Benchmark Specification for HTGR Fuel Element Depletion

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I. Introduction

There are currently several on-going High Temperature Gas-cooled Reactor (HTGR) development projects underway throughout the world with the U.S. DOE Next Generation Nuclear Plant (NGNP) representing a significant and growing activity in the United States. HTGR designs utilize graphite-moderated fuel forms and helium gas as a coolant. There are two main forms of HTGR fuels: pebbles are used in the Pebble Bed Reactor (PBR), while cylindrical rods (or compacts) are used in the modular high temperature gas cooled reactor (MHTGR). In PBRs, fuel elements are ~6-cm-diameter spheres; in MHTGRs, the fuel elements are graphite rods that are inserted into graphite hexagonal blocks. In both systems, fuel elements (spheres and rods) are comprised of tristructural-isotropic (TRISO) fuel particles. The TRISO particles are either dispersed in with the matrix of a graphite pebble for the pebble bed design or molded into compacts/rods that are then inserted into the hexagonal graphite blocks. In general, fuel grains have a density of a few hundred grains per cm^3.

The HTGR concept is a significant departure from LWR designs. As such, existing reactor analysis methods and data will be confronted by significant changes in the physics of neutron slowing down, absorption, and scattering. Furthermore, the use of localized fuel grains within a larger fuel element result in two levels of heterogeneity that will challenge many existing lattice physics methods. Hence, there is a need for advanced methods for treatment of both levels of heterogeneity effects. In doubly-heterogeneous (DH) systems, heterogeneous fuel particles in a moderator matrix form the fuel region of the fuel element (pebble or rod) and thus constitute the first level of heterogeneity. Fuel elements themselves are also heterogeneous with fuel and moderator or reflector regions, forming the second level of heterogeneity. The fuel elements may also form regular or irregular lattices.

Continuous energy (CE) methods are able to explicitly represent the dynamics of neutron slowing down in a heterogeneous environment with randomized grain distributions, but traditional tracking simulations can be extremely slow, and the large number of grains in a fuel element may often represent an extreme burden on computational resources. A number of approximations or simplifying assumptions have been developed to simplify the computational process and reduce the effort. Multigroup (MG) methods, on the other

hand, require special treatment of DH fuels in order to properly capture resonance effects, and generally cannot explicitly represent a random distribution of grains due to the excessive computational burden resulting from the spatial grain distribution. The effect of such approximations may be important and has potential to misrepresent the spectrum within a fuel grain.

Depletion methods utilized in lattice calculations typically rely on point depletion methods, based on the isotopic inventory of fuel depleted, assuming a single localized neutron flux. This flux is generally determined using either a CE or MG transport solver. Hence, in application to DH fuels, the primary factor influencing the accuracy of a depletion calculation will be the accuracy of the local flux calculated within the transport solution and the cross sections

The current lack of well-qualified experimental measurements for spent HGTR fuel elements limits the validation of advanced DH depletion method. Because of this shortage of data, this benchmark has been developed as the first, simplest phase in a planned series of increasingly complex set of code-to-code benchmarks. The intent of this benchmark is to encourage submission of a wide range of computational results for depletion calculations in a set of basic fuel cell models. Comparison of results using independent methods and data should provide insight into potential limitations in various modeling approximations. The benchmark seeks to provide the simplest possible models, in order to minimize the effect of competing and potentially offsetting phenomena that might mask weaknesses in given methods.

II. Benchmark Specification

This benchmark consists of three parts – a calculation of depletion in an infinite lattice of TRISO fuel grains, a depletion calculation for pebbles representative of PBMR fuel, and a similar calculation for an infinite lattice supercell representative of a prismatic MHTGR assembly lattice. The grain and pebble calculations may be performed in one or three dimensions; the prismatic lattice calculation is essentially a two-dimensional, infinite height model suitable for two- and three-dimensional methods. Participants are urged to perform and submit calculations for any or all configurations, based on available code capabilities. Participants are also encouraged to provide multiple submissions using different codes or data, where available.

