Application of Chord Length Sampling to VHTR Unit Cell Analysis

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Abstract

When the chord length sampling (CLS) method is used to analyze radiation transport in a finite region consisting of a stochastic distribution of microspheres in a background medium, boundary interference due to avoiding overlap of the external boundary by the sampled microspheres causes an intrinsic difficulty for obtaining accurate simulation results. In order to solve this problem, a self-consistent correction algorithm is developed and used in the chord length sampling method. It employs an iteration procedure to obtain an effective volume packing fraction that represents the actual geometry as seen by the CLS method, and this volume fraction is then used to perform the Monte Carlo simulation with CLS.

In this paper, the CLS method with the new correction algorithm is applied to analyze Very High Temperature Reactor (VHTR) unit cells representative of both prismatic and pebble bed designs. Comparisons with benchmark calculations and alternative boundary correction schemes show that the new correction algorithm is a promising approach for treating boundary interference.

1. Introduction

In the Very High Temperature Reactor (VHTR), TRISO fuel particles (microspheres) are randomly distributed in fuel pebbles for pebble bed reactors or in fuel compacts for prismatic reactors, forming stochastic mixtures of fuel particles which are strong absorbers of resonance neutrons, leading to the well-known "double heterogeneity." A number of methods have been developed to analyze TRISO fuel [Brown and Martin 2004], including chord length sampling (CLS), the subject of this

work. The CLS method has been used to analyze TRISO fuel particles in VHTR-like configurations [Murata et al 1996 and 1997, Donovan and Danon 2003, Ji and Martin 2007] with good results. The basic idea of the CLS method is to use chord length sampling to sample the distance to the next fuel particle when neutrons exit a fuel particle or are emitted by a source or a scattering collision within the background medium. Within a fuel particle, regular Monte Carlo simulation is performed. There are two advantages to this approach – (1) the Monte Carlo tracking does not need to account for the

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presence of the fuel particles, and (2) only one simulation is needed to account for the stochastic distribution of the fuel particles, avoiding multiple realizations.

In previous work [Ji and Martin 2007], a theoretical chord length probability density function (PDF) for the distance between microspheres (the chord length) was obtained based on assuming the PDF was exponential:

$$p(\lambda) = \frac{3}{4R} \cdot \frac{frac}{1 - frac} \cdot e^{-\lambda \cdot \frac{3}{4R} \frac{frac}{1 - frac}} \tag{1}$$

where R is the radius of microsphere and $frac$ is the volume packing fraction. A more careful literature review has shown that Torquato and Lu [1992,1993] derived a general formula of chord length distribution between n-dimensional hard spheres with a statistically isotropic distribution in a background medium using statistical-mechanical concepts. In 3D, their result is identical to Eq. (1). This PDF was then used with the CLS method to predict the transport of resonance energy neutrons incident on a large box of TRISO microspheres with various enrichments and packing fractions characteristic of both pebble bed and prismatic VHTR designs. Excellent agreement was obtained compared to analog Monte Carlo benchmark results for this configuration [Ji and Martin 2007].

However, "boundary effects" are a major issue for using the CLS method to analyze finite geometries. In CLS, the next microsphere is always sampled "on-the-fly". If the sampled microsphere overlaps the external boundary, it is rejected and a re-sampling is performed. This yields a smaller packing fraction near the boundary since some fraction of the microspheres are missing from the simulation. This must be accounted for in the CLS simulation.

This work addresses the boundary effect. The PDF used in the CLS method is still based on Eq. (1) but with an effective packing fraction that is determined by iterating a simple CLS calculation of the geometry until the predicted packing fraction from the CLS calculation agrees with the specified packing fraction. With this correction, CLS calculations of the transport of neutrons in both fuel pebbles and fuel compacts were performed and the results are compared to the cases of no boundary correction and the simple boundary correction suggested by [Murata et al 1996]. The results of our

CLS predictions are excellent, showing the success of our boundary correction. In addition, the modified CLS method was used to compute intra-pebble and intra-compact Dancoff factors for VHTR configurations and these compare very well with benchmark results, further evidence that our boundary correction approach is reasonable.

