CHORD LENGTH SAMPLING METHOD FOR ANALYZING VHTR UNIT CELLS IN CONTINUOUS ENERGY SIMULATIONS

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ABSTRACT

The chord length sampling method (CLS) is studied in the continuous energy simulations by applying it to analyzing two types of Very High Temperature Gas-cooled Reactor (VHTR) unit cells: the fuel compact cell in the prismatic type VHTR and the fuel pebble cell in the pebble-bed type VHTR. Infinite multiplication factors of the unit cells are calculated by the CLS and compared to the benchmark simulations at different volume packing fractions from 5% to 30%. It is shown that the accuracy of the CLS is affected by the boundary effect, which is induced by the CLS procedure itself and results in a reduction in the total volume packing fraction of the fuel particles. To mitigate the boundary effect, three correction schemes based on the research of 1) Murata et al. 2) Ji and Martin 3) Griesheimer et al. are used to improve the accuracy by applying a corrected value of the volume packing fraction to the CLS. These corrected values are calculated based on 1) a simple linear relationship, 2) an iterative self-consistent simulation correction method, and 3) a theoretically derived non-linear relationship, respectively. The CLS simulation using the corrected volume packing fraction shows excellent improvements in the infinite multiplication factors for the VHTR unit cells. Ji and Martin’s self-consistent correction method shows the best improvement.

Key Words: Chord Length Sampling, VHTR, Monte Carlo method, stochastic media, volume packing fraction.

1. INTRODUCTION

The research on the radiation transport simulation in the stochastic media has received great attention in the past decades [1-9]. In the nuclear engineering field, one of the typical stochastic media systems is the Very High Temperature Gas-cooled Reactor (VHTR) configuration [10,11], where tens of thousands of TRISO particles are randomly embedded in a fuel pebble or a fuel compact, with graphite as the background material. Monte Carlo methods have been used to analyze the VHTR by explicitly modeling the stochastic distribution of the TRISO fuel particles [12,13]. Usually, such analyses are based on simulations over a large number of physical realizations and the ensemble-average solutions are calculated. In practice, the ensemble-average solution is very expensive to obtain due to: (i) the huge memory cost for the explicit model of

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every fuel particle, and (ii) the time-consuming boundary search in determining the next nearest fuel particle. In the past decades, much effort has been made to develop alternative and less expensive methods to simulate radiation transport in the stochastic media. The Chord Length Sampling (CLS) method has been shown the most successful one [1-9].

Zimmerman and Adams [1] firstly proposed the CLS algorithms for a transmission problem in 1-D rod geometry. By sampling a distance from a probability density function, the next material interface is determined on the fly. Algorithms with memory concerns were investigated, and good agreement with benchmark in transmission/reflection rates was obtained. Brantley [2] followed and extended this original work to calculate the scalar flux distribution in 1-D slab geometry for a fixed source problem. Both works showed the successful application of the CLS method in the 1-D geometry. Murata et al. [3,4] and Donovan et al. [5] applied the CLS method to calculating multiplication factors in the configurations of high temperature gas-cooled reactors. Good agreements were also obtained compared with benchmark but the use of an empirically determined chord length PDF limits the application of CLS in practice. Ji and Martin proposed a theoretical chord length PDF to verify the application of CLS in a general 3-D geometry [6] and applied it to analyzing the VHTR unit cells [7]. Good accuracy of the CLS simulation was obtained. More recently, Reinert et al. [8] incorporated the CLS into a hybrid methodology framework in solving transport problems involving randomly densely packed, optically thick absorber systems. Generally speaking, previous work has been focusing on the demonstration of the CLS method by performing a series of simulations for specific systems. Little has been done to provide a systematic analysis on the accuracy of the CLS for practical applications, especially under the continuous energy simulations. To assure the high confidence in the application of CLS, more insightful understanding of the effects on the accuracy of the CLS and the strategies in mitigating these effects becomes very necessary. This motivates the research topic presented in this paper.

