEutroniCS (FENNECS) [1], [2] code is being developed at GRS.

This paper considers the Heat Pipe Micro Reactor (HPMR) core proposed in the publicly available document [3]. It is structured as follows: First, a brief summary of the FENNECS code is given with focus on the meshing of unstructured geometries. The study case, i.e. the HPMR, is described in section 3. Section 4 gathers the results of the simulations performed with the Monte Carlo code Serpent and are compared to those given in the benchmark. The model of the HPMR core in FENNECS and comparison with the reference Monte Carlo calculation are presented in section 5. Section 6 draws the conclusion of the study.
2. FENNECS code

2.1. Solution method
FENNECS solves the time-dependent and steady-state three-dimensional few-energy group diffusion equation in the Galerkin finite element representation using upright triangular prisms with linear basis functions as spatial elements. The implementation of the finite element solution of the diffusion equation largely follows standard approaches as given by, e.g., [4]. Both direct and adjoint neutron flux distributions can be evaluated. Wielandt iteration is applied for convergence acceleration of the eigenvalue problem. The time integration of both transport and delayed neutron precursor equations is carried out implicitly which provides unconditional numerical stability. FENNECS is also coupled [2] with the GRS thermal-hydraulic system code ATHLET [5] for thermal-hydraulics feedback. FENNECS uses macroscopic cross section libraries in NEMTAB-like format [6] which may be parameterized with respect to up to six thermal-hydraulic feedback parameters with linear cross section interpolation. In addition, it includes graphical pre- and postprocessing capabilities for displaying the input geometry and material distribution as well as output power density, neutron flux and thermal-hydraulic parameter distributions. FENNECS has been first applied to and assessed against other neutronics codes for the prismatic (or block type) high-temperature reactor MHTGR-350MW within an OECD/NEA benchmark activity [7] and the sodium cooled fast reactor concept ASTRID [8] within the EU project ESNII+.

2.2. Spatial meshing
For spatial meshing, FENNECS includes an internal meshing module for regular Cartesian and hexagonal lattices. It also reads lists of nodes and elements connectivities from external ASCII files. For the meshing of the irregular geometries of (v)SMRs, an external meshing tool is being developed as a Python software module which generates the mesh data required by FENNECS. It processes as shown in Figure 1: Every step (gray boxes) corresponds to a specific Python class which can be replaced by another one to adapt the tool. First, it reads the input of FENNECS. As alternative, a specific input for the external meshing tool in a YAML format is also developed. Then, it performs the 3-d meshing in two steps: the first step is to perform the axial meshing (1-d) and the second step is to perform the radial meshing (2-d). Concerning the radial meshing, rectangles can be divided either into 4 or 16 isosceles triangles and hexagons can be divided either into 6 or 24 equilateral triangles. Then, the ASCII files required by FENNECS are written.
Figure 1. Python software module scheme for meshing geometries and generating ASCII files required for FENNECS.

The challenge of meshing the HMPR core lies in properly meshing the control drums which surround a regular hexagonal lattice of the fuel elements. For this study, the implementation of the meshing of a circle embedded in a hexagonal lattice is required. The circular shape is approximated by regular polygons. Two polygons are tested: a 12-edges polygon and a 24-edges polygon which are centred into a 7-hexagon lattice (see figure 2). Moreover, the radius of the polygon is adjusted so that the polygon area is equal to the circle area.

Figure 2. A 12-edges polygon (left) and a 24-edges polygon (right) for approximating a circle (displayed in black dashed line) into a 7-hexagon lattice.

3. Heat Pipe Micro Reactor specifications
This paper considers the HPMR core proposed in the publicly available document [3]. The specification provides a detailed description of all geometries. The core layout is composed of 192 hexagonal fuel elements surrounded by six control rod drums (see figure 3).
All fuel elements are identical: each one has a pitch of 5.4 cm and has central cylindrical heat pipe with a 3 cm diameter surrounded by the fuel contained within a hexagonal stainless steel (SS-316) can. Axially, each fuel element consists of two 15 cm axial reflector zones, composed of beryllium oxide (BeO), directly placed above and below the 100 cm fuel zone. The fuel element lattice pitch is 5 cm. The fuel is of metallic type consisting of 18.1% enriched uranium with a 10% weight fraction of zirconium (U-10Zr), assuming to have a porosity of 10% to allow for the swelling due to fission gas release.

