PBR Pebble Sensitivity Analyses for Material Accountancy Purposes

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ABSTRACT

Pebble bed reactors (PBR) are one of several advanced reactor designs being developed by multiple commercial entities. While there are many benefits to PBR, the fact that the fuel consists of thousands of relatively small pebbles creates material accountancy challenges. Modeling and simulation work is being conducted in an attempt to address this issue, but a fundamental challenge in opensource modeling is the ability to get precise data. Information such as uranium enrichment, densities, elemental compositions, and number of TRISO particles per pebble are all examples of key modeling parameters that could be proprietary, not yet defined, or vary due to limitations in manufacturing. Because of this, a fuel pebble in a generic PBR is modeled in MCNP6.2 and key modeling parameters varied to assess the impact of key metrics, such as criticality. This sensitivity analyses will allow other PBR opensource modelers to identify which parameters are of greatest importance in their models. Understanding and minimizing these sources of potential bias is essential in any material accountancy activities.

INTRODUCTION

Models and simulations are only as good as their input data. Radiation transport simulations of nuclear fuel are no exception to this rule, with values such as density and thickness often being key input parameters. Of particular interest to safeguards, facility operation, waste management, material control and accountancy, and others is how changes in these input parameters can change the criticality of the fuel as well as the radionuclide masses in the used fuel. Established nuclear fuel forms, such as light water reactor fuel, has been well characterized with variations in each vendor's fuel geometry and composition well documented as well as expected tolerances in the physical properties of the fuel during manufacturing. This however is not true for new fuel forms, such as Generation IV gas cooled reactors that use TRISO particle fuel in either pebble or cylindrical compact form.

TRISO Particle Based Fuels

TRISO particle fuel consists of thousands of TRISO particles imbedded in a graphite matrix, which is used to moderate the neutrons. The coolant for these reactors can vary, but generally consists of helium or molten salt. The physical form of the fuel consists of cylindrical pellets that are placed inside a prismatic graphite block to form a fuel assembly or spherical pebbles. These two fuel geometries are show in Fig. 1 [1].

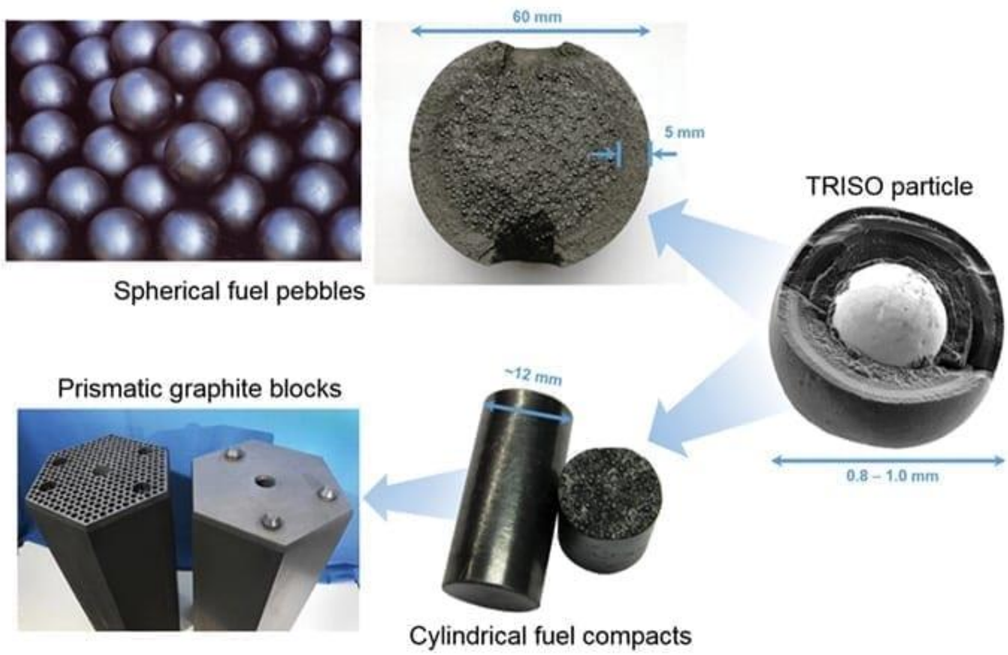

Figure 1. Diagram illustrating pebble and cylindrical compact based TRISO particle fuel forms [1].

