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PERFORMANCE OF HYBRID FUSION-FISSION REACTOR – A COMPARISON BETWEEN OPENMC AND MCNP

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ABSTRACT

This study evaluates the application of an external fusion source in a simple hybrid fusion-fission system modeled using the MCNP6 and OPENMC codes, both based on the Monte Carlo method for particle transport. The neutron source was derived from an isotropic fusion spectrum calculated in the Affordable Robust Compact (ARC) reactor and applied as an external source at the center of the SFF1 system (modeled with MCNP6) and the SFF2 system (modeled with OPENMC). The JEFF3.3 nuclear data library (Joint Evaluated Fission and Fusion File) was used for both models. The study compared key neutronic parameters of the two systems, such as the effective multiplication factor (keff) and neutron flux, to evaluate the performance of the model developed in OPENMC with the external fusion source. The results showed that the small differences in neutron flux between the systems confirm that OPENMC produces results consistent with the well-established MCNP6 code. Despite the slight differences observed, influenced by factors such as tally normalization and server execution environments, the OPENMC model demonstrated potential for future studies in fusion-fission hybrid reactor designs, providing reliable data and consistent behavior with MCNP6.

1. INTRODUCTION

In recent years, open-source Monte Carlo codes, such as OPENMC [1]-[3], Geant4 [4], ROLL [5], and SCONE [6], have gained popularity in nuclear reactor analysis. The advantage of these codes lies in their free availability, user-modifiable versatility, and benefits such as flexibility, traceability, portability, and compatibility with various platforms. These benefits allow researchers to perform reactor analyses more collaboratively and efficiently [1]. However, these codes must undergo rigorous validation processes and comparison with experimental data and other codes to ensure that the simulation results produced accurately reflect the expected physical phenomena from research. This comparison is crucial, as it reassures us about the accuracy and reliability of our research. Additionally, by comparing the simulation results with experimental data or benchmark results, developers can identify discrepancies and improve the predictive capabilities of the code.

OPENMC is one of the most widely used open-source Monte Carlo codes for nuclear reactor analysis. The code was developed by members of the Computational Reactor Physics Group at the Massachusetts Institute of Technology in 2011 and is currently being developed by the community for neutron and photon transport simulations [3]. Using constructive solid geometries or CAD representations, this code enables fixed-source calculations, eigenvalue problems, and subcritical problems. Additionally, the code uses a native HDF5 format [7] to store continuous-energy particle interaction data, which can be generated from ACE files [8] through NJOY [9]. OPENMC supports continuous-energy and multigroup transport and features high performance, parallelism, modularity, and extensibility [3].

Despite the advancements brought by this open-source code, challenges remain, particularly regarding validation through experimental data and comparison with other codes to ensure accuracy and reliability. Furthermore, the increasing complexity of nuclear reactor models demands continuous improvements in these open-source codes to handle more detailed and precise simulations.

Therefore, this study evaluates the performance of OPENMC and compares it to the Monte Carlo N-particle (MCNP6) code. MCNP6 is a closed-source general-purpose code that can be used for problems of transport of particles such as neutrons, photons, electrons, or neutrons/photon/electrons, including the capability to calculate eigenvalues for critical systems [8]. Additionally, MCNP6 has undergone some validations in different applications, demonstrating its reliability and accuracy in neutron transport simulations [8]. Previous studies on hybrid fusion-fission reactors based on the Affordable Robust Compact reactor (ARC), developed by the Department of Nuclear Engineering (DEN/UFMG) using MCNP6, have demonstrated the use of high-energy neutron flux of 14.1 MeV produced by deuterium-tritium (D-T) fusion reactions to increase the probability of fission in a transmutation layer [10]. As a result, reprocessed fuels can be introduced into this fission layer to achieve greater transmutation of transuranic elements.