For control of reactivity, six cylindrical control drums are provided at the corners of the hexagonal shaped core. The control drums are cylinders of 10.8 cm diameter. They are composed of reflector material (aluminium oxide ceramic - Al₂O₃) and absorber material placed in 150° annular sectors of 2 cm thickness at the edge of the control drums. The absorber material is boron carbide (B₄C) with 90% enriched B-10.

The central position of the core is a safety control rod which fits within a single fuel element hexagonal can. Its diameter is 4.65 cm. It is composed of B₄C with 90% enriched B-10.

The radial reflector is composed of Al₂O₃. The cooling fluid is potassium (K). The total thermal power is 5 MW.

![Figure 3](image_url)

**Figure 3.** HMPR core description. From left to right: fuel element vertical cross section, fuel element horizontal cross section, cross section of the micro-reactor core.

### 4. Serpent Monte Carlo model and results

#### 4.1. HMPR core model in Serpent

The purpose of the Serpent Monte Carlo model is twofold. First, it serves as a reference model to compare with the FENNECS simulation results presented in Section 5. Second, it is used to generate few-group macroscopic cross section data for different material zones (e.g. fuel cells, control drums, etc.) which will be used for the deterministic calculations with FENNECS. While the specification provides a detailed description of all geometries, no mass density of any material is given and must be gathered from open literature which is summarized in Table 1.

| Material   | Density (g/cm³) |
|------------|----------------|
| U-10Zr     | 13.9032        |
| BeO        | 3.01           |
| SS-316     | 7.970          |
| Al₂O₃      | 3.987          |
| B₄C        | 2.52           |
Monte Carlo Serpent models are developed for two configurations:

- **All Rods Out – ARO – configuration:** This configuration is the most reactive state of the core where the absorber faces of all control drums are turned out of the core (see Figure 4 on the left). This control drum position results in minimizing the absorption while maximizing the reflection.

- **All Rods In – ARI – configuration:** This configuration is the less reactive state of the core where the absorber faces of all control drums are turned towards the core (see Figure 4 on the right). This control drum position results in maximizing the absorption while minimizing the reflection.

In both configurations, the central safety control rod is fully withdrawn from the core and modelled as a hexagonal can full of coolant (no absorber material). In order to reduce the statistical uncertainties to an acceptable level, each Serpent calculation is performed with 5,000 cycles (and 100 inactive cycles) of 50,000 source neutrons per cycle. This provides an uncertainty of less than 5.0E-05 for the multiplication factor. All calculations are performed using the JEFF-3.1.1 continuous energy library.

The homogenised macroscopic cross section libraries required for FENNECS have been generated using the 12-energy group structure shown in Table 2. It is based on the 8-energy group structure suggested in [10] which has been extended by additional group subdivisions. This 12-energy group structure has already been applied successfully in several SFR analyses (see [11] and [12]).

![Figure 4. HMPR core model in Serpent. Left: All Rods Out (ARO) core configuration. Right: All Rods In (ARI) core configuration.](image)
### Table 2. Lower boundaries of the 12-energy group structure used for cross section generation with Serpent.

| Group Index | Lower boundary [MeV] | Group Index | Lower boundary [MeV] | Group Index | Lower boundary [MeV] |
|-------------|----------------------|-------------|----------------------|-------------|----------------------|
| 1           | 6.0653E+00           | 5           | 1.1109E-01           | 9           | 2.0347E-03           |
| 2           | 2.2313E+00           | 6           | 4.0868E-02           | 10          | 7.4852E-04           |
| 3           | 8.2085E-01           | 7           | 1.5034E-02           | 11          | 1.4894E-04           |
| 4           | 3.0197E-01           | 8           | 5.5309E-03           | 12          | 1.0000E-11           |

4.2. Serpent Monte Carlo results

The multiplication factors taken from [3] and those obtained with Serpent are shown in Table 3. The difference between the multiplication factors is less than 40 pcm in ARO configuration and about 140 pcm in ARI. This demonstrates that both models are in good agreement with those performed in [3] and can be used for the cross sections’ generation required for FENNECS and can also be taken as reference for comparison purposes with FENNECS.

