MCNP Simulations of Various Pebble Models for Pebble Bed Gas Cooled Reactors

Zachary Crouch*, Braden Goddard, Zeyun Wu, Ben Impson

Department of Mechanical and Nuclear Engineering
Virginia Commonwealth University, 401 West Main Street, Richmond, VA 23284 USA
*crouchzc@vcu.edu

INTRODUCTION

Pebble Bed Reactors (PBRs) are high-temperature gas-cooled (or molten salt-cooled) reactors. Thousands of pebbles cycle through the nuclear reactor, at a relatively slow speed, to fuel the reactor. These pebbles are spherical and vary from a golf ball to tennis ball in size, depending on the reactor design. Contained within these pebbles are thousands of TRISO particles. These reactors claim to have high efficiency (40-50%) and claim that the pebbles cannot melt. Accurate data is needed to ensure the safety and security of PBRs. This includes, for example, waste management, nuclear safeguards, nonproliferation, and reactor criticality safety. Reactor criticality safety is of the upmost importance to avoid accident chain reactions, such as the demon core accidents that occurred in the mid-1940s.

The goal of this research is to create a pebble bed library that will contain useful information such as the burnup of spent fuel in the pebbles, isotope signatures such as gamma ray energies and neutron flux from spent fuel, the isotopic composition of the pebbles, the k-effective of spent fuel at different burnups, and the amount of fissile material in the spent fuel. Much of this work will be simulated using the MCNP (Monte Carlo N- Particle) software.

MODEL SPECIFICATIONS

TRISO Particle Specification

TRISO particles are much smaller than pebbles with thousands of TRISO particles fitting into a pebble. TRISO particles have a spherical shape and typically contain up to 20 wt.% ^{235}U enrichment. TRISO particles traditionally have 5 layers (as seen in Figure 1): the fuel kernel in the center composed of either UO_2 or UCO, a porous carbon buffer layer, an inner pyrolytic carbon layer, a silicon carbide layer, and an outer pyrolytic carbon layer. The Xe-100 is a PBR under development by X-energy which uses TRISO particles and pebbles as the fuel type. The uranium enrichment of fuel is between 15 and 20 wt.% ^{235}U.

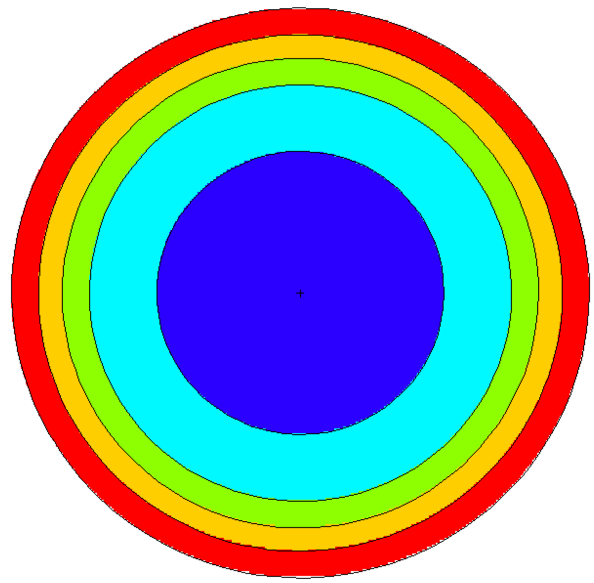

Figure 1. 2-D view of the TRISO fuel particle in the Xe-100 reactor. From inside to out the layers are: fuel kernel (blue), porous carbon (cyan), inner pyrolytic carbon (green), silicon carbide (orange), outer pyrolytic carbon (red).