A. Fuel Specifications

This benchmark consists of depletion calculations for three different configurations – the first an infinite lattice of grains, the second representative of a generic pebble-bed configuration, and the third based on the characteristics of an MHTGR prismatic fuel element. For simplicity, all models will be based on a single TRISO fuel element type design, although with different particle densities within the fuel element types (the density of the infinite grain-lattice model is based on the density of grains in the pebble design). Configurations 2 and 3 are based on an infinite lattice representation of fuel elements. Note that at 8.2 wt% enrichment, these TRISO fuel particles have a lower enrichment than anticipated for an MHTGR fuel design, which are expected to be at greater than 10% enrichment,

Data for the grain dimensions used in all three configurations are provided in Table 1, Table 2 provides isotopic concentrations for all compositions used in all configurations. Isotopic compositions and particle coating parameters have been selected based on specifications provided for a related benchmark [Ref 1]. The infinite lattice of grains and the pebble-bed fuel design have also been drawn from this reference; a representative design for a prismatic fuel lattice has been developed based on specifications available in Ref 2. For the purposes of this benchmark, all materials in all models are assumed to be at a uniform temperature of 293.6K. Details of the three models are provided below.

1. Infinite Lattice Grain Model

This model is intended to provide a baseline comparison on methods without requiring the complexity of a doubly-heterogeneous treatment. Effectively, it represents an infinite lattice of coated particles with a density based on that of the pebble bed fuel element described below. For straightforwardness, a cubic lattice is assumed such that a 9.043% packing fraction is attained. The fuel grains are spaced within the graphite matrix defined for both pebble bed and prismatic fuel models. Dimensions of this lattice are provide in Table 3, with grain dimensions and and isotopic concentrations as provided in Tables 1 and 2, respectively.

2. Pebble Bed Model

The pebble-bed model consists of a single fuel pebble in an infinite lattice. A cubic lattice is assumed for simplicity. Specifications for the pebble are provided in Table 3. The fuel pebble consists of a 2.5 cm radius fuel volume encased in a 3.0 cm radius (0.5cm thick) outer coating. The fuel volume contains a random dispersion of coated fuel particles within a graphite matrix. Regions outside the pebble are filled with coolant, helium. Pebbles are assumed to be in direct contact; i.e., the pebble-to-pebble pitch is 6.0 cm. Table 3 provides the pebble-to-pebble pitch for a cubic lattice for use in three-dimensional models; however, the equivalent coolant radius is also provided for use in one-dimensional models.

3. Prismatic Fuel Model

The prismatic fuel model is somewhat more complicated, requiring a supercell model including both fuel and coolant channels. Figure 1 shows a portion of the repeating lattice pattern. A rectangular, triangular, or hexagonal supercell may be used, taking advantage of symmetry with reflective boundary conditions. Fuel compacts are radially centered within each fuel channel; coolant channels and the fuel/channel gap are filled with helium. Because the fuel is assumed to be infinite in height, the model is essentially two-dimensional. The compact height given in Table 4 is for volume and particle density calculations only.

Table 1: Coated Particle Specification

Item	Units	Value
UO_2 fuel density	g/cm^3	10.4
Uranium enrichment (by mass ^{235}U / (^{235}U+^{238}U)	%	8.2
Fuel natural boron impurity by mass	ppm	1
Outer coated particle radius	mm	0.455
Fuel kernel radius	mm	0.25
Coating materials	-	C / C / SiC / C
Coating thickness	mm	0.09 / 0.04 / 0.035 / 0.04
Coating densities	g/cm^3	1.05 / 1.9 / 3.18 / 1.9

Table 2: Material Specifications

Material	Nuclide	Atoms per barn•cm
UO_2 fuel	U-238	2.12877e-02
	U-235	1.92585e-03
	O	4.64272e-02
	B-10	1.14694e-07
	B-11	4.64570e-07
Inner low-density carbon kernel coating	C (nat)	5.26449e-02
Pyro carbon kernel coatings (inner and outer)	C (nat)	9.52621e-02
Silicon carbide kernel coating	C (nat)	4.77240e-02
	Si (nat)	4.77240e-02
Pebble/compact carbon matrix	C (nat)	8.77414e-02
	B-10	9.64977e-09
	B-11	3.90864e-08
Pebble outer coating/Prismatic block	C (nat)	8.77414e-02
	B-10	9.64977e-09
	B-11	3.90864e-08
Helium coolant	He-3	3.71220e-11
	He-4	2.65156e-5

