



# On the improvements in neutronics analysis of the unit cell for the pebble-bed fluoride-salt-cooled high-temperature reactor



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## ABSTRACT

The stochastic characteristics of the randomly distributed coated-fuel particles, the thermal-neutron scattering effect of the fluoride-salt and the resonance elastic scattering effect of heavy nuclides were neglected in early neutronics studies on the Pebble-Bed Fluoride-salt-cooled High-temperature Reactor (PB-FHR). In order to assess the impact of these effects on the neutronics calculation, the stochastic effect is analyzed by applying the explicit random modeling approach and Chord Length Sampling method, the thermal-neutron scattering effect of the fluoride-salt is quantified by evaluating and processing a new thermal-neutron scattering data library, and the resonance elastic scattering effect is covered by using the Doppler Broadening Rejection Correction (DBRC) method in this work. According to the critical calculations of the PB-FHR pebble unit cells with different TRISO Packing Factor (TPF), the different stochastic modeling methods lead to a difference of  $k_{inf}$  by tens of pcm, the thermal scattering effect of  $2\text{LiF-BeF}_2$  results in a decrease of  $k_{inf}$  by 104–290 pcm and the resonance elastic scattering effect leads to a decrease of  $k_{inf}$  by 107–437 pcm, respectively. In addition, the thermal-neutron scattering effect and resonance elastic scattering effect can be additive, the total impact of the thermal scattering effect of  $2\text{LiF-BeF}_2$  and the resonance elastic scattering effect of heavy nuclide leads to a decrease of  $k_{inf}$  by 204–747 pcm.

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## 1. Introduction

The Pebble-Bed Fluoride-salt-cooled High temperature Reactor (PB-FHR) is a novel design which adopts low-pressure liquid fluoride-salt and high-temperature randomly distributed Tristructural-isotropic (TRISO) coated-fuel particles. Recent studies of fluoride-salt-cooled high-temperature reactor conceptual designs cover the Pebble Bed Advanced High Temperature Reactor (PB-AHTR) at UCB (Fratoni, 2008), Sm-AHTR at ORNL (Greene et al., 2010), large central-station AHTR at ORNL (Holcomb et al., 2011; Varma et al., 2012), the Pebble-Bed FHR at UCB (Krumwiede et al., 2013; Scarlat and Peterson, 2013), and the experimental pebble-bed fluoride-salt-cooled high-temperature reactor at Shanghai Institute of Applied Physics which will be constructed as an initial step to test and verify the technical feasibility of a large-scale reactor in the next years (SINAP, 2012; Xiao et al., 2014; Liu et al., 2016). However, some significant neutronics effects are

ignored in early neutronics analysis of the PB-FHR. In addition, the distinctive characteristics of the PB-FHR are as follows:

The first characteristic of the PB-FHR is that the pebble-bed reactor core consists of randomly distributed fuel pebbles which are made of randomly distributed TRISO coated-fuel particles. This special structure is the so-called 'double-level random distribution'. However, in the preliminary neutronics analysis of the fluoride-salt-cooled high-temperature reactor (Qin et al., 2016), only regular lattice modeling method is applied. Recently some random modeling methods have been developed, for example, the explicit random modeling method is shown to be the most precise one among the Random Lattice Method, Chord Length Sampling (CLS) method and explicit random modeling method (Liu et al., 2015a). The explicit random modeling method has been implemented in the Monte-Carlo codes such as MONK (Smith et al., 2001), RMC (She et al., 2015; Liu et al., 2015b) and Serpent (Leppänen, 2012). In this work, the coordinates of the TRISO coated-fuel particles were read from a separate file generated by the in-house packing code PACK, then the coordinate file is used by Serpent to perform the Monte-Carlo simulation of PB-FHR pebble unit cell. Because the explicit

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random model costs huge memory and needs reading the positions of the particles from a separate file, the CLS method as an alternative and less expensive method has been widely studied (Murata et al., 1996, 1997; Mori et al., 2000; Reinert, 2010), but the challenge of the CLS method is the boundary effect (Murata et al., 1996) which would influence the accuracy. Three kinds of correction technique have been proposed to improve the accuracy of the CLS method (Murata et al., 1996; Ji and Martin, 2008; Griesheimer, 2010), the latest nonlinear relationship correction technique (Griesheimer, 2010) is adopted when the TPF is high in this work. Since the explicit random model and CLS method have their advantages and disadvantages, the Monte-Carlo simulation results of the two methods are compared to analyze the stochastic effect of the PB-FHR and to decide which random method is adopted to obtain accurate Monte-Carlo transport calculation results for all the PB-FHR pebble unit cells in the following sections in this paper.

The second characteristic of the PB-FHR is that the coolant of the core is high-temperature fluoride-salt (2LiF-BeF<sub>2</sub>). It is found that the moderating properties of 2LiF-BeF<sub>2</sub> are not negligible and the impact of the thermal-neutron scattering effect of 2LiF-BeF<sub>2</sub> on the neutronics calculation of MSRE is significant (Mei et al., 2013). However, the impact of the thermal-neutron scattering effect of 2LiF-BeF<sub>2</sub> on the neutronics calculation of PB-FHR has not been studied (Qin et al., 2016). The thermal-neutron scattering effect of the 2LiF-BeF<sub>2</sub> is quantified by re-evaluating and processing a new thermal-neutron scattering data library. In addition, the fuel of the PB-FHR core works at high temperatures. Recent studies show that the energy-dependent elastic scattering kernel of <sup>238</sup>U would considerably improve the precision of critical calculations for high-temperature reactors such as HTR and HTTR (Becker et al., 2009a). However, the impact of the resonance elastic scattering effect on the neutronics of PB-FHR has not been studied in early studies (Qin et al., 2016). In this study, the resonance elastic scattering effect of the <sup>238</sup>U is calculated by the Doppler Broadening Rejection Correction (DBRC) method.