Our previous work [9] has performed a series of parameter sensitivity simulations for one group eigenvalue problems in cubic systems packed with mono-sized or poly-sized fuel kernels. It has shown that the accuracy of the CLS changes at different system size, fuel kernel cross sections, and fuel kernel volume packing fractions. The change in the accuracy has been discussed and related to the boundary effect, which is always present when applying the CLS in a finite stochastic media system. This is due to not allowing the overlap of the sampled fuel kernel with the system boundary. Re-sampling is performed in the CLS if an overlap happens [3,7]. However, this would decrease the volume packing fraction (VPF) of the fuel kernels, and the accuracy of the CLS is decreased. In the literature, the boundary effect was first mentioned by Murata et al. [3], where a simple correction method was proposed to calculate a corrected VPF in the CLS simulation in order to preserve the total mass of the fuel particles. Later, Ji and Martin [11] developed a self-consistent correction technique to calculate the VPF needed in the CLS simulation to preserve the nominal VPF of the benchmark configuration. More recently, Griesheimer et al. [14,15] derived a nonlinear relationship between the effective inclusion VPF and the true inclusion VPF for the 1-D slab binary stochastic system. It can be naturally extended with certain approximations to the 3-D system packed with spherical fuel particles and provide a relationship of the volume packing fractions between the CLS and the benchmark simulations. Although each correction method has been used to show good agreement between the CLS and the benchmark simulations, a thorough investigation is still needed to have a full comparison of
these methods in analyzing a practical system configuration, especially in the continuous energy simulations.

In this paper, we first extend the previous parameter sensitive study [9] to the infinite lattice configurations of two VHTR unit cells. The accuracy of the CLS method is investigated at different fuel particle VPFs in the continuous energy simulation. A series of simulations will be done using a modified production Monte Carlo code MCNP [16] with the CLS capability implemented. Benchmark simulations are done by explicitly modeling the VHTR unit cells using MCNP. Infinite multiplication factors are calculated for the comparison between the CLS and the benchmark methods. Then, the three correction schemes from Murata et al., Ji and Martin, and Griesheimer et al. [3,7,14,15] are used to improve the accuracy of the CLS simulation, and the improvements are compared among the three schemes.

The remainder of the paper is organized as follows: In Section 2, the accuracy study of the CLS simulations in analyzing two VHTR unit cells is performed. In Section 3, three correction schemes for the CLS accuracy improvement are examined. In Section 4, the general conclusions and future possible work are given.

2. PARAMETER SENSITIVITY STUDY IN ANALYZING VHTR UNIT CELLS

In this section, we first describe the VHTR unit cell configurations and the material compositions used for the study. Then a general introduction of the CLS procedure is provided. Finally, the predicted multiplication factors in the CLS and the benchmark computations are compared in terms of relative errors at different volume packing fractions.

2.1. Monte Carlo Simulation Model: VHTR Unit Cell Configurations

Two types of the VHTR design are studied: prismatic type and pebble-bed type designs. The unit cells for the two designs are the infinite lattice of the fuel compact cell and the fuel pebble cell. The fuel compact cell consists of a cylindrical fuel zone packed with TRISO fuel particles. The cylindrical fuel zone has a radius of 0.6225 cm and a height of 4.9276 cm, surrounded by a hexagonal graphite region with reflecting boundary conditions on each side. The flat-to-flat distance of the hexagonal graphite region is 2.1958 cm. The fuel pebble cell consists of a 2.5 cm radius spherical fuel zone and a 0.5 cm thick graphite shell. TRISO fuel particles are packed in the fuel zone. White boundary conditions are applied to the outer surface of the cell. Figure 1 shows one physical realization of each unit cell. The stochastic packing of the fuel particles in each cell is implemented by the Random Sequential Addition (RSA) method [17]. For the RSA procedure, two steps are performed: 1) uniformly sample a sphere within the container; 2) when the newly sampled sphere is overlapped with any existing spheres in the container, it is rejected and a new sphere is sampled until no overlap occurs. The two steps continue until the desired VPF is reached. The values of the TRISO fuel geometry dimensions and the material composition/density in each unit cell are listed in Table I based on Refs. [10] and [18]. The spherical TRISO fuel particles consist of a fuel kernel and four coating layers. They are embedded into graphite matrix background region in each fuel zone.
(a) Fuel compact cell at 28.92% VPF   (b) Fuel pebble cell at 5.76% VPF

