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WPPMI-CPR(18) 21109

B Colling et al.

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Preprint of Paper to be submitted for publication in Proceeding of
30th Symposium on Fusion Technology (SOFT)



This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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Assessment of Serpent 2 application to fusion neutronics

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Radiation transport models for fusion neutronics analysis are becoming increasingly complex, further exacerbating problems in the creation and integration of neutronics models found in traditional analysis methods using MCNP. Serpent 2, an alternative radiation transport code developed at VTT Technical Research Centre of Finland, is considered as a potential method for neutronics analysis in fusion relevant problems. Advantages of Serpent 2 include a more robust universe implementation with capability for the use of a mixed geometry definition with of a combination of constructive solid geometry and mesh-based geometry, making it an excellent candidate as an alternative transport code for fusion neutronics, particularly in the case of complex models [1]. Therefore, investigation into the use of Serpent 2 for fusion relevant neutronics analysis is ongoing with important computational and experimental benchmarking.

In this paper computational Serpent 2 results have been compared with both computational MCNP results and experimental data, following on from previous preliminary investigations with the ITER reference model [2]. A spherical model was employed for a basic benchmark of the fusion application of Serpent 2 and its corresponding nuclear data library showing good agreement. Comparison of computational results of tritium production in a fusion DEMO [demonstration] reactor has also been performed with results within 3σ . Experimental results from the activation foils in the Frascati Neutron Generator HCLL [helium cooled lithium lead] benchmark have been compared with Serpent 2 and promising results observed.

1. Introduction

Nuclear fusion is entering a ‘nuclear phase’ with significant emphasis on nuclear safety, shielding and activation. Neutronics analysis is required to support the successful design and development of nuclear fusion facilities such as ITER and DEMO [demonstration reactor]. Some important quantities include neutron flux, nuclear heating, absorbed dose rate, gas production, tritium breeding, radiological inventory and shutdown dose rates.

Radiation transport models for fusion neutronics analysis are becoming increasingly complex putting additional demands on traditional 3D computational analysis methods using MCNP [1], [2]. Investigations into potential alternative and complementary analysis codes and tools are imperative to ensure neutronics analysis methods develop to meet analysis requirements and further the confidence in results through multiple calculation methods. To this end this paper reports on progress to assess the use of Serpent 2, developed at VTT Technical Research Centre of Finland, for fusion neutronics analysis.

Comparisons have been performed on computational results between Serpent 2 and MCNP for a basic model and the DEMO 2015 benchmark model [3]. Comparisons have also been performed with experimental data for the FNG benchmark.

2. Neutronics analysis

Traditionally neutronics analysis for 3D computational models has been performed using constructive solid geometry with MCNP [4] for particle transport. MCNP is an established code with significant history in radiation transport problems and is considered

the standard code for ITER related fusion neutronics. Complex models, such as the ITER neutronics reference model, has resulted in the MCNP geometry creation and integration process becoming increasingly time-consuming and inefficient. Significant time is required to produce a suitably simplified system model and successfully integrate into the ITER reference model. Some of the main issues regarding the implementation of large complex universe-based models was discussed in previous work [1] with some alternative CSG and mesh-based neutronics analysis approaches, including Serpent 2, also investigated. Initial results in comparison to the conventional MCNP constructive solid geometry method have proved agreeable [2].

In this paper further investigation of Serpent 2 for fusion neutronics has been performed using (1) a spherical elemental material model, (2) the DEMO 2015 benchmark with helium cooled lithium lead (HCLL) homogeneous blankets [5] and (3) experimental reaction rate data from the FNG benchmark. In order to carry out the analysis further developments of Serpent 2 and user source routines were required.

2.1 Transport code versions

MCNP version 6.1 [4] was used for benchmarking computational results with Serpent version 2.1.31 beta [6]. Constructive solid geometry models have been used in this work.

2.2 Spherical elemental material model

Analysis has been performed using a spherical model with a 14 MeV neutron source and repeated for a Co60 gamma source with each of the elements from hydrogen to lead. The FENDL3.1b [7] nuclear data library was used with both Serpent 2 and MCNP. Total neutron /

photon leakage through a spherical shell has been compared along with the flux per energy bin and volumetric heating.

2.3 DEMO 2015 benchmark model

The 2015 DEMO benchmark model with homogeneous HCLL blanket materials [5] was used for comparison. The MCNP geometry model was converted to Serpent 2 input file format (Figure 1) using a previously developed tool. The MCNP DEMO model can be used with either an 'sdef' source or the parametric plasma source. For use in Serpent 2, the parametric plasma source code was rewritten in C-programming language and implemented as a user defined source with the Serpent 2 code.