The remainder of the paper is organized in the following manner: the methods of modeling the randomly distributed TRISO coated-fuel particles to quantify the stochastic effect are described in Section 2. Section 3 introduces the methods of re-evaluating and processing thermal-neutron scattering data libraries of the 2LiF-BeF<sub>2</sub>. The ACE format continue-energy and WIMS format multi-group thermal-neutron scattering cross-section libraries are used by the Monte-Carlo code Serpent and deterministic code SUGAR to quantify the thermal-neutron scattering effect. Section 4 describes the DBRC method to quantify the resonance elastic scattering effect. Section 5 discuss the total impact of the thermal-neutron scattering effect and resonance elastic scattering effect. Finally conclusions and future work plans are given in Section 6.

## 2. Stochastic modeling methods

The PB-FHR adopts fuel pebbles with a 0.5 cm thickness graphite shell outside and 2.5 cm thickness graphite matrix inside which contains a large number of TRISO coated-fuel particles. The TRISO packing factor (TPF) is defined as the volume fraction of the TRISO coated-fuel particles in the matrix. The TPF of the PB-FHR fuel pebble in this paper varies from 5.02% to 30% which covers most of the existing PB-FHR designs. The TRISO coated-fuel particle, from inner to outer, consists of a UO<sub>2</sub> fuel kernel, porous carbon buffer layer, dense inner pyrolytic carbon layer, chemically vapor deposited silicon carbide layer, and dense outer pyrolytic carbon layer. A binary molten salt system of the 2LiF-BeF<sub>2</sub> (0.005% <sup>6</sup>Li) is used as the primary coolant. The volumetric filling fraction of pebbles in core is set to be 60.46%. The calculated atomic densities of the pebble unit cell (IAEA, 2003) are summarized in Table 1.

In order to quantify the stochastic effect of the PB-FHR pebble unit cell, the following two models are compared.

The first model is the explicit random modeling method, as shown in Fig. 1. Before performing the Monte-Carlo calculations, the random coordinate sampling for TRISO coated-fuel particles is calculated by the in-house packing code PACK. The calculation procedure is as follows: 1) uniformly sample a TRISO coated-fuel particle within the fuel zone of the pebble; 2) compare with all the other existing TRISO coated-fuel particles in the fuel zone to check if the newly sampled TRISO coated-fuel particles overlaps with any one of them; 3) the new particle will be accepted if there is no overlap, otherwise reject and resample. These steps continue until the desired TRISO packing factor is reached. The coordinates of the randomly distributed TRISO coated-fuel particles are then used as the input for subsequent Monte-Carlo calculations. The explicit random modeling method of Serpent treats the distributions of TRISO coated-fuel particles explicitly.

In order to obtain the actual  $k_{inf}$  of the PB-FHR pebble unit cell, 10 types of randomly distributed TRISO coated-fuel particles for one pebble unit cell are simulated. The coordinates of the randomly distributed TRISO coated-fuel particles of each type are randomly generated by the packing code PACK. The average value of the 10 types is used as the practical  $k_{inf}$ . The criticality calculation is performed by Serpent. Each Monte-Carlo calculation uses 100,000 neutrons per cycle, 10,500 active cycles and 500 inactive cycles. The standard deviation of  $k_{inf}$  is 0.00004. The results of these configurations are summarized in Table 2. It is found that the uncertainty  $\sigma(k_{inf})$  caused by different types of random distribution is quite small.

The second random model called CLS method which is also implemented in the Monte Carlo code Serpent. A flag is set for the stochastic medium region, the CLS method is used when a neutron enters the flagged region. When a neutron enters a TRISO fuel particle, regular Monte Carlo procedures are applied. A chord length PDF (Liang et al., 2012) given by Eq. (1) is applied in the CLS to sample the distance to a TRISO fuel particle: 1) when a neutron enters the stochastic fuel zone; or 2) after a neutron flies off a TRISO fuel particle; or 3) after a neutron scatters in the graphite matrix.

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

where TRISO Packing Factor (TPF) is the TRISO fuel particle volume packing fraction in the pebble unit cell,  $r$  is the radius of the TRISO fuel particle.

The change of the CLS method is the accuracy related to the boundary effect (Murata et al., 1996), which is unavoidable when the CLS method is used in a finite stochastic media system (Liang and Ji, 2011). The boundary effect results from not allowing the overlap of the sampled fuel kernel with the system boundary. Re-sampling is performed in the CLS if an overlap happens (Murata et al., 1996; Ji and Martin, 2008), that would reduce TRISO Packing Factor (TPF) and finally lead to bring down the accuracy of the CLS method. Three kinds of correction technique has been proposed to improve the accuracy of the CLS method (Murata et al., 1996; Ji and Martin, 2008; Griesheimer, 2010), the latest nonlinear relationship correction technique (Griesheimer, 2010; Liang et al., 2012) is adopted when the TPF is high in this work. The corrected TPF and true TPF has a nonlinear relationship given by Eq. (2) which was derived based on modified Poisson approximation.

$$TPF' = 1 - \frac{R}{r} + \sqrt{\left(\frac{R}{r} - 1\right)^2 + 2 \frac{R}{r} \cdot TPF} \quad (2)$$

where  $TPF'$  is the corrected TRISO packing factor and  $TPF$  is the true

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