DOUBLE-HETEROGENEITY MODELLING OF HIGH TEMPERATURE REACTORS CONTAINING PARTICULATE FUEL

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ABSTRACT

There is substantial current interest in gas-cooled high temperature reactors (HTRs) utilizing coated particle (TRISO) fuels, both in the UK and abroad. Several small modular HTRs are under development. TRISO fuel modelling presents unique challenges for both deterministic and Monte Carlo radiation transport approaches.

Amec Foster Wheeler has developed multi-scale techniques within the ANSWERS code suite for modelling TRISO particulate fuels. In the deterministic code WIMS, a subgroup calculation is used to derive resonance-shielded cross sections for fissile isotopes in the pins containing TRISO particles. The collision probability method is used to derive fluxes and cross sections for a representative pin containing TRISO particles, which can then be used to perform an assembly or core calculation. In the Monte Carlo code MONK, neutron transport through regions containing TRISO particles is generally treated using Woodcock Tracking. Both WIMS and MONK have been extensively validated, for HTR applications.

The particular case of the liquid-salt-cooled Small Modular Advanced HTR (SmAHTR) is analysed using the deterministic reactor physics code WIMS in collaboration with researchers at the University of Cambridge. The SmAHTR concept was proposed in 2010 by Oak Ridge National Laboratory as a small fluoride-cooled HTR with passive decay heat removal. Burn-up dependent k-infinity and fuel and coolant temperature reactivity coefficients are in excellent agreement with reference calculations performed using the Monte Carlo code Serpent with explicit modelling of TRISO particles and with results reported in the literature.

1. Introduction

The UK has unique experience in operational and associated gas-cooled reactor fuel performance amassed over 50 years from operation of its fleet of Magnox reactors and AGRs. This experience extends to coated particle fuels that have been developed for utilisation in high temperature reactor (HTR) systems. In particular, such fuels were fabricated in the UK as early as the 1960s and irradiated in the DRAGON HTR at Winfrith. TRISO coated particle fuels consist of microscale fuel particles encompassing U/Pu oxides (or other fuel-related materials) within several graphite layers; these may be contained in pebbles or prismatic cans. TRISO fuel could be suitable for high temperature thermal or fast reactor systems, for molten salt and for recycled fuel and waste transmutation.

US and Russian designs of HTR have generally used prismatic fuel blocks. The Peach Bottom and Fort St. Vrain HTRs operated in the USA in the 1960s-1980s. While Peach Bottom was broadly successful, Fort St. Vrain experienced numerous technical difficulties [1]. More recently, the gas-turbine, modular helium reactor (GT-MHR) has been developed by a consortium of companies [2].

The pebble bed modular reactor (PBMR) was pioneered in Germany with the AVR (Arbeitsgemeinschaft Versuchsreaktor). However, this experienced technical problems associated with local hot spots and inadequate fuel quality [3], which led to the structural integrity of the fuel being compromised and significant contamination of the reactor with Cs-137 and Sr-90. The PBMR design was under active development in South Africa, which had plans to construct a demonstration 400 MWth unit [4], although this was cancelled in 2010. A prototype 10 MWth PBMR, the HTR-10, operates in China, with two scaled-up 250 MWth versions currently under construction [5] [6]. In the United States, researchers at MIT, University of California, Berkeley (UCB) and University of Wisconsin are also looking at the utilisation of pebble TRISO fuels in their 236 MWth fluoride-salt-cooled HTR (FHR) concept [7]. In addition, Oak Ridge National laboratory (ORNL) is developing a 3600 MWth advanced HTR (AHTR) concept using TRISO particles that are compacted into fuel plates [8]. Associated experimental work, such as irradiation and high-temperature testing of TRISO fuels, is currently being carried out at the INL and ORNL. Preliminary testing has shown promising results, proving the TRISO fuel is able to retain fission products at temperatures of 1800 °C [9].

Amec Foster Wheeler have developed multi-scale techniques within the ANSWERS codes' suite for modelling TRISO fuels and examples of these are described in this paper. The ANSWERS codes WIMS [10] and MONK [11] have been extensively validated for reactor physics applications. The particular case of the liquid-salt-cooled Small Modular Advanced HTR (SmAHTR) is analysed using the deterministic reactor physics code WIMS by researchers at the University of Cambridge. The SmAHTR concept was originally proposed in 2010 by ORNL as a 1-batch small size 125 MWth fluoride-cooled HTR with passive decay heat removal. The design concept uses graphite as a moderator and a hexagonal fuel assembly with a single circular coolant channel for FLiBe liquid salt coolant. Within an assembly, fuel pins containing TRISO particles are arranged in a triangular lattice.

