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Physics Evaluation of Alternative Uranium-based Oxy-Carbide Annular Fuel Concepts for Potential Use in Compact High-Temperature Gas-cooled Reactors

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9 **ABSTRACT**

10 *Lattice physics calculations have been carried out to evaluate the performance and safety characteristics of a*
11 *modified high temperature gas-cooled reactor (HTGR) prismatic fuel block concept, based on the MHTGR-350*
12 *benchmark problem. Key changes were to replace the conventional Tri-Structural ISotropic (TRISO)-filled fuel*
13 *compacts with heterogeneous, multi-layer annular fuel pellets made with UCO, ThCO, or (U,Th)CO. These fuel*
14 *pellets have multiple protective cladding layers of pyrolytic carbon and silicon carbide, which will give it robust*
15 *qualities. With the increased loading of U-235 in the fuel block, it was necessary to replace up to 78 fuel holes and*
16 *42 coolant holes with a hydrogen-based moderator (⁷LiH), in order to ensure a thermal neutron energy spectrum in*
17 *the lattice. Calculation results demonstrate that the modified fuel concept has several advantages and some*
18 *challenges relative to the conventional MHTGR-350 design concept. With the increased uranium loading, and the*
19 *reduced neutron leakage due the use of ⁷LiH moderator rods, higher burnup levels and lower natural uranium*
20 *consumption levels can be achieved with the same level of uranium enrichment. In addition, the expected fuel*
21 *residence time increased by a factor of 20 or more, making such a concept very attractive for use in small, modular,*
22 *“nuclear battery” HTGRs that would only need to be fueled once. Calculation results for the current concept indicate*

23 *positive graphite and hydrogen moderator temperature coefficients, and further modifications will be required to*
24 *ensure a negative power coefficient of reactivity.*

25 **1. INTRODUCTION**

26 There is interest among governments, industry, and reactor vendors in the deployment of small
27 modular high temperature gas-cooled reactors (SM-HTGRs) [1], [2], [3], [4] for various
28 applications. The HTGRs that are currently under development use helium gas as the primary
29 coolant, and are moderated using graphite. Thus, HTGRs can operate at temperatures ($\geq 700^{\circ}\text{C}$)
30 that are much higher than in water-cooled reactors such as pressurized water reactors (PWRs)
31 and pressure tube heavy water reactors (PT-HWRs). With high operating temperatures, HTGRs
32 are well-suited for providing heat for a wider range of industrial processes and for higher
33 efficiency electrical power generation. A drawback for most HTGRs currently under
34 development, especially those with small cores, is their relatively high neutron leakage, and
35 their high fissile fuel consumption, which is much higher per unit energy generated than that of
36 PWRs [7], or PT-HWRs [8], [9], [10]. Their higher fissile consumption is primarily a consequence
37 of using tri-structural isotropic (TRISO) fuel particles and graphite moderator, which gives a
38 relatively low loading density of uranium. Hence, higher enrichments of uranium (typically
39 between 10 wt.% U-235 and 19.75 wt.% U-235) are needed to get sufficiently high burnup
40 levels and fuel residence time / operating life in an SM-HTGR core.

41 A TRISO particle is composed of a spherical kernel of fissionable material that is surrounded by
42 layers of graphite and SiC, and is less than 0.1 cm in diameter. TRISO particles have been
43 designed to be very robust, tough, and durable, performing very well in retaining fission
44 products (FP) under postulated accident conditions. A small HTGR core comprises hundreds of

45 millions of TRISO particles, the manufacture of which presents challenges, especially with
46 respect to quality control, for such small particles. Since TRISO particles comprise ~12 vol.%
47 fissionable material, the use of TRISO particles also limits the mass of fissionable material that
48 can be loaded in the core, which in turn necessitates the use of higher fuel enrichments, and
49 limits fuel residence time.

50 An alternative to TRISO particles that is proposed in this study is a multi-layer heterogeneous
51 annular fuel element that is in the order of 1 cm in diameter and several centimetres long. It is
52 somewhat similar to a conventional fuel element used in PWRs and PT-HWRs, but as a
53 modification, it uses additional protective layers to prevent the migration of FPs. Drastically
54 fewer of such fuel elements would be required in the core, and they could be designed to
55 enable the loading of a higher volume and mass of fissionable material in the core. Such fuels
56 retain the multi-layer barrier feature of TRISO fuels, in that multiple coatings are used to help
57 retain FPs. The performance of the alternative fuel element concept with respect to FP
58 retention is not evaluated in this study, but may be the topic of future studies.

59 The higher loading of fissionable material in the core requires augmenting neutron moderation
60 to achieve sufficient fuel burnup and residence time. In this study, elements comprising lithium
61 hydride (LiH) encased in silicon carbide are added to the fuel block in place of some of the fuel
62 compacts and coolant holes to provide extra moderation. LiH (using 99.995 at.% Li-7/Li) has
63 previously been investigated as a moderator for small reactors, especially for space
64 applications, due to its thermal stability, the moderating characteristics of hydrogen, and the
65 relatively low neutron capture cross-section of lithium-7 [6].

66 The purpose of this study is to evaluate the impacts on fuel consumption and reactivity
67 coefficients of using the proposed annular fuel elements in a representative HTGR, the
68 MHTGR-350 [11], [12], [13], as an alternative to using fuel compacts made of thousands of
69 TRISO particles in a graphite matrix. This study relies on infinite lattice physics calculations and
70 a 2-group neutron diffusion leakage model with geometric buckling in-lieu of full core
71 calculations. The proposed annular fuel element is analyzed with different levels of uranium
72 enrichment and with uranium-thorium fuel perturbations.

73

74 **2. HTGR FUEL CONCEPTS**

75 **2.1 REFERENCE PRISMATIC FUEL BLOCK**

76 The reference concept is a prismatic fuel block based on the MHTGR-350 (350 MWth / 165
77 MWe), which is the basis of an international benchmark exercise for prismatic block HTGRs
78 [11]. The MHTGR-350 uses prismatic fuel blocks (analogous to fuel assemblies in PWRs, and fuel
79 bundles in PT-HWRs) made of graphite, with holes for coolant (such as helium) and holes for
80 fuel compacts (which are analogous to fuel elements). The fuel compacts are made of TRISO
81 particles embedded in a surrounding graphite matrix. Neutron moderation is provided by the
82 graphite in the fuel and reflector blocks, the fuel compact matrix, and the graphite found in the
83 TRISO particles. The core comprises a hexagonal lattice of blocks, which is shown in Fig. 1. The
84 focus of this study is on the prismatic fuel block, which is described in more detail in the
85 remainder of this section.

86 The reference prismatic fuel block, which is shown in Fig. 2, comprises a hexagonal lattice of
87 fuel compacts and coolant channels that are embedded in graphite. Each cylindrical fuel
88 compact comprises TRISO fuel particles that are randomly dispersed in graphite. The fuel kernel
89 is uranium oxycarbide ($UC_{0.5}O_{1.5}$), the uranium of which is 15.5 wt.% U-235/U. The
90 specifications of the TRISO particles are provided in Table 1, and those of the fuel compacts and
91 fuel block are provided in Table 2, which are obtained from [12]. Three additional levels of
92 uranium enrichment are also analyzed in this study: 5, 10, and 19.75 wt.% U-235/U.

93 The lattice physics model of the hexagonal prismatic fuel block comprises a single layer of fuel
94 compacts, each of which is 4.928 cm in length and contains 6416 TRISO particles. In this model

95 the total power is 36 kW, which is the power per compact (172 W) multiplied by the 210 fuel
96 compact locations per fuel block, and rounded to the nearest kW. The reference temperatures
97 of the materials in the fuel block are based on thermal-hydraulics calculations presented in [13],
98 the results of which are averaged and rounded to the nearest 5 K, and are shown in Table 3.
99 The composition of $UC_{0.5}O_{1.5}$ is identical to that of [13], and is shown in Table 4.

100 **2.2 PRISMATIC FUEL BLOCK WITH ANNULAR-TYPE FUEL PELLETS**

101 In a modified fuel block with annular-type fuel pellets, the fuel compacts of the reference fuel
102 block are replaced with heterogeneous, multi-clad, annular fuel elements in which the fuel is in
103 the form of two concentric, hollow cylinders as is shown in Fig. 3.

104 The purpose of having two annular fuel layers is for evaluating more heterogeneous fuel
105 element design concepts, such as those with enriched uranium on the outside (in the form of
106 UO_2 , UCO , UC , or UN) and using a fertile material on inside, either thorium (in the form of ThO_2 ,
107 $ThCO$, ThC , or ThN) or a mix of thorium and depleted uranium (DU) (in the form of $(Th,DU)O_2$,
108 $(Th,DU)CO$, $(Th,DU)C$ or $(Th,DU)N$).

109 A fuel element, including endcaps, extends from the bottom to the top of the 79-cm high
110 prismatic fuel block. The lattice physics model comprises a 4.928 cm long mid-section of this
111 element, which excludes the endcaps.

112 The materials that comprise the fuel element are listed in Table 5. The non-fuel material (i.e.,
113 the carbon-based materials and SiC) are identical to those in the TRISO fuel of the reference
114 concepts.

115 Table 6 lists the annular fuel element concepts that are analyzed in this study to evaluate the
116 effects of varying fissionable materials in the fuel annuli. Three of these concepts have 100%
117 uranium with enrichments of 5, 10, and 19.75 wt.% U-235/U, respectively. The other concepts
118 comprise roughly equal volumes of uranium and thorium, which are either blended or in
119 separate fuel annuli. One of these concepts includes depleted uranium blended with Th for the
120 purpose of reducing the weight fraction of U-233 in uranium in the spent fuel, to help improve
121 proliferation resistance. The nuclide compositions for each type of fuel are listed in Table 7.

122 Thorium is considered an attractive alternative fertile fuel, since it is abundant (nearly 3 to 4
123 times as abundant as uranium) and can be used to complement and extend uranium resources
124 [20]. Previous studies have shown that thorium-based fuels can help increase fuel burnup and
125 uranium utilization, and thorium-based fuels can give more negative fuel temperature reactivity
126 coefficients (FTRCs), which is advantageous for enhanced safety [8], [9], [10].

