Chord Length Sampling Correction Analysis for Dispersion Fuel in Monte Carlo Simulation

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Abstract

Due to their excellent safety performance, dispersion fuels are widely used in advanced reactors, such as high-temperature gas-cooled reactors (HTGRs). Compared with deterministic methods, the Monte Carlo method has more advantages in the geometric modeling of stochastic media. The explicit modeling method has high computational accuracy and high computational cost. The chord length sampling (CLS) method can improve computational efficiency by sampling the chord length during neutron transport using the matrix chord length's probability density function (PDF). This study shows that the excluded-volume effect in realistic stochastic media can introduce significant deviations into the CLS. A chord length correction approach is proposed to obtain the chord length correction factor by developing the Particle code based on equivalent transmission probability. Through numerical analysis against reference solutions from explicit modeling in the RMC code, it was demonstrated that CLS with the proposed correction method provides good accuracy for addressing the excluded-volume effect in realistic infinite stochastic media.

Full Text

Preamble

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Abstract

Due to their excellent safety characteristics, dispersion fuels are widely employed in advanced reactors, particularly high-temperature gas-cooled reactors (HT-

GRs). Compared with deterministic methods, the Monte Carlo method offers significant advantages for geometric modeling of stochastic media. While explicit modeling achieves high computational accuracy, it comes at substantial computational cost. The chord length sampling (CLS) method improves efficiency by sampling chord lengths during neutron transport using the probability density function (PDF) of matrix chord lengths. This study demonstrates that the excluded-volume effect in realistic stochastic media can introduce notable deviations into CLS. A chord length correction approach is proposed to obtain the correction factor by developing a Particle code based on equivalent transmission probability. Through numerical analysis against reference solutions from explicit modeling in the RMC code, it is shown that CLS with the proposed correction method provides good accuracy for addressing the excluded-volume effect in realistic infinite stochastic media.

Keywords: Stochastic media; Monte Carlo; Chord Length Sampling; Excluded-volume effect; Chord Length Correction

Introduction

Dispersion fuel can effectively prevent nuclear leakage and offers high safety performance, making it widely used in advanced reactors, especially high-temperature gas-cooled reactors (HTGRs). In traditional deterministic methods, the presence of stochastic media causes dispersion fuel to exhibit double heterogeneity, which poses a significant challenge for reactor physics calculations. The Monte Carlo method has distinct advantages for simulating stochastic media due to its flexible geometric modeling capabilities and continuous-energy nuclear cross-sections. Several approaches have been developed to simulate stochastic media by accounting for stochastic effects, including random explicit modeling and the chord length sampling (CLS) method.

The explicit modeling method can accurately describe the geometry of each grain, depending on the technique used to generate stochastic grains. Early studies [?] placed grains in regular lattices to represent stochastic media without considering the randomness of grain distribution. Brown et al. [?] introduced random translations into grain positions within repeated regular lattices and implemented this approach in MCNP. While this random lattice method incorporates some randomness, the grains remain relatively regular at the macroscopic level.

The explicit random modeling method can accurately describe each stochastic grain with minimal approximation, based on random packing methods such as Random Sequential Addition (RSA) [?], Close Random Packing (CRP) [?], and Discrete Element Method (DEM) [?]. However, the generation and storage of grains and the ray-tracing process incur substantial computational costs. Consequently, the random explicit modeling method, despite its highest accuracy, is often used to provide reference solutions and has been implemented in Monte

Carlo codes such as OpenMC [?], SERPENT [?], and RMC [?, ?].

Unlike explicit methods, CLS is an implicit method that samples the matrix chord length and entry angle to reach the next grain during neutron transport without explicitly describing the stochastic media. Zimmerman and Adams [?] proposed the CLS method based on 1D geometry. Murata et al. [?, ?] developed the MCNP-CFP code to simulate HTGRs based on the nearest neighbor distribution (NDD) method. CLS offers the advantage of simplifying geometric modeling and improving computational efficiency.

The CLS method uses the probability density function (PDF) of matrix chord lengths to sample the distance to the next grain, indirectly determining the grain packing fraction. The PDF of matrix chord length is inherently assumed to satisfy a Poisson distribution [?] because the transport process in CLS is a Markovian process where previous grains do not affect future grains (i.e., overlapping between grains is not considered).

