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Chord length sampling correction analysis for dispersion fuel in Monte Carlo simulation

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Abstract

Dispersion fuels, knowned for their excellent safety performance, are widely used in advanced reactors, such as high-temperature gas-cooled reactors. 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. This study shows that the excluded-volume effect in realistic stochastic media can introduce certain 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.

Keywords Stochastic media · Monte Carlo · Chord length sampling · Excluded-volume effect · Chord length correction

1 Introduction

Dispersion fuels, known for their ability to effectively prevent nuclear leakage and high safety performance, are widely used in advanced reactors, particularly high-temperature gas-cooled reactors (HTGRs). In traditional deterministic methods, the presence of stochastic media causes the dispersion fuel to exhibit double heterogeneity, which poses a challenge to reactor physics calculations. The Monte Carlo method has significant advantages in the simulation of stochastic media due to its flexible geometric modeling and continuous energy nuclear cross-section. Several approaches have been developed to simulate stochastic media by considering stochastic effects, such as random explicit modeling and the chord length sampling (CLS) method.

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The explicit modeling method can accurately describe the geometry of each grain, depending on the method of generating stochastic grains. Early studies [1–3] placed grains in regular lattices to describe stochastic media without considering the randomness of the grain distribution. Brown et al. [4] introduced random translations into the positions of grains within repeated regular lattices and implemented them in MCNP. This random lattice method considers some randomness; however, the grains remain relatively regular at the macro level. The explicit random modeling method can accurately describe each stochastic grain with the least approximation based on random packing methods such as random sequential addition (RSA) [5], close random packing (CRP) [6] and discrete element method (DEM) [7]. The generation and storage of grains and the ray tracing process incur significant computational costs. Therefore, the random explicit modeling method with the highest accuracy is often used to provide reference solutions and has been used in Monte Carlo codes such as OpenMC [8], SERPENT [9] and RMC [10, 11].

Unlike the explicit methods above, an implicit method called CLS 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 [12] proposed the CLS method based on 1D geometry. Murata et al. [13, 14] developed an MCNP-CFP code to simulate HTGR based on the nearest neighbor distribution (NDD) method. CLS has the advantage of simplifying geometric modeling and improving computational efficiency.

The CLS method uses the matrix chord length's probability density function (PDF) to sample the distance to the next grain, indirectly determining the grains' packing fraction. The PDF of matrix chord length is inherently assumed to satisfy a Poisson distribution [15–18], because the transport process of CLS is a Markovian process in which 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, influenced by the boundary effect of the external boundary and excluded-volume effect of the micro 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 external boundary. Thus, the total packing fraction is lower than expected. To address the boundary effect, many studies have focused on correction methods for the packing fraction influenced by finite boundaries, such as those by Murata [13], Ji [15], Griesheimer [19, 20] and Liang [21]. These studies were based on the assumption that the PDF follows an exponential distribution, and focused on the 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, the former grains have an excluded-volume effect on the latter grains during packing, resulting in a significant decrease in the proportion of matrix chord length near the grain size. The excluded-volume effect can cause the matrix chord length 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 the interactions between grains, especially at low packing fractions. The excluded-volume effect conflicts with the Poisson distribution assumption of the CLS, making it difficult to correct CLS.

In this study, we analyzed the mechanism of the excluded-volume effect on the matrix chord length PDF. Subsequently, the Particle code was developed to generate stochastic grains rapidly and perform chord length sampling analysis. Furthermore, a chord length correction method was proposed based on the matrix transmission probability equivalence to obtain the matrix chord length correction factor. The CLS method with correction was implemented in the RMC code [10, 11, 22]. 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: Sect. 2 introduces the basic principles and excluded-volume effect issues of the CLS method, and a correction approach for the chord length is proposed based on the Particle code. The verification of the CLS with chord length correction is presented in Sect. 3. Finally, the conclusions are presented in Sect. 4.

2 Methodology

2.1 Chord length sampling

There may be some differences in the implementation of CLS for different Monte Carlo codes. The CLS process in the RMC code [23] is shown in Fig. 1. After entering the stochastic media region, the neutrons pass through the matrix and grains 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 were also determined by sampling.

