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Analysis of different nuclear data libraries on the Fluoride-salt-cooled high-temperature reactor

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ABSTRACT

This work presents a comparison of Fluoride-salt-cool High-temperature Reactor (FHR) system calculations using the ENDF/B-VII.1, JEFF-3.2, JEFF-3.3 and ENDF/B-VIII.0 nuclear data libraries. Analysis of a simplified model of the Shanghai Institute of Applied Physics TMSR-SF1 reactor using both Serpent and MCNP was performed. Unit cell and full core models based on a specification developed at the University of California, Berkeley were used in this work. The use of the newer cross section libraries produced an increase of thermal fission of ^{235}U by 0.5–1%. The reactivity of the system in a fresh configuration was increased by 270–600 pcm, thermal flux was reduced by ~1% and the effect on reactivity of the system as a function of ^{7}Li purity of salt coolant was also reduced by ~2%. Neutron leakage, reaction rates, neutron flux spectra, thermal flux distributions and the effect of spatially homogenising regions of the system were also calculated and analysed.

1. Introduction

The aim of this work was to evaluate the variation in key figures of merit (FOM) calculated for a FHR system when using different cross section (XS) libraries. This system was defined in a benchmarking effort conducted at the University of California, Berkeley (UCB) as part of a larger national effort to develop FHR systems for eventual commercial deployment (Dept. Nuc. Eng., 2015, 2017). Without any reactors of this kind ever having been built, no operational data exists for integral validation of the system. The FHR is, in a sense, a hybrid of the Very-High-Temperature Reactor (VHTR) and the Molten Salt Reactor (MSR) with utilisation of graphite-matrix solid fuel and salt coolant. The FHR can also be viewed as a "stepping stone" technology to the MSR, providing valuable data and regulatory confidence in the new materials introduced into the power reactor regime.

The FHR benchmarking effort in the US is currently being undertaken by two consortia of US universities with considerable support from several US Department of Energy National Laboratories (Dept. Nuc. Eng., 2015). The preliminary neutronics benchmark is based on two geometries: a unit cell of fuelled pebbles immersed in salt and a simplified full core design based on the Shanghai Institute of Applied Physics (SINAP) TMSR-SF1 reactor, a 10 MW test reactor proposed as part of a pioneer project in 2011. The benchmark specification contained materials and geometry definitions for both scenarios along with results of several FOM. An analysis of the effect of spatial homogenisation of the materials, and thus simplification of geometry, was also provided.

This work aims to further examine the homogenisation of this system (Maul et al., 2016), and determine the level of homogenisation that maintains acceptable results compared to completely heterogeneous system. It also aims to examine the effect of different cross-section libraries on the key FOM, namely ENDF/B-VII.1 (E71) (Chadwick, 2011), JEFF-3.2 (J32), JEFF-3.3 (J33) and ENDF/B-VIII.0 (E80). Serpent v2.1.24 was used as the primary calculation suite in this work, the delta-tracking capability of which allows for the fast calculation of the neutron transport cycle. The FOM studied include k_{eff}, reaction rates of most materials in the system, flux spectra and flux distributions. In addition, the purity of ^{7}Li in the salt was considered and the impacts on the FOM analysed. Lastly, certain calculations were also performed using MCNP 6.1.1b with every effort made to maintain fidelity to the model used in Serpent, with the intent on providing some verification of the results.

2. Model description

The model specifications in this work are based on the benchmark specification from the UCB Neutronics Benchmark (Dept. Nuc. Eng., 2017). A single fuel element in the pebble-bed reactor system used in this work is a 6 cm diameter graphite pebble containing small fuel particles. Each particle contains a uranium dioxide (UO_2) fuel kernel with four layers of encapsulation surrounding it; these are called Tri-Isotopic (TRISO) particles, a common fuel form for high temperature reactor designs. The total diameter of each particle is ~1 mm and nominally 11,558 populate each pebble in the TMSR-SF1 design. The

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particles are embedded in a matrix of graphite. The outer 0.5 cm shell of the pebble is graphite containing no TRISO particles. While real pebbles have the fuel particles arranged stochastically, the benchmark focuses on a regular lattice geometry. While this has been shown to introduce some difference in some FOM (Dept. Nuc. Eng., 2017), namely k_{eff} and neutron leakage, for the purposes of comparison between XS libraries it was not considered important to consider at this stage. Instead, the particles were arranged in an FCC configuration.

Sections 2.1–2.3 include details about the TRISO unit cell, the pebble unit cell and the simplified core specifications. Additional details and approximations about these systems and the data used include:

- The differences in atomic weights between each library for a given isotope were so small that the material specifications in MCNP and Serpent input files were not adjusted from nominal values between calculations utilising different XS libraries.
- All carbon present in the system was treated with graphite thermal scattering XS.
- Edge effects for the TRISO lattice within a pebble and the pebble lattice in the full core scenario were not accounted for and some deviation from the nominal material specification from the original benchmark may be present. However, as this work is primarily a code and data verification exercise, this was not deemed significant enough to compensate for.
- The ENDF/B-VIII.0 library does not contain natural carbon and instead has separate evaluations for ^{12}C and ^{13}C. For the E71, J32 and J33 libraries, natural carbon was used and for E80 an atomic ratio of 98.9:1.1 $^{12}C/^{13}C$ was used. In the case of the latter, thermal scattering libraries were applied to both materials. Only crystalline graphite thermal scattering was used in this work, owing to abnormalities presented in testing results on the porous graphite data (Marquez Damian and Roubtsov, 2017).
- All silicon (SiC layer in TRISO) was treated as ^{28}Si in the material specification.

