Chord Length Sampling in Stochastic Media Packed with Poly-Sized Spheres

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INTRODUCTION

Previous work about chord length sampling (CLS) method focused on solving radiation transport problems in the media packed with mono-sized disks/spheres. These disks/spheres are randomly packed in 2D/3D containers. Good agreements were obtained between CLS and benchmark results, either using an empirical chord length probability density function (PDF) or using a theoretical chord length PDF [1-4]. CLS has shown a promising Monte Carlo (MC) method to analyze the stochastic distribution of mono-sized TRISO fuel particles in Very High Temperature Reactors (VHTR).

However, in certain radiation transport systems, the structural materials distributed in a background region, such as tissue and air structures in a lung model [5] or TRISO fuel particles in the Fort Saint Vrain (FSV) gas cooled reactor system [6], are poly-sized, not mono-sized. Much work has been done to verify CLS can predict accurate results in mono-sized sphere systems, but CLS has not been verified to do so in poly-sized sphere systems yet.

This paper will verify that CLS can be applied to analyze poly-sized structure system with accuracy. A theoretical chord length PDF was first derived for background material in the poly-sized sphere system. Eigenvalue and fixed-source problems were solved using CLS with this PDF. Good agreement between benchmark and CLS was obtained. In addition, infinite medium and finite medium Dancoff factors of poly-sized fuel kernels in stochastic medium were computed by CLS and compared very well with benchmark results. To authors' knowledge, these calculations and investigations have not been performed before.

METHODOLOGY DESCRIPTION

In mono-sized sphere systems, CLS is used to sample the next sphere's position while regular MC is performed inside the sphere. If a sampled sphere overlaps with external boundary, then it is discarded and the previous CLS and collision distance sampling are performed again [4]. When one comes to poly-sized sphere systems, the only difference in the CLS procedure between two systems is that once a neutron is determined to enter a new sphere at sampled position, additional sampling is needed to sample the size of the new sphere based on a known sphere size distribution function.

In current research, two types of sphere size distribution are assumed for CLS investigation: uniform and quadratic distribution in radii over an interval $[r_a, r_b]$. The PDFs of two distributions are described in Eq. (1).

$$s(r) = \begin{cases} 1/(r_b - r_a) & \text{uniform distribution,} \\ 3r^2/(r_b^3 - r_a^3) & \text{quadratic distribution.} \end{cases} \quad (1)$$

In CLS, a chord length PDF in background material is needed to sample the distance to the next sphere after neutron leaves current sphere or scatters in background. The chord length PDF is assumed an exponential function defined by

$$p(l_b) = (1/<l_b>)e^{-l_b/<l_b>}, \quad (2)$$

where the $<l_b>$ is the mean chord length in background material. The validation of the above equation has been demonstrated by many researchers in mono-sized and poly-sized sphere systems [7, 8]. It should be noted that a more accurate derivation of chord length PDF between spheres was recently proposed [9]. Generally, $<l_b>$ can be theoretically calculated by an infinite medium scaling relationship [7]:

$$<l_b> = <l_s>(1-frac)/frac, \quad (3)$$

where $<l_s>$ is the mean chord length in spheres and *frac* is the volume packing fraction of spheres. In mono-sized sphere system, $<l_s>=4r/3$, where r is the sphere radius. However, in poly-sized sphere system, $<l_s>$ depends on the distribution of sphere size and must be calculated by deriving the PDF of l_s. Based on Olson et al. [8], the conditional chord length distribution function in a sphere at a fixed radius r is given by:

$$f(l_s; r) = \frac{l_s}{2r^2} \quad \text{for } l_s < 2r. \quad (4)$$

If a new PDF is introduced and defined by

$$t(r) = (r^2/<r^2>)s(r), \quad (5)$$

where $<r^2> = \int_{r_a}^{r_b} r^2 s(r)dr$, then the chord length PDF for spheres having a distribution in radii over $[r_a, r_b]$ can be derived following the similar procedure as Olson et al. [8] did:

$$f(l_s) = \begin{cases} \int_{r_a}^{r_b} f(l_s; r)t(r)dr & \text{for } 0 \le l_s \le 2r_a, \\ \int_{l/2}^{r_b} f(l_s; r)t(r)dr & \text{for } 2r_a \le l_s \le 2r_b, \end{cases} \quad (6)$$

It should be emphasized that Eq. (1) is the size distribution function for all the spheres populated in the container while Eq. (5) is the size distribution function for spheres that are seen by neutrons traveling along straight lines in space [8]. Equation (1) is used to construct benchmark realizations and Eq. (5) is used to sample sphere size in CLS.

Introducing Eqs. (1) and (4) into Eq. (6), one obtains the chord length PDFs in spheres with uniform and quadratic distributions in radii, respectively. The mean chord length can be calculated by

$$< l_s > = \int_0^{2r_b} l_s f(l_s) dl_s \ .$$

Using Eq. (3), after straightforward calculations, one finally obtains the mean chord length in background:

$$< l_b > = \frac{r_b^4 - r_a^4}{r_b^3 - r_a^3} \frac{1 - frac}{frac}, \tag{7}$$

for uniform distribution, and

$$< l_b > = \frac{10}{9} \frac{r_b^6 - r_a^6}{r_b^5 - r_a^5} \frac{1 - frac}{frac}, \tag{8}$$

for quadratic distribution.

Equation (2) is used in CLS to solve eigenvalue and fixed-source problems. Effective multiplication factor (K_{eff}) and absorption rate are calculated, respectively. Also, average Dancoff factors for a fuel kernel in an infinite medium and a finite medium are computed using CLS. This is an extension of previous work [4] from mono-sized fuel kernel system to poly-sized kernel system. The results from CLS are compared to benchmark Monte Carlo results.