2. UK Context for TRISO Fuel

The first generation of UK reactors were the Magnox reactors, which contain U metal fuel with Mg-Al cladding. Unenriched fuel is employed, leading to low discharge burn-ups. At the time of writing, a single Magnox reactor remains operational at Wylfa in Wales. The high chemical reactivity of the Mg-Al cladding means that the fuel can only be stored for a limited time following fuel discharge, necessitating reprocessing of Magnox fuel [12].

The second generation of UK power reactors were the advanced gas-cooled reactors (AGRs), which utilise stainless-steel cladding, and as a result require low-enriched uranium (LEU) fuel. The use of stainless-steel cladding, gas coolant and graphite moderator allows high temperature operation to be maintained, leading to relatively high thermal efficiency of ~40% [12].

TRISO fuel was originally developed and deployed at the DRAGON test reactor at Winfrith. The fuel was produced on site [13], and consisted of LEU, but thorium and plutonium fuels were also tested.

More recently, URENCO has proposed the U-Battery®, a small micro-reactor utilizing TRISO fuel [14] and a helium-cooled primary circuit. A 10 MWth cartridge-style core is envisaged. The U-Battery® is being developed in a consortium with Amec Foster Wheeler and Atkins, and motivates continued development of TRISO fuel analysis methods in the UK, in the particular context of a small core.

3. Modelling of TRISO Fuel

TRISO fuel consists of an essentially randomly distributed set of small particles inside a graphite matrix. This geometry is challenging to model, both in deterministic and Monte Carlo neutron transport codes, due to:

- the random distribution of particles within the compact (which introduces some uncertainty);
- the large number of particles to be modelled;
  the multiple length scales involved (particles within a compact);
- the ‘double heterogeneity’ of the problem (i.e. small spheres within a containing body which may not be spherical). In particular, an explicit 2D representation of the geometry is not possible.

The TRISO compact is itself surrounded by coolant. Various different geometric configurations have been proposed:

- cylindrical or annular TRISO compacts surrounded by coolant channels (e.g. DRAGON, GT-MHR) [13] [15];
- spherical 'pebbles' of fuel as in the PBMR [16]. This design introduces its own challenges as the exact distribution of the pebbles in the reactor is uncertain;
- a recently proposed configuration of the AHTR utilizes TRISO fuel contained in plates [17].

Deterministic and Monte Carlo approaches to modelling these geometries have been implemented in WIMS and MONK respectively. The methodologies in MONK and WIMS have been validated against each other for array and core PBMR geometries [18]. WIMS and MONK agreed within 50 pcm for an infinite array of heterogeneous fuel pebbles, while calculations were within 250 pcm for a full-core calculation. The WIMS calculation route has been validated using data from the ASTRA critical facility, and been benchmarked for the HTR-10 and PBMR-400 designs [16].

3.1. Implementation in WIMS

In deterministic transport theory, it is necessary to take into account this heterogeneous geometry in order to calculate accurate multigroup shielded cross sections for use in a flux solution. In WIMS, this is accomplished by splitting the broad group cross sections over the fuel isotope resonances into a number of 'subgroups.' The contribution of each subgroup is weighted by the background cross-section-dependent resonance integral, and the flux in each subgroup. The flux is calculated by solving the transport equation. This differs from alternative approaches which involve calculating geometry-specific Dancoff factors for particular TRISO geometries (e.g. Ref. [19] for PBMRs, Ref. [20] for a prismatic block design).

For TRISO fuel, WIMS solves the transport equation using the collision probability method. Annular, spherical and plate geometries are available. The collision probabilities between different shells of the TRISO particle are first evaluated, followed by the cross particle transmission probability. This collision probability solution is used first to derive shielded multigroup cross sections, and then to solve the flux equation.

The solution to the transport equation can then be used to calculate effective 'particle + matrix' cross sections. These can be used to construct lattice or full-core calculations as shown in Fig. 1.