Thus, an external fusion source will be used in a simple fusion-fission system modeled using the OPENMC and MCNP6 codes. The models are referred to as SFF1 and SFF2, respectively. The external fusion neutron source originates from an isotropic source with a deuterium-tritium (^2H-^3H) neutron spectrum calculated in the fusion plasma region of the ARC reactor, which has a D-shaped configuration with a major radius of 3.3 m, a minor radius of 1.3 m, and a volume of 141 m^3 [10]. This source was obtained using the MCNP6 code and subsequently added to the center of both SFF1 and SFF2 systems. For the comparison of the codes, the same geometry, composition, physical condition, and nuclear data library "Joint Evaluated Fission and Fusion File" (JEFF 3.3) [11] are employed to ensure there are no differences attributable to the data. These systems are then compared based on neutronic parameters in steady-state.

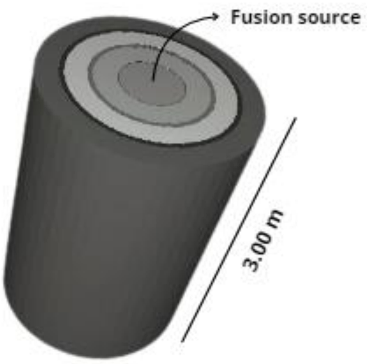
2. METHODOLOGY

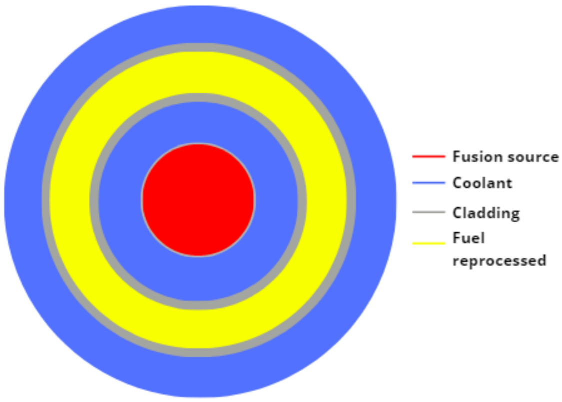
Starting from previously developed studies on the hybrid reactor based on the ARC fusion reactor [10], a simple fusion-fission system was designed, containing a fusion source and a fission transmutation layer. The JEFF3.3 nuclear data library was used in this study in all systems. This cross-section library was processed using the Nuclear Data Processing System NJOY code, according to the characteristic temperatures of each material [9, 11]. Tab. 1 presents the components and volume of each material inserted in the transmutation layer for the simple hybrid system and the working temperature for each component.

Tab.1. Parameters used in the design of the fission transmutation layer.

Components	**Material**	**Volume (cm^3)**	**Mass (ton)**	**Temperature (K)**
Fuel	Fuel reprocessed	2.7043×10^6	28.3951	1200
Cladding	HT-9	1.3719×10^6	10.7010	900
Coolant	Lead-Bismuth Eutectic (LBE)	5.9498×10^6	61.1166	650
Total volume		1.0026×10^7		

Two systems were developed, called SFF1 and SFF2. Initially, the SFF1 system was modeled using the MCNP6 code [8], and the SSF2 was developed using the OPENMC code [3]. These systems (SFF1 and SFF2) have a diameter of 2.5 m and an effective core height of 3.00 m. Thus, the same geometry elaborated in MCNP6 and OPENMC, can be compared to observe any differences between the two systems, such as the processing of input data. In MCNP6, the input file consists of a series of commands structured in ASCII text, known as 'cards'. Each card comprises keywords and data entries defining the simulation conditions. In OPENMC, the input is configured through the Application Programming Interface (API) in Python provided by OPENMC. In this approach, the user can define functions and classes corresponding to the input commands and elements. These data are then exported and read in XML format, facilitating the execution of the simulation. Fig. 1 shows the design of the simple system with the external fusion source elaborated to SFF1 and SFF2 in (a) 3D view and (b) XY view with color-coded components.





(a) (b)

Fig. 1. (a) 3D view of the model with location of the external fusion source and (b) XY view with indications of the materials.