### Table 3. Multiplication factors obtained with Serpent in ARO and ARI configurations and comparison with the benchmark results.

|                  | ARO       | ARI       |
|------------------|-----------|-----------|
|                  | k-eff     | uncertainty | k-eff     | uncertainty |
| Benchmark k-eff  | 1.02321   | 3.60E-05   | 0.98953   | 3.60E-05   |
| Serpent k-eff    | 1.02362   | 4.10E-05   | 0.99092   | 4.30E-05   |
| Deviation from the benchmark k-eff (k-eff_bench)\(^{-1}\) – (k-eff_serpent)\(^{-1}\) \[pcm\] | 39        | -         | 142       | -          |

5. FENNECS deterministic model and results

5.1. HPMR core model in FENNECS

In radial direction, the meshing is derived from the regular lattice of the hexagonal fuel cells and the central safety rod cell. The hexagonal lattice is extended to the region of the radial reflector. Each hexagonal cell is represented by six equilateral prisms. The radial reflector elements are arranged in such a way as to best approximate the circular shape of the reactor vessel. Figure 5 shows the radial meshing of the core in both ARO and ARI configurations. The black circle depicts the actual circular vessel boundary to illustrate the geometrical approximation of the radial reflector elements. The control drums are placed into the regular hexagonal lattice by replacing groups of seven hexagons. They are meshed according to the method described in section 2. Both 12-edges polygon meshing and 24-edges polygon meshing to approximate the control drums are applied. For each configuration, the sensitivity of the control drum meshing is tested as follows: one test with the control drums approximated by a 12-edges polygon and another one with the control drums approximated by a 24-edges polygon. The axial discretization consists of 27 equally sized meshes of 5 cm height.
Figure 5. HMPR core model in FENNECS (Control drums are modelled with a 12-edges polygon). Left: All Rods Out (ARO) core configuration. Right: All Rods In (ARI) core configuration.

5.2. FENNECS deterministic results
The multiplication factor is evaluated with FENNECS for both ARO and ARI configurations and results are given in Table 4. The multiplication factors are compared to those obtained with the Serpent simulations.

Table 4. Multiplication factor obtained with FENNECS in ARO and ARI configurations with control drums approximated with 12-edges polygon and 24-edges polygon and comparison with the Serpent results.

|          | ARO        | ARI        |
|----------|------------|------------|
|          | 12-edges   | 24-edges   | 12-edges | 24-edges |
| k-eff    | 1.02252    | 1.02272    | 0.99275  | 0.99296  |
| Deviation from Serpent k-eff | -105 [-105 pcm] | -86 [-86 pcm] | 186 [186 pcm] | 207 [207 pcm] |

It can be observed that the FENNECS results are in good agreement with the reference Serpent results. For the ARO configuration, FENNECS slightly underestimates the multiplication factor: the deviation is about -105 pcm and -86 pcm for 12-edges and 24-edges approximation, respectively. For the ARI configuration, the multiplication factor is slightly overestimated by FENNECS: the deviation is about 186 pcm and 207 pcm for 12-edges and 24-edges approximation, respectively. It can be also concluded from Table 4 that the approximation of the control drums with a 12-edges polygon or a 24-edges polygon has little impact on the multiplication factor.

These preliminary results are very promising and prove that the FENNECS code can properly model very small micro reactors, and yields results in good agreements with Monte Carlo codes.

To further improve the current results, two possible areas are identified as future work:

- Some tests will be performed on the generation of the cross sections. It is well known that for SFR applications, the application of the SPH method [13] for consistent cross sections of
absorber materials is recommended for full core simulations, so improvement also for the HPMR results could be expected.

- The approximation of the reactor vessel is quite rough in the above FENNECS models. To improve the model, it is required to extend the Python software module for an improved meshing of the circular reactor vessel boundary.