The JEFF3.2 nuclear data [8] was used with both Serpent 2 and MCNP.

The tritium production within 10 equally spaced layers of an equatorial, inner upper and outer lower blanket has been compared between Serpent 2 and MCNP.

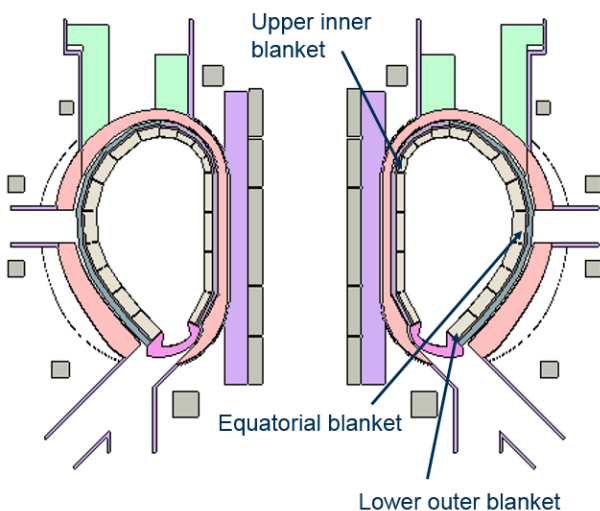


Figure 1: DEMO 2015 benchmark model [5] (Serpent 2 plot)

2.4 FNG HCLL benchmark model

The FNG benchmark model and experimental data from 36 activation foil measurements has been used for comparison with Serpent 2. The MCNP model was converted to Serpent 2 input file format. As yet we have no specific tool to convert any MCNP sdef source to a Serpent 2 source definition. To produce some preliminary data for comparison a source particle file was generated from an MCNP PTRAC simulation. This source file contained the x, y, z position, u, v, y direction, energy, weight and time for 1×10^7 neutrons.

Calculations were performed using FENDL3.1b [7] for transport and reaction rate estimations apart from niobium that used lldos [9]. The nuclear data selected was inline with that used in previous work to review the FNG HCLL benchmark data for inclusion in the SINBAD database. Calculations have been performed in

this study with other nuclear data and this is an ongoing area of research.

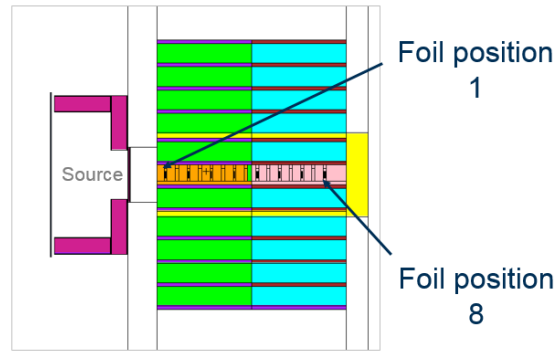


Figure 2: MCNP model of the FNG HCLL benchmark

3. Results

3.1 Spherical elemental material model

The Serpent 2 results have been compared with those from MCNP for a number of different quantities. A scripted approach using Python was utilized to create the input files, read the output data and perform the comparison. A criterion was set, requiring 90% of results within a tally to be within 3σ . A summary of the tallies compared are shown below where a tick denotes the tally has passed the criteria test.

Tally tests with neutron source:

Neutron flux	✓
Photon flux	✓
Neutron spectrum	✓
Photon spectrum	✓
Heating (neutron)	✓
Heating (photon)	✓

Tally tests with photon source:

Photon flux	✓
Photon spectrum	✓

An example of the data comparison is shown in Figure 3 and Figure 4. Where Figure 3 shows the difference (Serpent 2 - MCNP / MCNP) in the neutron (top) and photon (bottom) leakage in each of the spherical elemental material models using a neutron source. The majority of the results have less than 2% difference and all are within 3σ of the combined statistical error.

Figure 4 compares the neutron flux spectrum for the spherical model containing lithium. Only results with a statistical error less than 30% have been compared; most results have a statistical error of less than 5%. The results are within 3σ with a relative difference of less than 5% in most energy bins.