The fuel inserted into the transmutation layer comes from spent fuel from the Angra I reactor (PWR type). This spent fuel had an initial enrichment of 3.1%, which, after a burnup of 33,0000 MWd/t, is then kept for an additional 5 years in a cooling pool. Afterward, the spent fuel is reprocessed through the GANEX (Group Actinide Extraction) process and spiked with thorium [12],[13]. The composition of the normalized fuel is described in Tab. 2, which contains 11 percent fissile material.

Tab. 2. Fuel composition (normalized) spent reprocessed by the GANEX method and spiked with thorium.

Nuclide	Weight fraction	Nuclide	Weight fraction	Nuclide	Weight fraction
^{232}Th	7.20072E-01	^{239}Np	1.28346E-05	^{242}Cm	7.05030E-06
^{233}U	5.67791E-13	^{238}Pu	2.79157E-03	^{244}Cm	8.08245E-06
^{234}U	2.34330E-06	^{239}Pu	7.30995E-02	^{245}Cm	2.81247E-07
^{235}U	1.21955E-04	^{240}Pu	2.49899E-02	^{143}Nd	1.86502E-03
^{236}U	6.23415E-05	^{241}Pu	2.34968E-02	^{150}Sm	3.74004E-04
^{237}U	1.60815E-09	^{242}Pu	8.87993E-03	^{153}Eu	7.95299E-05
^{238}U	1.48252E-02	^{241}Am	2.26418E-05	^{16}O	1.20738E-01
^{237}Np	6.85264E-03	^{242}Am	4.16683E-08		
^{238}Np	2.03273E-07	^{243}Am	1.69817E-03		

2.1 Fusion source definition

The external fusion neutron source used in the SFF1 and SFF2 systems originates from an isotropic source, with the neutron spectrum of deuterium-tritium (D-T) reactions calculated at the first internal wall of the ARC reactor [10]. For the calculated spectrum, the energy range considered is from 10^{-6} to 14.1 MeV, using the MCNP6 neutron transport code. This neutron flux is normalized over the total flux and projected as an external source at the center of the SFF1 and SFF2 systems, whose volume is $9\text{x}10^5 \text{cm}^3$. The neutrons released in the ^2H-^3H fusion reactions at a temperature of 10 keV are represented by a Gaussian energy spectrum:

$$p(E) = C\ exp\left[-\left(\frac{(E-b)}{a^2}\right)\right] \tag{1}$$

In the ARC reactor this spectrum is described with the SDEF source definition card of the MCNP6 code, where a is the width in MeV and b is a parameter that defines the average energy in MeV. Width here is defined as the energy ΔE equal -0.01 MeV; and b equal to -1.00 MeV; and maximum neutron energy of 14.1 MeV [8],[10]. Fig. 2 shows the normalized neutron spectrum obtained from the fusion source, calculated in the ARC reactor. The external fusion source presents a neutron flux that remains in the hardened neutron range (energy above 3 MeV), due to the neutrons with energy 14.1 MeV emitted in the D-T fusion reaction.

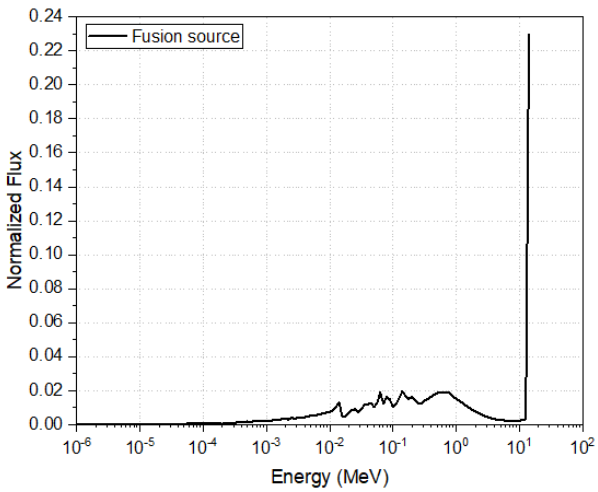


Fig. 2. Neutron spectrum normalized at the fusion source calculated at the first inner wall of the ARC fusion reactor used for the SFF1 and SFF2 systems.

