Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

MONTE CARLO SIMULATION OF VHTR PARTICLE FUEL WITH CHORD LENGTH SAMPLING

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ABSTRACT

The Very High Temperature Gas-Cooled Reactor (VHTR) poses a problem for neutronic analysis due to the double heterogeneity posed by the particle fuel and either the fuel compacts in the case of the prismatic block reactor or the fuel pebbles in the case of the pebble bed reactor. Direct Monte Carlo simulation has been used in recent years to analyze these VHTR configurations but is computationally challenged when space dependent phenomena are considered such as depletion or temperature feedback. As an alternative approach, we have considered chord length sampling to reduce the computational burden of the Monte Carlo simulation. We have improved on an existing method called “limited chord length sampling” and have used it to analyze stochastic media representative of either pebble bed or prismatic VHTR fuel geometries. Based on the assumption that the PDF had an exponential form, a theoretical chord length distribution is derived and shown to be an excellent model for a wide range of packing fractions. This chord length PDF was then used to analyze a stochastic medium that was constructed using the RSA (Random Sequential Addition) algorithm and the results were compared to a benchmark Monte Carlo simulation of the actual stochastic geometry. The results are promising and suggest that the theoretical chord length PDF can be used instead of a full Monte Carlo random walk simulation in the stochastic medium, saving orders of magnitude in computational time (and memory demand) to perform the simulation.

Key Words: stochastic geometry, Monte Carlo, chord length sampling

1. INTRODUCTION

The Very High Temperature Gas-Cooled Reactor (VHTR) is a potential Generation IV design. Two types of designs are considered for the VHTR, the prismatic block reactor and the pebble bed reactor [1,2]. Both designs use TRISO fuel, which is a stochastic mixture of coated microspheres (of diameter 0.78 mm) that are randomly distributed in a background graphite matrix with a volume packing fraction of 28.9% for prismatic fuel and 5.76% for pebble bed fuel. The TRISO fuel particles present a prohibitive computational challenge to traditional neutronic analysis because they are strong absorbers for resonance energy neutrons, resulting in the well-known "double heterogeneity" caused by the fuel particles at the first level and the fuel compacts (or fuel pebbles) at the second level. Methods for treating the double heterogeneity range from the calculation of Dancoff factors in order to augment traditional resonance integral calculations to detailed Monte Carlo simulations that take into account the detailed geometry of the VHTR including resolution of individual microspheres. [3,4,5,6,7]

Explicit Monte Carlo simulation of the VHTR is very time-consuming and may not be feasible when space-dependent phenomena are accounted for, such as depletion and temperature feedback. We have studied an alternative methodology to analyze particle fuel that is based on chord length sampling (CLS).

The CLS method was proposed in 1D geometry [8] to avoid explicitly modeling the stochastic mixture. The basic idea of CLS is to treat the stochastic geometry as a binary stochastic mixture whose two components are characterized by chord length probability distribution functions (PDFs). The Monte Carlo simulation proceeds by sampling a distance to collision in the current medium and comparing to a distance to boundary that was sampled from the chord length PDF for that medium. If a neutron crosses a boundary, this process is repeated in the second medium.

A variation on CLS, called limited chord length sampling (LCLS) [9] was examined in 2D geometry for stochastic mixtures similar to TRISO fuel. For LCLS, chord length sampling is only done in the background medium, and conventional Monte Carlo is performed in the fuel region, which is a microsphere in the case of TRISO fuel. The results were promising but there were several areas that warranted further investigation: the results were limited to 2D, the chord length PDFs were based exclusively on empirical chord length distributions, microspheres near the external boundary needed to be treated carefully to avoid overlap with the boundary, and one needed to account for the fact that a neutron leaving a microsphere may backscatter into the same microsphere.

A method very similar to LCLS had been developed earlier by Murata et al. [6,7] for the analysis of TRISO fuel. This method included chord length sampling to find the next microsphere, and then conventional Monte Carlo within the microsphere. Two of the same issues as noted above for LCLS were present, including boundary overlap and backscattering into the same microsphere.

To address these issues and yield a method capable of analyzing realistic TRISO fuel configurations, we have based the chord length PDF for the background medium on a theoretical model rather than an empirical model. We have validated the theoretical chord length PDF for the background medium with benchmark Monte Carlo simulations. These chord length PDFs were then used in a stochastic mixture representative of TRISO fuel with neutrons at the 6.67 eV resonance of U238. These calculations were performed using packing fractions ranging from pebble bed reactors (~ 5%) to prismatic block reactors (~ 29%) and the results were compared with a benchmark Monte Carlo code. The results are very promising and suggest that the LCLS method with theoretical PDFs can be used to analyze TRISO fuel for both pebble bed and prismatic block reactors.