While the macroscale geometries of these two fuel forms are very different, their TRISO particles are the same. This is due to the fact that certifying new nuclear fuel forms through a regulatory body is a financially costly and time-consuming process. Four of the main vendors looking to use TRISO particles in their fuel forms, X-energy [2], BWXT, Kairos Power [3], Ultra Safe Nuclear Corporation [4], and Westinghouse, have all adopted the specifications tested in the AGR-5/6/7 program [5][6][7][8][9]. One of the main goals of this program was to irradiate TRISO particles in the Advanced Test Reactor and analyze the particles pre and post irradiation properties. This work was done to help certify TRISO particle-based fuel forms to reduce the financial burden on vendors and shorten the time for their fuel certification. Additional information on vender specific TRISO particle fuel certification can be found on the United States Nuclear Regulatory Commission website [1].

<u>TRISO Particle Specification</u>

The TRISO particles used in the AGR-5/6/7 program had specific fuel fabrication specifications as shown in Table 1. As part of the program, fuel particles were measured for conformity with the results also shown in Table 1. Particles that were misshapen during the fabrication process, shown in Figure 2, where identified and rejected, thus not contributing their variations to the "Manufactured" results shown in Table 1.

Table 1. TRISO particle specified and manufactured properties for the AGR-5/6/7 program [7].

	Specified		Manufactured		Percent Difference	
Material	**Density (g/cm^3)**	**Thickness (μm)**	**Density (g/cm^3)**	**Thickness (μm)**	**Density (g/cm^3)**	**Thickness (μm)**
Outer Pyrolytic Carbon	1.9 ± 0.05	40 ± 4	1.897 ± 0.004	35.03 ± 1.99	0.16%	12.43%
Silicon Carbide	≥ 3.19	35 ± 3	3.195 ± 0.002	36.15 ± 0.65	-0.16%	-3.29%
Inner Pyrolytic Carbon	1.9 ± 0.05	40 ± 4	1.897 ± 0.099	39.24 ± 1.26	0.16%	1.90%
Porous Carbon Buffer	1.05 ± 0.05	100 ± 15	1.031 ± 0.022	100.4 ± 5.6	1.81%	-0.40%
UCO	≥ 10.4	212.5 ± 5	11.048 ± 0.044	212.89 ± 5.21	-5.94%	-0.18%
Graphite Matrix	≥ 1.65	N/A	1.75 ± 0.01	N/A	-6.06%	N/A

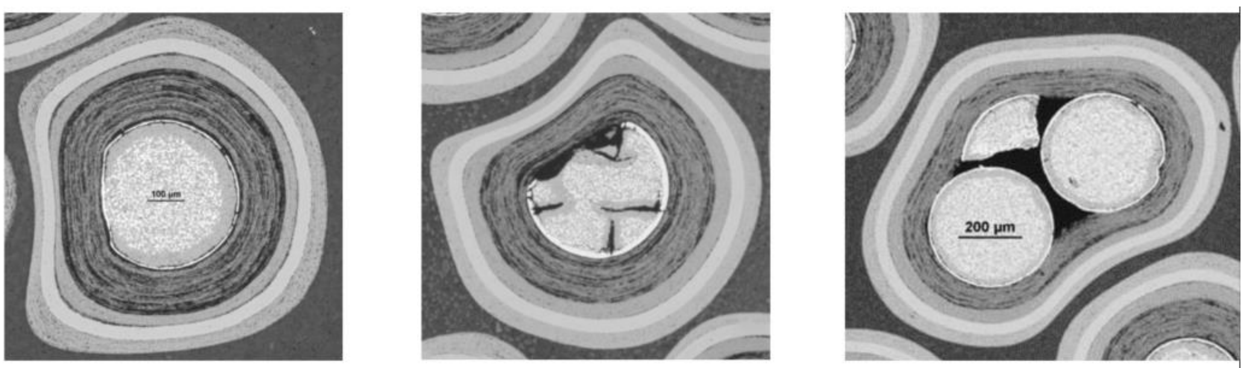

Figure 2. Misshapen TRISO particles identified during the AGR-5/6/7 program [7].