In SFF1, this fusion source distribution is inserted as a source through the SDEF card, in MNCP6 code, which allows the input of distribution values using the SP card. In SFF2, the external source is defined as a fixed source, and the neutron flux distribution from the fusion source is included in the source description as a class. Therefore, the fusion source used in SFF1 and SFF2 systems is the same.

2.2 Simulation

The simulations were conducted using two different neutron transport codes: MCNP6 for the SFF1 model and OPENMC for the SFF2 model. The neutron behavior of the SFF1 and SFF2 systems was evaluated in steady-state conditions. The effective multiplication factor (k_{eff}) was determined for both systems, along with the relative error of this estimate. In addition, the neutron flux on the inner surface of the first wall of the systems was calculated, as well as the neutron flux in the transmutation layer volume of the SFF1 and SFF2 models. For the simulations, 10^6 neutrons per second and 550 cycles were established for both systems. However, it is important to note that the simulations were run on different servers, which may have influenced the generation of random numbers used in the calculations.

3. RESULTS AND DISCUSSION

Fig. 3 shows, in a view in the XZ plane, approximately 10^6 neutrons per second emitted from the external fusion source in the SFF1 reactor, modeled using MCNP6. In this figure, it is possible to observe the distribution of neutrons throughout the region of the central volume.

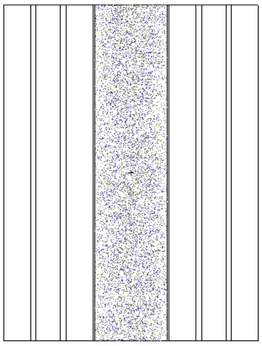


Fig. 3. Neutrons emitted from the external fusion source in the SFF1 model, located at the center of the system (view in the XZ plane).

Figure 4 presents the neutron spectrum calculated on the surface of the first wall inner of the SFF1 and SFF2 systems. This neutron flux represents the spectrum of the external fusion source inserted into the respective systems. The neutron flux in the SFF1 and SFF2 systems shows similar behavior, predominantly within the intermediate and fast neutron energy ranges. The difference between the spectra is small, amounting to approximately 4.23% of the total calculated flux. The intermediate neutron spectrum (0.625 eV - 100 keV) is slightly more in the SFF1 model than the SFF2, with a difference of ~0.006 percentage points. In the fast neutron range (>100 keV), the spectrum of SFF2 shows a more hardened than SFF1, particularly in the energy range of 10 to 14.1 MeV, where the largest calculated difference between the systems is also around ~0.006 percentage points.

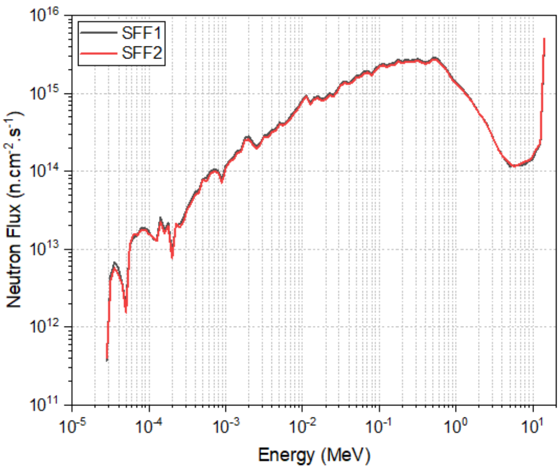


Fig. 4. Calculated neutron flux in the first inner wall of the SFF1 and SFF2 systems.