Figure 1. VHTR unit cell configurations

Table I. Fuel geometry and composition in VHTR unit cells

<table>
<thead>
<tr>
<th>Fuel Compact Cell</th>
<th>Radius(cm)</th>
<th>Isotope and atom density (atom/barn·cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel kernel</td>
<td>0.0175</td>
<td>$^{235}$U: 2.4749E-3; $^{238}$U: 2.1142E-2; C: 1.1809E-2; O: 3.5426E-2</td>
</tr>
<tr>
<td>Carbon buffer layer</td>
<td>0.0275</td>
<td>C: 5.2645E-2</td>
</tr>
<tr>
<td>Inner pyrolytic carbon layer</td>
<td>0.0315</td>
<td>C: 9.5262E-2</td>
</tr>
<tr>
<td>Silicon carbide layer</td>
<td>0.0350</td>
<td>C: 4.8060E-2; Si: 4.8060E-2</td>
</tr>
<tr>
<td>Outer pyrolytic carbon layer</td>
<td>0.0390</td>
<td>C: 9.5262E-2</td>
</tr>
<tr>
<td>Graphite matrix</td>
<td></td>
<td>C: 8.7441E-2</td>
</tr>
<tr>
<td>Hexagonal graphite shell</td>
<td></td>
<td>C: 8.7241E-2; $^{10}$B: 1.4369E-7; $^{11}$B: 5.7838E-7</td>
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<table>
<thead>
<tr>
<th>Fuel Pebble Cell</th>
<th>Radius(cm)</th>
<th>Isotope and atom density (atom/barn·cm)</th>
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<td>Fuel kernel</td>
<td>0.0250</td>
<td>$^{235}$U: 1.8788E-3; $^{238}$U: 2.1334E-2; O: 4.6425E-2</td>
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<tr>
<td>Carbon buffer layer</td>
<td>0.0340</td>
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<td>Outer pyrolytic carbon layer</td>
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<td>C: 9.5262E-2</td>
</tr>
<tr>
<td>Graphite matrix</td>
<td></td>
<td>C: 8.7441E-2</td>
</tr>
<tr>
<td>Pebble shell</td>
<td></td>
<td>C: 8.7441E-2</td>
</tr>
</tbody>
</table>

2.2. Implementing CLS into MCNP

To analyze the VHTR unit cells in the continuous energy simulations, CLS is implemented into the production Monte Carlo code MCNP. A flag is set for the stochastic medium region, such as the spherical or cylindrical fuel zone in each unit cell. Each time a neutron enters the flagged stochastic region, CLS is applied. When a neutron enters a TRISO fuel particle, regular Monte
Chord Length Sampling Method for Analyzing VHTR Unit Cells in Continuous Energy Simulations

Carlo procedures are used. An exponential chord length PDF given by Eq. (1) is employed in the CLS [6] to sample the distance to a TRISO fuel particle: 1) when a neutron enters the stochastic fuel zone; or 2) after a neutron leaves a TRISO fuel particle; or 3) after a neutron scatters in the graphite matrix background. The chord length PDF is shown below:

$$f (l) = \frac{3}{4 \cdot r} \frac{\text{frac}}{1 - \text{frac}} \cdot e^{-\frac{3}{4 \cdot r} \frac{\text{frac}}{1 - \text{frac}}}$$

(1)

where \(\text{frac}\) is the fuel particle volume packing fraction in the benchmark system, \(r\) is the radius of the TRISO fuel particle. The accuracy of the Eq. (1) as the chord length PDF has been verified by comparing with the actual chord length distribution obtained by a direct ray emitting method [19].

Each time a TRISO fuel particle is sampled by the CLS, a collision distance in the graphite matrix is also sampled. The smaller distance is selected to advance the neutron to the next location. If a neutron is to enter a TRISO fuel particle, the fuel particle’s center location is determined by assuming a cosine current distribution around the entering location [3,6]. If the sampled TRISO fuel particle is overlapped with the fuel zone boundary, it is rejected and the neutron is moved back to the original site before the chord length sampling. Then a re-sample is performed [3,7], i.e. sampling distances to the next TRISO fuel particle and the collision site in graphite matrix. By using the CLS method, there’s no need to store location information for each TRISO fuel particle, and spend time in searching boundaries of every TRISO fuel particle to determine the next nearest one, as done in the benchmark MCNP simulation. Also, only one simulation is needed to account for the stochastic distribution of the fuel particles rather than a large number of simulations for different realizations. The CLS simulations have shown significant time efficiency improvement compared to the conventional MCNP simulations for VHTR unit cells, with a speedup of 300 to 1000 in a single threaded run compared to a single realization simulation using MCNP.