6. Conclusion
In this paper, as an up-to-date example for a (v)SMR, the Heat Pipe Micro Reactor (HPMR) core, whose specifications are to be found in the publicly available document [3], is modeled with the recently developed deterministic finite element 3-d neutron kinetics code FENNECS. Few-group cross section data are generated by a full core Monte Carlo Serpent model which also serves as a reference solution for two studied core configurations All Rods Out (ARO) and All Rods In (ARI). The multiplication factors obtained with Serpent are in good agreement with the results provided in the specifications document [3]. Concerning the model of the HPMR core in FENNECS, the meshing of the control drums is a challenge: the external Python meshing tool, dedicated to mesh irregular geometries and to provide data required by FENNECS, is further developed to approximate control drums with a 12-edges polygon or a 24-edges polygon. FENNECS multiplication factors are in good agreement with the reference Serpent results. Moreover, the multiplication factor is almost insensitive on whether the control drums are discretized with a 12-edges polygon or a 24-edges polygon.

These preliminary results are very promising and prove that the FENNECS code can properly model very small modular reactors and yields results in good agreement with a Monte Carlo code reference solution.

For further improvements, it is planned, among others, to apply the SPH method to the cross sections of absorber materials and to further develop the Python software module to properly mesh the reactor vessel into a circle shape. Future work will also focus on further development of FENNECS and its verification and validation.

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References
[1] Seubert A 2020 A 3-D finite element few-group diffusion code and its application to generation IV reactor concepts Proceedings of PHYSOR2020 (Cambridge, United Kingdom).
[2] Seubert A, Bousquet J and Henry R 2021 Recent advances of the FEM neutronics code for safety assessment of (v)SMR, generation IV and other innovative concepts Proceedings of MC2021 (Raleigh, North Carolina, USA) to be published (abstract submitted).
[3] Hu G, Hu R, Kelly J M and Ortensi J 2019 Multi-Physics Simulations of Heat Pipe Micro Reactor, United States: N. p. Web. doi:10.2172/1569948, ANL-NSE-19/25.
[4] Zienkiewicz O C and Tayler R L 1994 The Finite Element Method. Vol. 1: Basic Formulation and Linear Problems. 4th edition MacGraw-Hill Book Company.
[5] Austregeilo H, Bals C, Langenfeld A, Lerchl G, Schöffel P, Skorek T, Von der Cron D, and Weyermann F 2019 ATHLET 3.2 Models and Methods. Technical Report GRS-P-1/Vol. 4, Rev. 5, Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) gGmbH.
[6] Kostadin I, Beam T, Baratta A, Irani A and Trikouros N 1999 Pressurised Water Reactor Main Steam Line Break (MSLB) Benchmark:Volume I: Final Specifications. Technical report NEA/NSC/DOC(99)8, NEA/OECD, Paris, France.
[7] Ortensi J 2018 OECD/NEA Coupled Neutronic/Thermal-Fluids Benchmark of the MHTGR-350 MW Core Design: Results for Phase-I Exercise 1 NEA/OECD.
[8] F. Varaine et al. 2012 Pre-conceptual design study of ASTRID core Proceedings of ICAPP ’12, (Chicago USA).
[9] Leppänen J et al. 2015 The Serpent Monte Carlo code: Status, development and applications in
2013, *Annals of Nuclear Energy*, pp. 142-150, **82**.

[10] Waltar A E, Todd D R, and Tsvetkov P V 2012 Fast Spectrum Reactors. *Springer Science+Business Media LLC, Boston, MA*.

[11] Bousquet J, Seubert A, and Henry R, 2019, 3-d coupled PARCS/ATHLET transient simulation of SFR using detailed expansion modeling, *Proceedings of MC2019, (Portland OR, USA)*.

[12] Bousquet J, Henry R and Seubert A, 2020, 3-d transient coupled simulation of Superphenix with PARCS/ATHLET, *Proceedings of PHYSOR2020, (Cambridge, United Kingdom)*.

[13] Hébert A and Mathonnière G 1993 Development of a Third-Generation Superhomogenisation Method for the Homogenization of a Pressurized Water Reactor Assembly, *Nuclear Science and Engineering*, pp. 129-141, **115**.