

# STOCHASTIC GEOMETRY AND HTGR MODELING WITH MCNP5

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## ABSTRACT

The MCNP5 Monte Carlo code has been frequently used to model HTGRs with explicit geometric representation of fuel compacts or pebbles, including the microscopic fuel kernels within them. The random locations of fuel kernels within each fuel compact or pebble, and of pebbles within the core, however, present difficulties. A new, on-the-fly, stochastic geometry model for MCNP5 has been developed for modeling the random fuel kernels within the graphite matrix. This model is compared to both fixed lattices and multiple realizations of explicit random kernels. In addition, the effects of infinite vs. finite lattices on full-core geometries are investigated, including the effects of stochastic geometry modeling.

*Key Words:* MCNP, Monte Carlo, stochastic geometry, HTGR

## 1 INTRODUCTION

Coated particle fuel (TRISO fuel) is the likely fuel candidate for the Next Generation Nuclear Plant, which is expected to be a high temperature gas reactor (HTGR) using either a prismatic or pebble-bed design [1]. Pebble bed or prismatic designs for HTGRs present a significant challenge for geometry modeling due to their multiple levels of heterogeneity. Prismatic HTGRs are composed of hexagonal fuel assemblies that contain fuel compacts, burnable poison compacts, and He coolant channels in a graphite matrix. The fuel compacts are cylindrical and contain coated microscopic fuel kernels (~ 1 mm diameter) embedded in a graphite matrix. Each fuel kernel typically has a spherical uranium oxycarbide region surrounded by layers of graphite, pyrolytic graphite, and silicon carbide. Pebble bed HTGRs contain randomly located fuel pebbles which in turn are filled with randomly located fuel kernels in a graphite matrix. Either core configuration results in the well known "double heterogeneity", with the fuel kernels constituting one heterogeneity and the fuel pebbles (~ 6 cm diameter spheres) or fuel compacts (~ 1 cm diameter cylinders) causing the second heterogeneity. This paper primarily concerns the analysis of the stochastic particle heterogeneity which is applicable to both prismatic and pebble-bed designs.

The MCNP5 Monte Carlo code [2] has been frequently used to model HTGRs with explicit geometric representation of fuel compacts or pebbles, including the microscopic fuel kernels within them [3,4,5,6]. The random locations of fuel kernels within each fuel compact or pebble,

and of pebbles within the core, however, present difficulties. To date, three approaches have been tried for handling the randomness: (1) A regular lattice arrangement, ignoring any randomness [3,4,5,6], (2) The chord-length sampling approach in MVP [7,8,9] and recent research [10,11], (3) The explicit approach in MONK using "hole geometry" with a single realization of the entire random geometry [12].

We have developed an approach to stochastic geometry modeling for MCNP5 which roughly combines the 3 previous approaches. For embedded geometry (universe or lattice), we have introduced the notion of a random translation. That is, when a neutron enters an embedded universe flagged as stochastic, its coordinates are transformed randomly. Different translation parameters can be declared for different levels of the geometry, and the random translations are performed only upon entering universes which the user declares as stochastic. In addition, when a fission occurs and the site parameters are saved in the fission bank, the current values of the random translation parameters must be saved along with the normal fission site data. The stochastic variations may be applied independently at multiple levels of the geometry hierarchy, such as for the locations of both individual fuel pebbles and the fuel kernels within them. There are some advantages to this approach: simplicity of setting up a regular lattice, randomly displacing geometry rather than using less-intuitive chord-length distributions, and avoiding possible repetitions in the single-realization approach. Numerical results are presented which verify the MCNP5 stochastic treatment.

The MCNP5 stochastic geometry does not require any significant memory storage, nor does it noticeably increase running time. It provides a relatively simple method for modeling stochastic HTGR geometry.

## 2 DETAILED MCNP5 MODELING OF PARTICLE FUEL

In this section, we discuss the detailed modeling of HTGR particle fuel in MCNP5, without regard to the higher-level geometry of pebbles or compacts, or full core arrangement. After a brief review of MCNP5 geometry modeling capabilities, four different modeling approaches are described, and then numerical results are presented.