3.2. Implementation in MONK

In MONK, neutron transport through regions containing TRISO particles is generally treated using Woodcock Tracking. This is an efficient representation of the geometry, as there may be several thousand particles in any given region, and explicitly tracking neutrons across such a large number of surfaces is computationally expensive. TRISO particles are randomly placed into a containing body. Neutrons are tracked through the containing body, and 'pseudo collisions' are used to distinguish between different regions of the particles and surrounding matrix, avoiding the need for explicit surface tracking. Alternatively, an explicit surface-tracking treatment, where the user directly specifies the coordinates of every particle, is obviously possible.

MONK can be used to perform a standalone calculation, to generate effective multigroup cross sections for use in WIMS, or to perform a 3D flux solution using multigroup cross sections prepared by WIMS. MONK can perform calculations using continuous energy data libraries, or perform self-shielding for TRISO particles based on subgroup theory.

In particular, MONK contains dedicated geometry options for PBMRs, which generate random distributions of pebbles within a containing cone or annulus body. In a PBMR, the locations of all the pebbles in the reactor are not known. It is possible to approximate the geometry using a regular array of pebbles, but this is unrealistic, and leads to the presence of neutron streaming paths due to the regularity of the array. A more realistic approach can be used in MONK, where each layer of pebbles in turn is randomly oriented and dropped into the spaces in the layer beneath it. In this manner, a realistic core geometry is built up layer by layer. This has been shown to lead to reduced leakage relative to a regular array of pebbles [21]. An example pebble packing model is shown in Fig. 2.