Firstly, the matrix chord length l_0 between the grains is sampled based on the PDF in Eq. (1).

$$p\left(l_0\right) = \frac{1}{\overline{l_0}} e^{-\frac{l_0}{\overline{l_0}}} \tag{1}$$

Here, the PDF is assumed exponential, and the matrix mean chord length $\overline{l_0}$ is defined by Eq. (2).

$$\overline{l_0} = \frac{4}{3} \frac{1 - \sum_j f(j)}{\sum_j \frac{f(j)}{r_j}} \tag{2}$$

This matrix mean chord length is different from it in traditional CLS because it considers the case of a stochastic media containing multiple grains, such as fuel and poison

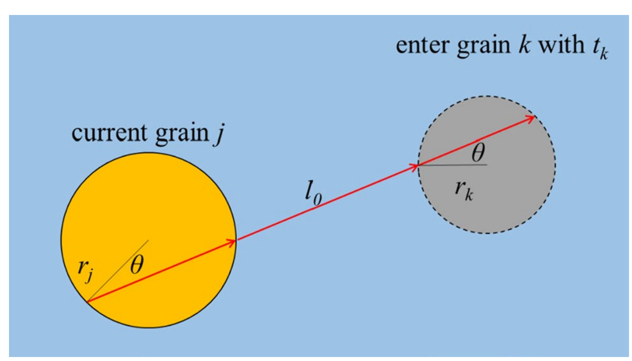

Fig. 1 Schematic diagram of CLS

grains, where $f(j)$ represents the packing fraction of grain j with radius r_j.

Secondly, the type of the next entering grain is sampled, entering grain j with probability t_j using Eq. (3).

$$t_j = \frac{f(j)}{r_j} / \sum_m \frac{f(m)}{r_m} \tag{3}$$

Thirdly, based on the assumption that neutrons enter grains isotropically, the angle θ in 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 $\mu = \cos(\theta)$ from Eq. (4).

$$\mu = \sqrt{\xi} \tag{4}$$

where ξ is a random number between (0, 1).

2.2 Excluded-volume effect

The excluded-volume effect is a problem in realistic stochastic media. Because of the hard-sphere assumption, grains cannot overlap with other grains. The excluded-volume effect impacts both the explicit modeling and CLS methods.

In the explicit modeling method, owing to the hard-sphere assumption, the newly sampled grain is rejected and resampled when overlapping with any existing grain, resulting in a matrix chord length that is not equal to 0. 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.

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

We noticed that a correction treatment is used in some codes to determine whether the grains overlap, considering that the next grain may overlap with the current grain when the chord length is small, as shown in Fig. 3. When an overlap occurs between grains, the current sampling result is rejected, and the chord length and angle are resampled.

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 the previous grains. In other words, there is no need to consider the overlapping problem of previous grains in the CLS. Suppose it is necessary to consider the overlap between grains; not only the previous one but also all grains in history should be considered, which violates the principle of the CLS. This correction causes many smaller chord lengths to be rejected, whereas larger ones are retained, increasing the mean chord length, which is equivalent to a reduction in the packing fraction of the grains.

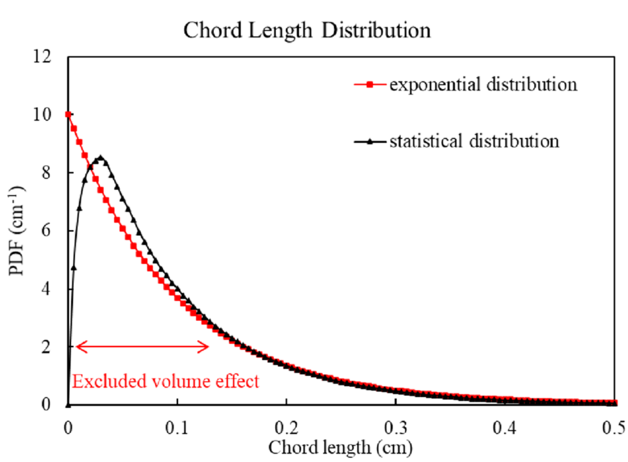

Fig. 2 Schematic diagram of matrix chord length distribution in realistic stochastic media influenced by excluded-volume effect

2.3 Particle code

The Particle code was developed to quickly model realistic stochastic grains and sample matrix chord lengths to address the excluded-volume effect. As shown in Fig. 4, the implementation of the Particle code includes the following processes.