### 2.1 Review of MCNP5 Geometry Modeling

MCNP5 permits a very general, detailed representation of 3D geometry. Volumes in space called *cells* are defined in terms of their bounding *surfaces*. Surface types include planes, quadrics, and tori (aligned with a major axis). Alternatively, users may specify *macrobodies* (e.g., sphere, finite cylinder, ellipsoid, etc.), which are converted internally into individual surfaces. *Boolean operators* (union, intersection) and *surface-senses* (inside, outside) may be used with the surface specifications to precisely define the volume enclosed by a cell. Cells may also include the *complement* of another cell and may be composed of non-convex or disjoint volumes.

Hierarchical geometry may be modeled using the MCNP5 concept of a *universe*. One or more cells may be declared as belonging to a universe, and that universe can then be embedded inside of another cell. If the universe geometry is larger than the cell it is embedded in, it is clipped by the enclosing cell. Up to 10 levels of embedding are permitted. A variation on the

universe concept is a *lattice*, where a cell (which may have an embedded universe) is repeated in 1, 2, or 3 dimensions. Lattice cells may be hexahedra (i.e., “bricks”) or hexagonal prisms.

## 2.2 MCNP5 Modeling Schemes for Particle Fuel

There are four basic approaches to representing the graphite matrix and embedded fuel kernels in MCNP5:

### 2.1.1 Homogenization

Simple homogenization of the graphite matrix and fuel kernels leads to significant errors in  $k$ -effective. In the numerical examples below, simple homogenization results in underpredicting  $k$ -effective by 6%. Partial homogenization, where the fuel kernel coatings are homogenized with the graphite matrix but the UCO fuel region is represented explicitly, can give negligible errors in  $k$ -effective of less than 0.1% and can significantly reduce computer running time [13]. In the present work, we consider only exact geometry representations and do not examine partial homogenization schemes.

### 2.1.2 Multiple realizations of explicit random geometry

Using auxiliary programs or scripts, fuel kernel locations in the graphite matrix may be chosen randomly and used to create an input file for MCNP5. This single realization of the geometry is then used for running an MCNP5 calculation. If this process is repeated, choosing many different realizations and then averaging the results from the separate runs, then the overall results will approach those for a true random geometry. This process is expensive since many separate Monte Carlo runs are needed. The specific algorithm used for constructing the multiple realizations of geometry for MCNP5 input may involve simple randomness (e.g., the Random Sequential Addition (RSA) process [14]) or may incorporate knowledge of the physical processes used in manufacturing the fuel [8,15]. Regardless, the approach can not be used for modeling entire cores due to limitations in the number of cells permitted in MCNP5 – a few thousand fuel kernels can be modeled explicitly, but not a few million.

### 2.1.3 Lattice models

The fuel kernels can be placed on a regular lattice, either cubic or hexagonal, such that the packing fraction of fuel kernels in the graphite matrix is preserved. This is the approach most often used in explicit representation of the fuel kernels and matrix [3,4,5]. A single fuel kernel is defined in a fixed position and then used as the “universe” which fills each cell of a lattice. In general, infinite lattices have been used and then clipped by the bounding surface (e.g., a cylinder for prismatic cores or a sphere for pebble cores). The MCNP5 infinite lattice approach can handle an essentially unlimited number of fuel kernels, without significant increases in memory storage. Extra memory storage is required for finite lattices, where the numbers of lattice elements in each direction are specified explicitly and different “universes” may be specified in each lattice element, but there are no particular MCNP5 limits on the number of kernels permitted.

MCNP5 has the flexibility to model many different types of regular lattice arrangements of fuel kernels: simple cubic (with a fuel kernel at the center of each lattice element), body-centered cubic (with kernels at the center and each corner), face-centered cubic (with kernels at each corner and at the center of each side), simple hexagonal (stacked hexagons), and hexagonal close-packed (hexagons stacked in interstices of alternate layers). Some basic characteristics of these lattice types are given in Table I [16]. The effects of lattice arrangement will be examined in the next section.