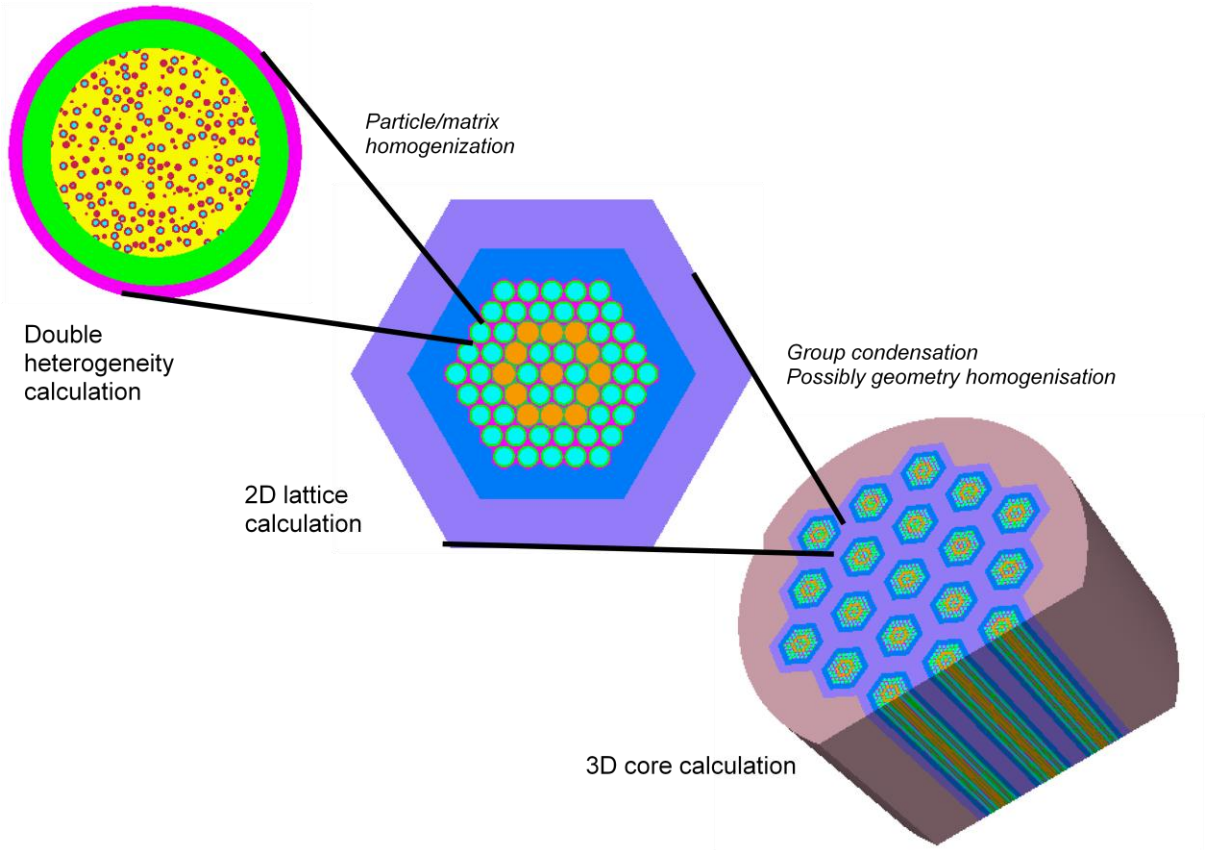

Fig. 1. Multi-scale core modelling approach in WIMS. HTR pebbles, cylinders and plates can be analysed using double-heterogeneity modelling. A lattice calculation can then be used to model complicated assembly geometries. This allows equivalent cross sections to be generated for multigroup core diffusion theory calculations, or alternatively a full 3D multigroup transport solution of the core.

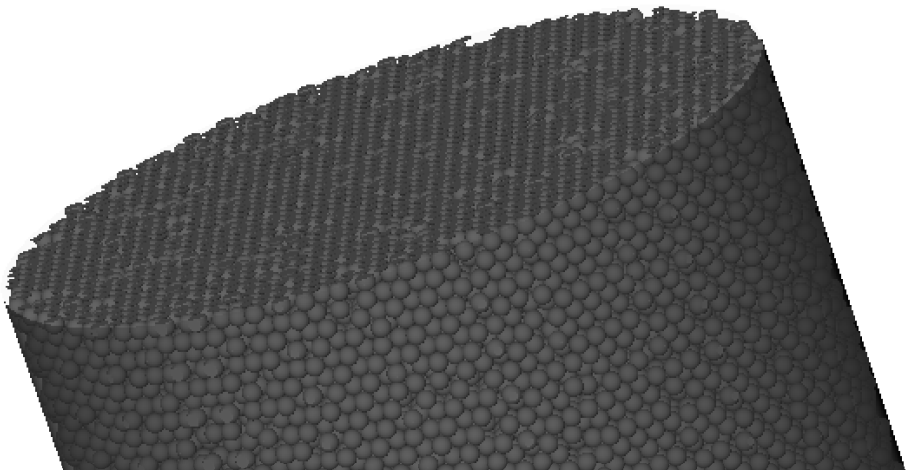

Fig. 2. MONK model of pebbles packed into a cylindrical vessel

3.3 Effect of particle heterogeneity

The effect of modelling the TRISO particles and matrix explicitly relative to considering them as a homogenized medium is known to be large – of the order of 1000s of pcm. This is demonstrated here with WIMS and MONK for a simple test case of a square pincell containing a graphite cylindrical compact fuel element with enriched UO_2 TRISO particulate fuel and helium coolant (Fig. 3). The inner and outer pin radii were 2.5 cm and 3 cm respectively, the TRISO packing fraction was 9% and the

TRISO particle outer radius was 0.0455 cm. MONK was run with the WIMS 172-group data library rather than a continuous energy data library to isolate the effect of differences in geometry modelling and self-shielding treatment.

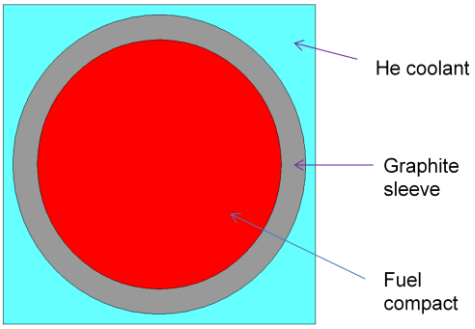

Fig. 3. Simple lattice model used for particle heterogeneity study

Results for k-infinity in WIMS10 and MONK10 are given in Table 1. Results are given for treatment of TRISO particles, and for a case where the TRISO particles and matrix material are homogenized. WIMS and MONK were generally in good agreement. Homogenizing the TRISO particles and matrix gives a substantial underestimate in k-infinity of more than 3000 pcm. This effect is consistent with published results for particulate geometries (e.g. Ref. [22]). This difference increases slightly with burn-up in this case: in WIMS the difference becomes ~4000 pcm at a burn-up of 40 GWd/t.