MODELING AND SIMULATIONS

To understand how variations in TRISO particle parameters can impact criticality and used fuel composition, Monte Carlo N Particle (MCNP) version 6.2 simulations were performed on various perturbations of fuel parameters [10]. MCNP is a general-purpose radiation transport code that uses Monte Carlo methods to track interactions of particles, including neutrons, in complex 3D geometries. The code can also perform a series of criticality (k-code) calculations to determine the energy dependent neutron flux distribution within a geometry to determine which nuclides will fission during a user-defined time step. This process can be combined and repeated with internal MCNP depletion calculations until the desired burnup is achieved [11]. The fuel geometry that was modeled, shown in Fig. 3, is based on public information of X-energy's Xe-100 fuel pebble [2]. The pebble sphere was surrounded by a cube of helium 6x6x6 cm^3 with mirror reflective boundary conditions. This approximates the neutron flux a pebble in the center of a reactor would experience. Criticality results from this geometry represent the k_∞ value of this fuel pebble. The 18,949 heterogeneous TRISO particles were modeled within the body of the pebble in a uniform lattice shape. Special attention was taken to ensure that no particles on the outer edge of the lattice were cut in the model, although previous work has shown that cut particles have statistically no impact on criticality calculations [12]. The UCO fuel was modeled at 1200K with all other materials modeled at 900K. The enrichment of the uranium was 15.5 wt.% ^{235}U. The ENDF/B-VII.1 cross-sections were used for all materials in the MCNP simulations [13].

The graphite moderation treatment was applied to all graphite materials to account for molecular effects of neutron scattering. The MCNP k-code specifications were to simulate 200,000 particles per cycle for 600 cycles, with the first 10 cycles being excluded from mean k_∞ calculation. Select simulations were run with fewer particles to reduce computational time. There was a total of 42 burnup time steps over a duration of 1304 days with each burnup duration time step consisting of no more than 40 days. The final burnup of the fuel was 168,000 MWD/MTU. Fission product tier 3 was used for all burnup simulations. In order to assess the precision of the MCNP simulations for radionuclide content in spent fuel calculations, ten identical simulations were performed with different initial random number seeds.

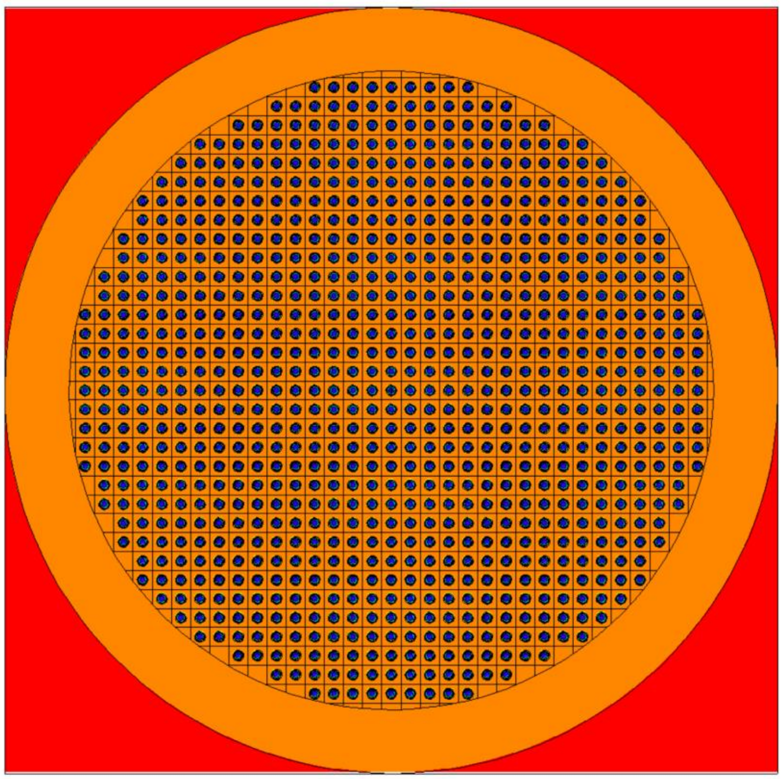

Figure 3. Cross-sectional view of X-energy's Xe-100 pebble modeled in MCNP. Red is helium, Orange is graphite, and the small spheres are heterogeneous TRISO particles.