127 The annular fuel element contains a larger volume of fuel than that of the reference fuel
128 compact, with the fuel element and fuel compact comprising 3.88 cm³ and 0.26 cm³ of fuel,
129 respectively. The difference in fuel volume is substantial, differing by a factor of $\sim 3.88/0.26$
130 ~ 14 . The larger volume of fuel in the annular fuel element design concept permits longer fuel
131 residence times due to reduced specific power, since the total power is the same as in the
132 reference concept.

133 The added fuel also replaces a large quantity of graphite in the compact. This change, combined
134 with the large increase in fuel volume, significantly reduces the ratio of carbon to fissile
135 uranium atoms (or any fissile atoms), C/U-235, and thus significantly reduces moderation, and
136 thus makes the neutron energy spectrum become harder, faster, and non-thermal. As a result,

137 the hardening of the neutron energy spectrum will make the fuel block sub-critical (k -effective
138 ≤ 1.000 ; k -infinity ≤ 1.000) due to insufficient moderation.

139 The reference fuel design for the MHTGR-350 with TRISO fuel particles has already been
140 optimized (or nearly optimized) to achieve the C/U-235 ratio that achieves sufficient
141 moderation to create a thermal neutron energy spectrum, and also achieves sufficiently high
142 reactivity (k -infinity). Thus, any significant changes to the loading of fissile fuel in the prismatic
143 fuel block is going to require other modifications to maintain a thermal neutron energy
144 spectrum.

145 Thus, the replacement of fuel compacts with annular fuel elements also requires the
146 replacement of several fuel elements and coolant channels with special moderator elements to
147 improve moderation to achieve a fuel block that is super-critical in the core at the beginning of
148 cycle (BOC). The configuration of moderator elements in the fuel block is shown in Fig. 4. This
149 alternative configuration has 108 moderator holes on the outside, 12 moderator holes on the
150 inside, 132 fuel holes, and 66 coolant holes. The number of fuel and coolant holes have been
151 reduced from the original reference design (210 fuel holes, 108 coolant) holes by approximately
152 40% ($132/210 \sim 0.63$; $66/108 \sim 0.61$).

153 Each moderator element comprises a cylindrical ${}^7\text{LiH}$ pellet (0.73 cm radius) encased in SiC
154 cladding (0.794 cm outer radius). Lithium hydride (${}^7\text{LiH}$) is chosen for the additional moderation
155 since it is a more “efficient” moderator than carbon in graphite, with a much shorter slowing-
156 down distance. The Li is enriched to 99.995 at.% Li-7/Li to reduce neutron capture in Li-6 nuclei.

157

158 **3. EVALUATION CRITERIA**

159 **3.1 FUEL CONSUMPTION**

160 Annual fuel consumption (Q_{EU}) for a full SM-HTGR core is calculated for each concept using
161 Equation (1). In a 3-batch fueling scheme, the mass of fresh fuel that is loaded into the core
162 during refueling is 1/3 of the mass of fuel in the core, and the interval of time between
163 refueling is 1/3 of the fuel residence time. Equations (2) and (3) are used to calculate the annual
164 natural uranium (NU) consumption (Q_{NU}), where \mathbf{R} is the NU feed to enriched uranium product
165 ratio.

$$Q_{EU} = \frac{L_{EU}}{T} \quad (1)$$

$$\mathbf{R} = \frac{\mathbf{x}_p - \mathbf{x}_t}{\mathbf{x}_f - \mathbf{x}_t} \quad (2)$$

$$Q_{NU} = Q_{EU} \mathbf{R} \quad (3)$$

L_{EU} is the mass of enriched uranium that is loaded into the core during refueling (i.e.,
1/3 of the core for 3 batch refueling).

T is the duration between refueling (i.e., 1/3 of the fuel residence time for 3 batch
refueling).

\mathbf{x}_p is the wt.% of U-235 in enriched uranium.

\mathbf{x}_f is the wt.% of U-235 in NU, which is assumed to be 0.711 wt.% U-235/U.

x_t is the wt.% of U-235 in the enrichment tails, which is assumed to be 0.2 wt.%
U-235/U.

166 In this study there are four grades of enriched uranium that are used in the fuel concepts: 5
167 wt.% U-235/U ($R = 9.4$), 10 wt.% U-235/U ($R = 19.2$), 15.5 wt.% U-235/U ($R = 29.9$), and 19.75
168 wt.% U-235/U ($R = 38.3$).

169 **3.2 REACTIVITY COEFFICIENTS**

170 Fuel, graphite, and hydrogen moderator temperature coefficients of reactivity are calculated
171 over a range of temperatures and burnups. For each annular fuel concept, Table 8 shows the
172 burnups and material temperatures at which k_{inf} (infinite multiplication factor) is calculated
173 using SERPENT 2. The same values, excluding the hydrogen-based moderator compact
174 temperature variations, are also used for the reference TRISO fuel concepts. Within each row of
175 Table 8, a SERPENT 2 calculation is conducted for each combination of burnup fraction (i.e., the
176 associated fuel composition at a given burnup level) and temperature of the material in the
177 right-most column, with the temperatures of all other materials set to their respective
178 reference values. The k_{inf} are then used to calculate the temperature coefficients of reactivity
179 over the range of temperatures $[T_1, T_2] = [300 \text{ K}, 600 \text{ K}]$, $[600 \text{ K}, 900 \text{ K}]$, $[900 \text{ K}, 1200 \text{ K}]$, and $[1200$
180 $\text{ K}, 1500 \text{ K}]$ at the indicated burnup (B) using Equation (4).

$$C(B, T_1, T_2) = \frac{k_{inf}(B, T_1) - k_{inf}(B, T_2)}{T_1 - T_2} \quad (4)$$

181 **4. METHODS**

182 **4.1 LATTICE PHYSICS CALCULATIONS**

183 The lattice physics calculations are performed using the SERPENT 2 (version 2.1.31) Monte
184 Carlo (MC) neutron transport and burnup/depletion code [15]. SERPENT 2 calculates the
185 continuous energy neutron flux in two-dimensional (2D) or three-dimensional (3D) geometries
186 using MC methods to simulate neutron histories, and it calculates the evolution of fuel
187 composition with burnup.

188 All results presented in this document are calculated using the ENDF/B-VII.0 nuclear data library
189 that is distributed with SERPENT 2. The results are calculated on the Minerva cluster using 550
190 generations (or cycles), with 2 million neutrons per generation. The first 50 generations are
191 used to achieve convergence of the criticality source calculation and are not included in the
192 calculation of the reaction rates and output data statistics.

193 The cross-section and thermal scattering data that is used for the given material temperature
194 are listed in Table 9. Each material temperature matches the temperature at which the
195 corresponding cross-section data were evaluated. With respect to thermal scattering data,
196 there is no graphite data at 300 K, 900 K, or 1500 K. Instead, the thermal scattering data
197 evaluated at the nearest lower temperature is used at these material temperatures. The
198 material densities in the model are not modified in these calculations.

199 No thermal scattering data is used for the LiH moderator compacts due to there being no such
200 data for Li-bound hydrogen.

201 **4.2 CALCULATION OF K-EFFECTIVE**

202 All SERPENT calculations of the lattice physics model of a single prismatic fuel block are
 203 conducted using reflective boundary conditions on a fuel block. To calculate the effective
 204 neutron multiplication factor (k-effective, or k_{eff}) considering expected neutron leakage in a full,
 205 finite-sized reactor core, a 2-group diffusion leakage model with homogenized cross-sections
 206 generated by SERPENT 2 is used along with a user-defined geometric buckling value associated
 207 with the full finite core geometry. The formula for calculating k_{eff} is given in Equation (5). This
 208 calculation provides an approximate value of k_{eff} for comparison purposes in this study. A more
 209 accurate value of k_{eff} will be calculated using a full core physics model with SERPENT (or a
 210 deterministic core physics code) in future work.

$$k_{\text{eff}} = \frac{\nu\Sigma_{f1} + \nu\Sigma_{f2} \frac{\Sigma_{S(1\rightarrow2)}}{(D_2B^2 + \Sigma_{R2})}}{(D_1B^2 + \Sigma_{R1}) - \Sigma_{S(2\rightarrow1)} \frac{\Sigma_{S(1\rightarrow2)}}{(D_2B^2 + \Sigma_{R2})}} \quad (5)$$

B^2 is the geometric buckling, assuming $B_1^2 = B_2^2$.

$\nu\Sigma_{fn}$ is the fission neutron production cross-section for group n .

$\Sigma_{S(n\rightarrow m)}$ is the neutron scattering cross-section from group n to m .

D_n is the diffusion coefficient for group n .

Σ_{Rn} is the removal cross-section for group n .

211 The value of B^2 is calculated using Equation (6), assuming a cylindrical, homogeneous core with
 212 active height (H_a) of 793 cm [11] and an effective radius (R_a) of 153.5 cm. The effective radius is

213 approximated based on the horizontal area of 66 fuel blocks, which are shown in Fig. 1. Each
214 fuel block is hexagonal with a flat-to-flat length of 36 cm (Fig. 2), and thus is 1122.4 cm² in area.
215 A circle with an area of 1122.4 x 66 = 74,076.3 cm² has an effective radius of 153.5 cm. Thus,
216 the geometric buckling is calculated to be 2.61E-4 cm⁻². This value of geometric buckling
217 neglects the effect of the inner and outer graphite reflectors in reducing neutron leakage, thus
218 it is likely an overestimate of the neutron leakage.

$$B^2 = \left(\frac{2.405}{R_a}\right)^2 + \left(\frac{\pi}{H_a}\right)^2 \quad (6)$$

219
220 The use of SERPENT for performing lattice physics calculations, and then imposing a geometric
221 buckling that is based on the bare cylindrical core dimensions, with zero extrapolation distance,
222 and using a diffusion-based leakage model to estimate the core k_{eff} is considered a conservative
223 approximation, in that it will over-estimate leakage, and under-estimate exit burnup. In a full-
224 core SERPENT model, with the presence of radial and axial reflectors, the core leakage will be
225 reduced. For the purpose of carrying out initial scoping and exploratory calculations to
226 evaluate fuel behavior, exit burnup, reactivity coefficients, and other performance and safety
227 characteristics, this more simplified and approximate approach using lattice physics calculations
228 is considered both practical and satisfactory. The results from these lattice physics calculations
229 and their extrapolation to full-core behavior are a pre-cursor to performing more detailed full-
230 core analyses with complete modeling of both radial and axial reflectors.