Table 3 presents the effective multiplication factor (k_{eff}) for the analyzed SFF1 and SFF2 systems. The k_{eff} value between the systems has a small difference of 2.76 pcm, and it is noted that with the same simulation parameters, SFF2 showed a lower relative error than SFF1, with a difference in the error propagation of 0.027 pcm. Figure 5 presents the neutron flux calculated in the fission transmutation layer volume in the systems SFF1 and SFF2, where it is noted that the flux between the systems exhibits a similar behavior. The percentage difference between the thermal, intermediate, and fast neutron energy regions is presented in Tab.4. The neutron flux remains in the fast neutron region, and the difference between the systems is ~0.0003 percentage points, whose value is higher for SFF2. In the intermediate neutron region, the SFF1 system is more than the SFF2 system, with a difference at the second decimal point.

Tab. 3. k_{eff} values calculated in SFF1 and SFF2 systems.

System	k_{eff} value	Code difference
SFF1	0.98231 ± 0.000060	2.76 ± 0.027 pcm
SFF2	0.98507 ± 0.000029	

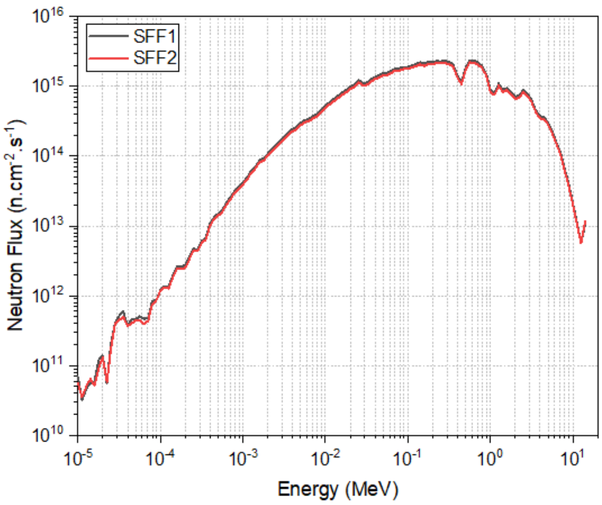


Fig. 5. Calculated neutron flux in the fuel volume of the SFF1 and SFF2 systems.

Tab. 4. Neutron flux calculated in in the fission transmutation layer volume for SFF1 and SFF2.

Neutron flux	SFF1	SFF2	Difference
Thermal (0.625 eV)	4.188E-06%	1.070E-05%	0.00 pp
Intermediate (0.625 eV - 100 keV)	37.5297%	37.5031%	0.0003 pp
Fast (>100 keV)	62.4690%	62.4969%	0.0003 pp
Total	8.0427E+16	8.4217E+16	4.71%

*pp = percentage points

4. CONCLUSION

The MCNP6 and OPENMC codes, based on the Monte Carlo method for particle transport, were compared in a simple hybrid fusion-fission system. The SFF1 and SFF2 systems used the same geometry and parameters, and differences between the codes were demonstrated by calculating the k_{eff} value and the neutron flux in the systems. Although the SFF1 and SFF2 systems were executed with the same parameters, these were executed on different servers, which may have influenced the differences indicated between the systems. Another difference that may have influenced the results is due to the normalization of the specific tallies in each code in the neutron flux calculation. Both OPENMC and MCNP provide several tallies for flux calculation. However, MCNP tallies are typically normalized to a source particle, while OPENMC tallies are normalized by the total weight of the simulated source particles.

The steady-state analysis indicated a lower relative error for the k_{eff} calculated in SFF2, which may indicate better performance in this system. The characteristic neutron flux spectrum of the external source calculated in the models influences the neutron flux reaching the transmutation layer volume. The small difference observed in the neutron flux between the two systems demonstrates that the open-source code OPENMC produces results consistent with MCNP6. Therefore, the data obtained from the model developed in OPENMC, using an external fusion source, is consistent with the model already established in MCNP6. This enables future studies on fusion-fission hybrid reactors using the open-source code OPENMC.

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