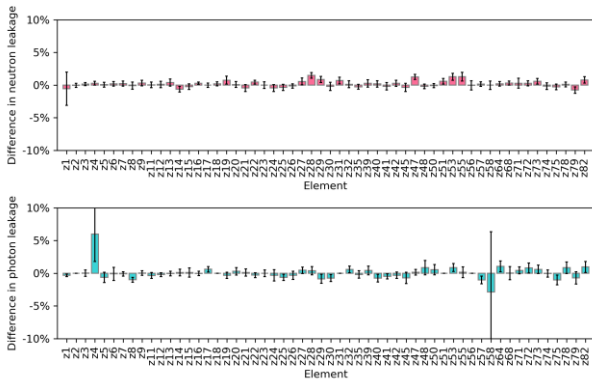


Figure 3: Comparison of neutron (top) and photon (bottom) flux leakage with elemental material model

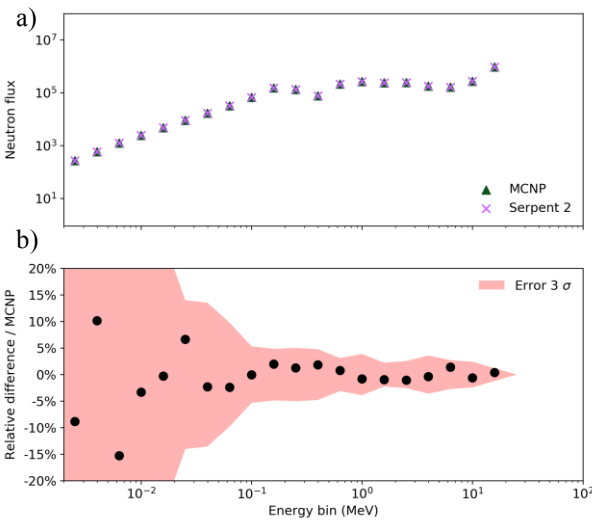


Figure 4: a) Comparison of flux spectrum leakage through lithium model, b) relative difference and combined statistical error

3.2 DEMO 2015 benchmark model

A comparison of the source data used with the DEMO 2015 benchmark model is shown in Figure 5, with a plot of the normalized neutron flux and comparison of the x, y, z profile. The profile comparisons were performed by plotting the frequency of 10000 starting particles within 33 equally spaced bins in the x, y and z direction. The sources show good agreement.

The tritium production within 10 equally spaced layers of an equatorial, inner upper and outer lower blanket has been compared between Serpent 2 and MCNP. All results are within 3σ . A comparison of the fraction of tritium production per layer for the equatorial blanket is shown in Figure 6 along with the relative difference which is below 0.2%.

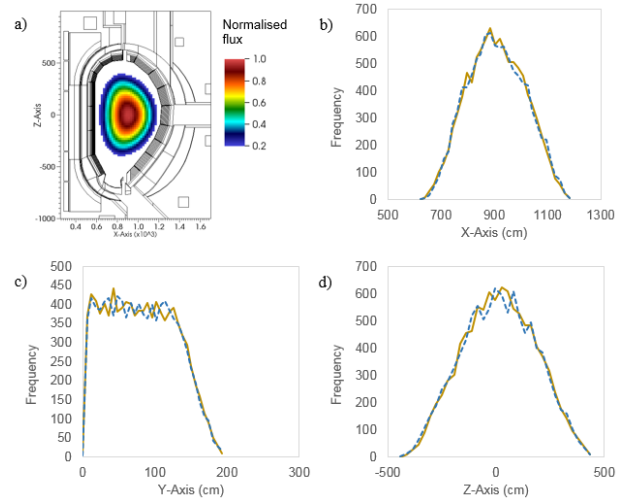


Figure 5: Comparison of parametric plasma source: a) radiation map of normalized neutron flux and histogram plots of 1000 starting particle positions in b) x-axis, c) y-axis, d) z-axis (orange solid line = Serpent 2, blue dashed line = MCNP)

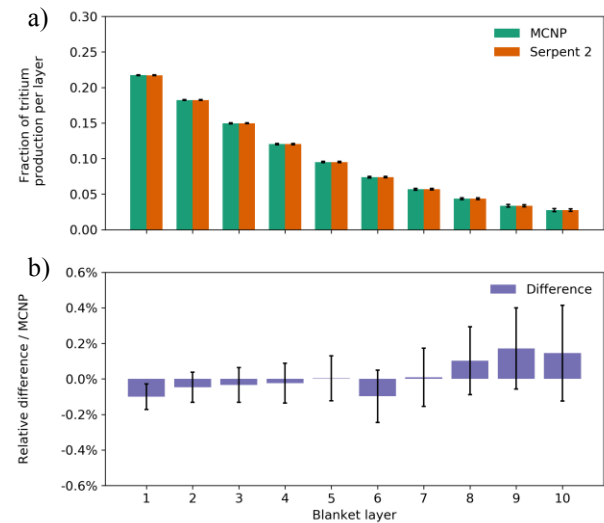


Figure 6: a) Comparison of tritium production in equatorial blanket layers of DEMO model, b) relative difference in tritium production with combined statistical error bars