RESULTS AND ANALYSES

The parameters that were varied are shown in Table 2, with perturbations from the specification values ranging from ±90%. While it is unrealistic to fabricate TRISO particles with 90% higher UCO density, these extreme situations that can only be done with simulations provide insights into the physical phenomenon that is driving trends in the data for smaller (±5%) realistic perturbations. All trend lines and best fit linear equations are only for data ranging from ±15%. Values outside of this range are considered unrealistic and bias the linearity of the trend line for data near the specification value.

Table 2. k_∞ results from MCNP simulations with various parameter perturbations. Values with larger uncertainties were generated from simulations with fewer histories.

Parameter	-90%	-50%	-25%	-15%	-5%	Specified	+5%	+15%	+25%	+50%	+90%
Fuel Density	1.51621 ±0.00004	1.59116 ±0.00028	1.54091 ±0.00007	1.52245 ±0.00007	1.50507 ±0.00007	1.49667 ±0.00007	1.48874 ±0.00007	1.47335 ±0.00007	1.45905 ±0.00007	1.42662 ±0.00033	1.38324 ±0.00007
Graphite Matrix Density	1.33654 ±0.00007	1.41939 ±0.00030	1.46147 ±0.00007	1.47643 ±0.00007	1.49023 ±0.00007	1.49667 ±0.00007	1.50322 ±0.00006	1.51539 ±0.00007	1.52665 ±0.00007	1.58477 ±0.00006	1.58477 ±0.00006
Uranium Enrichment	1.02211 ±0.0008	1.42023 ±0.00031	1.46965 ±0.00007	1.48215 ±0.00007	1.49235 ±0.00007	1.49667 ±0.00007	1.50099 ±0.00006	1.50830 ±0.00007	1.51469 ±0.00007	1.54512 ±0.00006	1.54512 ±0.00006
Number of TRISO Particles (fresh)	N/A	N/A	N/A	N/A	1.51353 ±0.00211	1.49698 ±0.00088	1.48212 ±0.00212	N/A	N/A	N/A	N/A
Number of TRISO Particles (spent)	N/A	N/A	N/A	N/A	0.90507 ±0.00232	0.90677 ±0.00062	0.90534 ±0.00241	N/A	N/A	N/A	N/A

All results shown in Figs. 4-7, based on data from Table 2, have a linear trend for perturbation values in the range of ±25%. Changing the graphite matrix density by 1% from the specification value results in an approximate 130 pcm reactivity change in the fresh fuel. This result is to be expected as the reactor is under moderated and increasing graphite density increases moderation, thus reducing the energy of neutrons in the reactor towards more optimal thermal values.

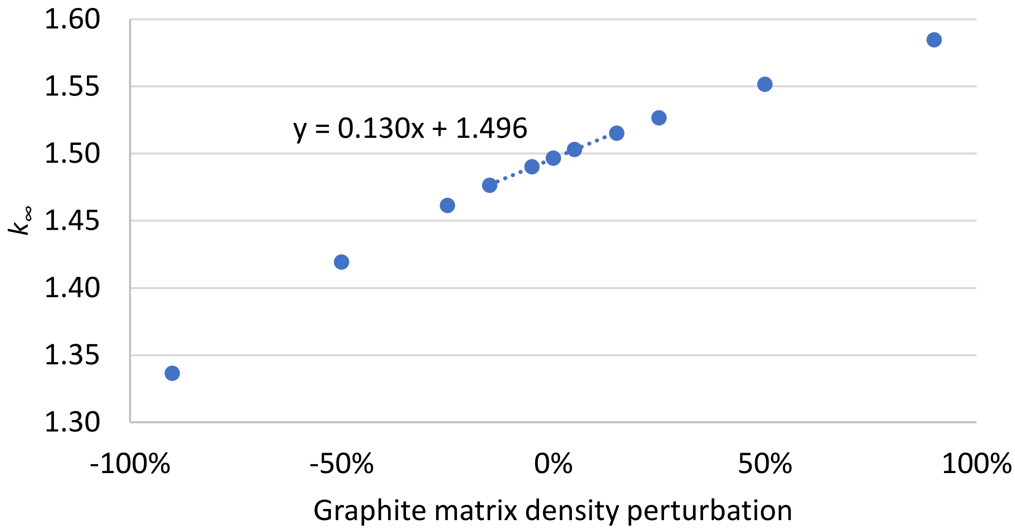

Figure 4. Change in k_∞ with changing graphite matrix density.