Table 3. Fuel Grain Lattice Data

Item	Units	Value
Unit cell grain square array pitch (cubical outer boundary)	cm	0.16341
Unit cell grain outer radius (spherical outer boundary)	cm	0.10137
Grain outer radius	cm	0.0455
Packing fraction of coated particles	%	9.043
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
UO_2 fuel mass per pebble	g	6.806E-4

Table 4. Pebble Bed Fuel Lattice Data

Item	Units	Value
Unit cell pebble square array pitch (cubical outer boundary)	cm	6.0
Unit cell coolant outer radius (spherical outer boundary)	cm	3.53735
Pebble radius	cm	3.0
Radius of fuel zone	cm	2.5
Pebble outer carbon coating thickness	cm	0.5
Pebble outer carbon natural boron impurity by mass	ppm	0.5
Number of coated particles per pebble	-	15,000
Packing fraction of coated particles	%	9.043
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
Pebble outer carbon coating density	g/cm^3	1.75
UO_2 fuel mass per pebble	g	10.210

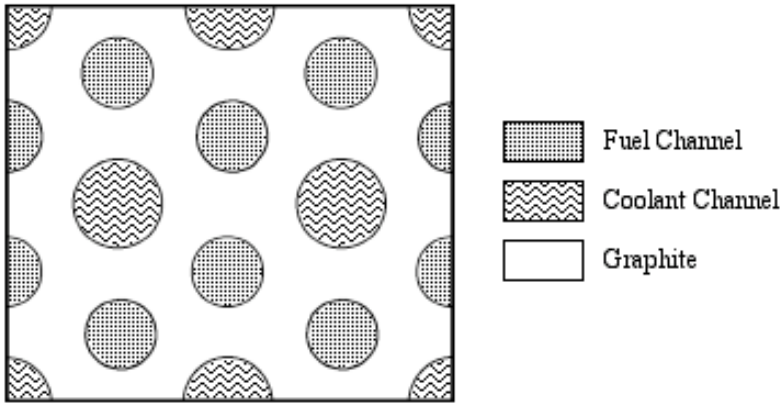

Figure 1. Prismatic assembly lattice pattern.

Table 5. Prismatic Fuel Lattice Data

Item	Units	Value
Triangular pitch (coolant channel-rod channel and rod channel-rod channel)	cm	1.880
Fuel channel diameter	cm	1.270
Coolant channel diameter	cm	1.588
Fuel compact (centered in fuel channel) diameter	cm	1.245
Compact height	cm	4.93
Number of coated particles per compact	-	6,000
Packing fraction of coated particles	%	12.560
Graphite matrix density	g/cm^3	1.75
Graphite matrix natural boron impurity by mass	ppm	0.5
UO_2 fuel mass per compact	g	4.084

B. Depletion Calculations

Depletion calculations are to be performed for each model. Results (described below) are to be reported for fresh fuel and for burnup steps of 0.5, 5, 10, 20, 40, 80, and 120 GWd/tonne initial uranium (intermediate burnup steps should be performed as appropriate to ensure accurate depletion). Depletion is to be performed at a constant power of 62 MW/tonne initial uranium, assuming continuous burnup with no downtime. Both fuel and the graphite matrix (boron impurities) should be depleted.

Reported results are as follows:

- Infinite multiplication factor
- Spectral indices (assuming a fast/thermal boundary at 0.625eV)
  - $\rho^{238} = {}^{238}U_{cap}(fast) / {}^{238}U_{cap}(thermal)$
  - $\delta^{235} = {}^{235}U_{fis}(fast) / {}^{235}U_{fis}(thermal)$
  - $\delta^{238} = {}^{238}U_{fis} / {}^{235}U_{fis}$
  - $c/f^{235} = {}^{238}U_{cap} / {}^{235}U_{fis}$
- Nuclide concentrations (grams/tonne initial U)
  - Actinides: ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{244}Cm, and ^{245}Cm
  - Fission Products: ^{85}Kr, ^{90}Sr, ^{110m}Ag, ^{137}Cs, ^{135}Xe, ^{149}Sm, and ^{151}Sm
- Volume-averaged energy-dependent spectrum in fuel pebble/compact (using participant's own group structure).