Table 1. Effect of Particle Heterogeneity on k-infinity

	WIMS	**MONK**	**Difference (pcm)**
TRISO k-infinity	1.463119	1.471311	–381
Homogeneous k-infinity	1.399399	1.399824	–21
Difference (pcm)	–3112	–3471	

4. Application to SmAHTR

4.1 Background

The AHTR is being developed by ORNL, Sandia National Laboratory and UCB [23]. The reactor concept is similar to the gas-cooled VHTR concept, except that it is filled with liquid salt coolant instead of gaseous coolant, and utilises TRISO fuel in plates. The liquid salt coolant is advantageous for passive decay heat removal, as the liquid salt can still efficiently remove decay heat in the event that the primary circuit is depressurized. There is also a lower temperature difference across the core, leading to improved thermodynamic efficiency relative to gas-cooled reactors. The proposed salt is a mixture of lithium fluoride and beryllium fluoride ('FLiBe'). One of the main advantages of the FLiBe is its high boiling point, which is above 1400 °C. Moreover, it also has a high volumetric heat capacity of 4670 kJ/m^3 °C [24]. These features allow the AHTR to achieve a very high core power density and to operate at significantly low system pressure (less than 1 MPa) while producing a high outlet temperature, more than ~700 °C. Furthermore, this high operating temperature extends the functionality of the reactor for other high temperature applications, such as hydrogen production. Nevertheless, the main disadvantage of the AHTR is the requirement for a novel coolant, which introduces potential corrosion issues and leads to the production of undesirable activation products.

The SmAHTR is a small modular version of the AHTR developed by ORNL [25]. It has a thermal power of 125 MW. It is envisaged to have 9 fuel assembly columns in a hexagonal layout. The design considered here utilises solid cylindrical fuel elements, although recent designs include plate-type assemblies [17]. The core dimensions are given in Table 2. A diagram of the core is shown in Fig. 4.

ORNL calculations of the equilibrium core utilize 3D Monte Carlo multigroup depletion within SCALE. The Dancoff factor is calculated by finding a value for the multigroup solution which reproduces the

multiplication factor of the reference continuous energy KENO-VI Monte Carlo solution [17]. This has been shown to be in excellent agreement with continuous energy Monte Carlo reference results [22].

Table 2. Solid cylindrical fuel SmAHTR core component dimensions. (Data from Ref. **[26]**)

Component	Subcomponent	Dimension	Size (cm)
Fuel pins (72 fuel pins per fuel assembly)	Fuel pin	Radius	1.1
		Pitch	3.08
		Height	80
	Fuel pin cladding	Outer radius	1.4
Graphite pins (19 pins per fuel assembly)	Graphite pin	Radius	1.4
		Pitch	3.08
		Height	80
Graphite fuel block (5 blocks arranged vertically)	Coolant cylinder	Radius	16.94
		Height	80
		Pitch	45
Radial Reflector	Graphite Reflector	Outer radius	150
		Height	400