2. Methodology

Fig. 1 illustrates the spherical fuel pebble and cylindrical fuel compact cells in pebble bed and prismatic VHTRs, respectively (red regions represent fuel zones and light blue regions represent graphite zones). The CLS simulations assume a uniform, isotropic source (stars represent neutron sources as shown in the picture) in the graphite regions. Vacuum boundary conditions are assumed for the outer boundaries of the sphere or cylinder except the upper and lower cylindrical faces are assumed to be reflecting boundaries. If Eq. (1) is used without modification within the CLS method, the results will underestimate the resonance absorption in the fuel region and overestimate the flux integral in the non-fuel region.

A straightforward explanation for these poor estimates is that the CLS method based on Eq. (1) does not preserve the actual volume packing fraction. This is due to the fact that microspheres are not allowed to overlap the external boundary when the next microsphere is sampled with the CLS method, effectively reducing the packing fraction near the boundary, hence reducing the amount of fuel in the lattice. In order to preserve the overall (specified) packing fraction, we need to replace $frac$ with a higher packing fraction $frac*$ in Eq. (1):

$$p(\lambda) = \frac{3}{4R} \cdot \frac{frac^*}{1 - frac^*} \cdot e^{-\lambda \cdot \frac{3}{4R} \frac{frac^*}{1 - frac^*}} \tag{2}$$

Murata et al [1996,1997] first noticed this boundary interference and suggested a simple way to get $frac*$ by shrinking the stochastic region away from each surface by a distance $t=R$, the microsphere radius, which leads to $frac*= (V/V*) \cdot frac$, where V is the original volume and $V*$ is the reduced volume. The choice of R is motivated physically by noting that the center of a microsphere cannot be placed within R of a boundary. This higher packing fraction $frac*$ was then used with

R1=2.5cm   R2=3.0cm   R=0.039cm   r=0.0175cm   Rc=0.6225cm   H=100cm   P=2.196cm

Fuel-pebble cell   TRISO fuel particle   Fuel compact cell
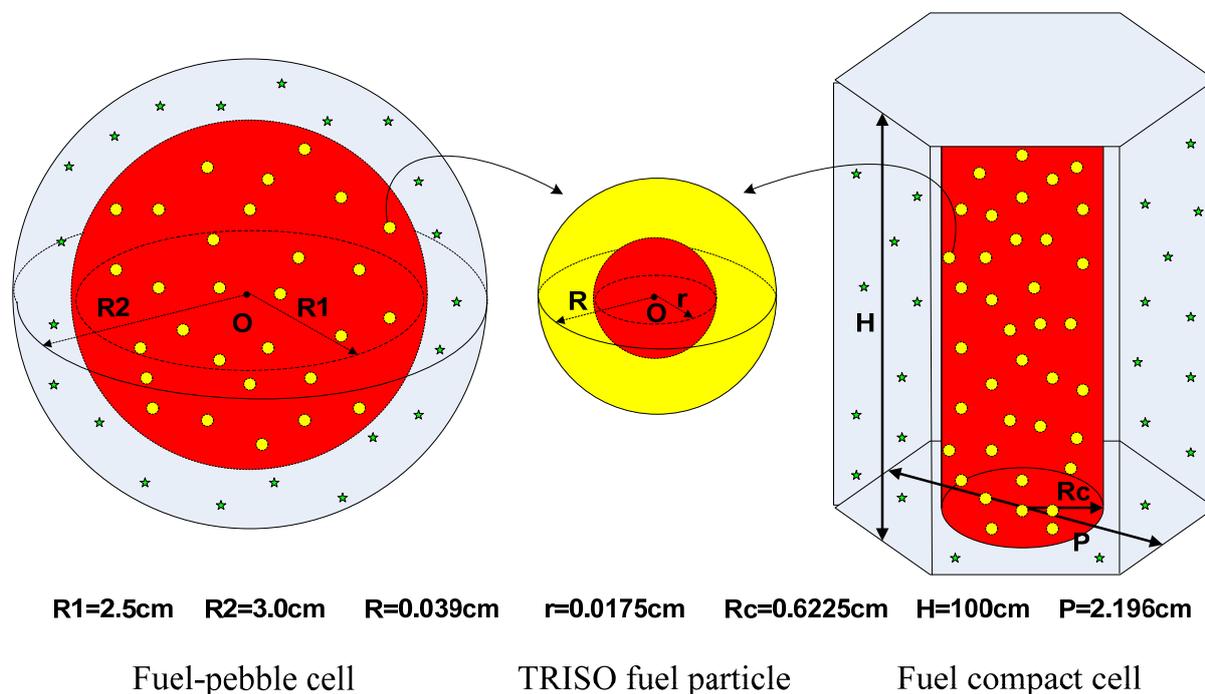
Fig. 1. Illustration of VHTR unit cells and TRISO fuel particles.