Changing the uranium enrichment by 1% from the specification value of 15.5 wt.% ^{235}U (i.e. 15.5 ±0.155) results in an approximate 87 pcm reactivity change in the fresh fuel. This result is to be expected as more fissile nuclides will increase the likelihood of a neutron resulting in fission.

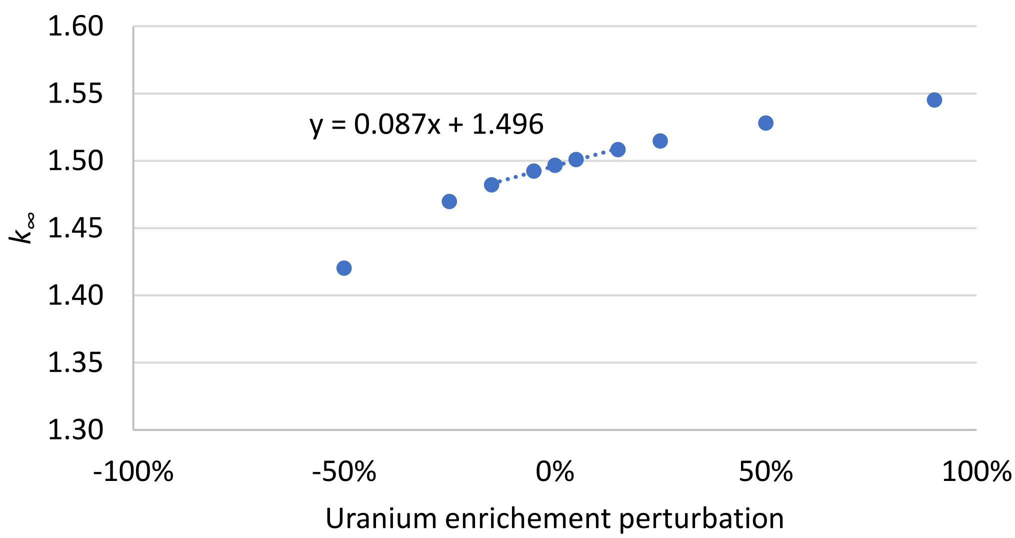

Figure 5. Change in k_∞ with changing uranium enrichment.

Changing the UCO fuel density by 1% from the specification value results in an approximate -164 pcm reactivity change in the fresh fuel. This result may seem counter intuitive in that adding more UCO atoms decreases the reactivity. k_∞ is defined as the number of neutrons created divided by the number of neutrons absorbed, as shown in Eq. 1. Since the thermal neutron absorption cross sections of the non-fuel regions, helium (^{4}He, ~0 mb), graphite (^{12}C, 3.53 mb), and silicon carbide (^{28}Si, 177 mb), are negligible compared to that of uranium, the atom density value in Eq. 1 (*N*) represents that of the fuel region. This allows k_∞ to be represented by the average number of neutrons emitted from fission times the ratio of the microscopic fission cross section to the microscopic absorption cross section. This value should be constant for all UCO densities, unless a change in density changes the energy distribution of the neutron flux. It can be imagined that an increase in the number of UCO atoms would preferentially absorbed thermal neutrons, thus hardening the neutron spectrum. Since the reactor is under moderated this would decrease reactivity.

$$k_\infty = \frac{\nu\Sigma_f}{\Sigma_a} = \frac{\nu N\sigma_f}{N\sigma_a} = \frac{\nu\sigma_f}{\sigma_a} \quad (1)$$