Pebble Specification

The pebble is the final fuel product that will be inserted into the nuclear reactor. The specifications used in this research include a carbon matrix density of 1.75 g/cm^3 [1], 19,000 TRISO particles per pebble [2], an outer pebble diameter of 60 millimeters [**Error! Reference source not found.**], and an outer pebble carbon layer thickness of 5 millimeters [**Error! Reference source not found.**]. In order to assess the accuracy of modeling a pebble as a homogeneous object (shown in Figure 2), the 19,000 TRISO particles and the graphite matrix between these TRISO particles were combined into one homogeneous material. The outer carbon layer of the pebble was not homogenized due to its simplistic geometry.

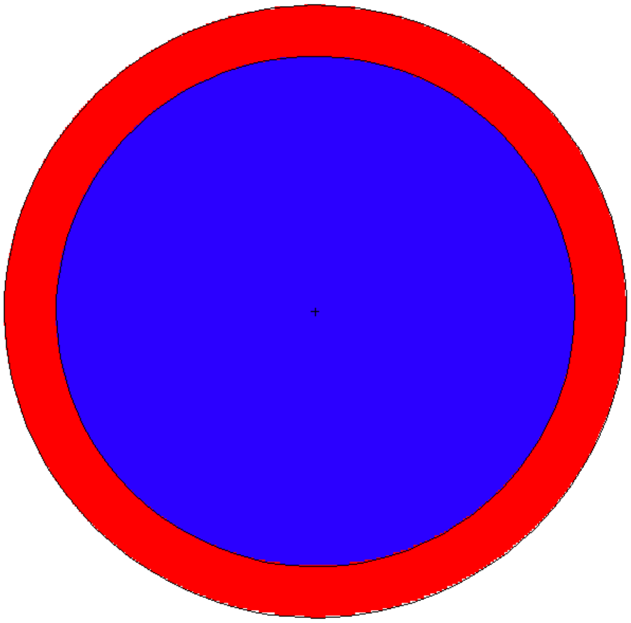

Figure 2. 2-D view of the homogeneous fuel pebble in the Xe-100 reactor. From inside to out the layers are: homogenized TRISO particle carbon matrix material (blue), outer carbon layer (red).

RESULTS AND DISCUSSION

The k-values of each of these models, shown in Tables I-IV, were run for various boundary conditions. The values from these simulations provide validation that the models are correct (k-inf values must be greater than 1) and identify what modeling assumptions create a statistical difference in the pebble's criticality.

Homogeneous Pebble, Heterogeneous (Clipped) Pebble, and Heterogeneous (Unclipped) Pebble

Clipped Pebble Model refers to the TRISO particles in the pebble which were clipped at the particle core boundary of 2.5 cm. Unclipped Pebble Model refers to the TRISO particles in the pebble that were not included in the pebble model because the particles were clipped at the boundary. Heterogeneous pebble model refers to the physical actual pebble model where realistic TRISO particles are placed uniformly in the particle core of the pebble, as shown in Figure 3. Homogeneous pebble model refers to the mixing of all elements and isotopes in the particle core and each atom is distributed evenly in the particle core. The homogeneous pebble contains the mass of 19,045 TRISO particles. The number of TRISO particles in the heterogeneous (clipped) pebble is unknown but contains 19,000 +/- 1,000 TRISO particles. The heterogeneous (unclipped) pebble model contains exactly 19,045 TRISO particles. The k-values and their respective standard deviations for these models are shown in Table I.

Table I: k-infinity values of homogeneous and heterogeneous pebble models with different boundary conditions.

Pebble Model	k-inf (plus)	k-inf (plus) std. dev.	k-inf (star)	k-inf (star) std. dev.
Homogeneous	1.39962	0.00063	1.41510	0.00055
Clipped Heterogeneous	1.50473	0.00077	1.51247	0.00063
Unclipped Heterogeneous	1.50631	0.00068	1.51638	0.00054

The statistical difference of the plus (+) reflective condition and the star (*) reflective condition is hypthesized to be due to the biasing of neutrons toward the core. If more neutrons are reflected from the boundary to the core, then the k-infinity is increased. The plus (+) reflective condition in MCNP reflects neutrons isotropically and does not consider the angle at which the neutron is reflected at the surface. The star (*) reflective condition in MCNP is more realistic because the angle of the neutron is taken into account during calculations. With the star reflective condtion, on average the netrons are coming from a center bias and thus are reflected back into a center bias.