231

232 **4.3 EXIT BURNUP**

233 The single-batch exit burnup and fuel residence time correspond to the burnup step in which
234 $k_{\text{eff}} = 1.0$. A two-point linear interpolation is used to estimate the burnup and fuel residence
235 time that correspond to $k_{\text{eff}} = 1.0$ using the values of k_{eff} , burnup, and fuel residence time at the
236 last burnup step where $k_{\text{eff}} > 1.0$ and at the first burnup step where $k_{\text{eff}} < 1.0$. In this study a 3-
237 batch refueling scheme is used, which is also used in previous studies of the MHTGR-350 [12]
238 [15]. The linear reactivity model is used to estimate the exit burnup and fuel residence time for
239 a 3-batch refueling scheme, which is $3/2$ times the single-batch exit burnup and fuel residence
240 time, respectively. The formula for the linear reactivity model is: $BU(n) = BU(1) \times 2n/(n+1)$. For a
241 3 batch scheme, $n = 3$, and $BU(3) = BU(1) * 6/4 = 1.5 * BU(1)$.

242

243 **4.4 ESTIMATED FULL CORE FUEL MASS**

244 The fuel and NU consumption in this study are calculated from the mass of fuel in a core. The
245 total mass of fuel in the core is calculated based on a description of the MHTGR-350 from [11],
246 which describes the two types of fuel blocks in the core: a standard block and a reserve
247 shutdown control (RSC) block, which are referred to as “fuel elements” in that document. The
248 RSC block has fewer fuel holes than the standard block in order to make room for control
249 devices. In total, there are 660 prismatic fuel blocks in the MHTGR-350 core. There are 540 (54
250 fuel columns \times 10 blocks per column) standard and 120 (12 fuel columns \times 10 blocks per
251 column) RSC blocks in the core, each of which has 210 and 186 fuel holes, respectively, in the
252 reference MHTGR-350 design. Each fuel hole contains 15 fuel compacts in a 79-cm high
253 prismatic fuel block. Thus, there are $15 \times (210 \times 540 + 186 \times 120) = 2,035,800$ fuel compacts in the
254 reference core. Each fuel compact comprises 6416 TRISO particles, which is 2.5 gU/compact. As
255 such, the reference core contains 5,086 kgU.

256 Due to the replacement of some fuel compacts with moderator compacts in the annular fuel
257 block, there are 156 and 134 fuel holes per standard and RSC block, respectively. Thus, there
258 are a total of $156 \times 540 + 134 \times 120 = 100,320$ annular fuel elements in the core. The length of
259 an annular fuel element is 73.92 cm, thus, there is 29.1 cm^3 of fuel in each of the inner and
260 outer annuli of a fuel element. Given the make-up of each annular fuel concept in Table 6 and
261 the composition of each fissionable material in Table 7, the total mass of fuel in a core for each
262 annular fuel concept is listed in Table 10.

263 **5. RESULTS**

264 **5.1 REFERENCE VERSUS BENCHMARK CALCULATIONS**

265 The calculated value of k_{inf} versus burnup for the benchmark MHTGR-350 model and the
266 reference model developed for this study are shown in Fig. 5. The data for the benchmark case
267 is taken from [13]. The values of k_{inf} calculated using the reference model in this study are very
268 similar to those from the benchmark calculations, with a difference of 3.6 mk at 0 burnup and a
269 maximum difference of 8.0 mk, which occurs at 100 MWd/kgHM.

270 **5.2 ANNULAR VERSUS REFERENCE FUEL BLOCK**

271 In this section the reference fuel concepts R5, R10, and R19.75 with 5, 10, and 19.75 wt.% U-
272 235/U, respectively are compared with the annular fuel concepts A5, A10, and A19.75.

273 **5.2.1 NEUTRON ENERGY SPECTRUM**

274 The differences between the reference and annular fuel blocks affect the neutron energy
275 spectra. The plot in Fig. 6 shows that the annular concepts have a lower proportion of neutron
276 flux in the epithermal range, between 10^{-6} MeV and 0.1 MeV, which is due to their reliance
277 on LiH as the primary moderator. Neutrons require fewer interactions with hydrogen in order
278 to be slowed down to thermal energies than with carbon, thus neutrons reach thermal energies
279 in much less time. This figure also shows that the annular concepts have higher neutron flux in
280 the fast range, above 0.1 MeV, which is due to their larger volume and mass of fissionable
281 material. Unlike the epithermal and fast energy ranges, the differences in thermal neutron flux
282 between the reference and annular fuels vary substantially with enrichment. As shown in Fig.
283 6, as the fissile content is increased, the ratio of C/U-235 and H/U-235 are decreased, making

284 the neutron energy spectrum harder, which is true for both reference and annular-type fuels.
285 However, due to the more heterogeneous design and arrangement of moderator rods in the
286 annular-type design, which experiences neutron moderation due to hydrogen, graphite, and to
287 a lesser degree, lithium, there is a shift in the thermal flux between low-enrichment (5 wt% U-
288 235/HM) and high enrichment (19.75 wt% U-235/U) fuel.

289 For example, the thermal flux for R5 is much higher than that of A5 but the thermal flux of
290 A19.75 is higher than that of R19.75. The data shown appears to indicate that the reference
291 fuel concepts are somewhat under-moderated, and so when the U-235 content is doubled from
292 5 wt% U-235/U to 10 wt% U-235/U, the thermal neutron flux drops significantly, and when the
293 fissile content is doubled again to 19.75 wt% U-235/U, the spectrum in the TRISO fuel becomes
294 harder still. In contrast, it appears that the fuel block with annular-type fuel elements and LiH
295 moderator rods may actually be slightly over-moderated, since it experiences smaller changes
296 in the thermal neutron flux when the fissile content is doubled from 5 wt% U-235/U to 10 wt%
297 U-235/U.

298 **5.2.2 NEUTRON MULTIPLICATION FACTOR**

299 For each level of uranium enrichment, the infinite neutron multiplication factor (k_{inf}) is over 90
300 mk higher for the annular fuel at 0 burnup, as is shown in Fig. 8. These higher values are due to
301 the higher concentration of U-235 in the annular fuel which leads to a greater influence of the
302 spatial self-shielding effect. Neutron leakage in the annular fuel is reduced by over 90 mk,
303 shown in Fig. 8, due to the addition of LiH moderator compacts on the periphery of the fuel
304 block. The increased k_{inf} and reduced leakage combine to increase the effective multiplication
305 factor (k_{eff}) by over 200 mk, which is shown in Fig. 9.

306 The higher values of k_{eff} lead to higher exit burnups for each of the annular fuel concepts
307 relative to the reference concept with the same initial uranium enrichment, as shown in Fig. 10.
308 Due to this higher exit burnup and the larger mass of uranium in the annular fuel concepts, the
309 fuel residence times for the annular concepts are all over 20 years longer than those of the
310 reference fuel. Note that such long residence times may not be feasible due to limits on the fast
311 neutron fluence that graphite can experience before having to be removed from the core. Due
312 to its higher burnup, using the annular fuel reduces the annual NU consumption (Fig. 12) by
313 between 48 and 72%, where the reduction is highest for 5 wt.% U-235/U and lowest for 19.75
314 wt.% U-235/U. The lowest NU consumption is achieved using 10 wt.% U-235/U, which is 4% less
315 than using 5 wt.% U-235/U: the annular concept with the highest NU consumption.

316 **5.2.3 REACTIVITY COEFFICIENTS**

317 An apparent tradeoff of using the current annular fuel concepts is the resulting increase in
318 temperature reactivity coefficients. The plot in Fig. 13 shows that the average of the FTTCs over
319 burnup and temperature are as much as 0.064 mk/K higher, although still negative at all
320 temperatures and burnups. The average graphite temperature reactivity coefficients (GTRCs)
321 are also higher by as much as 0.015 mk/K, as shown in Fig. 14, and are slightly positive, ranging
322 between +0.002 mk/K and +0.004 mk/K. Although conventional HTGR fuel designs with TRISO
323 fuel particles and graphite moderator have a negative GTRC, the annular fuel design concept in
324 this study, combined with the use of a hydrogen-based moderator leads to the slightly positive
325 GTRC. For comparison, other HTGR-type reactors with alternative coolants and moderators,
326 such as the SmaHTR, a molten FLiBE-cooled reactor, have also demonstrated slightly positive
327 GTRC values, ranging from +0.0002 mk/K to +0.0011 mk/K [17].

328

329

330 Since the GTRCs are smaller in magnitude than the FTRCs, which means that the core
331 temperature coefficient of power would likely be negative but for the positive (~ 0.090 mk/K)
332 hydrogen temperature reactivity coefficients (HTRCs) shown in Table 11. This result concurs
333 with other studies of alternative moderators, which have also found that hydrogen-based
334 moderators have positive reactivity coefficients [16]. These results are attributed to the
335 reduced neutron absorption in hydrogen with increasing temperature, along with slight
336 changes in the neutron energy spectrum which will lead to reduced neutron absorption in U-
337 235, U-238 and other actinides.

338 However, the present evaluation of HTRCs does not consider the effects of density changes in
339 solid LiH with temperature. Given that the density of solid LiH decreases with temperature by
340 between 1.1×10^{-4} and 1.4×10^{-4} g/cm³/K [18], as illustrated in Fig. 16, it is expected that the
341 calculated HTRC would still be quite positive if the density changes were considered for solid
342 LiH, but would become much less positive, or perhaps even negative for temperatures beyond
343 its melting point of 692°C / 965 K [5], [18]. In this concept it is assumed that each LiH rod
344 extends the full height of the core, and that there is space at the axial ends of each moderator
345 compact to allow for thermal expansion. It is also noted that the LiH moderator rods will be at
346 a temperature between that of the helium coolant (750 K) and the graphite block (835 K), (see
347 Table 3) which is well below the melting point of LiH (~ 965 K).