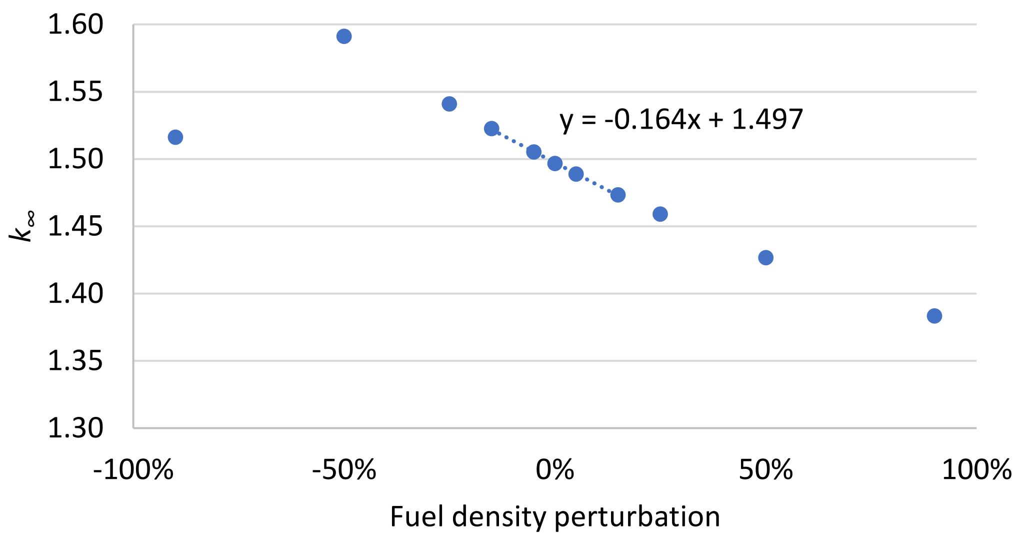

Figure 6. Change in k_∞ with changing UCO fuel density.

Changing the number of TRISO particles in the pebble by 1% from the specification value results in an approximate -314 pcm reactivity change in the fresh fuel. This result is to be expected as adding more TRISO particles will both increase the number of UCO atoms, thus hardening the neutron energy spectrum, as well as displace the graphite moderator, which will reduce the moderating ability of the pebble.

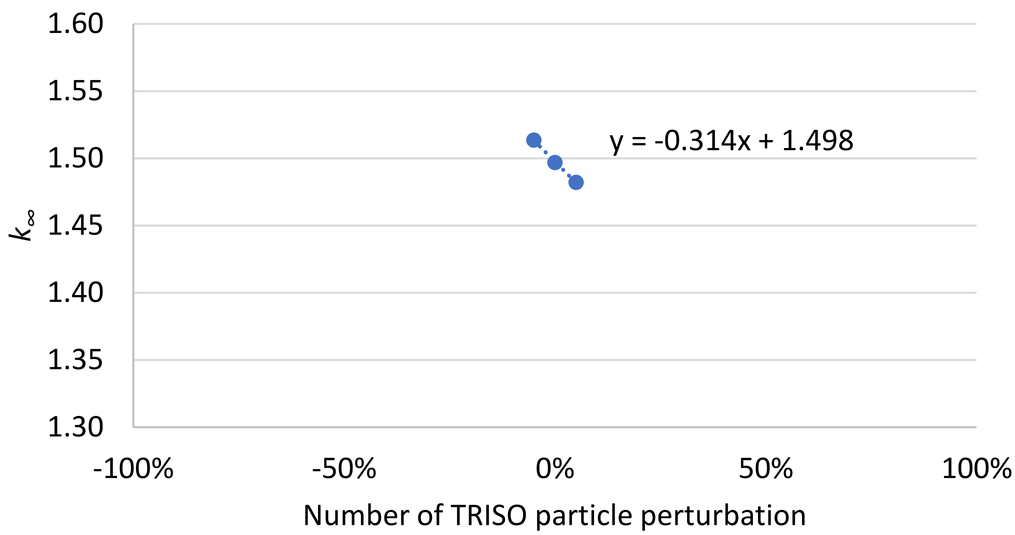

Figure 7. Change in k_∞ with changing the number of TRISO particles.