In realistic stochastic media, the chord length distribution deviates from the Poisson distribution due to two effects: the boundary effect of the external boundary and the excluded-volume effect of micro-scale grains. A major problem in finite stochastic media is the boundary effect, which reduces the local packing fraction near an external boundary to avoid overlap between grains and the boundary, resulting in a total packing fraction lower than expected. To address this boundary effect, many studies have focused on correction methods for the packing fraction influenced by finite boundaries, such as those by Murata [?], Ji [?], Griesheimer [?, ?], and Liang [?]. These studies were based on the assumption that the PDF follows an exponential distribution and focused on methods for correcting the packing fraction to balance the boundary effect.

The excluded-volume effect is an existing but unresolved problem in realistic stochastic media. To avoid overlapping between grains, earlier grains exert an excluded-volume effect on later grains during packing, resulting in a significant decrease in the proportion of matrix chord lengths near the grain size. This excluded-volume effect can cause the matrix chord length distribution to deviate from the exponential distribution. However, this effect has been neglected in previous studies because the grain size is usually sufficiently small to ignore interactions between grains, especially at low packing fractions. The excluded-volume effect conflicts with the Poisson distribution assumption of CLS, making it difficult to correct.

In this study, we analyzed the mechanism of the excluded-volume effect on the matrix chord length PDF. Subsequently, a Particle code was developed to rapidly generate stochastic grains and perform chord length sampling analysis. Furthermore, a chord-length correction method was proposed based on matrix transmission probability equivalence to obtain the matrix chord length correction factor. The CLS method with correction was implemented in the RMC code [?, ?, ?]. Cases with infinite stochastic media were used to verify the accuracy of the modified CLS method while avoiding the influence of boundary effects.

The remainder of this paper is organized as follows: Section 2 introduces the basic principles and excluded-volume effect issues of the CLS method, and proposes a correction approach for chord length based on the Particle code. The verification of CLS with chord length correction is presented in Section 3. Finally, conclusions are presented in Section 4.

2.1 Chord Length Sampling

There may be differences in CLS implementation across various Monte Carlo codes. The CLS process in the RMC code [**?**] is shown in Fig. 1 [Figure 1: see original paper]. After entering the stochastic media region, neutrons pass through the matrix and particles until they experience their first collision. A characteristic of CLS is using a PDF to describe the matrix chord length, which is the length of the matrix path traveled by neutrons leaving the current grain to reach the next grain. The type and position of the next grain are determined by sampling.

Firstly, the matrix chord length l_0 between grains is sampled based on the PDF in Eq. MATH_0 . Here, the PDF is assumed exponential, and the matrix mean chord length $\bar{l}_0$ is defined by Eq. MATH_1 . This matrix mean chord length differs from traditional CLS because it considers the case of stochastic media containing multiple grain types, such as fuel and poison grains, where $f^{(j)}$ represents the packing fraction of grain j with radius r_j.

Secondly, the type of the next grain entered is sampled, entering grain j with probability t_j using Eq. MATH_2 . Thirdly, based on the assumption that neutrons enter grains isotropically, the angle θ at which the neutron enters the next sphere is sampled, and then the spherical center of the next grain is determined. The angle θ can be sampled by its cosine value from Eq. MATH_3 , where x is a random number between (0, 1).

2.2 Excluded-Volume Effect

The excluded-volume effect is a fundamental problem in realistic stochastic media. Due to the hard-sphere assumption, grains cannot overlap with other grains. This effect impacts both explicit modeling and CLS methods. In explicit modeling, when a newly sampled grain overlaps with any existing grain, it is rejected and resampled, resulting in a matrix chord length that is not equal to zero. When the matrix chord length is extremely small and close to zero, the number of small chord lengths decreases significantly, causing the matrix chord length distribution to deviate from the exponential distribution, as shown in Fig. 2 [Figure 2: see original paper].

In the CLS method, the physical process is assumed to be a Markov process in which newly sampled grains do not need to consider previous grains, and the PDF follows an exponential distribution. This physical process conflicts with correction methods that consider overlap between grains, making it difficult to correct the PDF for the excluded-volume effect.

We noticed that some codes employ a correction treatment to determine whether grains overlap, considering that the next grain may overlap with the current grain when the chord length is small, as shown in Fig. 3 [Figure 3: see original paper]. When overlap occurs between grains, the current sampling result is rejected, and the chord length and angle are resampled. However, this correction treatment is unnecessary, although it appears more consistent with realistic stochastic media.