348 Since the HTRC decreases with increasing mass of U-235 in the fuel, it is expected that reducing
349 the volume of LiH moderator in the core, and hence further reducing the H/U-235 ratio, would
350 further reduce the HTRC, although it will have an impact on the exit burnup and NU
351 consumption. Reducing the H/U-235 ratio can be achieved simply by removing ${}^7\text{LiH}$ moderator
352 rods, and replacing them with fuel rods.

353

354

355 **5.3 ANNULAR FUEL BLOCK: URANIUM VERSUS URANIUM-THORIUM FUEL**

356 In this section the uranium and uranium-thorium annular fuel concepts are compared. The
357 uranium fuel with 5 wt.% U-235/U (A5) is compared with the heterogeneous uranium-thorium
358 fuel concept (U10|Th) that is 50 vol.% uranium (10 wt.% U-235/U), both of which have fissile
359 content of ~5 wt.% U-235/HM. The other uranium-thorium concepts, U19.75+Th and
360 U19.75|DU+Th, are 50 vol.% uranium that is 19.75 wt.% U235/U, for a fissile content of ~10
361 wt.% U-235/HM. Thus they are compared with A10, which has 10 wt.% U-235/HM. Since Th in
362 ThCO is 11% less dense than U in UCO, the thorium-uranium concepts have 6% less mass of HM
363 than the uranium concepts.

364 The plot in Fig. 15 shows that replacing 50 vol.% of the uranium with thorium reduces k_{eff} for
365 fresh fuel due to neutron absorption in Th and slows the decline in k_{eff} with burnup due to U233
366 build-up. These effects influence the exit burnup, fuel residence time, and NU consumption,
367 which are shown in Table 12. The difference in k_{eff} for fresh fuel between the uranium and
368 uranium-thorium fuels is largest (83 mk) for the 5% fissile fuel concepts A5 and U10|Th. The
369 U10|Th fuel has 2% lower exit burnup, which indicates that U-233 is not being bred quickly
370 enough to compensate for the initial drop in k_{eff} before the fuel block becomes subcritical. This
371 concept also has a 8% shorter fuel residence time, which is a consequence of its lower burnup
372 and lower mass of HM. This reduction in residence time, and the more than 2 times higher NU
373 feed to product ratio (R) for the uranium in U10|Th (10 wt.% U-235/U) than that of uranium in
374 A5 (5 wt.% U-235/U), combine to increase NU consumption by 11%.

375 The differences in k_{eff} between the 10% fissile uranium and uranium-thorium concepts for fresh
376 fuel are 59, 66, and 57 mk, for U19.75|Th, U19.75+Th, and U19.75|DU+Th, respectively. The
377 exit burnup of each of these concepts is ~5% higher than that of A10, but the NU consumption
378 of each concept is also slightly (< 1%) higher than that of A10. This increased NU consumption is
379 due to the 0.6 to 0.7% reduction in fuel residence time, which more than offsets the 0.2% lower
380 NU feed required to produce enriched uranium for a uranium-thorium fuel block.

381 For the heterogeneous and homogenous fuel concepts, U19.75|Th and U19.75+Th,
382 respectively, the differences in exit burnup, fuel residence time, and NU consumption are small.
383 The homogeneous concept has 0.2% higher exit burnup and fuel residence time, and 0.2%
384 lower NU consumption, which indicates that the homogeneous fuel results in more breeding of
385 U-233 than that of the heterogeneous fuels.

386 The replacement of 10 vol.% of the Th in the inner annulus of the U19.75|Th concept with DU
387 causes a 2 mk increase in k_{eff} at 0 burnup, a 0.6% reduction in exit burnup, and negligible
388 differences in fuel residence time and NU consumption.

389 Replacing half of the uranium with thorium in the annular fuel concepts causes a reduction in
390 the average fuel, graphite, and hydrogen temperature reactivity coefficients, as is shown in
391 Table 13. The FTRCs of the uranium-thorium fuel concepts are all more than 0.005 mk/K less
392 than those of the uranium-only fuel concepts due to the greater increase in Th-232 capture
393 cross-section with temperature relative to that of U-238, which was also observed in [19].

394 There is also a reduction of 0.005 mk/K, or more, in the HTRCs. The reduction in GTRCs is
395 0.001 mk/K.

396 **6. SUMMARY AND CONCLUSIONS**

397 SERPENT lattice physics calculations have been carried out to evaluate the performance and
398 safety characteristics of a modified HTGR prismatic fuel block concept, based on the MHTGR-
399 350 benchmark problem. The key changes were to replace the conventional TRISO-filled fuel
400 compacts with heterogeneous, multi-layer annular fuel pellets made with UCO, ThCO,
401 (U,Th)CO, or (DU,Th)CO. These fuel pellets have multiple protective cladding layers of pyrolytic
402 carbon (PyC) and silicon carbide (SiC), which is anticipated to give it robust qualities similar to
403 TRISO particles, but at a more macroscopic scale. With the increased loading of uranium in the
404 fuel block, it was necessary to replace up to 78 fuel holes and 42 coolant holes (120 holes total)
405 with a hydrogen-based moderator (^7LiH), in order to ensure a thermal neutron energy spectrum
406 in the lattice.

407 Results demonstrate that the modified fuel concept has several advantages and challenges
408 relative to the conventional MHTGR-350 design concept. With the increased uranium loading
409 (almost by a factor of 10), and the reduced neutron leakage (by 60 mk or more) due to the use
410 of a hydrogen-based moderator (^7LiH), much higher burnup levels and lower natural uranium
411 consumption levels can be achieved with the same level of uranium enrichment. For example,
412 the annular-type fuel pellets made with UCO with 19.75 wt.% U-235/U can achieve nearly
413 double the burnup (~ 201 MWd/kgU), as TRISO-loaded fuel compacts (~ 105 MWd/kg).

414 Estimated uranium consumption in a full reactor core is reduced from ~ 46.5 tonnes-NU/year
415 for the TRISO-based fuel down to ~ 24.0 tonnes-NU/year for the annular-type fuel. In addition,
416 the expected fuel lifetime / residence time in a HTGR core before the fuel must be replaced is
417 increased dramatically, to values as high as 76.6 years (with 3-batch refuelling) for annular –

418 type fuel made with 19.75 wt.% U-235/U in the form of UCO. By comparison, fuel blocks with
419 TRISO-type fuel in compacts will need to be replaced after ~4.2 years. Hence, the modified fuel
420 design could be very attractive for developing HTGR-SMRs as “nuclear batteries” that are
421 fuelled only once, although this may be limited due to irradiation damage to various materials
422 in the core, including the fuel, moderator, graphite, and other components.

423 The use of thorium as a fertile material in either homogeneous annular fuel pellets ((U,Th)CO in
424 outer and inner fuel annuli), or heterogeneous annular fuel pellets (UCO in outer fuel annulus,
425 ThCO or (Th,DU)CO in inner fuel annulus) gives a comparable or slightly higher burnup than
426 UCO fuels with the same average fissile content (wt.% U-235/HM). The residence time is slightly
427 smaller for thorium-based fuels, due to the lower density of ThCO relative to UCO. The annual
428 NU consumption rate for thorium-based fuels is slightly higher (up to 10%) in comparison with
429 UCO fuels with the same average fissile content, although at a high fissile content level (~10
430 wt.% U-235/(U+Th), there is essentially no difference between the UCO and the (U,Th)CO fuels.

431 The challenge of the current design concept of the modified HTGR fuel concept with annular-
432 type fuels, and ⁷LiH moderator rods, is that in comparison to the conventional MHTGR-350
433 design with TRISO-based fuel compacts, it has less negative fuel temperature reactivity
434 coefficients, FTRC, (as small as -0.028 mk/K), and slightly positive graphite and hydrogen
435 moderator temperature coefficients, with values as high as +0.015 mk/k (for graphite MTC) and
436 +0.19 mk/K (for hydrogen MTC). Thorium-based annular fuels made with (U,Th)CO appear to
437 have more negative FTCs, and less positive graphite and hydrogen temperature coefficients
438 relative to annular fuels made with UCO, which is advantageous from a reactor safety
439 perspective.

440 It is speculated that the current concept is “*over-moderated*”, and the number of ^7LiH rods need
441 to be reduced. Although full-core physics calculations would need to be performed to better
442 quantify and assess the resulting power coefficient of reactivity (PCR), it is anticipated that the
443 PCR could be too high, and an active control system would be required to prevent a power
444 transient. Thus, further modifications to the design concept will be required to ensure smaller
445 or negative moderator temperature coefficients and a negative PCR.

446

447 **7. OPTIONS FOR FUTURE WORK AND IMPROVEMENTS**

448 Based on what has been learned from the current studies of uranium and uranium-thorium
449 oxy-carbide fuels in modified prismatic HTGR fuel blocks with annular-type fuel pellets (instead
450 of conventional TRISO-based fuel compacts) and ^7LiH moderator fuel rods, the following are
451 potential options for future work:

- 452 • Evaluate the effects of using graphite thermal scattering libraries at more appropriate
453 temperatures on the lattice physics calculations.
- 454 • Evaluate alternative fuel matrix materials, including oxides, nitrides, and carbides.
- 455 • Evaluate plutonium/thorium fuels in the form of oxides, nitrides, carbides, and oxy-
456 carbides. The plutonium isotopic composition could be based on either spent LEU fuel
457 from a pressurized water reactor (PWR) fuel or spent NU fuel from a pressure tube
458 heavy water reactor (PT-HWR).
- 459 • Evaluate alternative materials for moderator rods, including ^7LiD , $^7\text{LiOH}$, and NaOH.
460 Hydroxides are potentially advantageous over hydrides, since they can operate at much
461 higher temperatures before boiling or undergoing decomposition. For example, NaOH
462 boils at 1,388 °C, well above the expected maximum operating temperature of an HTGR.
463 Recent studies have shown that hydroxides could be an attractive moderator material
464 for compact SMRs [21].
- 465 • Adjust the number of ^7LiH moderator rods to a lower number to potentially reduce the
466 hydrogen moderator temperature coefficient, such that the modified HTGR lattice will
467 have a negative power coefficient of reactivity.