CLS and the results showed very good agreement with benchmark results.

However, when Murata's boundary correction method is used, the results were not always satisfactory depending on the geometry, packing fraction, and microsphere radius. So shrinking the stochastic volume may give a first order correction but does not seem to work in general. As a result, an alternative approach to compute *frac** was developed.

Since the packing fraction is only a function of geometry and not a function of material composition, the CLS method can be used to compute the packing fraction for the given geometry by assuming all regions (microspheres and background) are voided and using the track length estimator to estimate the volumes of the microsphere and background regions. This yields the effective packing fraction for this geometry as experienced by the CLS method. This effective packing fraction is the actual packing fraction seen by the CLS method for that geometry and the idea is to force this to equal the specified packing fraction. This is done by changing the input packing fraction for the special CLS calculation until the resulting packing fraction equals the desired packing fraction. This input packing fraction is then used in the actual CLS simulation of the stochastic geometry. The special CLS calculation is performed with a monodirectional plane source on one side of the stochastic geometry with all internal regions voided. This is done for both the cylindrical and spherical VHTR cells.

The CLS method can also be used to estimate the finite medium Dancoff factors (intra-pebble and intra-compact) for these two geometries. The Dancoff factor is defined as the average probability that a neutron escaping an absorber (fuel kernel) enters another absorber (fuel kernel) without having a collision in the intervening moderator (non-fuel) region. Since the Dancoff factor depends on the location of the fuel kernels, not the coatings, it can be calculated by treating the fuel kernels as stochastically distributed microspheres in a background medium consisting of the graphite matrix and the homogenized coatings. The PDF for the distance to the next fuel kernel is given by

Table 1 Results for CLS Simulations of VHTR Configurations

Configuration	Method	Res. absorption rate in kernel (at 5.76% packing fraction)	Res. absorption rate in kernel (at 28.92% packing fraction)
Fuel pebble	benchmark	0.154	0.2806
	CLS w/o correction	0.148	0.2794
	relative error	**-4.2%**	**-0.43%**
	CLS with Murata's correction	0.152	0.2814
	relative error	**0.6%**	**0.29%**
	CLS with proposed correction	0.150	0.2804
	relative error	**-2.9%**	**-0.07%**
Fuel compact	benchmark	0.0692	0.200
	CLS w/o correction	0.065	0.195
	relative error	**-6.07%**	**-2.7%**
	CLS with Murata's correction	0.0724	0.206
	relative error	**4.62%**	**3.0%**
	CLS with proposed correction	0.0692	0.199
	relative error	**0.00%**	**-0.5%**

$$p(\lambda) = \frac{3}{4r} \cdot \frac{frac^*(r/R)^3}{1 - frac^*(r/R)^3} \cdot e^{-\lambda \cdot \frac{3}{4r} \cdot \frac{frac^*(r/R)^3}{1 - frac^*(r/R)^3}} \quad (3)$$

where r is the radius of a fuel kernel and R is the radius of the overall microsphere. Eq. (3) accounts for the fact that the overall microsphere radius R determines the stochastic arrangement of microspheres but the fuel kernel packing fraction is needed to determine the chord length PDF between fuel kernels. As before, the effective packing fraction $frac^*$ needs to be used by the CLS method and is calculated using the methodology described above.