**Table I. Basic Characteristics of Lattice Types**

Lattice Type	Number of kernels per lattice element	Maximum packing fraction
Simple cubic	1	.524
Body centered cubic	2	.680
Face centered cubic	4	.740
Simple hexagonal	3	.605
Hexagonal close-packed	4	.740

#### 2.1.4 MCNP5 stochastic geometry

For embedded geometry (universe or lattice), we have introduced the notion of a random translation. That is, when a neutron enters an embedded universe flagged as stochastic, the universe coordinates are transformed randomly according to

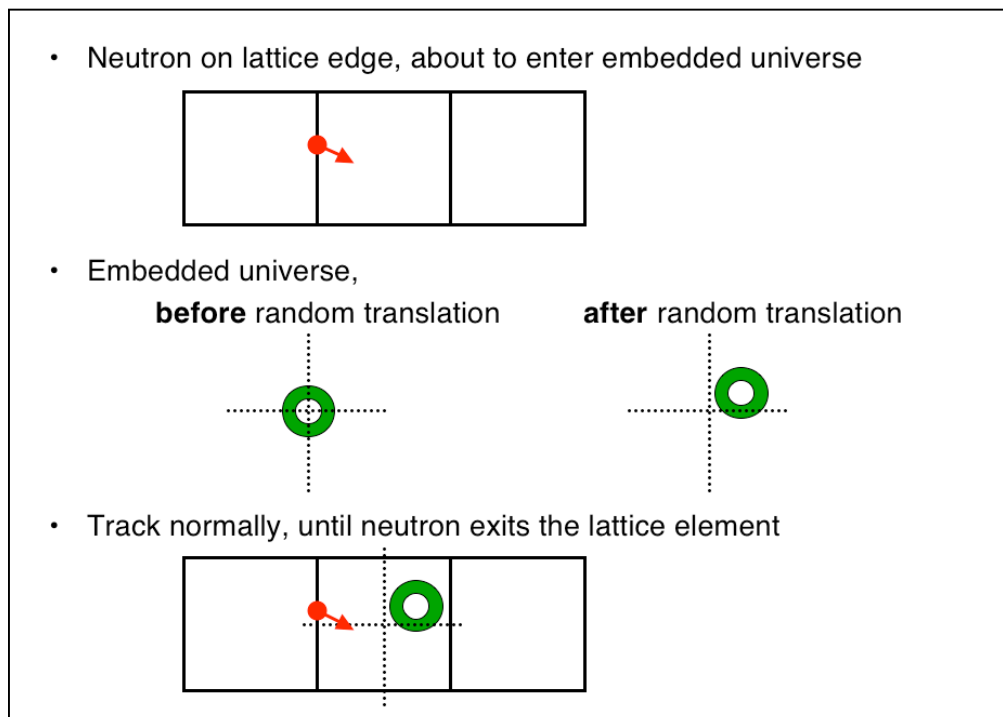
$$x = x + (2\xi_1 - 1) \cdot \delta_x$$

$$y = y + (2\xi_2 - 1) \cdot \delta_y$$

$$z = z + (2\xi_3 - 1) \cdot \delta_z$$

where  $\xi_1$ ,  $\xi_2$ ,  $\xi_3$  are random numbers uniformly distributed on (0,1), and  $\delta_x$ ,  $\delta_y$ ,  $\delta_z$  are user-defined parameters. Different translation parameters can be declared for different levels of the geometry, and the random translations are performed only upon entering universes which the user declares as stochastic. To preserve mass and packing fractions, the translation parameters should be chosen such that fuel kernels or other objects are not displaced beyond the edges of the enclosing cell or lattice element. This capability has been implemented for simple cubic lattices and is equivalent to "jiggling" the sphere randomly within the cubical cell every time the cell is entered (see Figure 1). If  $\delta_x$ ,  $\delta_y$ ,  $\delta_z$  are chosen to be less than or equal to the distance between the kernel and the lattice edge, then the sphere will stay entirely within the cell. We are examining the application of this methodology to other lattice types (fcc, bcc, hcp).