2.3. Infinite Multiplication Factor as a Function of Volume Packing Fraction

A series of criticality calculations are performed at the volume packing fractions ranging from 5% to 30% for each unit cell. The infinite multiplication factors, denoted as \(k_{\text{inf}}\), in the benchmark are calculated by averaging \(k_{\text{inf}}\) from 100 independent physical realizations. In each realization, a total of 80 cycles with 50 inactive are simulated. In each cycle, a total of 100,000 histories are tracked. The standard deviation of the ensemble-average \(k_{\text{inf}}\) is less than 1e-5. The same number of cycles and a million histories per cycle are used in the CLS simulation. The standard deviation of \(k_{\text{inf}}\) is also kept less than 1e-5. Table II summarizes the solutions for both the benchmark and the CLS simulations. It is interesting to see that there is a maximum value of the \(k_{\text{inf}}\) for the fuel compact cell at the packing fraction of 17%. For the fuel pebble cell, the value of the \(k_{\text{inf}}\) decreases from low to high packing fractions.
Table II. Simulation solutions of $k_{\text{inf}}$ for VHTR unit cells ($1\sigma = 1\text{E-5}$)

<table>
<thead>
<tr>
<th>VPF</th>
<th>Fuel compact unit cell</th>
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<th>Fuel pebble unit cell</th>
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<td></td>
<td>Benchmark</td>
<td>CLS</td>
<td>Benchmark</td>
<td>CLS</td>
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<tr>
<td>5.00%</td>
<td>1.35255</td>
<td>1.31890</td>
<td>1.62321</td>
<td>1.62769</td>
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<tr>
<td>5.76%</td>
<td>1.39633</td>
<td>1.36754</td>
<td>1.60268</td>
<td>1.60815</td>
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<tr>
<td>7.00%</td>
<td>1.44817</td>
<td>1.42573</td>
<td>1.56839</td>
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<tr>
<td>9.00%</td>
<td>1.49986</td>
<td>1.48500</td>
<td>1.51451</td>
<td>1.52024</td>
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<td>11.00%</td>
<td>1.52857</td>
<td>1.51899</td>
<td>1.46487</td>
<td>1.47279</td>
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<tr>
<td>13.00%</td>
<td>1.54390</td>
<td>1.53851</td>
<td>1.41950</td>
<td>1.42791</td>
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<td>15.00%</td>
<td>1.55127</td>
<td>1.54868</td>
<td>1.37837</td>
<td>1.38713</td>
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<tr>
<td>17.00%</td>
<td>1.55342</td>
<td>1.55324</td>
<td>1.34118</td>
<td>1.34976</td>
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<td>19.00%</td>
<td>1.55191</td>
<td>1.55366</td>
<td>1.30729</td>
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<td>21.00%</td>
<td>1.54826</td>
<td>1.55165</td>
<td>1.27637</td>
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<td>23.00%</td>
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<td>1.24800</td>
<td>1.25696</td>
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<td>25.00%</td>
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<td>1.54266</td>
<td>1.22206</td>
<td>1.23127</td>
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<td>27.00%</td>
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<td>30.00%</td>
<td>1.51743</td>
<td>1.52639</td>
<td>1.16580</td>
<td>1.17488</td>
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</tbody>
</table>

Figure 2 plots the relative error of $k_{\text{inf}}$’s between the benchmark and the CLS simulations as a function of packing fraction. The relative errors are calculated by:

$$\text{relative errors} = \frac{\text{CLS} - \text{Benchmark}}{\text{Benchmark}} \times 100\%.$$  \hspace{1cm} (2)

Figure 2. Relative errors of $k_{\text{inf}}$ between the CLS and the benchmark
From Figure 2, it can be seen that for the fuel compact cell, the $k_{\text{inf}}$ is underestimated by the CLS method below the packing fraction of 17% and overestimated above 17%. As the packing fraction increases or decreases further from 17%, the relative errors become larger. This tendency is consistent with the previous research for a cubic system in one group simulations, where the boundary effect and the associated chord length PDF accuracy were considered major factors affecting the CLS accuracy [9]. For the fuel pebble cell, the CLS method overestimates the $k_{\text{inf}}$ over all the packing fractions with a trend that the relative errors increase as the packing fraction increases. The boundary effect is also the major factor that causes the larger relative errors for the fuel pebble cell.