The physical process of CLS is a Markov process in which neutrons leave the current grain and enter the matrix without considering the history of previous grains. In other words, there is no need to consider the overlapping problem of previous grains in CLS. If it were necessary to consider overlap between grains, not only the previous grain but all grains in history should be considered, which violates the principle of CLS. This correction causes many smaller chord lengths to be rejected while larger ones are retained, increasing the mean chord length, which is equivalent to a reduction in the grain packing fraction.

2.3 Particle Code

The Particle code was developed to rapidly model realistic stochastic grains and sample matrix chord lengths to address the excluded-volume effect. As shown in Fig. 4 [Figure 4: see original paper], the implementation of the Particle code includes the following processes: (1) The geometry of a finite region is defined, and a virtual acceleration mesh is established around the entire geometry. (2) With the virtual grid acceleration, RSA and CRP are combined to quickly generate the coordinates of stochastic grains while establishing an index between grains and the virtual grid. (3) Randomly sample the matrix chord length to the entry grain and angle based on ray tracing and white boundary condition, search for the nearest grain on the path, and record the chord length information. This chord length sampling process is repeated N times to obtain the distribution of matrix chord lengths. (4) To reduce random error, we replace the random seed and repeat steps (1)–(3) to obtain stable statistical results.

The Particle code is based on geometric chord length sampling of realistic stochastic media without considering real nuclear physics reactions. The calculation time of the Particle code is much shorter than that of Monte Carlo neutron transport simulation based on explicit modeling. Therefore, its simulation efficiency is very high, typically taking only a few seconds on a single core at low packing fractions, which can be almost ignored.

2.4 Chord Length Correction

The Particle code is based on geometric chord length sampling of realistic stochastic media, and it is not appropriate to use the statistical matrix mean chord length directly in the exponential distribution after obtaining the matrix chord length distribution because it no longer satisfies the exponential distribution. The matrix chord length corresponds to the matrix transmission probability for a physical process in stochastic media. Therefore, a chord length correction method based on equivalent transmission probability is proposed, which ensures conservation of the matrix transmission probability by correcting the matrix chord length. This correction method has been implemented in the chord-length-based double heterogeneity model in the XPZ code [?] and has demonstrated high accuracy and application prospects.

After the chord length sampling procedure in the Particle code is completed, the mean transmission probability of the matrix is calculated using Eq. MATH_4 , and the matrix mean chord length $\bar{l}_0$ is calculated by Eq. MATH_5 , where l_i is the sampled chord length with index i among N sampling results.

Graphite or SiC is commonly chosen as the matrix material for dispersion fuels in HTGRs, compact gas-cooled reactors, or FCM [?] fuel in PWRs, and the cross-section is usually insensitive to energy. The cross-section can be discretized into a multigroup problem based on energy if it is sensitive to energy. It is assumed that the macroscopic total cross-section of the matrix material is a constant value Σ_t^0 within an energy range.

Assuming an exponential distribution, the theoretical matrix transmission probability can be expressed using Eq. MATH_6 . By equating T_0 with $\bar{T}_0$, the corrected chord length $\bar{l}_0^c$ can be derived using Eq. MATH_7 .

The boundary effect is unavoidable when the Particle code generates stochastic grains. Therefore, stochastic grains should be generated in the largest possible region until the statistical matrix mean chord length $\bar{l}_0$ approaches the theoretical value obtained using Eq. MATH_1 . Finally, a dimensionless matrix chord length correction factor is defined by Eq. MATH_8 , which is used to correct the matrix mean chord length under the assumption of an exponential distribution. This factor is multiplied by the sampled chord length to obtain the corrected chord length in CLS. Because the excluded-volume effect is considered in the Particle code's modeling procedure, the corrected CLS is more consistent with the explicit modeling method in infinite stochastic media.

Additionally, to improve computational efficiency, an interpolation table can be established in advance to avoid calling the external code. We found that the chord length correction factor correlates with the grain radius r and packing fraction f; thus, it can be established as shown in Table 1 . The macroscopic total cross-section Σ_t^0 was set to 0.412/cm in the full energy range when the matrix material was graphite with a density of 1.73 g/cm^3.

3.1 Test Case

The CLS and its correction methods discussed in this paper were implemented in the RMC code using efficient computational convergence methods [?]. A set of infinite stochastic media cases was designed to validate the effectiveness of the proposed method in addressing the excluded-volume effect. Numerical results from explicit modeling in RMC were used as reference solutions and compared with the CLS method. The same cross-sections from the ENDF/B-VIII.0 nuclear data library were adopted for calculations in RMC to ensure a direct comparison of transport methods. RMC uses settings of 40,000 particles, 2,000 generations, and 50 inactive generations to reduce the standard deviation of the infinite multiplication factor (k_{inf}) to within 10 pcm.