In addition to the random translation applied to a neutron entering a stochastic universe, special treatment is needed for saving the fission sites in an eigenvalue calculation. When a



**Figure 1. Illustration of MCNP5 Stochastic Geometry Treatment**

fission occurs and the site parameters are saved in the fission bank, the current values of the random translation parameters must be saved along with the normal fission site data. In the next cycle of the calculation, these saved translation parameters are used for the neutron starting at that fission site, so as to continue the flight from the same stochastic realization in effect when the site was saved.

This approach retains the simplicity of setting up a regular lattice in the MCNP5 input. Randomness is introduced directly through displacing the universe geometry, and the conventional Monte Carlo random walk is utilized throughout the simulation. Each time a neutron enters a stochastic universe, a new random sample of the displacements is made, avoiding the possible repetitions which could occur in the single-realization approach. Finally, the use of on-the-fly random translations does not incur the large memory requirements of the single-realization approach.

The MCNP5 stochastic geometry approach does not require any significant memory storage, nor does it noticeably increase the running time for a problem. It provides a relatively simple method for modeling stochastic HTGR geometry.

### 2.3 Numerical Results for Modeling Particle Fuel

MCNP5 calculations were performed for fuel kernel configurations corresponding to an infinite array of fuel kernels in a graphite matrix. The fuel kernel geometry and composition were taken from the NGNP Point Design [1] and are reproduced in Table II for convenience. The packing fraction for all of these calculations was 0.289.

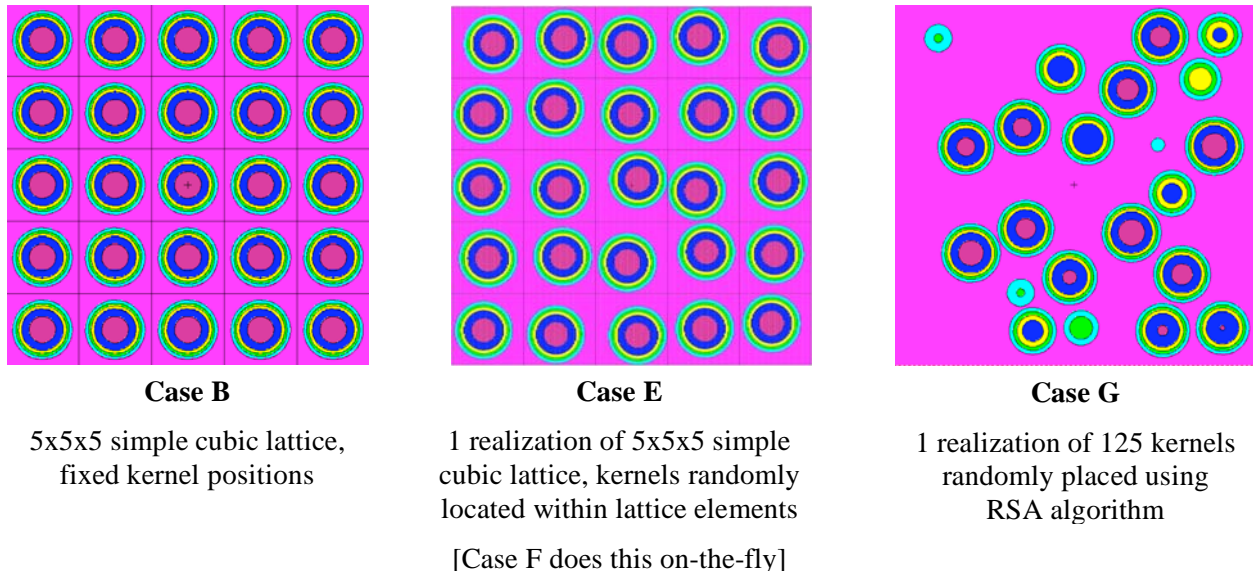
**Table II. TRISO Fuel Kernel Geometry and Composition**

Region #	Name	Outer radius ( $\mu$ )	Composition	Density (g/cc)
1	Uranium oxycarbide	175	UCO ( $UC^{.5}O^{1.5}$ )	10.5
2	Porous carbon buffer	275	C	1.0
3	Inner pyrolytic carbon	315	C	1.9
4	Silicon carbide	350	SiC	3.2
5	Outer pyrolytic carbon	390	C	1.9