(1) The geometry of a finite region was defined, and a virtual acceleration mesh was established around the entire geometry.
(2) With the virtual grid acceleration, RSA and CRP are combined to quickly generate the coordinates of stochastic grains to achieve the packing fraction of PF,

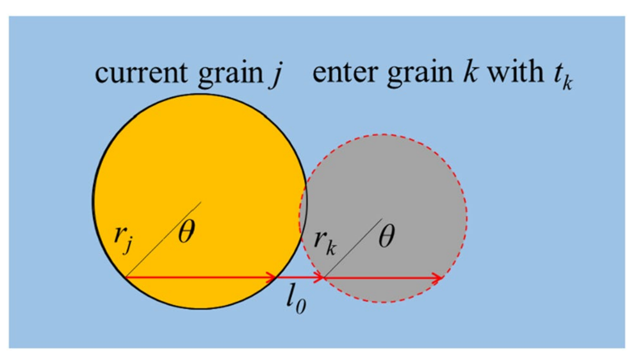

Fig. 3 Next grain overlapping with the current grain

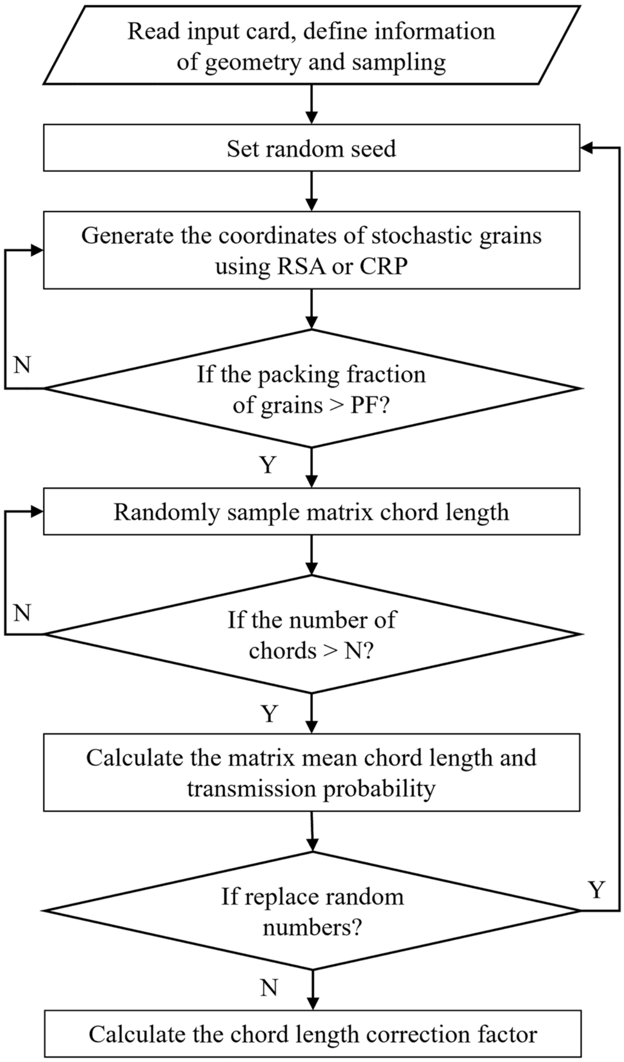

Fig. 4 The flowchart of the Particle code

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 was repeated N times to obtain the distribution of the matrix chord lengths.

(4) To reduce the random error, we replace the random seed and repeat (1)–(3) to obtain a stable statistical result.

The Particle code is based on geometric chord length sampling of realistic stochastic media without considering nuclear physics reactions. The calculation time of the Particle code is much shorter than that of the Monte Carlo neutron transport simulation based on explicit modeling. Therefore, its simulation efficiency is very high, usually taking a few seconds under one core at a low packing fraction, 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 in the exponential distribution directly 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 the stochastic media. Therefore, a chord length correction method based on the equivalent transmission probability is proposed, which ensures the 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 [24] and has shown high accuracy and application prospects.

