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Stochastic Geometry Capability in MCNP5 for the Analysis of Particle Fuel

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Abstract

A stochastic geometry capability has been implemented into the MCNP5 Monte Carlo code. This capability allows the analysis of TRISOL particle fuel, allowing for the random locations of the fuel kernels within the graphite matrix. The method has been compared to a MCNP5 benchmark calculation of randomly placed fuel kernels within a box with reflecting boundaries as well as multiple realizations of lattices where the microspheres are randomly located within the equivalent cubical cells. Comparisons are also made to MCNP5 calculations where the fuel kernels are fixed on a cubical lattice. Our preliminary results for infinite medium configurations indicate that the new stochastic geometry capability in MCNP5 is an accurate and efficient approach to analyze TRISO particle fuel configurations.

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 (MacDonald et al. 2003). 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 (~ 4 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.

We have developed a capability for treating the particle heterogeneity by developing a stochastic geometry capability in MCNP5 (X-5 Monte Carlo Team 2003) that accounts for the random locations of the fuel kernels within the graphite matrix. This method is a relatively straightforward modification to the MCNP5 tracking routines that effectively results in a random displacement of the microsphere within a cubical matrix cell whenever a neutron enters the cell. The method has been compared to a MCNP5 benchmark calculation of randomly placed fuel kernels within a box with reflecting boundaries. Comparisons are also made to MCNP5 calculations where the fuel kernels are fixed on a cubical lattice as well as multiple realizations of lattices where the microspheres are randomly located wholly within

the equivalent cubical cells. Our preliminary results for infinite medium configurations indicate that the new stochastic geometry capability in MCNP5 is an accurate and efficient approach to analyze TRISO particle fuel configurations.

2. Methods for the analysis of particle fuel

2.1. Effective Dancoff factor approach

The original methodology for analyzing TRISO fuel used effective Dancoff factors to compute heterogeneous resonance integrals that were then used within unit-cell transport-based spectrum codes (Massimo 1976 and MICROX-2 1999).

2.2 Explicit Monte Carlo on a lattice

Several investigators (Johnson et al. 2001, Plukiene and Ridikas 2003, Difilippo 2003) have analyzed particle fuel by placing the kernels on a lattice within the graphite matrix, with the lattice dimension determined to preserve the packing fraction. For example, Defilippo used MCNP4C to analyze a benchmark pebble bed configuration and was able to model over 50 million fuel kernels including detailed internal structure of the kernels.

2.3 Chord length sampling methods

In contrast to explicit Monte Carlo simulation, Murata et al. (Murata et al. 1996 and Murata et al. 1997) developed an empirical nearest neighbor distribution function for the fuel kernels using a sphere packing simulation and used this to sample the location of the next fuel kernel along a neutron trajectory in the fuel matrix. Within a fuel kernel, conventional Monte Carlo random walk was employed, resolving the detailed structure of the fuel kernel. This approach, which was implemented into MCNP4C and the MVP codes (Mori et al. 2000), avoids specifying the locations of the fuel kernels since they are encountered "on the fly" during the random walk within the fuel matrix.

Donovan et al. (Donovan and Danon 2003a, Donovan et al. 2003b, and Donovan and Danon 2003c) have modeled the particle fuel as a binary stochastic mixture and used chord length sampling to determine the location of the next sphere during the random walk within the fuel mixture, and applied this to a 2D fuel configuration. They extended this approach by treating the random walk within the fuel kernels by conventional Monte Carlo and used an empirical distribution function to sample the distance to the next fuel kernel. This method was applied to a benchmark fuel pebble cell with excellent results. The chord length distribution function within the fuel matrix was determined from a sphere packing simulation using random sequential addition (RSA) (Widom 1966 and Torquato 2002) to insert the kernels into the fuel matrix. This method is very similar to the method of Murata (Murata et al. 1996), with the primary difference being the way the empirical chord length distribution function was determined.

2.4 Single realization of stochastic geometry

An alternative approach is to generate a realization of the stochastic geometry and explicitly analyze this configuration with traditional random walk Monte Carlo. This is the approach taken in the Monk code (Armishaw et al. 2003).