It can be concluded that if the boundary effect, i.e. the reduction in the total volume packing fraction in the CLS simulation, can be corrected, the CLS accuracy would be improved. This can be done by applying a higher VPF than the actual one to the CLS simulation. How to choose a higher VPF will be discussed in the next section.

3. PACKING FRACTION CORRECTION IN THE CLS SIMULATION

Three correction schemes are investigated and employed [3,7,14,15] to correct the volume packing fraction, denoted as $\text{frac}$ in Eq. (1) and applied to the CLS simulations. For convenience, a correction factor defined by $c = \text{frac}' / \text{frac}$ is introduced to compare the three schemes, where $\text{frac}'$ is the corrected or effective VPF. It is expected that the CLS simulation using $\text{frac}'$ would produce more accurate solutions.

The first scheme was proposed by Murata et al. [3]. In order to reproduce the prescribed volume packing fraction, a simple way was suggested to correct the VPF by multiplying a volume ratio:

$$\text{frac}' = \frac{V}{V - \Delta V} \cdot \text{frac} \quad (3)$$

where $V$ is the original volume of the stochastic region, $\Delta V$ is the volume of the boundary region with the thickness of one fuel particle radius from $V$.

The second scheme was proposed by Ji and Martin [7]. Since the packing fraction is only a function of geometry and not a function of material composition, a special CLS simulation can be performed for the given geometry by assuming all regions (fuel particle and background) are voided and using the track length estimator to estimate the volumes of the fuel particle and background regions. This yields the packing fraction for this geometry as experienced by the CLS method. This 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 mono-directional plane source on one side of the stochastic geometry with all internal regions voided. This is done for both the fuel compact and fuel pebble VHTR cells. A total of $10^7$ neutrons are tracked each iteration in this study, reaching an accuracy of $1e-5$ standard deviation.
In practice, the corrected input packing fraction can be pre-calculated by Ji and Martin’s scheme before the actual CLS simulation.

The third scheme was proposed by Griesheimer et al. [14,15]. A nonlinear relationship between the effective (corrected) inclusion packing fraction and the true inclusion packing fraction was derived based on a modified Poisson approximation in a 1-D binary stochastic medium system:

\[
frac{\prime} = 1 - m + \sqrt{(m-1)^2 + 2m \cdot \frac{\prime}} ,
\]

where \(m = \frac{L}{l}\). \(L\) is the 1-D slab system length and \(l\) is the inclusion thickness. Although Eq. (4) is derived for 1-D system, it can be extended to the 3-D system, like the VHTR unit cell system studied in this paper, by redefining \(m = \frac{\langle L \rangle}{\langle l \rangle}\), where \(\langle L \rangle\) is the mean chord length of the fuel zone, and \(\langle l \rangle\) is the mean chord length of the TRISO fuel particle. This extension can be justified by the Figure 3: when a neutron enters a stochastic region, its path length along any flying direction can be regarded as a 1-D system. A neutron may penetrate several fuel particles in each path and these fuel particles can be regarded as the inclusion in the 1-D system. In this sense, a 3-D system can be regarded as a 1-D system assuming that the length of the system is \(\langle L \rangle\) and the inclusion thickness is \(\langle l \rangle\). Then as a first order approximation, Eq. (4) can be used to correct the VPF for the VHTR unit cells with the new definition of \(m\). It should be noted that exact derivation of Eq. (4) in 3-D should explicitly account for the size and shape of the fuel particles and fuel zones under consideration, as pointed by Griesheimer et al. [15]. The mean chord length of the TRISO fuel particle and the fuel zones in VHTR unit cells can be calculated as [20,21]:

\[
\langle l \rangle = \frac{4}{3} r, \quad \langle L \rangle = \begin{cases} 
2 \cdot R_c, & \text{fuel zone fuel compact cell} \\
(4/3) \cdot R, & \text{fuel zone fuel pebble cell}
\end{cases}
\]

where \(r\) is the radius of the TRISO fuel particle, \(R_c\) is the radius of the cylindrical fuel zone, and \(R\) is the radius of the spherical fuel zone in the fuel pebble.