The infinite stochastic media shown in Fig. 5 [Figure 5: see original paper] is simplified from the fuel region of standard fuel pebbles in the HTR-10 and HTR-PM reactors [?, ?]. The matrix of the infinite stochastic media is graphite, and fuel grains are randomly dispersed within it, with a UO_2 kernel outer radius of 250 m and a graphite coating layer outer radius of 455 m. The applicability across different neutron energy spectra was verified by varying the grain packing fraction from 1% to 30%.

The chord length correction coefficient C was calculated using the Particle code where 1,000,000 chords were sampled, the matrix macroscopic total cross-section was set to 0.412/cm, and the boundary radius was greater than 7.5 cm until the results converged.

3.2 Sensitivity Analysis

Because the CLS method does not require explicit modeling of grains, an external boundary with infinite radius was set to calculate k_{inf}. However, explicit modeling of infinite stochastic media is unrealistic. Therefore, a finite region of stochastic media with white boundary condition was used to simulate infinite stochastic media. To minimize the boundary effect, the sensitivity of k_{inf} was studied by increasing the outer radius of the finite region. The radius of the stochastic media was selected as 0.5, 1.5, 2.5, 5.0, 7.5, and 10.0 cm, with the result for 10.0 cm taken as the reference.

The difference curve of k_{inf} with radius for various packing fractions (PFs) is shown in Fig. 6 [Figure 6: see original paper]. It can be observed that there is a significant difference between the reference solution and calculated results, with a strong boundary effect at a boundary radius of 0.5 cm. Furthermore, when the explicitly modeled region was small, the proportion of the region near the boundary with lower packing fraction increased, while the region far from the boundary had a larger packing fraction. This leads to a more uneven spatial distribution of packing fraction and an enhanced boundary effect, causing the calculated result to deviate from the infinite reference solution. As the external boundary radius increased, the boundary effect weakened and the deviation of k_{inf} decreased. After the radius exceeds 2.5 cm, the deviation can be controlled within $±$20 pcm, indicating that the external boundary has almost no effect on the stochastic media. Stochastic media with a radius of 10 cm can therefore be used as a reference solution for infinite stochastic media.

3.3 Numerical Results

Table 2 compares the numerical results of explicit modeling and CLS methods. First, the numerical results of the original CLS method are not significantly different from those of explicit modeling, with a maximum deviation of -170 pcm, which is acceptable for engineering applications but slightly large for Monte Carlo simulations. In more complex finite stochastic media, the deviation is amplified when the excluded-volume effect is not considered.

The matrix chord length correction method for the excluded-volume effect is listed in Table 2. The chord length correction factor C was obtained using Eq. MATH_8 . It can be observed that the CLS method with chord length correction is more consistent with explicit modeling than the original CLS method. Across all calculated packing fractions, the deviations are within $±$50 pcm, indicating that the chord length correction method proposed in this paper can effectively reduce the influence of the excluded-volume effect. The micro-heterogeneity of local stochastic grains is the main reason for the minor differences in k_{inf}.

It should be noted that the accuracy of this correction method depends on the chord length sampling statistics and the matrix cross-section. If the scale of chord length sampling is increased or the cross-section is discretized according to energy to calculate the chord length correction factor, the results will be more consistent with explicit modeling.

4. Conclusions

CLS is an efficient implicit method for treating dispersion fuels with stochastic media in Monte Carlo simulations. A basic assumption of CLS is the Markov process without considering the excluded-volume effect between grains. This study highlighted the excluded-volume effect in realistic stochastic media and discussed its impact on the matrix chord length distribution. A chord length correction method was proposed based on equivalent transmission probability to eliminate this effect. Moreover, the Particle code with stochastic grain modeling and chord length sampling capabilities was developed to obtain the chord length correction factor. The corrected CLS method proposed in this study can be easily implemented using existing CLS-based Monte Carlo codes. Finally, cases of infinite stochastic media were established to verify the correction method with respect to the excluded-volume effect. Numerical comparative analysis with explicit modeling has proven that the chord-length correction method proposed in this study can overcome the defects of neglecting the excluded-volume effect between grains in the original CLS method and achieves higher accuracy.

In future work, we will focus on developing a correction method that considers both the boundary effect and the excluded-volume effect in realistic dispersion fuels with finite stochastic media, building upon previous works on boundary effect.

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Note: Figure translations are in progress. See original paper for figures.