The MCNP5 calculations for Cases A-F were performed for a 5x5x5 array of fuel kernels in graphite with reflecting boundary conditions, corresponding to an infinite lattice. In each case, the size of the lattice elements was chosen to preserve the correct packing fraction of 0.289 (e.g., for body-centered cubic, with 2 kernels per lattice element (see Table I), the element volume was twice the volume of a simple cubic lattice element). For Case G, where all the kernels were randomly placed for each realization using the RSA algorithm, the overall volume was that corresponding to 125 fuel kernels and matrix, with reflecting outer boundaries. Figure 2 illustrates the geometry for Cases B, E, and G. Table III gives results from the MCNP5 calculations.

The results in Table III clearly show the serious error introduced by simple homogenization of the fuel kernels and graphite matrix – Case A underestimates k-effective by 6% compared to Cases B-G.

Comparing Cases B, C, and D, it can be seen that the results are not sensitive to the type of lattice representation, simple cubic, body-centered cubic, or face-centered cubic. Previous results from Karriem et al. [13] similarly showed no difference between hexagonal vs. simple cubic lattice arrangements for the description of fuel kernels in graphite. (Ref. [13] considered a kernel-matrix packing fraction of 0.04, compared to 0.289 in the current work.) Since simple



**Figure 2. Geometry for MCNP5 calculations of fuel kernels in graphite matrix**

cubic lattices can be used for packing fractions up to a maximum of .524 (cf. Table I), they are more than adequate for representing the fuel kernels and graphite matrix in the present studies. There is no need to use bcc, fcc, or hcp lattice arrangements with their more complicated input setup and longer running times.

Comparing results for Cases E, F, and G in Table III shows that (1) the new stochastic geometry treatment (Case F, on-the-fly random positioning) is implemented correctly, since it gives results nearly identical to those for Case E, and (2) random positioning of kernels within simple cubic lattice elements gives the same effect on k-effective as does a completely random arrangement of kernels (using RSA, Case G). Comparing results for Cases B/C/D where the fuel kernels are at regular, fixed lattice positions with Cases E/F/G which introduce random locations for the fuel kernels, it can be concluded that stochastic geometry effects lower k-effective by about 0.1 – 0.2 % for an infinite graphite matrix with embedded fuel kernels (with packing fraction 0.289). This is a small effect which may reasonably be neglected for many design calculations, but should be included for benchmarking and high-precision calculations of HTGRs.

**Table III. MCNP5 Results for Infinite Graphite Matrix with Embedded Fuel Kernels**

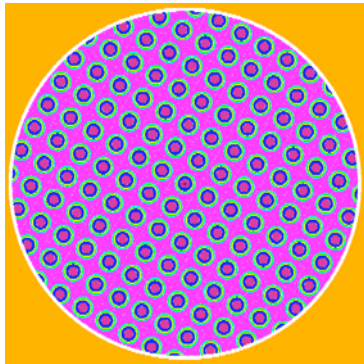
<b>Case</b>	<b>Configuration</b>	<b>K-effective <math>\pm 1\sigma</math></b>
<b>A</b>	Homogenized matrix & fuel kernel	1.0996 $\pm$ .0008
<b>B</b>	Simple cubic fixed lattice	1.1531 $\pm$ .0004
<b>C</b>	Body-centered cubic fixed lattice	1.1534 $\pm$ .0003
<b>D</b>	Face-centered cubic fixed lattice	1.1526 $\pm$ .0003
<b>E</b>	Multiple (25) realizations of simple cubic fixed lattice, with kernels randomly located within each lattice element	1.1513 $\pm$ .0004
<b>F</b>	New MCNP5 stochastic geometry, on-the-fly random location of kernels within simple cubic lattice elements	1.1515 $\pm$ .0004
<b>G</b>	Multiple (25) realizations of randomly located (RSA) kernels within a box	1.1510 $\pm$ .0003