3.3 FNG HCLL benchmark model

Serpent 2 calculated reaction rates have been compared with the FNG HCLL benchmark experimental results and show good agreement in the majority of cases (Figure 7a). All Serpent 2 $Al(n,\alpha)$ and $Au(n,\gamma)$ results fall within the experimental benchmark data. All Serpent 2 results apart from the entrance foil position for $Ni-58(n,p)$ fall within the experimental benchmark. All Serpent 2 results apart from the 7th foil position for $Ni-58(n,2n)$ fall within the experimental benchmark. None of the $Nb(n,2n)$ Serpent 2 results fall within the experimental benchmark.

Similar observations have been found when comparing MCNP results with the experiments (Figure 7b). The C/C plot of Figure 7c shows that the use of Serpent 2 has not introduced further discrepancies. It is proposed that the differences observed for the Nb(n,2n) results is due to the nuclear data used in the model.

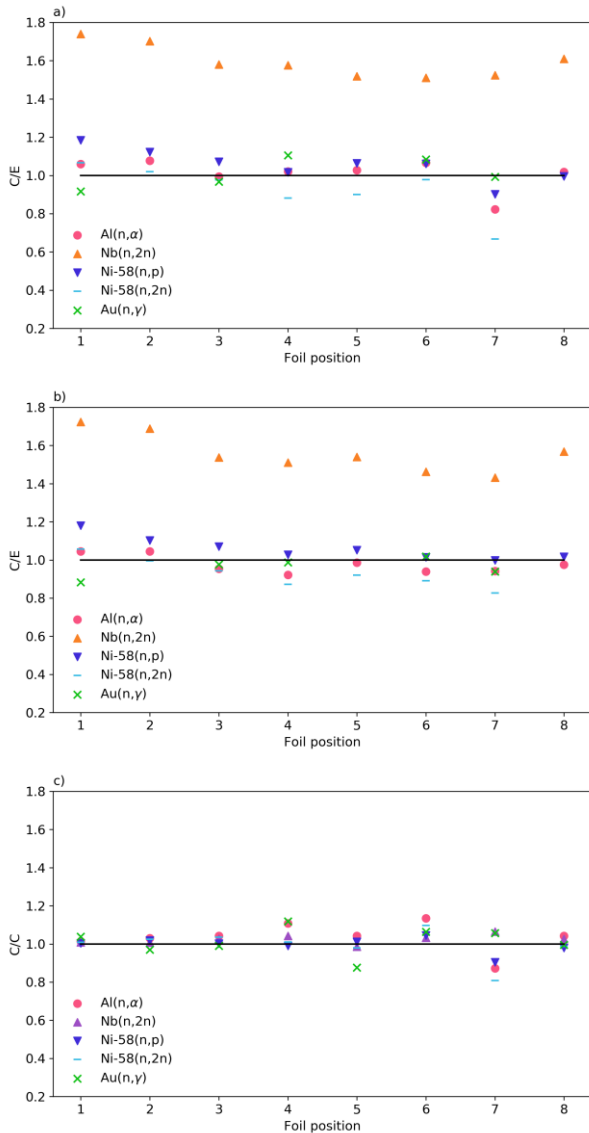


Figure 7: Comparison of FNG HCLL reaction rates: a) with Serpent 2 results, b) with MCNP results, c) between Serpent 2 and MCNP

4. Summary and conclusions

Comparisons have been performed between Serpent 2 and MCNP computational results for a spherical model and the DEMO 2015 benchmark model showing flux leakage and tritium production results within 3σ .

Promising results have also been observed when comparing Serpent 2 with experimental data from the FNG HCLL benchmark with the majority of results within 3σ .

Future and ongoing work includes the use of different nuclear data libraries, development of global

variance reduction methods through efficient weight window generation and further benchmarking.

Acknowledgments

This work has been funded by the RCUK Energy Programme [grant number EP/P012450/1]. This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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