2. MONTE CARLO SIMULATION

Figure 1 depicts a 3D binary stochastic mixture of microspheres within a box of background material. This is an actual realization of microspheres using the RSA algorithm

[10,11] to add spheres to the box. We will now derive the chord length distribution that characterizes the background material in Figure 1.

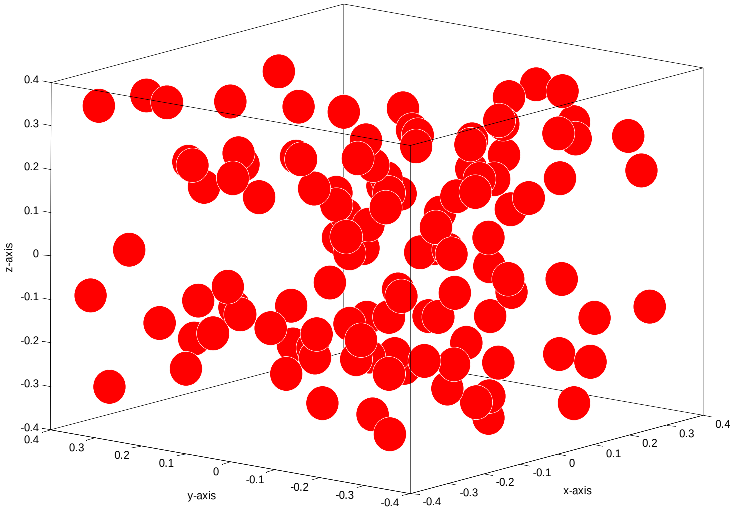

Figure 1. A Realization of Microspheres Randomly Located Inside a Cube

The key assumption we will make is that the distribution of chord lengths in the background material is exponential. This assumption will be confirmed with numerical results later in this paper. The following functional form for the chord length PDF may then be written:

$$p(\lambda_1) = \frac{1}{<\lambda_1>} \cdot e^{-\lambda_1/<\lambda_1>} \tag{1}$$

where λ_1 is the chord length between two microspheres and $<\lambda_1>$ is the mean chord length.

Consider a neutron trajectory that crosses N microspheres and background material regions in an infinite stochastic medium. Along this trajectory, the probability the neutron is in a microsphere region is given by:

$$p_2 = \frac{N\cdot<\lambda_2>}{N\cdot<\lambda_1>+N\cdot<\lambda_2>} \tag{2}$$

where $<\lambda_2>$ is the mean chord length inside a microsphere. This is identical to the volume packing fraction $frac$ if the microspheres are randomly distributed in the background medium:

$$frac = \frac{< \lambda_2 >}{< \lambda_1 > + < \lambda_2 >} \tag{3}$$

Inserting $< \lambda_2 >= \frac{4r}{3}$ into Equation (3) we find the following expression for $< \lambda_1 >$:

$$< \lambda_1 >= \frac{4 \cdot r}{3} \cdot \frac{1 - frac}{frac} \tag{4}$$

Inserting Equation (4) with Equation (1), an analytical chord length PDF is obtained:

$$p(\lambda_1) = \frac{3}{4 \cdot r} \cdot \frac{frac}{1 - frac} \cdot e^{-\lambda_1 \cdot \frac{3}{4 \cdot r} \cdot \frac{frac}{1 - frac}} \tag{5}$$

This is a general formula for the chord length PDF in the background medium as a function of the packing fraction and microsphere radius. An equivalent expression was derived earlier by Murata et al. [6] using the definition of the nearest neighbor distribution.

3. VALIDATION OF THE CHORD LENGTH PDF

The theoretical PDF given in Equation (5) was compared to a benchmark Monte Carlo simulation of the distribution of chord lengths between two microspheres in a medium of dispersed microspheres with a range of packing fractions. The Monte Carlo simulation proceeded by first using RSA [11] to construct a realization of a stochastic mixture similar to that depicted in Figure 1. A microsphere near the center of the cube is selected and an emission point is randomly chosen on the surface of the microsphere. An exiting neutron is then sampled with a cosine current distribution. A total of 4,000 realizations were constructed and for each realization, there were 50 sampled points and 100,000 sampled directions for each point, yielding 20 billion sampled chord lengths. The chord length was determined by tracking the neutron to the next microsphere. Figure 2 shows the resultant distribution of chord lengths as a function of packing fraction, along with the theoretical PDF (dotted lines) from Equation (5). The comparison between these two sets of results shows very good agreement with improved results for smaller packing fractions.