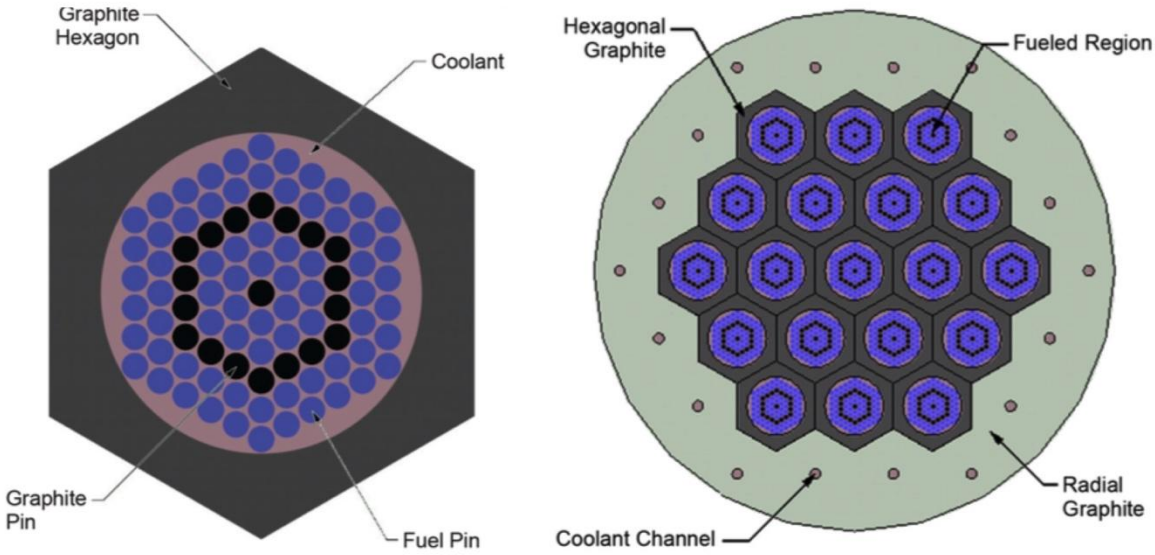

Fig. 4. (Left) Fuel assembly configuration. (Right) SmAHTR core cross section. (Reproduced from Ref. **[26]**)

4.2. Method

In WIMS, SmAHTR is analysed using the following calculation route:

- calculation of geometry-specific 172-group cross sections using subgroup theory;
- calculation of 172-group cross sections for remaining nuclides with equivalence theory;
- collision probability solution to double-heterogeneity problem using collision probability method to calculate effective 'smeared' TRISO-matrix cross sections;
- 2D method-of-characteristics solution to 172-group transport equation for hexagonal fuel assembly;
- reconstruction of fluxes and cross sections in fuel kernels for depletion calculation

A 'single heterogeneity' model of a single TRISO particle is used for the equivalence theory calculation, while a double heterogeneity model for the subgroup and collision probability calculations consist of TRISO particles within a single cylindrical fuel pin. The modelling of the surrounding environment in each of these models (e.g. whether to consider the influence of surrounding materials as equivalent shells or annuli) and the selection of equivalence theory model was to an extent selected using engineering judgement, so further work is required to justify the exact modelling

assumptions employed. The fuel assembly model created in WIMS is shown in Fig. 5. For simplicity, the WIMS model was designed with a hexagonal border, instead of a circular border for the coolant channel.[1] In doing so, the distance from the centre of the assembly to the hexagonal border was also adjusted in order to preserve the graphite moderator and coolant volumes of the original model. While this will have some effect on the power peaking within the assembly, it will not have a large impact on the reactivity or reactivity coefficients, which are the subject of the present study.

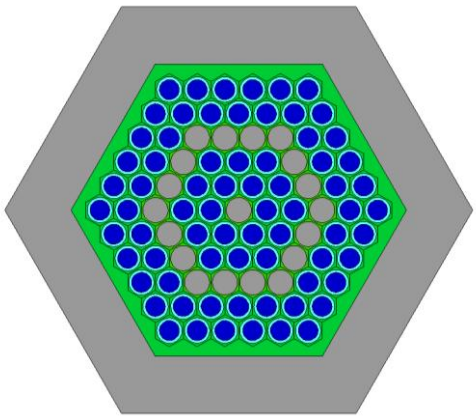

Fig. 5. WIMS model of the SmAHTR assembly

A 3D continuous-energy Monte Carlo reactor physics burn-up calculation code Serpent was also used to verify WIMS analysis. Serpent was initially developed at the VTT Technical Research Centre of Finland in 2004. Since then, it has been widely used for various applications, such as modelling of various reactors, including research reactors, small modular reactors and any closely coupled system, or performing fuel cycle studies involving assembly-level burn-up calculations, and many others [27].

For this study, an infinite lattice of the SmAHTR assembly was modelled and the criticality calculations throughout its depletion period were performed using ENDF/B-VII nuclear data libraries in order to be consistent with WIMS analysis. The statistical error in the Serpent calculations was around 32 pcm. To model the TRISO particles with the graphite matrix, Serpent allows users to explicitly specify the coordinate of each TRISO particle. Additionally, Serpent has a built-in feature, called 'disperse', that can help users to generate random particle or pebble distributions for a given packing fraction [28]. Interestingly, by implementing the SHAKE algorithm, Serpent can generate random coordinates for TRISO particle for relatively high packing fractions in various containing bodies (sphere, cylinder, cube, annular cylinder, cuboid and parallelepiped). Fig. 6 below shows the cross section of the compacted TRISO fuel pin with a 50% packing fraction that was created in Serpent.