After the chord length sampling procedure in the Particle code is completed, the mean matrix transmission probability is calculated using Eq. (5).

$$T_0^{\mathrm{MC}} = \frac{1}{N}\sum_{i}^{N} e^{-\Sigma_0 l_0^{(i)}} \tag{5}$$

And, the matrix mean chord length $\overline{l_0}^{\mathrm{MC}}$ is calculated by Eq. (6).

$$\overline{l_0}^{\mathrm{MC}} = \frac{1}{N}\sum_{i}^{N} l_0^{(i)} \tag{6}$$

where $l_0^{(i)}$ is the sampling 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 [25] 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 within an energy range. Assuming an exponential distribution, the theoretical matrix transmission probability can be expressed using Eq. (7).

$$T_0 = \int_0^{\infty} e^{-\Sigma_0 l_0} \frac{1}{\overline{l_0}} e^{-\frac{l_0}{\overline{l_0}}} dl_0 = \frac{1}{1+\Sigma_0 \overline{l_0}} \tag{7}$$

By equating T_0 with T_0^{MC}, the corrected chord length $\overline{l_0}^{\mathrm{Eq}}$ can be derived using Eq. (8).

$$\overline{l}_0^{\mathrm{Eq}} = \frac{1 - T_0^{\mathrm{MC}}}{T_0^{\mathrm{MC}} \Sigma_0} \tag{8}$$

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 $\overline{l}_0^{\mathrm{MC}}$ approaches the theoretical value obtained using Eq. (2). Finally, a dimensionless matrix chord length correction factor is defined by Eq. (9), which is used to correct the matrix mean chord length under the assumption of an exponential distribution.

$$C = \frac{\overline{l}_0^{\mathrm{Eq}}}{\overline{l}_0^{\mathrm{MC}}} \tag{9}$$

This factor is multiplied by the sampled chord length to obtain the corrected chord length in the 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 was correlated 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_0 was set to 0.412 cm^{-1} in the full energy range when the matrix material was graphite with a 1.73 $\mathrm{g/cm}^3$ density.

Table 1 The interpolation table of chord length correction factor

Radius (μm)	Packing fraction				
	1%	5%	10%	20%	30%
250	1.0051	1.0046	1.0044	1.0038	1.0029
500	1.0098	1.0093	1.0089	1.0077	1.0059
750	1.0154	1.0137	1.0132	1.0112	1.0087

Alternatively, based on the above interpolation table, it can be observed that there is a correlation between the parameters that can be fitted as a function, such as Eq. (10).

$$C^{\Sigma_0}(r,f) = 1 + 2r(-0.1338f + 0.09934) \tag{10}$$

where r is the radius of the grain (cm), and f is the packing fraction. This formula is suitable for use in specific problems, such as the fuel element of the HTGR, and requires reprocessing for new problems.

3 Numerical results and analysis

3.1 Test case

The CLS and its correction methods mentioned in this paper were implemented in the RMC code using efficient computational convergence methods [26]. A set of infinite stochastic media cases was designed to validate the effectiveness of the proposed method in addressing the excluded-volume effect. The numerical results from explicit modeling in the RMC were used as reference solutions and compared with the CLS method. The same cross-section from the ENDF/B-VIII.0 nuclear data library was adopted for the calculation in the RMC to ensure a direct comparison of the transport methods. The RMC uses settings of 40,000 particles, 2000 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 is simplified from the fuel region of the standard fuel pebble in the HTR-10 and HTR-PM reactors [27, 28]. The matrix of an infinite stochastic media is graphite and fuel grains are randomly dispersed within it, with a UO_2 kernel outer radius of