3. Description of stochastic geometry capability for MCNP5

3.1. MCNP5 geometry overview

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 that 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.

3.2. MCNP5 stochastic geometry

We have developed yet another approach to stochastic geometry modeling for MCNP5 which roughly combines the 3 previous approaches noted above. 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 ξ_1, ξ_2, ξ_3 are random numbers uniformly distributed on (0,1), and δ_X, δ_Y, δ_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 body-centered cubic (bcc) lattices and is equivalent to "jiggling" the sphere randomly within the cubical cell every time the cell is entered. If δ_X, δ_Y, δ_Z are chosen to be less than or equal to half the lattice edge, then the sphere will stay entirely within the cell. We are examining the application of this methodology to face-centered cubic (fcc) lattices as well as hexagonal close packed (hcp) lattices and will report on this at a later date.

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 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.

While this approach has similarities to the previous approaches noted above, there are some advantages: 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 conventional Monte Carlo random walk is utilized throughout the simulation, avoiding the determination and use of chord length distribution functions. 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.

4. Simulation results

4.1 Verification methodology

The stochastic geometry capability has been verified by comparison with several independent simulations of particle fuel configurations. The independent calculations are described next, followed by the numerical results. All fuel kernel configurations correspond to an infinite array of fuel kernels in a graphite matrix. The fuel kernel geometry and composition was taken from the NGNP Point Design (MacDonald et al. 2003) and is reproduced in Table 1 for convenience.

Table 1. TRISO Fuel Kernel Geometry and Composition

Region #	Name	Outer radius (μ)	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

- Fixed lattice with centered spheres. The first configuration analyzed was a 5x5x5 cubical lattice with fuel kernels centered within the cubical cells and reflecting boundaries on the outer surfaces. The lattice edge was chosen to preserve the specified packing fraction. Although this could have been accomplished with a single cubical cell with a centered sphere, the 5x5x5 lattice was chosen to be consistent with our other cases mentioned below.

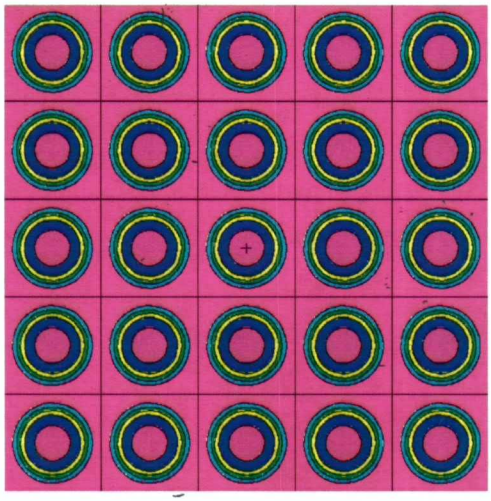

Figure 1. Fixed 5x5x5 Lattice with Centered Fuel Kernels

- Fixed lattice with randomly placed spheres. This is the same as the fixed lattice model except the stochastic geometry option is turned on, effectively moving the spheres randomly within the 5x5x5 cubical cells.

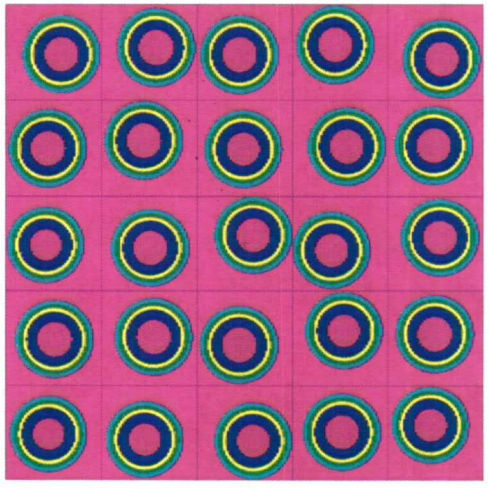

Figure 2. Fixed 5x5x5 Lattice with Randomly Placed Fuel Kernels

- Multiple lattice realizations. The *mcnp_pstudy* utility (Brown et al. 2004) was used to create 25 different input files for the 5x5x5 configuration, each a single realization of the stochastic lattice model above. These 25 cases were run independently and the k_{eff} results were averaged.