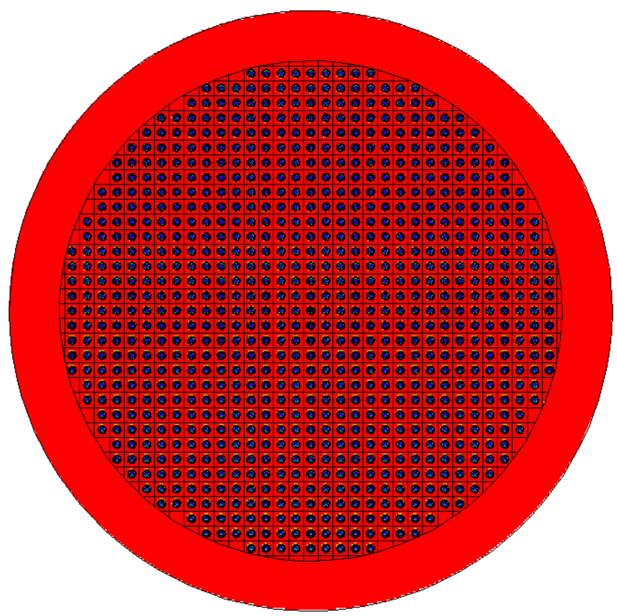

Figure 3. 2-D view of the heterogeneous (unclipped) pebble model in the Xe-100 reactor. Carbon matrix material (red), heterogeneous TRISO particles (blue spheres).

Heterogeneous Unclipped Pebble with Helium

This MCNP model, shown in Figure 4, consists of a 6 cm diameter sphere of the heterogeneous unclipped pebble placed inside a 6 cm x 6 cm x 6 cm cube. The region outside of the sphere and inside the cube was filled with natural helium with density (0.00286 g/cm^3), temperature (750°C), and pressure (6 MPa) of that found in the Xe-100 reactor [4]. The k-values for this model with and without helium are shown in Table II.

Table II: k-infinity Values of Heterogeneous Pebble Models with and without Helium.

Pebble Model	k-inf (plus)	k-inf (plus) std. dev.	k-inf (star)	k-inf (star) std. dev.
Unclipped Heterogeneous	1.50631	0.00068	1.51638	0.00054
Unclipped Heterogeneous w/ Helium	1.50816	0.00062	1.50822	0.00063

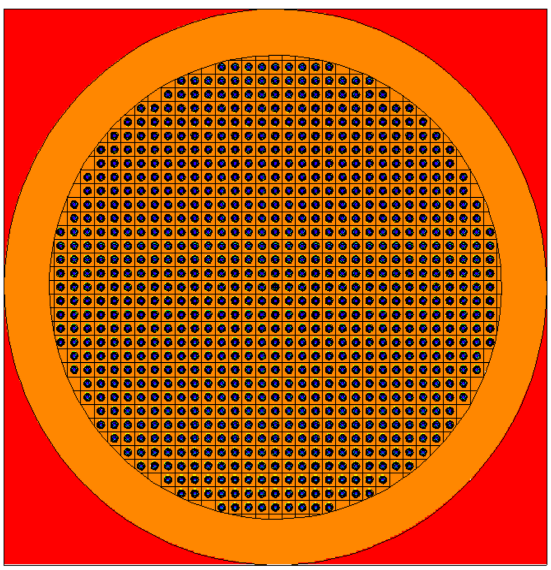

Figure 4. 2-D view of the unclipped heterogeneous pebble model with helium in the Xe-100 reactor. Carbon matrix material (orange), heterogeneous TRISO particles (blue spheres), helium (red).