### 3 FULL-CORE HTGR MODELING WITH MCNP5

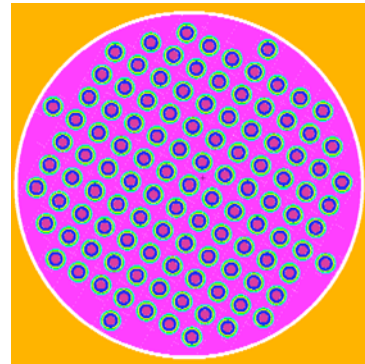
To investigate the impact of stochastic geometry for fuel kernels on overall results for full-core HTGR calculations, a detailed 3D model of the NGNP prismatic core design [1] was constructed for MCNP5. This model explicitly accounted for: each layer of the coated fuel particles, every individual fuel kernel in the fuel compacts, voids outside of each fuel compact, coolant holes, top and bottom reflectors, voids outside of the reflector column, etc. Several variations of this model were used to investigate the effects of (1) using an infinite lattice vs. a finite lattice, and (2) modeling the fuel kernels with stochastic geometry.

#### 3.1 Modeling Effects of Infinite vs. Finite Lattice of Fuel Kernels

As noted in Section 2.1.3, lattices may be defined as finite or infinite in MCNP5. If an infinite lattice is used, then the lattice geometry is clipped by the enclosing cylinder for prismatic HTGRs or by the enclosing sphere which forms the pebble boundary in pebble bed HTGRs. Using an infinite lattice, some of the fuel kernels in the lattice will be intersected by the enclosing sphere or cylinder, so that fragments of particles will exist in the MCNP5 model (see Figure 3a). If instead a finite lattice is used, then those lattice cells which intersect the bounding cylinder or sphere may be filled only with graphite matrix, i.e., without a fuel kernel (see Figure 3b).



3a. Infinite lattice of fuel kernels, with partial kernels due to clipping by the enclosing cylinder



3b. Finite lattice of fuel kernels, with graphite matrix in lattice elements which intersect the enclosing cylinder

**Figure 3. Fuel cylinder containing graphite matrix with embedded fuel kernels, for prismatic NGNP core**

Clearly, the fragments of kernels at the cylinder boundary in Figure 3a do not realistically model the geometry. Figure 3b is more realistic, containing only whole fuel kernels. Note that since there are fewer kernels in Figure 3b than in Figure 3a, the vertical spacing of the fuel kernels (along the cylinder axis) should be adjusted so as to yield the correct overall packing fraction for the fuel cylinder. That is, the packing fraction for the fueled lattice region needs to be increased, so that the overall packing fraction for the compact is correct when the graphite-only regions near the cylinder boundary are included.



Most reported MCNP models use infinite lattices and distort the geometry (as in Figure 3a) [3,4,5], even though earlier work [8] makes note of the effect and recommends a model similar to Figure 3b. The effect on computed k-effective results is discussed in the next section.

### 3.2 Numerical Results for Full-core HTGR Calculations

Table IV presents the results of a number of full-core HTGR calculations performed with MCNP5. For all of these calculations, the fission source distribution entropy was used in MCNP5 to ensure that a converged fission source was achieved prior to beginning the problem tallies [17]. Discussion of significant effects follows below.

**Table IV. MCNP5 Results for Full-core HTGR Calculations**

Case	Configuration	K-effective $\pm 1\sigma$
<b>A</b>	Fully homogenized core	1.0155 $\pm$ .0004
<b>B</b>	Heterogenous core, with homogenized fuel kernels & matrix in fuel cylinders	1.0583 $\pm$ .0004
<b>C</b>	Heterogeneous core, with simple cubic fixed infinite lattice (with partial kernels at cylinder boundary) [U. Mich]	1.0953 $\pm$ .0004
<b>D</b>	Heterogeneous core, with simple cubic fixed infinite lattice (with partial kernels at cylinder boundary) and with fuel kernel coatings homogenized into graphite matrix [U. Mich]	1.0949 $\pm$ .0004
<b>E</b>	Heterogeneous core, with simple cubic fixed infinite lattice (with partial kernels at cylinder boundary) [LANL]	1.0948 $\pm$ .0002
<b>F</b>	Heterogeneous core, with simple cubic fixed finite lattice (with no partial kernels at cylinder boundary)	1.0974 $\pm$ .0002
<b>G</b>	New MCNP5 stochastic geometry, on-the-fly random location of kernels within simple cubic finite lattice elements (with no partial kernels at cylinder boundary)	1.0968 $\pm$ .0002