- 468 • Account for changes in the ${}^7\text{LiH}$ density with temperature, and implement thermal
469 scattering data appropriate for H bound in a hydride. Current calculations did not
470 account for such effects, which will have some impact on the evaluation of k_{inf} , k_{eff} and
471 reactivity coefficients.
- 472 • Carry out full-core physics calculations of an HTGR core with a number of selected
473 annular-type fuel concepts to get a better estimate of the power distributions and the
474 exit burnup of the fuel. Full core modeling will provide a better estimate of the effects
475 of radial and axial reflectors, neutron leakage, and the effect of control rods used for
476 excess reactivity control and adjusting power distributions.
- 477 • Carry out thermal-hydraulic and heat transfer calculations to obtain better estimates of
478 the temperature distributions in the fuel and moderator with annular-type fuel pellets
479 and hydrogen-based moderator rods (${}^7\text{LiH}$).
- 480 • Evaluate the performance of the annular fuel with respect to fission product retention.
- 481 • Investigate the replacement of fuel block graphite with materials that are more resistant
482 to radiation damage.
- 483

484

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494

495 **NOMENCLATURE**

496

D_n	diffusion coefficient for group n , m
B^2	geometric buckling for a core; $\left(\left(\frac{2.405}{R_a}\right)^2 + \left(\frac{\pi}{H_a}\right)^2\right)$, m^{-2}
$BU(n)$	exit burnup for n batch refueling, MWd/kg
$C(B, T_1, T_2)$	temperature coefficient of reactivity at burnup B , between temperatures T_1 and T_2 ; $\left(\frac{k_{inf}(B, T_1) - k_{inf}(B, T_2)}{T_1 - T_2}\right)$, mk/K
H_a	effective height of the cylindrical core, m
L_{EU}	mass of enriched uranium that is loaded into the core during refueling, kg
mk	unit for the difference between two values of neutron multiplication factors; $(10^{-3} \Delta k)$
MWd	derived unit of energy; $(10^6 \cdot 24 \cdot 3600)$, J
Q_{EU}	annual fuel consumption; $\left(\frac{L_{EU}}{T}\right)$, kg/y
Q_{NU}	annual natural uranium consumption; $(Q_{EU}R)$, kg/y
R_a	effective radius of the cylindrical core, m
T	duration between refueling, s
y	derived unit of time; $(3600 \cdot 24 \cdot 365)$, s

497

498 **Greek Letters**

Σ_{Rn}	removal cross-section for group n , m^{-1}
$\Sigma_{S(n \rightarrow m)}$	neutron scattering cross-section from group n to m , m^{-1}
$\nu \Sigma_{fn}$	fission neutron production cross-section for group n , n/m

499

500

501 **Non-Dimensional Numbers**

k_{eff}	Neutron multiplication factor for a finite core; $\left(\frac{\nu \Sigma_{f1} + \nu \Sigma_{f2} \frac{\Sigma_{S(1 \rightarrow 2)}}{(D_2 B^2 + \Sigma_{R2})}}{(D_1 B^2 + \Sigma_{R1}) - \Sigma_{S(2 \rightarrow 1)} \frac{\Sigma_{S(1 \rightarrow 2)}}{(D_2 B^2 + \Sigma_{R2})}}\right)$
k_{inf}	Neutron multiplication factor on an infinite lattice
R	Ratio of natural uranium feed to enriched uranium product; $\left(\frac{x_p - x_t}{x_f - x_t}\right)$
x_f	weight % U-235/U in natural uranium feed
x_p	weight % U-235/U in enriched uranium product
x_t	weight % U-235/U in depleted uranium tails

502

503 **Subscripts or Superscripts**

EU	enriched uranium
----	------------------

NU	natural uranium
eff	effective
inf	infinite
f	feed or fission
p	product
t	tails

504

505 **Acronyms and abbreviations widely used in text and list of references**

2D	Two dimensional
3D	Three dimensional
BOC	Beginning of Cycle
DU	Depleted Uranium
FP	Fission Products
FTRC	Fuel Temperature Reactivity Coefficient
GTRC	Graphite Temperature Reactivity Coefficient
HM	Heavy Metal
MC	Monte Carlo
NU	Natural Uranium
PT-HWR	Pressure Tube Heavy Water Reactor
PWR	Pressurized Water Reactor
RSC	Reserve Shutdown Control
SM-HTGR	Small Modular High Temperature Gas-cooled Reactor
TRISO	Tri-Structural ISOtropic
wt.%	weight percent

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508 **8. REFERENCES**

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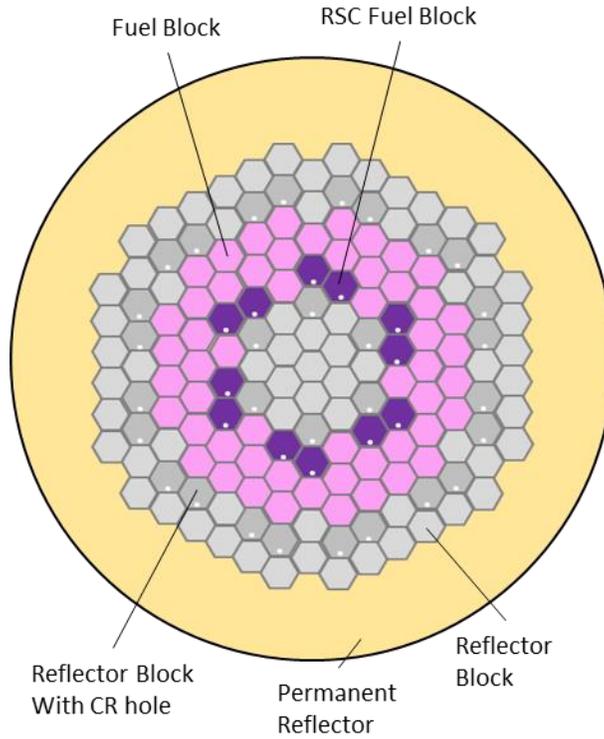
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* Note: there are 12 fuel columns with RCS Fuel Blocks (Purple).

623

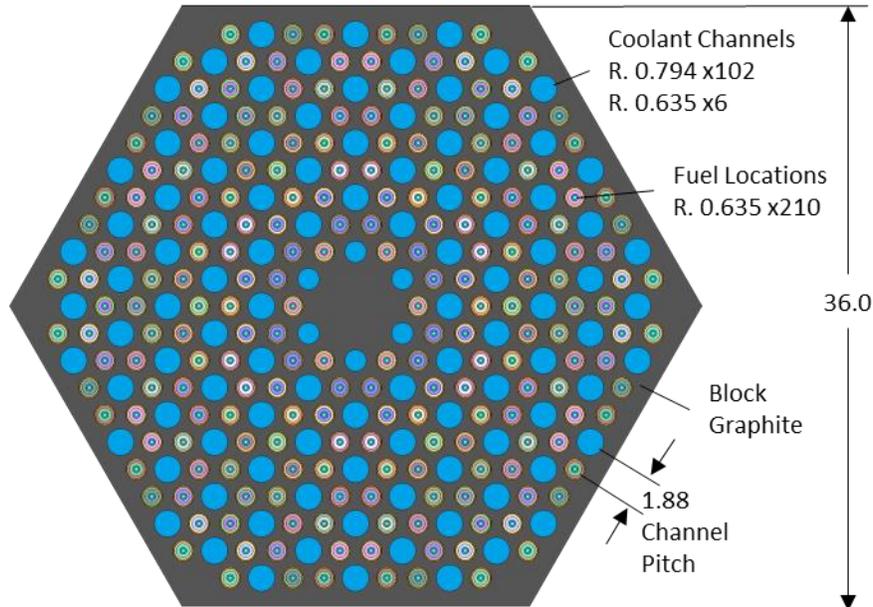
There are 6 (inner ring) + 24 (middle ring) + 24 (outer ring) = 54 fuel columns with regular Fuel Blocks (Pink).

624

Fig. 1: Core layout of MHTGR-350 (Adapted from Fig. 3 from [11])

625

626



627

628 *Note: There are 102 large coolant holes (0.793 cm in diameter), and 6 small coolant holes (0.635 cm in diameter).
629 There are 210 fuel holes, each 0.635 cm in diameter. To a first approximation, there is one coolant hole for every
630 two fuel holes.

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Fig. 2: Reference fuel block layout (Adapted from Fig. 2-2 from [12])

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Table 1: Specifications for TRISO Particles (adapted from Table 2-2 from [12])

Properties	Value	Unit
Particle layer outer radii		
Kernel	0.02125	cm
Buffer	0.03125	cm
IPyC	0.03525	cm
SiC	0.03875	cm
OPyC	0.04275	cm
Particle layer densities		
Kernel	10.9	g/cm ³
Buffer	1.0	g/cm ³
IPyC	1.9	g/cm ³
SiC	3.2	g/cm ³
OPyC	1.9	g/cm ³
Particle packing fraction	0.35	

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Table 2: Reference fuel compact and block specifications (from [12])

Properties	Value	Unit
Fuel compact radius	0.625	cm
Fuel compact height	4.928	cm
Power per compact	172	W
Fuel compact hole radius	0.635	cm
Number of fuel compact holes	210	
Large coolant hole radius	0.794	cm
Number of large coolant holes	102	
Small coolant hole radius	0.635	cm
Number of small coolant holes	6	
Block hexagon flat-to-flat length	36.0	cm

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Table 3: Assumed Material Temperatures of HTGR Components*

Material	Temperature (K)
Fuel Compact (TRISO particles and compact graphite)	875
Helium in gap surrounding fuel compacts	855
Block graphite	835
Helium in coolant channels	750
Lithium hydride (7LiH) in alternative HTGR design**	835

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* Note: Temperature data are taken from reference [13], which are averaged and rounded to the nearest 5 K

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** As a conservative approximation, the 7LiH is assumed to be at the same temperature as the graphite block, although it is anticipated that the equilibrium 7LiH temperature will be somewhere between that of the graphite block and the helium coolant. The temperature of the 7LiH (750 K to 835 K) is well below its melting point (~965 K).