FCC Homogeneous & Heterogeneous Pebble with Helium

A face centered cubic (FCC) structure unit cell with the equivalent of four homogeneous pebbles was created, as shown in Figure 5. The four pebbles are composed of six half spheres and eight one-eighth spheres. The dimensions of the unit cell are 8.4853 cm x 8.4853 cm x 8.4853 cm with a packing factor of 0.7402. In the gaps between the pebbles contain natural helium with a density of 0.00286 g/cm^3. One homogeneous pebble contains the uranium mass of 19,045 TRISO particles. This model was repeated with a heterogeneous structure, shown in Figure 6, with approximately 19,000 TRISO particles. The k-values from both models are shown in Table III.

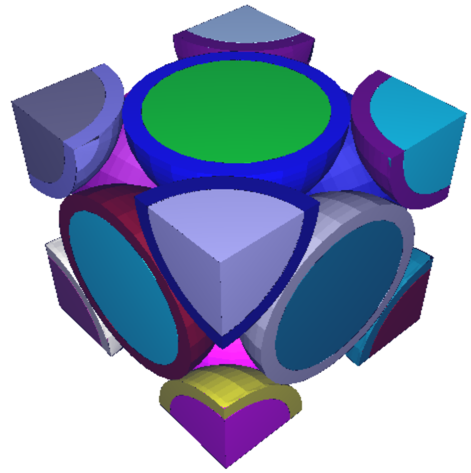

Figure 5. 3-D view of the FCC homogeneous pebble model with helium in the Xe-100 reactor.

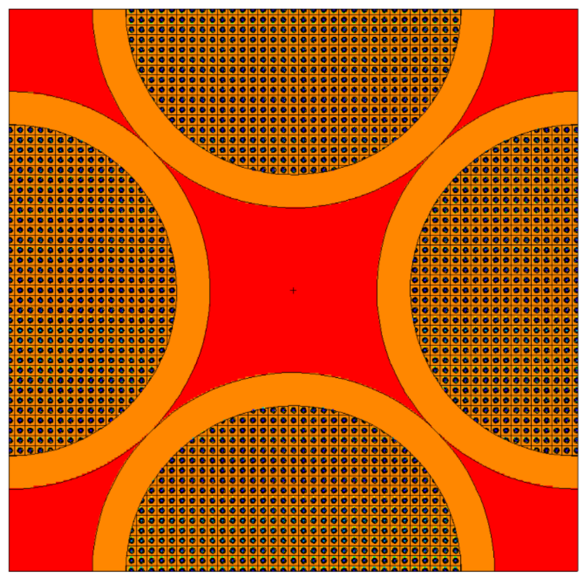

Figure 6. 2-D view of the FCC heterogeneous pebble model with helium in the Xe-100 reactor. Carbon matrix material (orange), heterogeneous TRISO particles (blue spheres), helium (red).

Table III: k-infinity values of the FCC homogeneous and heterogeneous pebble model with helium.

Pebble Model	k-inf (plus)	k-inf (plus) std. dev.	k-inf (star)	k-inf (star) std. dev.
FCC Homogeneous w/ Helium	1.40165	0.00078	1.39875	0.00063
FCC Heterogeneous w/ Helium	1.49654	0.00077	1.49598	0.00071

FCC Heterogeneous Semi-Unclipped Pebble with Helium

This simulation contains semi-unclipped TRISO particles which means all TRISO particles are whole except at the boundaries of the unit cell. On the edges of the unit cell, the TRISO particles are cut exactly in half on the half spheres and exactly in eighths for the one-eighth spheres. With this geometry, the TRISO particles can be reunited to form full TRISO particles when the unit cell connects to multiple unit cells in future MCNP simulations. This geometry can be seen in Figure 7 with k-values shown in Table IV.