In benchmark MC simulation, poly-sized spheres ranging from r_a=0.0195cm to r_b=0.039cm are randomly packed inside a 12*12*12cm cubic container at the packing fractions of 10% and 20%. Random Sequential Addition (RSA) method with a modified version of fast nearest neighbor search algorithm based on Ref. [11] is used to sample the sphere (center) position in the container. Once this position is determined, the radius of the sphere is sampled based on Eq. (1). If the sampled sphere overlaps with external boundary or an existing sphere, a new spatial position is sampled until no overlap exists. This procedure is performed until the total volume packing fraction of spheres reach the pre-determined value. Figure 1 shows one realization of packed spheres in a 2*2*2 cm container. K_{eff}, absorption rate and Dancoff factor are tallied using the collision estimator. Variance reduction techniques [11] are employed in the simulation. The results are ensemble-averaged over a total of 100 realizations.

In the simulation using CLS, sphere's position and size are sampled on the fly. When neutrons leave a sphere, no memory is kept about the sphere's position and size. Previous research [12] has shown this is the correct procedure in CLS.

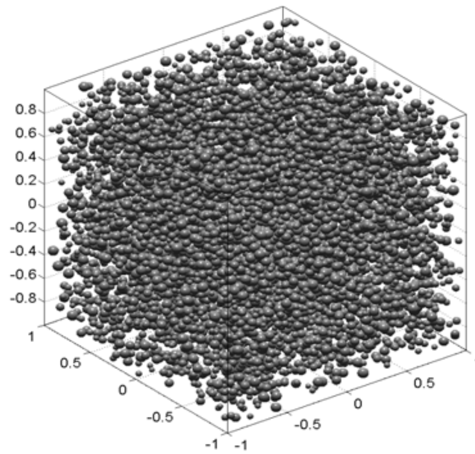

Figure 1. Poly-sized spheres packed in a 2*2*2cm cube at 10% packing fraction

RESULTS AND ANALYSIS

Table I shows the comparison of CLS and benchmark MC results.

In the eigenvalue problem, a total of 10M neutrons per cycle with 300 inactive and 100 active cycles are used for both benchmark simulation in each realization and CLS simulation. Very excellent agreement is obtained for K_{eff}. The relative error between CLS and benchmark is less than 0.1% over all the configurations. Furthermore, by comparing the benchmark results for uniform and quadratic distribution configurations, same results are obtained at the same volume packing fractions, while results are different at different volume packing fractions. This shows that K_{eff} is a parameter that is more sensitive to the total mass of fuel particles than the fuel particle size distribution.

In the fixed-source problem, a uniform source in the background material is assumed with 10M neutron emissions and the average absorption rate in spheres is tallied. It is shown that the relative errors of CLS results are within about 1.5% compared with benchmark results, with a better agreement at the higher packing fraction.

In the computation of Dancoff factors, the average probability that a neutron emitting from the surface of one sphere (representing a fuel kernel) will enter another sphere without collision in the background material is tallied. The benchmark is ensemble-averaged over 100 realizations with 100M neutron histories for each realization. A total of 100M neutrons are tracked in CLS. Both infinite and finite medium Dancoff factors are computed. From Table I, it can be seen that in all the configurations, the prediction of average Dancoff factors in infinite medium and finite medium using CLS shows very good agreement with benchmark results, within about 1% relative errors.

TABLE I Comparison of results between CLS and benchmark

(background material) $\Sigma_{t,1}$=0.4137cm^{-1}, $\Sigma_{a,1}$=0cm^{-1}, $\Sigma_{s,1}$=0.4137cm^{-1}; (poly-sized spheres) $\Sigma_{t,2}$=400.0cm^{-1}, $\Sigma_{a,2}$=200.0cm^{-1}, $\Sigma_{f,2}$=80.0cm^{-1}, $\Sigma_{s,2}$=200.0cm^{-1}, ν=2.5					
Distribution		Uniform		Quadratic	
Packing fraction		10%	20%	10%	20%
K_{eff} σ =2e-5	Benchmark	0.99904	0.99965	0.99908	0.99967
	CLS	0.99957	0.99980	0.99960	0.99983
	Relative Error	**0.053%**	**0.025%**	**0.052%**	**0.016%**
Average absorption rate σ =2e-4	Benchmark	0.9414	0.9670	0.9385	0.9686
	CLS	0.9556	0.9796	0.9533	0.9786
	Relative Error	**1.51%**	**1.30%**	**1.58%**	**1.03%**
Infinite medium Dancoff factor σ =2e-4	Benchmark	0.8653	0.9357	0.8598	0.9328
	CLS	0.8651	0.9352	0.8592	0.9321
	Relative Error	**-0.023%**	**-0.053%**	**-0.070%**	**-0.075%**
Finite medium Dancoff factor σ =2e-4	Benchmark	0.8229	0.9111	0.8151	0.9067
	CLS	0.8310	0.9173	0.8235	0.9132
	Relative Error	**0.98%**	**0.68%**	**1.03%**	**0.72%**

CONCLUSIONS

By applying the CLS method to solving eigenvalue and fixed-source problems in a 3D stochastic medium packed with poly-sized spheres, CLS shows very good accuracy in predicting the multiplication factor, the absorption rate and the Dancoff factors compared to the benchmark results. It verifies that the CLS method with derived theoretical chord length PDFs in this paper can be applied to solving radiation transport problems in the poly-sized sphere systems, which are characteristic of the lung model or the FSV gas cooled reactor system, and it can accurately predict radiation particles behavior.

ACKNOWLEDGMENT

This work performed under the auspices of the U.S. Nuclear Regulatory Commission Faculty Development Program under contract NRC-38-08-950.

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