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Table 4: Reference composition of $UC_{0.5}O_{1.5}$ (from [13])

Isotope	Wt.%
U-235	13.78
U-238	75.11
O-16	8.97
C (natural)	2.14

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Table 5: Description of regions in heterogeneous annular fuel element

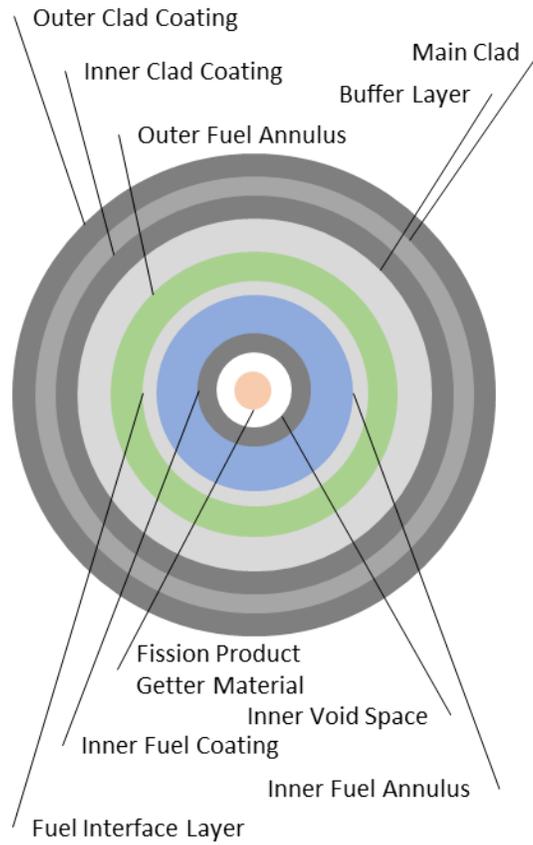
Region	Materials	Outer Radius (cm)	Inner Radius (cm)
1. Outer Clad Coating	Pyrolytic Carbon (OPyC)	0.625	0.621
2. Main Clad	Silicon Carbide (SiC)	0.621	0.561
3. Inner Clad Coating	Pyrolytic Carbon (IPyC)	0.561	0.557
4. Buffer Layer	Low Density Carbon Buffer	0.557	0.547
5. Outer Fuel Annulus	(U,Th)CO (see Table 6)	0.547	0.417
6. Fuel Interface Layer	Low Density Carbon Buffer	0.417	0.413
7. Inner Fuel Annulus	(U,Th)CO (see Table 6)	0.413	0.213
8. Inner Fuel Coating	Pyrolytic Carbon	0.213	0.209
9. Inner Void Space	Vacuum	0.209	0.109
10. Fission Product Getter Material	Porous Graphite	0.109	0

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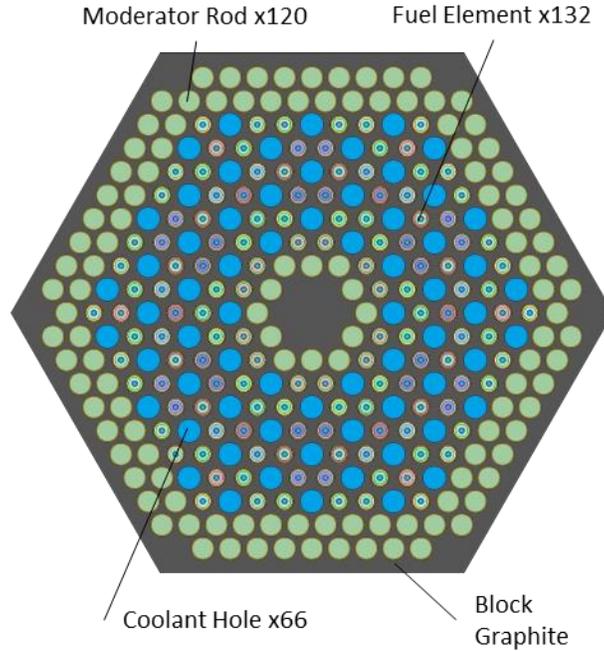
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* Note: Diagram is not to scale. Radial thickness of various coatings and clad regions and other non-fuel regions are exaggerated for better visual understanding.

Fig. 3: Radial cross section view of fuel element geometry (not to scale)

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666 * Green rods represent fuel and coolant holes that have been filled with a hydrogen-based moderator, such as
667 ⁷LiH. There are 108 Moderator holes on the outside, and 12 Moderator holes on the inside.

668 ** There are 132 Fuel Holes, and 66 Coolant Holes (Blue). The fuel holes are filled with heterogeneous, annular
669 fuel pellets instead of TRISO-based fuel compacts

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Fig. 4: Modified HTGR Fuel Block Concept with Moderator Elements

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Table 6: Fuel Specifications for Annular Fuel Pellet Concepts

Fuel Type	Homogeneous or Heterogeneous	Outer Annulus	Inner Annulus
A5	Homogeneous*	LEU (5 wt.% U-235/U)	LEU (5 wt.% U-235/U)
A10	Homogeneous*	LEU (10 wt.% U-235/U)	LEU (10 wt.% U-235/U)
A19.75	Homogeneous*	HALEU (19.75 wt.% U-235/U)	HALEU (19.75 wt.% U-235/U)
U10 Th	Heterogeneous **	LEU (10 wt.% U-235/U)	Th
U19.75 Th	Heterogeneous **	HALEU (19.75 wt.% U-235/U)	Th
U19.75+Th	Homogeneous*	50 vol% HALEU (19.75 wt.% U-235/U), 50 vol% Th	50 vol% HALEU (19.75 wt.% U-235/U), 50 vol% Th
U19.75 DU+Th	Heterogeneous **	HALEU (19.75 wt.% U-235/U)	90 vol% Th, 10 vol% DU (0.2 wt.% U-235/U)

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* Homogeneous – Inner & Outer fuel annuli are made of the same material

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** Heterogeneous – Outer fuel annulus contains higher fissile content. Inner fuel annulus contains low fissile, high fertile content.

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Table 7: Uranium and thorium oxy-carbide isotopic compositions (g/cm³)

Nuclide	Density of Nuclide in Fuel Material					
	UCO 5 wt.% U-235/U	UCO 10 wt.% U-235/U	UCO 19.75 wt.% U-235/U	ThCO	(U,Th)CO	(DU,Th)CO
Th-232				8.66E+00	4.33E+00	7.80E+00
U-234	3.71E-03	7.42E-03	1.47E-02	0.0	7.33E-03	1.48E-05
U-235	4.88E-01	9.76E-01	1.93E+00	0.0	9.64E-01	1.95E-03
U-238	9.26E+00	8.78E+00	7.82E+00	0.0	3.91E+00	9.74E-01
C	1.94E-01	1.95E-01	1.95E-01	1.77E-01	1.86E-01	1.79E-01
O-16	9.45E-01	9.45E-01	9.46E-01	8.60E-01	9.03E-01	8.68E-01
O-17	3.82E-04	3.82E-04	3.82E-04	3.47E-04	3.65E-04	3.51E-04
Total	1.09E+01	1.09E+01	1.09E+01	9.70E+00	1.03E+01	9.82E+00

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* What is shown in the table is the mass density (in g/cm³) of each isotope in each fuel material

682 **Table 8: Burnups and temperatures that are used to calculate reactivity coefficients**

Material	Burnup fraction^a	Material Temperatures (K)
Fuel	0, 1/3, 2/3, 1	600, 900, 1200, 1500
Graphite	0, 1/3, 2/3, 1	300, 600, 900, 1200
Hydrogen-based Moderator ^b	0, 1/3, 2/3, 1	300, 600, 900, 1200

^a Zero (0) burnup fraction corresponds to fresh fuel, and burnup fraction of 1 corresponds to the exit burnup.

^b Hydrogen-based moderator compact. Note that the melting point of ⁷LiH is 688°C (961 K), and the boiling point is ~950°C (1,223 K)

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Table 9: Cross-section and thermal scattering data

Material Temperature (K)	Cross-section Data (temperature)*	Thermal Scattering Data (temperature)
300	*.03c (300 K)	gre7.00t (294 K)
600	*.06c (600 K)	gre7.12t (600 K)
900	*.09c (900 K)	gre7.18t (800 K)
1200	*.12c (1200 K)	gre7.22t (1200 K)
1500	*.15c (1500 K)	gre7.22t (1200 K)

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Note: * is the name of the isotope. For example, 92225.03c is the data file for U-235 evaluated at 300 K.

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Table 10: Annular concepts core fuel mass

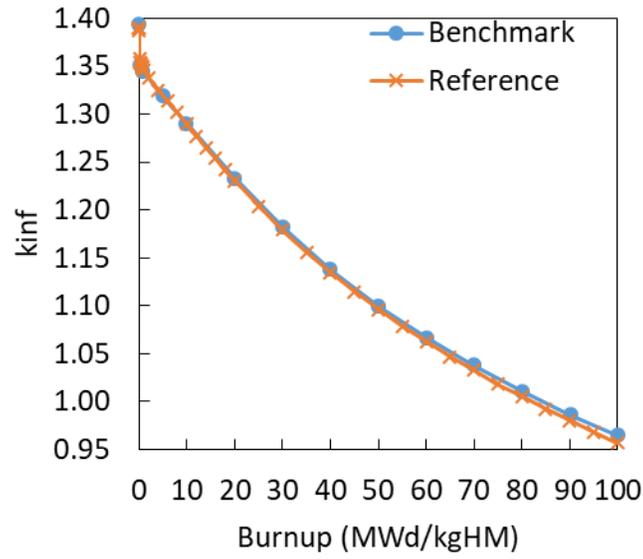
Mass of Fuel in Core with Fuel Type (refer to Table 6)							
Element	Uranium Fuel			Uranium-Thorium Fuel			
	A5	A10	A19.75	U10 Th	U19.75 Th	U19.75+Th	U19.75 DU+Th
U (kgU)	47969	47966	47960	23995	23991	23980	23991*
Th (kgTh)				21278	21278	21288	19150
Total (kgHM)	47969	47966	47960	45272	45269.	45268	45539

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* DU is not included here.