3. Results

Table 1 shows the results using the CLS method to simulate both a fuel pebble and a fuel compact. The CLS results are tallied for three different choices of the corrected packing fraction to account for the external boundary – no correction, Murata's correction, and the proposed correction scheme discussed above. The results contained in Table 1 show that both Murata's scheme and the new correction scheme improve the results compared to no correction. Other cases have also been analyzed that are not reported here but the results show that in general the new iteration scheme gives more improvement than Murata's scheme for most cases except for the fuel pebble with a low packing fraction.
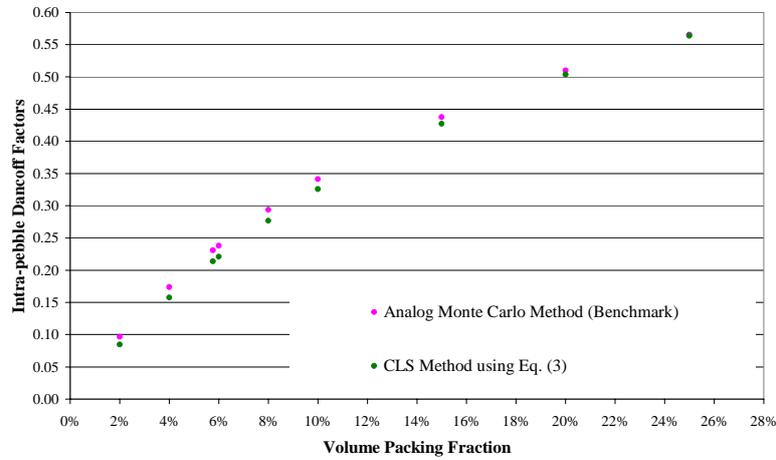
Intra-pebble Dancoff factors
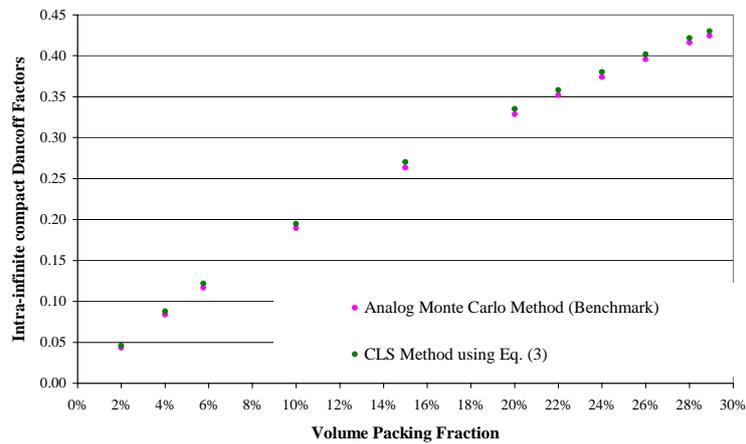
Intra-compact Dancoff factors

Fig. 2. Intra-Dancoff factors comparison between CLS and analog Monte Carlo methods

Fig. 2 shows the Dancoff factors as a function of packing fraction for both fuel pebbles and fuel compacts. The results from the CLS simulation with the new correction scheme are compared to results from an analog Monte Carlo benchmark calculation. The agreement is quite good over a range of packing fractions for both geometries, with slightly worse results for the fuel pebbles at low packing fractions.

4.   Conclusions

The CLS method has been shown previously to be a promising method for the analysis of stochastic geometries such as TRISO fuel configurations characteristic of the VHTR. However the CLS method has an intrinsic difficulty in modeling finite geometries due to boundary interference caused by avoiding the overlap of external boundaries with sampled microspheres. A

self-consistent correction scheme has been developed that is easy to implement and gives good results for a range of packing fractions. This scheme is still not optimal for all VHTR configurations and packing fractions but appears to be a promising method for correcting for boundary interference and we plan to refine this method in the near future.

5. Acknowledgement

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