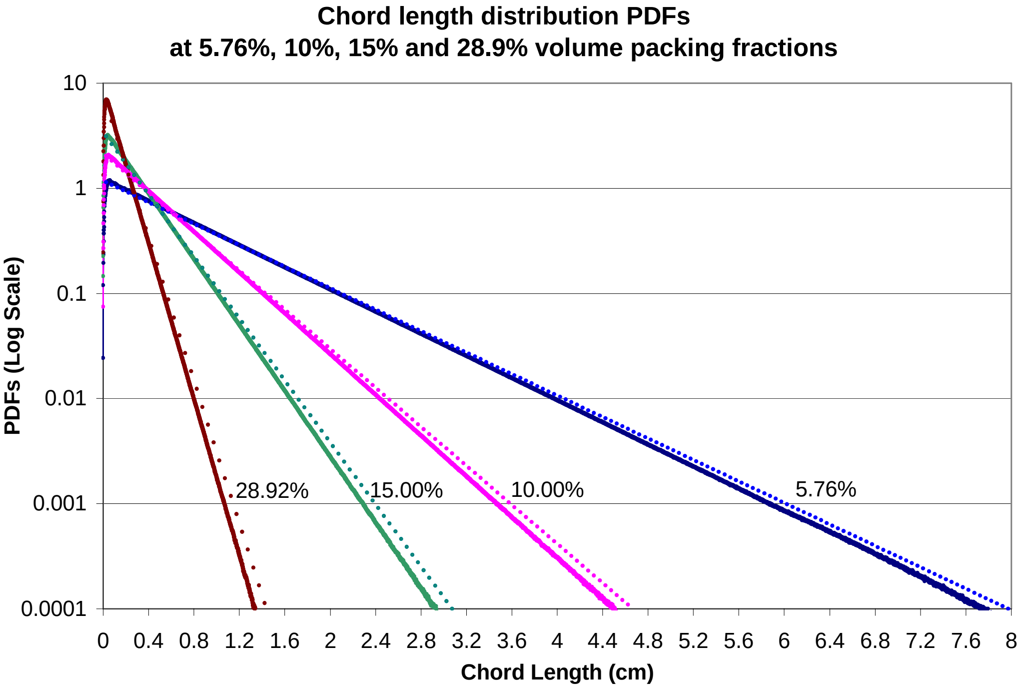

Figure 2. Comparison of Theoretical and Benchmark Chord Length Distributions

4. MONTE CARLO SIMULATION OF STOCHASTIC MEDIA USING LCLS

The chord length PDF given in Equation (5) was then used to simulate neutron transport in stochastic mixture of microspheres with a range of packing fractions. The microsphere geometry is representative of TRISO fuel for the NGNP [1]. The microsphere outer diameter is 0.78 mm and the fuel kernel diameter is 0.350 mm. The cross sections for the graphite matrix region and the microspheres were obtained from the BNL website [12] for neutrons at 6.67 eV. The four microsphere coatings were lumped into a single coating. Although the coating region and the graphite matrix region were distinct regions for the Monte Carlo simulation, these regions had identical cross sections obtained by homogenizing the materials in these two regions [3].

The stochastic mixture of microspheres and graphite matrix was contained in a cubical box with edge 8 cm. The microspheres were added to the box using RSA with packing fractions ranging from 5.76% to 29.8%. Incoming neutrons were emitted from a point at the center of the left side with a cosine current angular distribution. The average absorption rate in the microspheres was tallied, along with three leakage rates: reflection out the left wall, transverse leakage across the upper, lower and side walls, and transmission leakage across the right wall. These benchmark Monte Carlo results were then compared with the results using chord length sampling for the stochastic mixture. The benchmark Monte Carlo results were based on 100 realizations (different stochastic mixtures using RSA) with 10,000,000 particle histories per realization. The results are given in Table I.

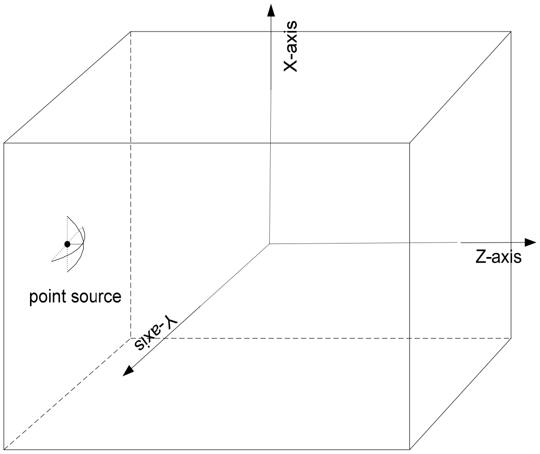

Figure 3. Monte Carlo Simulation Geometry

The results in Table I show very good agreement between the LCLS method and the benchmark Monte Carlo simulations. For all packing fractions, the absorption rate was within 0.15%, with no apparent dependence on packing fraction. For the reflection and transverse leakage rates, the agreement is within 1% for the low packing fractions and somewhat higher for high packing fractions, but it seems that the higher relative errors occur with relatively small absolute leakage rates, such as the transmission rates for all cases, and the transverse leakage rates for the high packing fraction cases.