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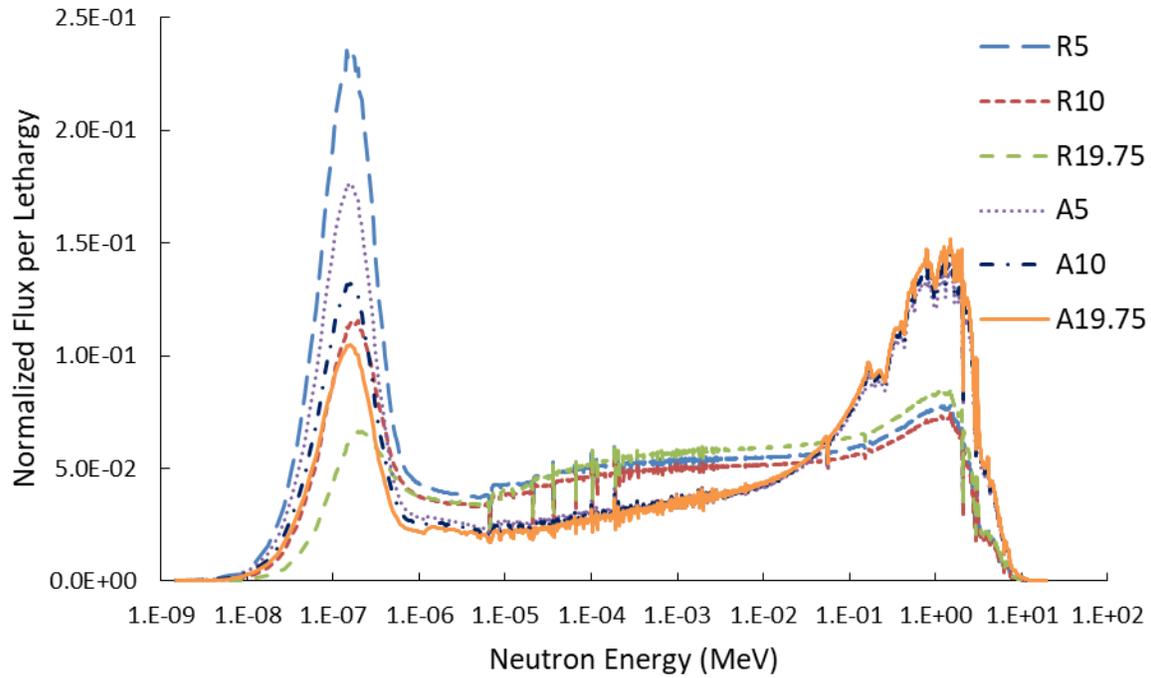
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Fig. 5: Calculated values of k_{inf} from the benchmark and reference models

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697 * Notice that R19.75, which uses TRISO fuel compacts with 19.75 wt% U-235/U, has a neutron energy spectrum
698 that is beginning to resemble a fast-spectrum reactor, due to a lower C/U-235 ratio, and insufficient moderation.

699 **Fig. 6: Normalized neutron energy spectrum ($n \cdot \text{cm}^{-2} \cdot \text{s}^{-1} / \text{total flux}$) for the reference (TRISO
700 particles in fuel compact) and annular pellet uranium-based oxycarbide fuel concepts**

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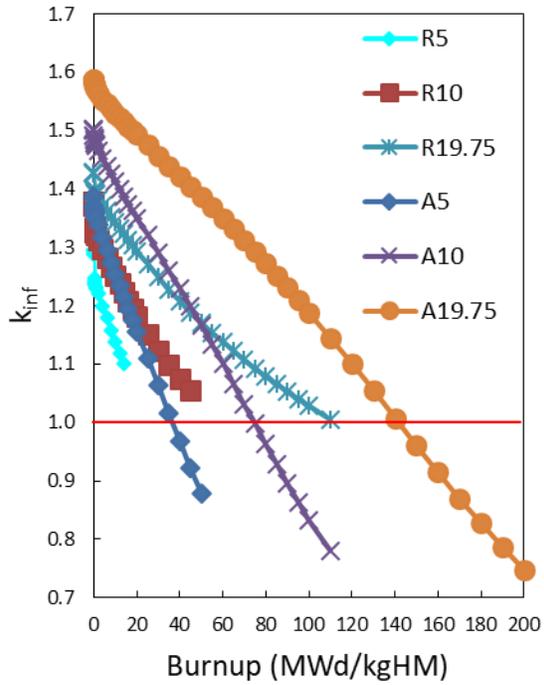
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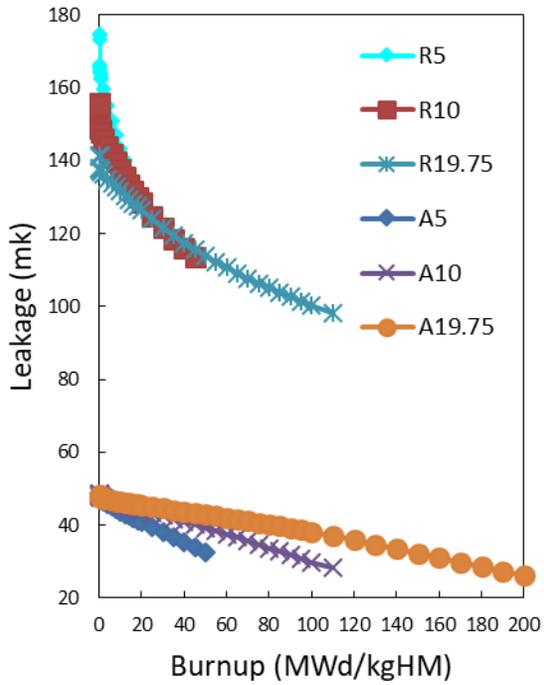
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708 **Fig. 7: k_{inf} of the reference (TRISO particles in fuel compact) and annular pellet uranium-based**
709 **oxycarbide fuel concepts**

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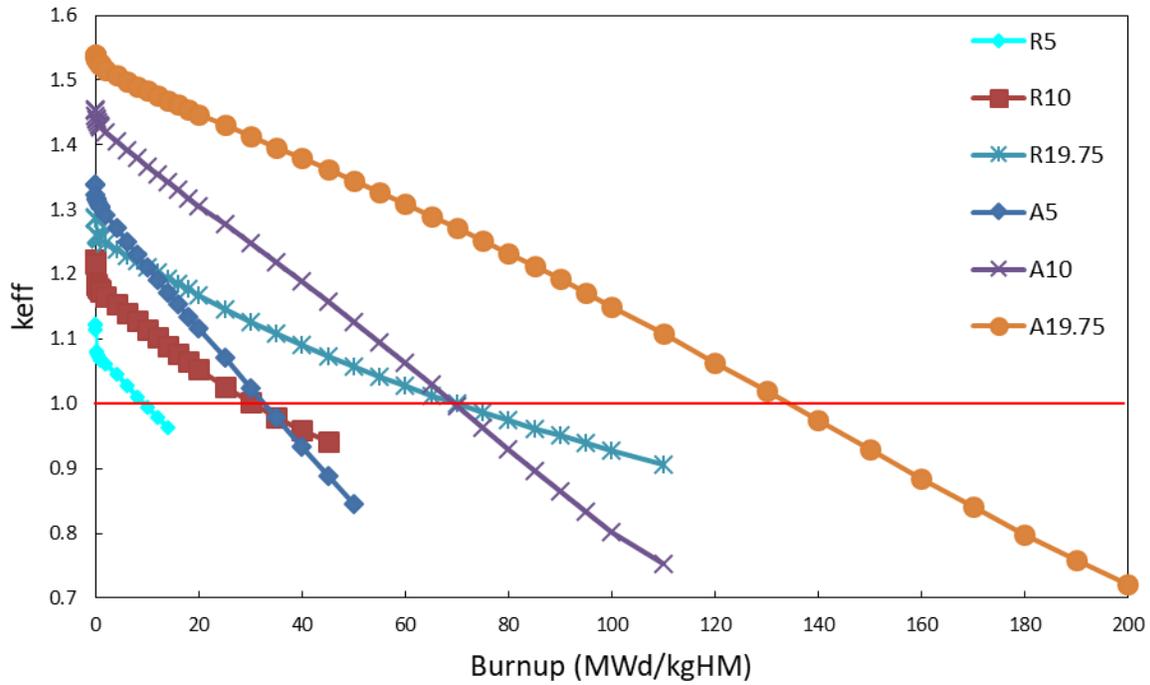
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Fig. 8: Neutron leakage of the reference (TRISO fuel compact) and annular pellet uranium oxycarbide fuel concepts

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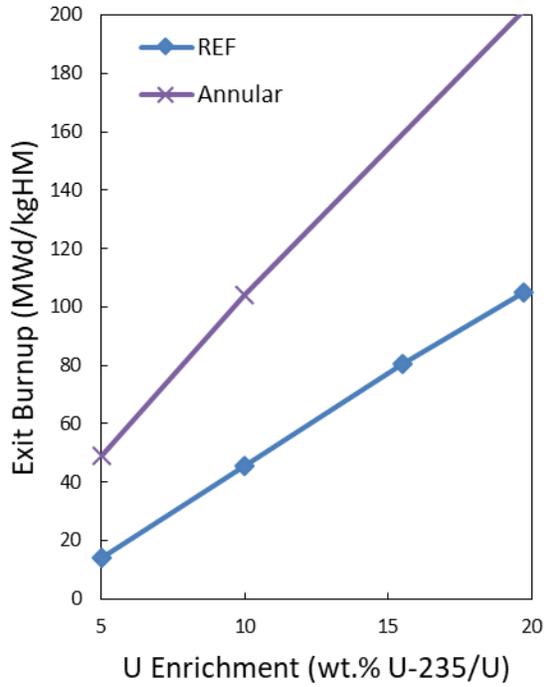
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Fig. 9: k_{eff} of the reference (TRISO fuel compact) and annular pellet uranium oxycarbide fuel concepts



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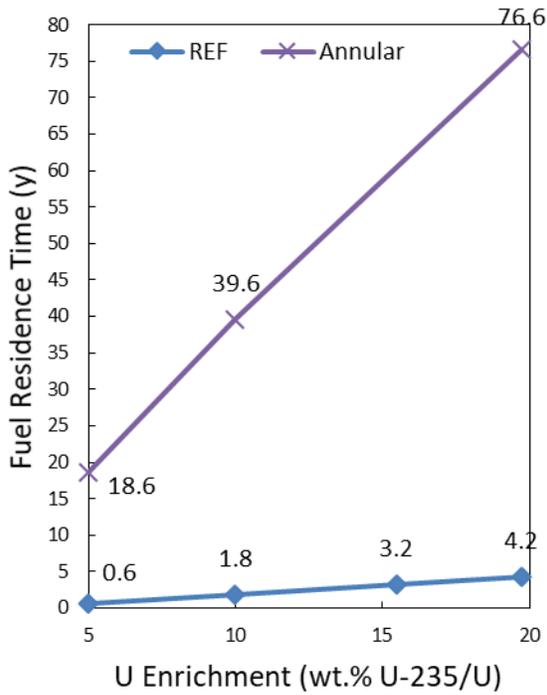
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Fig. 10: Exit burnup of the reference (TRISO fuel compact) and annular pellet uranium oxycarbide fuel concepts