**Figure 3. Extension of Eq. (4) to a 3-D system**
Figure 4 plots the correction factor as a function of the volume packing fraction for the three correction schemes that are applied to the VHTR unit cells analysis. It shows that the Murata et al.’s scheme predicts much larger corrected VPF than the other two schemes. The scheme of Ji and Martin predicts higher but close corrections to the scheme of Griesheimer et al. over the range of the VPF.

![Graph showing correction factor vs volume packing fraction for fuel compact and pebble unit cells.](image)

**Figure 4. Comparison of the three correction schemes for the volume packing fraction**

Using these three schemes, the corrected VPF $\frac{\text{f}}{\text{ac}'}$ can be obtained and a new chord length PDF for the CLS method can be written as:

$$f(t) = \frac{3}{4 \cdot r} \frac{\text{f}}{\text{ac}'} \cdot \frac{\text{f}}{\text{ac}'} \cdot e^{-\frac{3}{4 r} \frac{\text{f}}{\text{ac}'} \cdot \frac{\text{f}}{\text{ac}'}} \cdot t$$

Applying the new chord length PDF to the CLS simulations for the VHTR unit cells analysis, the improvements of the accuracy on the $k_{\text{inf}}$ can be compared among the three correction schemes. Figure 5 shows the relative errors of the $k_{\text{inf}}$ between the CLS simulation using the corrected VPF and...
and the benchmark simulation. With the standard deviation of 1e-5 for $k_{\text{inf}}$’s, the accuracy of the relative errors can be kept within 0.001%. It can be seen that Murata et al.’s scheme overcorrects the VPF, causing the overcorrection of the $k_{\text{inf}}$’s in the CLS simulation. This verifies the conclusion that this scheme overestimates the effective VPF [14,15]. The other two schemes both show excellent improvements of the accuracy, and Ji and Martin’s scheme is a little superior to Griesheimer et al.’s scheme. The improvement of the CLS accuracy can also be measured by calculating the mean value of the relative errors over all the VPFs:

$$<|R|> = \frac{1}{N} \sum_{n=1}^{N} \left| n^{\text{th}} \text{ relative error} \right|$$

Table III lists the mean value of the relative errors for the three corrections schemes. It shows that in both schemes of Ji and Martin and Griesheimer et al., $<|R|>$ is significantly reduced for both VHTR unit cells. For both fuel compact and fuel pebble cells, Murata et al.’s scheme overestimates the effective VPF, which induces a significant inaccuracy in the CLS simulations.

Figure 5. Comparison of three correction schemes in improving the accuracy of CLS
Table III. The value of $|R|$ for three correction schemes

<table>
<thead>
<tr>
<th></th>
<th>No correction</th>
<th>Murata et al.</th>
<th>Ji and Martin</th>
<th>Griesheimer et al.</th>
</tr>
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<tr>
<td>Fuel compact cell</td>
<td>0.74%</td>
<td>0.67%</td>
<td>0.19%</td>
<td>0.40%</td>
</tr>
<tr>
<td>Fuel pebble cell</td>
<td>0.61%</td>
<td>0.48%</td>
<td>0.17%</td>
<td>0.28%</td>
</tr>
</tbody>
</table>

4. CONCLUSIONS

We present a parameter sensitivity study on the accuracy of the CLS method under continuous energy simulations for the analysis of two VHTR unit cell designs. The infinite multiplication factors are calculated by the CLS method and compared with the benchmark simulation based on the RSA-generated geometry configuration. The CLS simulation shows significant deviation from the benchmark simulations over the range of volume packing fractions under consideration. This deviation is due to the boundary effect in the CLS procedure that causes the reduction in the total fuel particle volume packing fraction. In order to mitigate the boundary effect and assure the applicability of the CLS method, three correction schemes are studied in the CLS simulations by correcting the VPF. From the numerical calculation, the improvement with different degree is obtained under each scheme. The scheme of Murata et al. is the simplest correction scheme, but overestimates the VPF and leads to a further deviation from the benchmark. The theoretically derived correction scheme of Griesheimer et al. for the 1-D system is extended to the 3-D system and presents excellent improvement on the CLS accuracy. The scheme of Ji and Martin is the most flexible way to treat VPF correction for the systems of any geometry and size, and this scheme shows the highest level of improvement of the CLS accuracy.

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