The impact on the k_∞ value throughout the pebble's burnup lifespan with respect to different TRISO partial numbers is shown in Fig. 8. The difference in the k_∞ values converge at the end of the pebble's life with the max burnup of 168 GWD/MTU. This convergence is caused by the harder neutron spectrum (+5% more TRISO particles) causing more fissions and radiative captures in the ^{238}U, which results in more ^{235}U and ^{239}Pu at the end of the pebble's life. This harder neutron spectrum also results in more even plutonium isotopes being fissioned and relatively fewer odd (more fissile) plutonium isotopes being fissioned. These mass values are shown in Table 3 along with the plutonium isotopic composition.

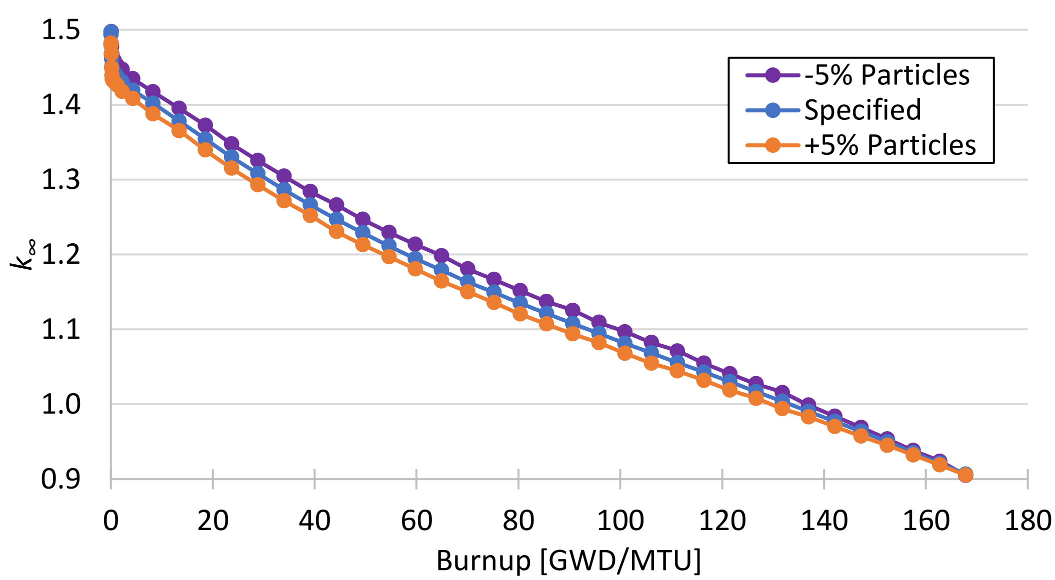

Figure 8. Pebble criticality with respect to burnup for different number of TRISO particles per pebble.

Table 3. ^{235}U and total plutonium masses in used pebble fuel along with the plutonium isotopic composition.

Number of TRISO Particles	-5%	Specified	+5%
^{235}U mass [g]	0.1435 ± 0.0005	0.1653 ± 0.0002	0.1858 ± 0.0005
Pu_{tot} mass [g]	0.1406 ± 0.0004	0.1599 ± 0.0001	0.1795 ± 0.0005
^{238}Pu [%]	6.42 ± 0.02	6.20 ± 0.01	6.05 ± 0.02
^{239}Pu [%]	30.68 ± 0.17	32.64 ± 0.05	34.39 ± 0.16
^{240}Pu [%]	22.49 ± 0.09	21.40 ± 0.02	20.39 ± 0.08
^{241}Pu [%]	18.09 ± 0.10	18.95 ± 0.03	19.65 ± 0.08
^{242}Pu [%]	22.31 ± 0.07	20.81 ± 0.02	19.52 ± 0.06

CONCLUSIONS

Having multiple fuel designs can be challenging for opensource modeling, however, for TRISO based fuels all TRISO particles have the same specifications. Based on the AGR-5/6/7 program results it can bee seen that TRISO particle manufacturing is good at meeting specifications, with the outer pyrolytic carbon thickness being the one statistically significant deviation. Perturbations in fuel parameters of 1% resulted in an approximate ±300 pcm change or less in the Xe-100 fresh pebble fuel. Changes in moderation appear to have large impacts on nuclear fuel content at the end of the pebble's life, but additional simulations and analysis are needed to make more confident and broad conclusions about this.

ACKNOWLEDGEMENTS

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