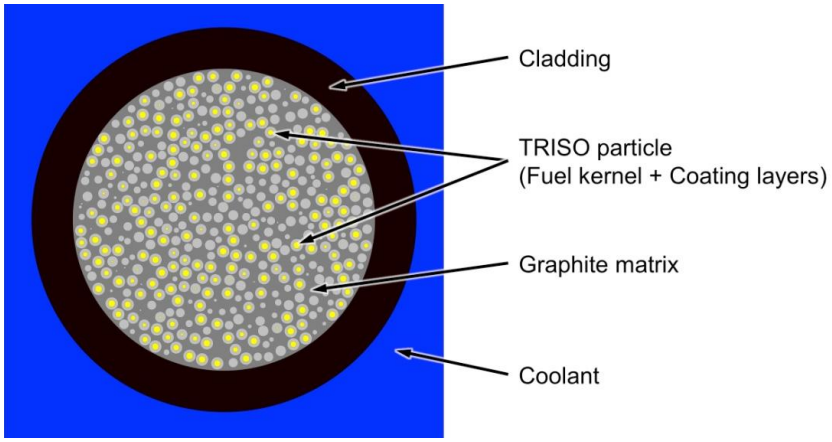

Fig. 6. Cross section of TRISO fuel pin that is modelled in Serpent.

[1] It should be noted that WIMS is also capable of modelling the plate-fuelled SmAHTR core geometry with a circular coolant channel.

4.3. Results

Beginning of life (BOL) k-infinity values found using WIMS10 and Serpent are given in Table 3. Results are presented for the heterogeneous representation of the TRISO fuel, and for the model where the TRISO particles and surrounding matrix are homogenized. The codes are in excellent agreement for both models. The flux spectrum in the TRISO particles from WIMS is shown in Fig. 7.

Table 3. Beginning of life WIMS and Serpent results for the SmAHTR assembly

Code	Heterogeneous	Homogenous	Difference between Heterogeneous and Homogenous (pcm)
WIMS	1.500685	1.467786	–1494
Serpent	1.49762	1.47378	–1080
Discrepancy (pcm)	61	–277	

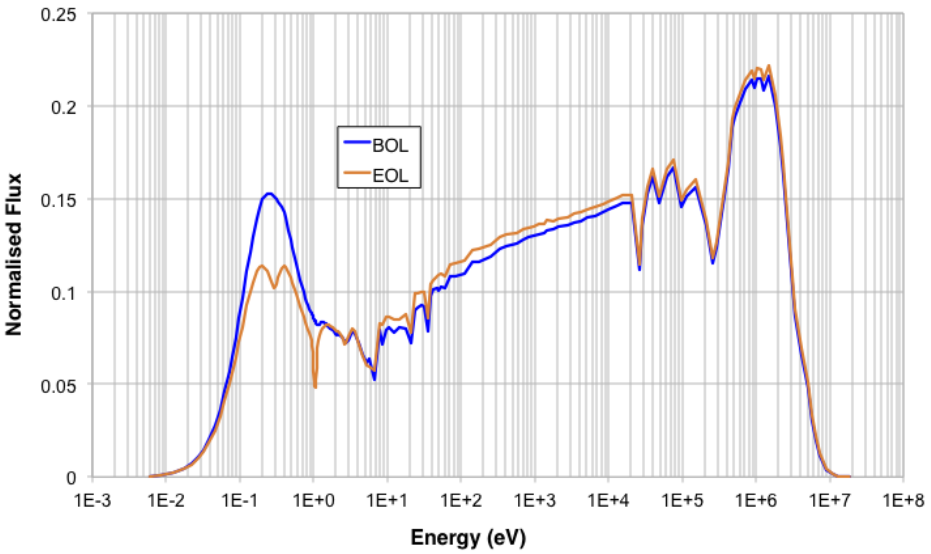

Fig. 7. Flux spectrum at BOL and end of life (EOL) in the TRISO particles

The variation in k-infinity with operating time is plotted in Fig. 8. The discrepancy between WIMS and Serpent remains under 200 pcm until 1000 effective full power days (EFPD), although beyond this the discrepancy increases somewhat. With the homogeneous fuel model, the discrepancy in k-infinity between WIMS and Serpent remains low throughout the depletion. As before, the heterogeneous effect of the TRISO particles increases slightly with burn-up, and k-infinity for the homogeneous fuel model is ~1700 pcm lower than with explicit particle modelling after 1400 EFPD.