We have also considered two extensions to the LCLS method for the analysis of TRISO fuel. The first is to account for the fact that a neutron exiting a microsphere in a highly scattering medium will have a reasonable probability of scattering back into the same microsphere. This was accounted for in LCLS by “remembering” the last microsphere the neutron exited and including its boundary as a potential surface to be tracked to along with a sampled chord length. If a neutron enters another microsphere, this memory is erased. This results in an improvement in the range of 0.1% to 2.0% depending on the specific configuration. Normally, for cases with low scattering cross sections ($<1.0\text{cm}^{-1}$) in background material, the effect is very small (< 0.5%). For cases with high scattering cross sections ($>1.\ 0\text{cm}^{-1}$) in background material, the backscatter effect can approach 2.0%.

The second extension is to account for microspheres that are close to the outer boundary of the box. If a neutron enters a microsphere in the interior of the box, the incoming direction is sampled uniformly on the unit hemisphere with respect to the outer normal. However, for a microsphere near the boundary, the resultant direction may be equivalent to letting the microsphere overlap the boundary. This was addressed by rejection sampling until the microsphere was wholly inside the boundary. Preliminary results indicate this is an important effect for realistic TRISO applications.

Table I. The results for VHTR geometry model

(matrix) $\Sigma_{t,1}$=0.4137cm^{-1}, $\Sigma_{a,1}$=0.0cm^{-1}, $\Sigma_{s,1}$=0.4137cm^{-1}; (coatings) $\Sigma_{t,2}$=0.4137cm^{-1}, $\Sigma_{a,2}$=0.0 cm^{-1}, $\Sigma_{s,2}$=0.4137cm^{-1}; (fuel kernel) $\Sigma_{t,3}$=228.4cm^{-1}, $\Sigma_{a,3}$=189.7cm^{-1}, $\Sigma_{s,3}$=38.7cm^{-1}				
Solution Method	absorption rate $\oint_{V_3} \Sigma_a \cdot \phi(r)dr$ in fuel kernels 1σ	reflection leakage via (–z) 1σ	transverse leakage via (±x, ±y) 1σ	transmission leakage via (z+) 1σ
Volume packing fraction at 5.76%				
Benchmark (time:120,695s)	**0.668 ± 0.001**	**0.2293 ± 0.0004**	**9.80e-2 ± 0.01e-2**	**5.00e-3 ± 0.02e-3**
chord length (10,000,000) (time: 142s)	**0.667 ± 0.001**	**0.2279 ± 0.0001**	**9.97e-2 ± 0.01e-2**	**5.18e-3 ± 0.02e-3**
Volume packing fraction at 15.00%				
Benchmark (time:65,244s)	**0.856 ± 0.001**	**0.1332 ± 0.0003**	**1.102e-2 ± 0.001e-2**	**1.44e-4 ± 0.01e-4**
chord length (10,000,000) (time: 162s)	**0.856 ± 0.001**	**0.1320 ± 0.0001**	**1.149e-2 ± 0.001e-2**	**1.50e-4 ± 0.04e-4**
Volume packing fraction at 20.00%				
Benchmark (time:56,485s)	**0.886 ± 0.001**	**0.1101 ± 0.0002**	**3.71e-3 ± 0.01e-3**	**2.21e-5 ± 0.02e-5**
chord length (10,000,000) (time: 174s)	**0.886 ± 0.001**	**0.1094 ± 0.0001**	**3.85e-3 ± 0.01e-3**	**2.40e-5 ± 0.15e-5**
Volume packing fraction at 28.9%				
Benchmark (time:32,124s)	**0.9147 ± 0.0001**	**8.47e-2 ± 0.01e-2**	**5.75e-4 ± 0.01e-4**	**0.84e-6 ± 0.03e-6**
chord length (100,000,000) (time: 2,031s)	**0.9136 ± 0.0001**	**8.60e-2 ± 0.01e-2**	**6.10e-4 ± 0.01e-4**	**0.75e-6 ± 0.09e-6**

5. CONCLUSIONS

A chord length distribution PDF was derived for a binary stochastic mixture media in 3D geometry assuming the PDF had an exponential form. The exponential form of the PDF was validated against a benchmark calculation using a direct ray emitting method to determine the chord length distribution in stochastic mixtures with varying packing fractions.

As a specific application for VHTR geometry model, the transport of resonance energy neutrons in a stochastic mixture representative of VHTR fuel was analyzed with this method for several different volume packing fractions. The results were compared against a benchmark Monte Carlo simulation using 100 realizations and 10 million histories per realization. The results indicate that the LCLS method can be used for realistic VHTR configurations.

ACKNOWLEDGMENTS

This work was funded by U.S. DOE NERI Grant DE-FC07-06ID14745.

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