2.1. TRISO sub-unit cell

The TRISO unit cell is based on the benchmark specification established at UCB in 2017 (Dept. Nuc. Eng., 2017). The unit cell scenario contains 8 1/8th sections of a particle located in each vertex of the cube boundary of the cell and 6 1/2 sections of a particle located on the faces of the boundary of the cell. The regions within the cell outside of the particle boundaries contain graphite. The radii of the fuel kernel at the centre of each particle and it's encapsulating layers are contained in Table 1:

The side length of the cubic TRISO unit cell region is 0.2828 cm, which provides a particle packing factor of 6.97% in an infinite square lattice. A 2D view of the TRISO unit cell is shown in Fig. 1 as visualised by the Serpent plotting function.

2.2. Pebble unit cell

A pebble has an inner radius of 2.5 cm of TRISO particles embedded in a matrix of graphite, described above. This fuel region is contained within a 0.5 cm thick shell of graphite, taking the pebble total radius to 3 cm. The unit cell scenario contains 8 1/8th sections of a pebble located in each vertex of the cube boundary of the cell and 6 1/2 sections of a pebble located on the faces of the boundary of the cell. The regions within the cell outside of the pebble boundaries contain a 2:1 eutectic salt of LiF and BeF_2 called FLiBe. The side length of the cubic unit cell region is 9.2575 cm, which provides a pebble packing factor of 57% in an infinite square lattice. This unit cell structure was chosen for being a tightly packed regular configuration of pebbles and the packing factor chosen was based on calculated estimates of the global packing factor for a random configuration of particles; this model does not count for localised packing phenomena, such as edge effects. This model only serves as a reference case.

Table 1
Geometry of a TRISO particle.

Layer	Radius (cm)	Thickness (cm)
UO_2 Fuel Kernel	0.025	n/a
Buffer Carbon Layer	0.034	0.009
Inner Pyrolytic Carbon Layer	0.038	0.004
Silicon Carbide Layer	0.0415	0.0035
Outer Pyrolytic Carbon Layer	0.0455	0.004

The nominal atom and mass densities for each region are contained in Table 2.

All materials in the system were set at 900 K and all cross-sections used were processed at that temperature, with the exception of the graphite thermal scattering data, which was processed at 1000 K (as no 900 K data exists in the libraries). A 2D view of the pebble unit cell is shown in Fig. 2 as visualised by the Serpent plotting function.

2.3. Simplified full core

The simplified core is described by five unique regions and material definitions: the top, bottom and side reflectors, the fuelled region and the salt region. A cutaway view of the core is shown in Fig. 3.

The fuelled region is filled with the pebble unit cell lattice. The salt region located directly underneath the fuelled region is filled with FLiBe. The pebbles are less dense than the salt coolant and thus float to the top of the core. The top and bottom reflectors are a spatially homogenised mix of graphite and salt, a simplification of the truncated conical coolant flow aspects of these components in the actual TMSR-SF1 design. The nominal ratios of graphite:salt in the top and bottom reflectors are 3.7:1 and 3.08:1, respectively. These ratios are based off the more specific dimensions for the TMSR-SF1 at the time the original benchmark specification was written in mid-2016. While the conical flow region in the top reflector section would nominally be filled with pebbles, this homogenised approximation does not include any material from pebbles, so while this model would not be suitable for a core validation, it suffices for code-to-code verification and XS library verification. The side reflector is essentially the same material as other graphite used in the model with the exception of a marginally higher density of 1.75 g/cm^3.

These five geometric regions are all cylindrical with a common centreline. The top reflector, fuelled region, salt region and bottom reflector are stacked together in that order from top to bottom and share a common radius. The side reflector is an annular region that fits around this stack of inner core regions like a sleeve, spanning the combined height of the assembly. The geometric parameters for the simplified core are contained in Table 3.

The location of the centroid of the pebble unit cell is located at the centroid of the fuelled region. The boundary conditions for the simplified core are black. The nominal atom and mass densities for each region in the simplified core are contained in Table 4.

2.4. Spatial homogenisation of the pebble unit cell

13 different levels of spatial homogenisation were defined by blending key geometric features together from the standard unit cell specification. Atom numbers were conserved and density was calculated based on the aggregation of the masses and volumes of all materials in each constituent region. Input files were created based on these altered specifications for Serpent and MCNP. Seven of these specifications considered only geometry at the TRISO level: an infinite cell of TRISO particles in a graphite matrix. Table 5 contains the description of each of these scenarios. Cases 2–4 examine a single particle in an infinite square lattice and cases 5–7 examine particles arranged in an FCC configuration in an infinite square lattice. Relative material