Table IV: k-infinity values of the FCC heterogeneous semi-unclipped pebble model with helium

Pebble Model	k-inf (plus)	k-inf (plus) std. dev.	k-inf (star)	k-inf (star) std. dev.
FCC Heterogeneous Semi-Unclipped	1.51061	0.00069	1.50827	0.00056

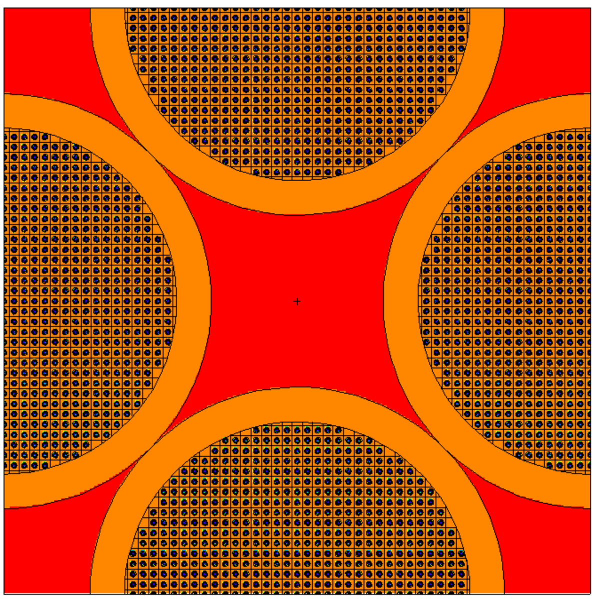

Figure 7. 2-D view of the FCC heterogeneous semi-unclipped pebble model with helium in the Xe-100 reactor.

CONCLUSIONS

Results from Table I indicate there is a statistical difference in a pebbles criticality when its material composition is homogenized. There is also a statistical difference depending on if the boundary condition is isotropic reflection (plus) or mirror (star) reflection. Having clipped particles in the model appears to make no statistical difference as long as the effective total number of particles is preserved.

From Table II, it can be seen that adding helium around a pebble has a slight statistical effect on criticality, but more importantly the difference in isotropic reflection and mirror reflection at the boundary statistical disappears when the reflective surface is changed from a sphere to a cube. This anomaly is believed to be due to a slight biasing reflected neutrons towards the center of the pebble when reflective boundary conditions are used on a spherical surface.

K-values from Table III reiterate that modeling pebbles, even as FCC unit cells, results in statistical differences between the homogeneous and heterogeneous.

Table IV illustrates that for a fixed amount of fissile material (effective whole particles) the unclipped model has a slightly higher k-infinity value. This is due to the fact that in order to remove the clipped particles while maintaining fissile material the particles must be packed slightly closer together which results in a higher density of fissile material in the inner part of the pebble surrounded by more moderating material.

FUTURE WORK

Future work will consist of MCNP modelling of the whole Xe-100 nuclear reactor including thousands of pebbles and nuclear reactor materials including reflectors. Simulations of the burnup of the pebbles will provide information about the isotopic composition of the pebbles as well as the gamma ray energies and neutron flux.

ACKNOWLEDGMENTS

This work is performed with the support of U.S. Department of Energy's Nuclear Energy University Program (NEUP) with the Award No. DE-NE0009304.

REFERENCES

1. D. W. MARSHALL, J. T. MAKI, P. A. DEMKOCWICZ, T. R. MITCHELL, and M. T. SHARP, "AGR-5/6/7 Fuel Specification," Idaho National Laboratory (2017).

2. C. LU, Z. WU, E. MULDER, and S. SEN, "A Direct Comparison of High-Order and Low-Order Neutronics Calculations of the 165MWth Xe-100 Reactor," *Trans. Am. Nucl. Soc.*, Vol. **124**, pp. 563-566 (2021).

3. C. LU and Z. WU, "A New Method to Efficiently Estimate the Equilibrium State of Pebble Bed Reactors," *Nuclear Technology*, Vol. **208**(10), pp. 1577-1590 (October 2022).

4. Xe-100, X-Energy, https://x-energy.com/reactors/xe-100, accessed on January 1, 2023