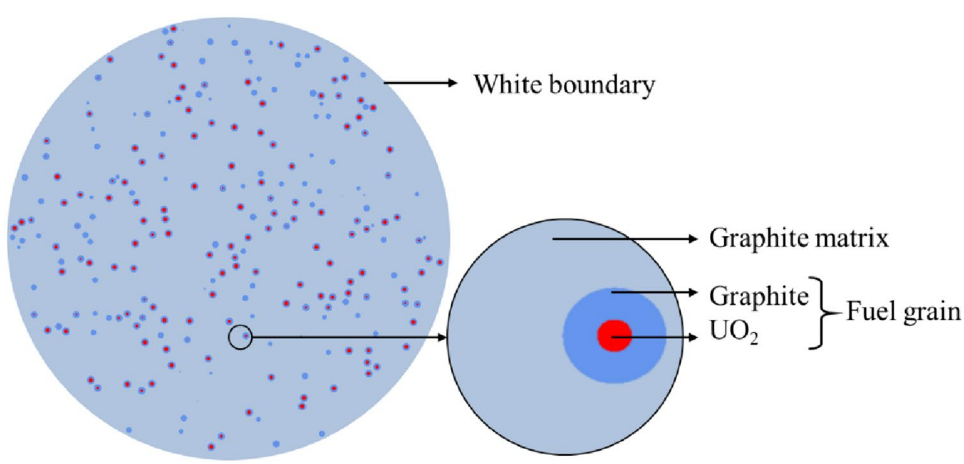

Fig. 5 Simplified infinite stochastic media by explicit modeling

250 μm and a graphite coating layer outer radius of 455 μm. The applicability of different neutron energy spectrum was verified by changing 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^{-1}, 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 an infinite radius was set to calculate k_{inf}. However, the explicit modeling of infinite stochastic media is unrealistic. Therefore, a finite region of stochastic media with white boundary condition was used to simulate an 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, and the result for 10.0 cm was taken as the reference.

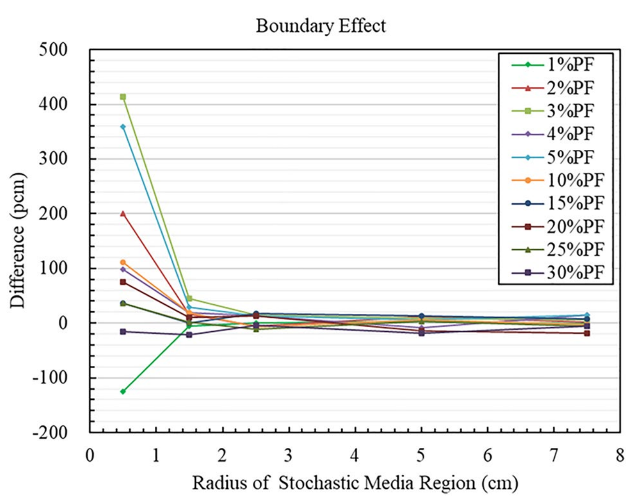

Fig. 6 Sensitivity curve of boundary effect

The difference curve of k_{inf} with the radius for the various packing fractions (PFs) is shown in Fig. 6. It can be observed that there is a significant difference between the reference solution and the calculated result, 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 a lower packing fraction increased. In contrast, the other region far from the boundary had a larger packing fraction. This leads to a more uneven spatial distribution of the packing fraction and an enhanced boundary effect, causing the calculated result to deviate from the infinite reference solution. As the radius of the external boundary increased, the boundary effect weakened, whereas 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 radius of 10 cm can be used as reference solution for infinite stochastic media.

3.3 Numerical results

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

The calculation result of matrix chord length correction method for the excluded-volume effect can be found in Table 2. The chord length correction factor, C, was obtained using Eq. (10). It can be observed that the CLS method with chord length correction is more consistent with

Table 2 k_{inf} of infinite stochastic media

Packing fraction	Explicit modeling	CLS				
		Original		Equivalent correction		
	k_{inf}	k_{inf}	Δk_{inf}(pcm)	k_{inf}	Δk_{inf}(pcm)	C
0.01	1.74386	1.74412	26	1.74352	− 35	1.00892
0.03	1.68906	1.68813	− 92	1.68942	37	1.00867
0.05	1.58367	1.58230	− 137	1.58416	49	1.00843
0.10	1.39134	1.38964	− 170	1.39180	46	1.00782
0.15	1.27505	1.27342	− 163	1.27518	13	1.00720
0.20	1.20278	1.20161	− 117	1.20258	− 20	1.00659
0.25	1.15726	1.15611	− 114	1.15689	− 37	1.00598
0.30	1.12860	1.12764	− 96	1.12818	− 42	1.00537

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 microheterogeneity of the 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 statistical method and the matrix's 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. In that case the results will be more consistent with explicit modeling.

4 Conclusion

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 of realistic stochastic media and discussed its impact on the matrix chord length distribution. A chord length correction method was proposed based on the 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, with respect to the excluded-volume effect, cases of infinite stochastic media were established to verify the correction method. 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 has higher accuracy.

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

Author contributions All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by ZYL, DS, YTW and LS. The first draft of the manuscript was written by ZYL, and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Data availability The data that support the findings of this study are openly available in Science Data Bank at https://cstr.cn/31253.11.sciencedb.j00186.00412 and https://doi.org/10.57760/sciencedb.j00186.00412.

Declarations

Conflict of interest Ding She is an editorial board member for Nuclear Science and Techniques and was not involved in the editorial review, or the decision to publish this article. All authors declare that there are no competing interests.

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