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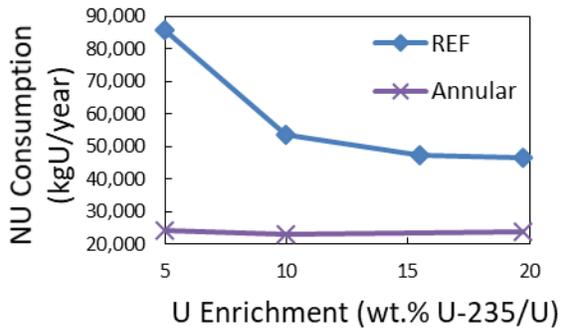
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725 **Fig. 11: Fuel residence time of the reference (TRISO fuel compact) and annular pellet uranium**
726 **oxycarbide fuel concepts**

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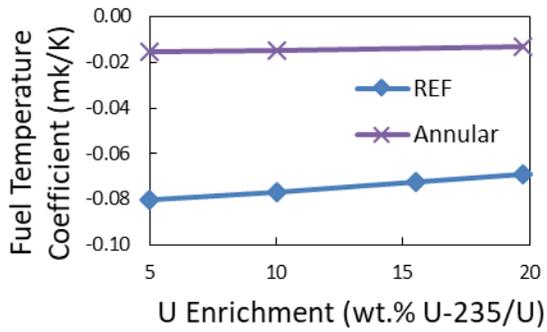


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731 **Fig. 12: NU consumption of the reference (TRISO fuel compact) and annular pellet uranium**
732 **oxycarbide fuel concepts**

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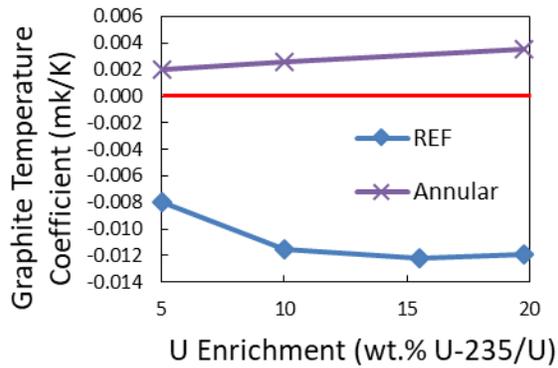
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736 * Note: The FTRCs shown in this plot are averaged over burnup and fuel temperature.

737 **Fig. 13: Fuel Temperature Reactivity Coefficient (FTRC) of the reference (TRISO fuel compact)**
738 **and annular pellet uranium oxycarbide fuel concepts**

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742 * Note: The GTRCs shown in this plot are averaged over burnup and graphite temperature.

743 **Fig. 14: Graphite Moderator Temperature Reactivity Coefficient (GTRC) reference (TRISO fuel**
744 **compact) and annular pellet uranium oxy-carbide fuel concepts**

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Table 11: Hydrogen-based Moderator Temperature Reactivity Coefficient (HTRC) of the annular pellet uranium oxy-carbide fuel concepts

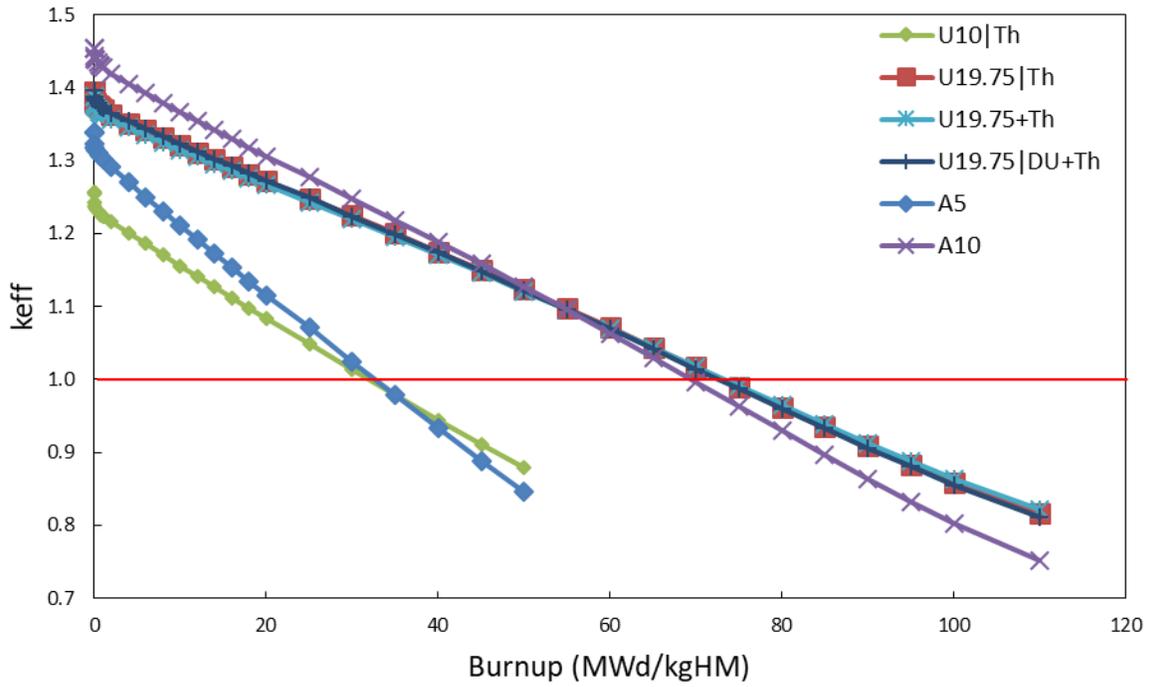
wt.% U-235/U	HTRC (mk/K)
5	0.094
10	0.088
19.75	0.085

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* Note: The HTRCs shown in this table are averaged over burnup and hydrogen temperature.

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753 **Fig. 15: Comparison of k_{eff} for the uranium and uranium-thorium annular fuel pellet concepts**

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756 **Table 12: Comparison of burnup, residence time and NU consumption for the uranium and**
757 **uranium-thorium annular fuel pellet concepts**

Fissile Content	Concept	Burnup (MWd/kgHM)	Residence Time (y)	NU Consumption (MTU/y)
5 wt.% U-235/HM	A5	49.0	18.6	24.2
	U10 Th	47.9	17.2	26.7
10 wt.% U-235/HM	A10	104.2	39.6	23.2
	U19.75 Th	109.6	39.3	23.3
	U19.75+Th	109.8	39.4	23.3
	U19.75 DU+Th	108.9	39.3	23.3

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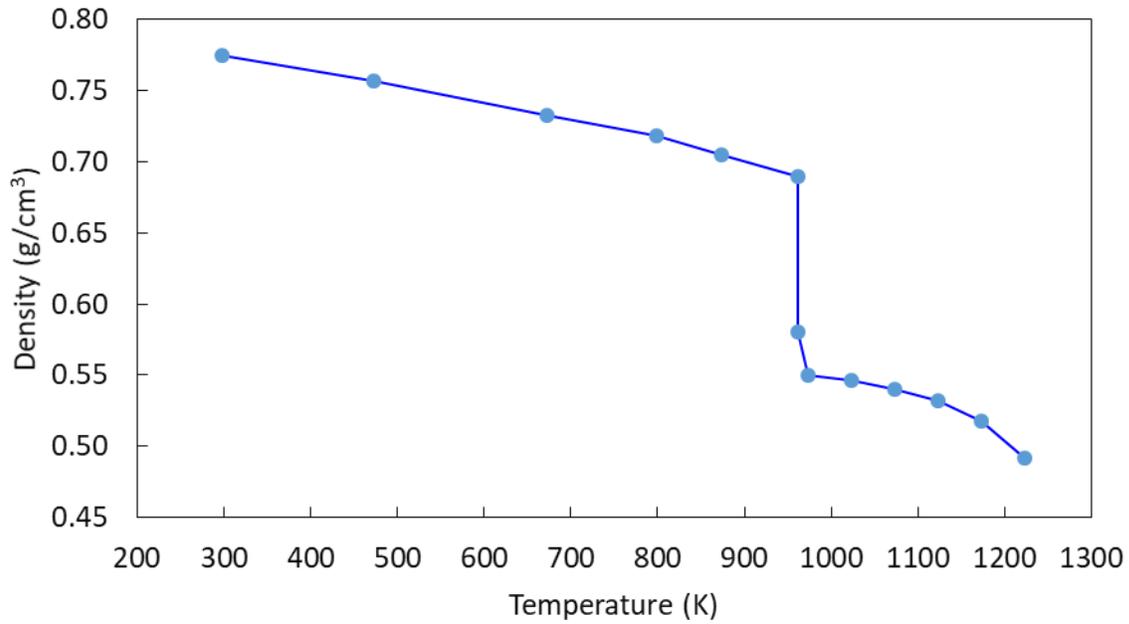
760 **Table 13: Comparison of temperature reactivity coefficients for the uranium and uranium-**
761 **thorium annular fuel pellet concepts**

Fissile Content	Concept	FTRC (mk/K)	GTRC (mk/K)	HTRC (mk/K)
5 wt.% U-235/HM	A5	-0.016	0.002	0.094
	U10 Th	-0.022	0.002	0.087
10 wt.% U-235/HM	A10	-0.015	0.003	0.088
	U19.75 Th	-0.021	0.002	0.083
	U19.75+Th	-0.022	0.002	0.083
	U19.75 DU+Th	-0.021	0.002	0.083

762 * Note: The temperature coefficients shown in this table are averaged over burnup and temperature.

763

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766 * Note: the melting point of LiH is $\sim 692^{\circ}\text{C}$ / 965 K

767 **Fig. 16: Density Variation with Temperature for Lithium Hydride (data obtained from [18])**

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