- Box of randomly placed fuel kernels. This configuration is a "box" equivalent to the 5x5x5 lattice that is packed randomly with 125 fuel kernels using RSA. The box has reflecting boundary conditions on all sides. The *mcnp_pstudy* utility was used to create MCNP5 input decks from 25 realizations of these randomly packed boxes. These 25 cases were run independently and the k_{eff} results were averaged.

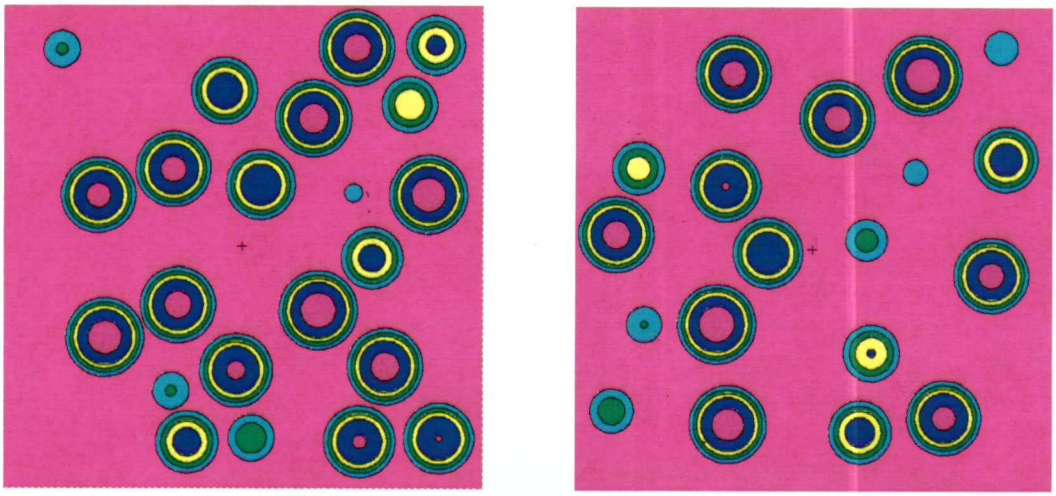

Figure 3. Two different planar slices through a single realization of the stochastic fuel box

4.2 Numerical results

Table 2 summarizes the results for the cases described above.

Table 2. MCNP5 Results for Infinite Lattices of Fuel Kernels

#	**Method**	**K-effective**
1	Fixed 5x5x5 lattice with centered spheres	1.1531 ± 0.0004
2	Fixed 5x5x5 lattice with randomly located spheres ("on the fly")	1.1515 ± 0.0004
3	Multiple (25) realizations of 5x5x5 lattice with randomly located spheres	1.1513 ± 0.0004
4	Multiple (25) realizations of randomly packed (RSA) fuel "box"	1.1510 ± 0.0003

There is remarkably close agreement among the three stochastic approaches (Methods 2-4) indicating that the stochastic geometry capability (Method 2) is working correctly. Furthermore, the effect of fixing the fuel kernels on a cubical lattice (Method 1) is relatively small, less than 0.2% Δk, at least for this configuration corresponding to a packing fraction of approximately 30% for the fuel

kernels. Considering only the innermost fuel region, this is equivalent to a 2.6% packing fraction, where the outer layers of the fuel kernel are included in the matrix region. The computational cost of turning on the stochastic geometry option is negligible (Method 1 vs. Method 2) for the lattice simulations reported here.

5. Conclusions

The new stochastic geometry treatment for MCNP5 provides an accurate and effective means of modeling the particle heterogeneity in TRISOL particle fuel. The results indicate that the neutronic effect of using a fixed lattice is negligible, and the effect of choosing either a centered spheres or randomly located spheres is also small, at least for the specific fuel geometry that was analyzed during this study. Future work will include examination of finite geometries, including cylindrical fuel compacts, hexagonal fuel blocks, and full core configurations. We will also consider lattices other than bcc lattices, such as fcc and hcp lattices.

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