Finally, the cycle length in WIMS was estimated by estimating the core leakage. For a cylindrical core of radius 1.5 m and height 4 m, a homogeneous buckling calculation gave an estimated leakage of 7%. This is very much a first approximation, and no substitute for a full-core calculation, but does allow results to be compared to the results in Ref. [26] (Table 4). Results for cycle length, initial reactivity and reactivity coefficients were generally in good agreement with the ORNL calculations, again increasing confidence in results.

Table 4. SmATHR cycle parameters in WIMS compared to ORNL calculations

Parameter	Reference Design [26]	WIMS analysis
Excess reactivity for fresh core (pcm)	26,940	26,750
BOL k-effective	1.368738	1.36518
Cycle length (years)	3.52	3.58
BOL fuel temperature coefficient (pcm/K)	–2.49	–2.34
BOL coolant temperature coefficient (pcm/K)	–0.3	–0.63

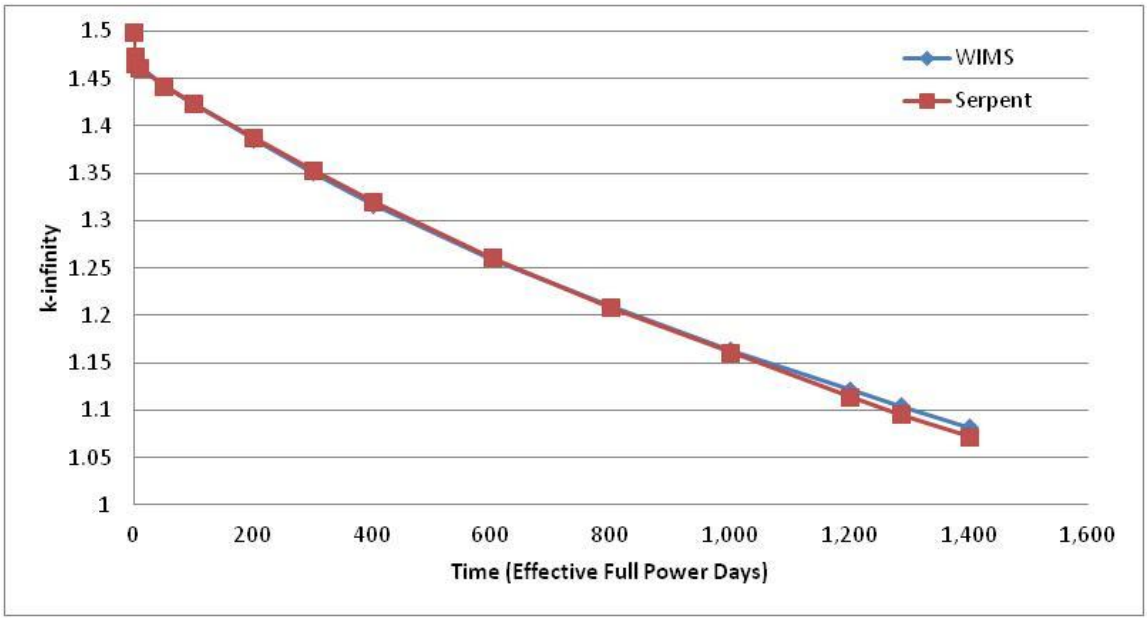

Fig. 8. k-infinity of a SmAHTR assembly (heterogeneous fuel model) in WIMS and Serpent

5. Conclusions

TRISO fuel modelling methods have been implemented in the ANSWERS deterministic reactor physics code WIMS and the Monte Carlo code MONK. The modular structure of WIMS allows these methods to be readily applied within the framework of a multi-scale approach, i.e. considering the particular environment of the TRISO fuel compact, an assembly (if applicable), and the full reactor core.

In this paper, a deterministic calculation methodology is developed for the SmAHTR design, which utilizes a liquid salt coolant, cylindrical fuel compacts and hexagonal assemblies. The subgroup method is used to generate multigroup cross section; the collision probability method is used to generate equivalent cross sections for the TRISO particles and surrounding matrix; and the method of characteristics is used to perform a lattice calculation for the assembly Burn-up dependent k-infinity is in excellent agreement with reference calculations performed using the VTT Monte Carlo code Serpent with explicit modelling of TRISO particles and with ORNL results reported in the literature. Cycle length and reactivity coefficients are also consistent with previously reported values. This methodology is readily applicable to other HTR designs. Future work will focus on progressing from the lattice calculations presented here to full-core deterministic transport calculations for small modular designs of HTR.

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