Cases A and B illustrate the substantial errors (versus Cases C-G) that are introduced by homogenization, with entire fuel assemblies homogenized in Case A and only the fuel kernels and matrix regions in Case B. Clearly, neither of these models should be used for HTGR calculations.

Cases C, D, and E involve modeling the fueled region of each compact as shown in Figure 3a, using an infinite lattice of fuel kernels clipped by the enclosing cylindrical boundary. All 3 cases yield essentially the same result within statistics. In Cases C and E, all layers of the fuel kernel coating were explicitly represented, whereas in Case D the coating layers were

homogenized into the graphite matrix. Thus, smearing the fuel coatings into the graphite matrix has no significant effect on results, and runs about 30% faster than the cases which explicitly model the fuel coatings. Cases C and E are identical models, run to verify that consistent versions of MCNP5 and its nuclear cross-section libraries were used at LANL and the University of Michigan.

Cases F and G were run using a finite lattice for the fuel kernel and graphite matrix, with only graphite (and not fuel kernels) in lattice elements intersecting the cylindrical boundary (as in Figure 3b). It can be seen by comparing Case F to Cases C/D/E that correctly modeling the boundary effects of the fuel kernels (i.e., by not allowing partial kernels at the boundary) leads to an increase in k-effective of about 0.2%. This is a small effect, but should certainly be included for benchmark or high-precision calculations.

Comparing Cases F and G, it can be seen that the stochastic geometry lowers k-effective by only about .06%. This is about half the size of the effect noted in Section 2.3 for infinite geometry. A possible explanation is that the spectrum is softer for the full-core geometry (due to the extra graphite in the block and reflectors), diminishing the effect of resonance absorption in the fuel kernels and thus reducing the stochastic effects on k-effective. Further investigation of the interaction between stochastic geometry and physics effects is in order.

As a final comment on the MCNP5 calculations described in this section and in Section 2.3, it should be noted that about *8-10 thousand* CPU hours of computations were performed on Pentium-IV or AMD Athlon processors in the course of this work. The principal tools which made this large amount of calculation feasible were the *mcnp\_pstudy* utility [18] (for submitting multiple MCNP5 jobs & combining results) and a large Linux cluster. Typically 50-100 MCNP5 jobs were submitted to the cluster using *mcnp\_pstudy* and ran concurrently.

## 4 CONCLUSIONS

We have investigated several geometric schemes for representing HTGR fuel with a graphite matrix and embedded fuel kernels. Homogenization of either the fuel assemblies or the fuel kernels and graphite matrix was shown to produce terrible results for k-effective, in error by ~5%. Clearly, homogenization should not be used for HTGRs. For infinite geometry, representing the geometry with a simple cubic lattice of fuel kernels results in overpredicting k-effective by about 0.1 – 0.2% compared to an explicit random representation of the kernels.

A new stochastic geometry treatment for MCNP5 was developed to randomly position fuel kernels "on-the-fly" for a neutron flight within each lattice element. This stochastic geometry treatment costs essentially nothing in computer time or storage, and yields k-effective results in agreement with a random representation (i.e., about 0.1 – 0.2% lower than for a fixed lattice in infinite geometry).

For full-core models of HTGRs, it is important to correctly model the boundaries of fueled regions, such that fuel kernels in lattices are not sliced into partial kernels. Correcting these geometry inaccuracies (so that there are no partial kernels at the boundaries) raises k-effective by about 0.2%. When the boundary effects are treated properly, the additional effect of the MCNP5 stochastic geometry treatment then lowers k-effective by about .06%, roughly half the size of the stochastic effect for infinite geometry.

## 5 ACKNOWLEDGMENTS

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