To be able to include calculations from as many different methods as possible, depletion calculations are to be performed without a critical spectrum correction.

Reflective/mirror boundary conditions should be used where available; white boundary conditions may be used where reflection is not an option.

C. Reporting of Results

Each submission should include the following information:

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- Date
- Organization
- Contact person
- E-mail address of the contact person
- Computer code(s) used
- Description of the analysis environment, including neutron data library source, group structure and data processing method (for MG), description of code system, geometry modeling approach, convergence limit or statistical errors for the eigenvalue calculations, assumptions/approximations in treating double heterogeneity, and any other relevant information.
- Keyword GRAIN, followed by results for infinite lattice grain (if grain depletion was performed

- Keyword PEBBLE, followed by results for pebble bed fuel (if pebble bed depletion was performed)
- Keyword PRISM, followed by results for prismatic fuel (if prismatic fuel depletion was performed).

A set of worksheets than may be used to report the above information is attached in the Appendix. This spreadsheet will also be provided electronically with this specification.

Results are to be transmitted electronically to: vhtr@ornl.gov. Multiple submissions calculations using different approaches or data are permitted and even encouraged.

III. References

1. G. Hosking and T. D. Newton, "Benchmark specification for an HTR fuelled with reactor grade-plutonium (or reactor-grade Pu/Th and U/Th): Proposal," NEA/NSC/DOC(2003)22, March 2005.

2. Y. Kim, C. Cho, and F. Venneri, "Long-Cycle and High-Burnup Fuel Assembly for the VHTR," Journal of Nucl. Sci. and Tech., pp 294-302, Vol. 44, No. 3, 2007.

Appendix

Worksheets are provided in which benchmark results can be recorded and reported. These worksheets will also be transmitted in electronic format.

Basic Information	
Date	
Organization	
Contact Person	
Contact Email	
Computer code(s) used	
Analysis Environment	
Neutron data library/source	
Group structure	
Data processing method	
Convergence limit or statistical error on eigenvalues	
Other related information	

GRAIN Results								
Burnup (GWd/t)	**0**	**0.5**	**5**	**10**	**20**	**40**	**80**	**120**
k-inf								
ρ^{238}								
δ^{235}								
δ^{238}								
c/f^{235}								
Actinide masses (g/t initial U)								
U-235								
U-238								
Pu-239								
Pu-240								
Pu-241								
Pu-242								
Am-241								
Cm-244								
Cm-245								

Fission product masses (g/t initial U)								
Kr-85								
Sr-90								
Ag-110m								
Cs-137								
Xe-135								
Sm-149								
Sm-151								
Volume-averaged spectrum in grain								
Group midpoint energy (eV) i = 1,ng								
Group flux (n/cm^2/sec), i = 1,ng								

PEBBLE Results								
Burnup (GWd/t)	**0**	**0.5**	**5**	**10**	**20**	**40**	**80**	**120**
k-inf								
ρ^{238}								
δ^{235}								
δ^{238}								
c/f^{235}								
Actinide masses (g/t initial U)								
U-235								
U-238								
Pu-239								
Pu-240								
Pu-241								
Pu-242								
Am-241								
Cm-244								
Cm-245								

Fission product masses (g/t initial U)								
Kr-85								
Sr-90								
Ag-110m								
Cs-137								
Xe-135								
Sm-149								
Sm-151								
Volume-averaged spectrum in grain								
Group midpoint energy (eV) i = 1,ng								
Group flux (n/cm^2/sec), i = 1,ng								

PRISM Results								
Burnup (GWd/t)	**0**	**0.5**	**5**	**10**	**20**	**40**	**80**	**120**
k-inf								
ρ^{238}								
δ^{235}								
δ^{238}								
c/f^{235}								
Actinide masses (g/t initial U)								
U-235								
U-238								
Pu-239								
Pu-240								
Pu-241								
Pu-242								
Am-241								
Cm-244								
Cm-245								

Fission product masses (g/t initial U)								
Kr-85								
Sr-90								
Ag-110m								
Cs-137								
Xe-135								
Sm-149								
Sm-151								
Volume-averaged spectrum in grain								
Group midpoint energy (eV) i = 1,ng								
Group flux (n/cm^2/sec), i = 1,ng								