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Original Article

# Treatment of non-resonant spatial self-shielding effect of double heterogeneous region

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ABSTRACT

A new approximation method was proposed for treating the non-resonant spatial self-shielding effects of double heterogeneous region such as the double heterogeneous effect of VHTR fuel compact in the thermal energy range and that of BP compact with BISO. The method was developed based on the effective homogenization method and a spherical unit cell model with explicit coated layers and a matrix layer. The self-shielding factor was derived from the relation between the collision probabilities for a double heterogeneous compact and the effective cross section for the homogenized compact. First, the collision probabilities and transmission probabilities for all layers of the spherical model were calculated using conventional collision probability solver. Then, the effective cross section for the homogenized sphere cell representing the homogenized compact was obtained from the transmission probability calculated using the probability density function of a chord length. The verification calculations revealed that the proposed method can predict the self-shielding factor with a maximum error of 2.3% and the double heterogeneous effect with a maximum error of 200 pcm in the typical VHTR problems with various packing fractions and BP compact sizes.


## 1. Introduction

The fuel of Very High Temperature Reactor (VHTR) contains TRi-structural ISOtropic (TRISO) particle fuels randomly dispersed in a graphite matrix. The unique neutronic characteristics of VHTR fuel is the so-called double heterogeneity (DH), which causes considerable complexity for the neutron transport calculation.

The lattice code developed at Korea Atomic Energy Research Institute (KAERI), DeCART (Deterministic Core Analysis based on Ray Tracing) [1] has two options for dealing with the spatial self-shielding effect of a DH region. One is the Sanchez-Pomraning method [2,3], with which the method of characteristics (MOC) can be applied to the explicit DH region of VHTR fuel. However, it needs self-shielded multi-group cross-section library which is prepared through resonance treatment procedure using external codes. The other is the Pin-based pointwise energy Slowing-down Method for Double Heterogeneity (PSM-DH) [4,5], which was developed for improving the inaccuracy and system-dependency of the pre-generated library in the resonance energy range. The method provides an effective homogenized cross section to reflect DH effect in the resonance energy range and the MOC calculation in the option is performed on the homogenized compact region.

The Sanchez-Pomraning method can treat the spatial self-shielding effect for a DH region including resonant and non-resonant nuclide regardless of energy range and the PSM-DH is, however, dedicated to handle the self-shielding effect of a DH region with resonant nuclide in the resonance energy range. Thus, PSM-DH cannot treat the spatial self-shielding effect of a non-resonant DH regions such as a VHTR fuel compact in the thermal energy range and a DH compact composed of non-resonant burnable poison (BP). In our previous work on PSM-DH [5], the DH effect of fuel compact in the thermal energy range was ignored, because the effect was very small in case of the problems composed of only fuel compact. However, it was found that the effect is not negligible in a fuel compact near burnable poison. Furthermore, it is necessary to properly treat the spatial self-shielding effect of a non-resonant BP compact with Bi-structural ISOtropic (BISO) particle used in conventional VHTRs. The spatial self-shielding effect of a BP compact with BISO containing boron in thermal energy range cannot be ignored and should also be treated properly.

Therefore, for reflecting the spatial self-shielding effect of non-resonant DH region while maintaining consistent MOC

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calculation region with the PSM-DH, it is needed to homogenize a DH compact based on the effective homogenization method.

There are some previous studies [6–8] for the effective homogenization method. Originally, Shmakov [6] proposed the effective homogenization method for a particle-dispersed medium model with only two regions, a matrix layer and a spherical fuel particle. The method has the assumptions that the thickness of the matrix is the same with the diameter of the particle sphere and that the first collision probability should be preserved in the medium model. To improve the Shmakov method, Yamamoto [7] proposed more realistic DH compact model. It was assumed that the model has three regions, a double-layered particle and a matrix, and that the thickness of the matrix can be larger than the diameter of the particle. Afterwards, She [8] proposed an effective homogenization method based on a transmission model with multi-layered particle and a matrix. It was assumed that the thickness of the matrix is the same with the diameter of the particle as in the Shmakov method. However, these models need complicated derivation of formula for calculating the collision probability depending on the number of the particle layers and the geometrical shape of the matrix.

In this work, an easily accessible effective homogenization method is proposed to treat the spatial self-shielding factor for a non-resonant DH region such as VHTR fuel compact in the thermal energy range and a BISO BP compact. The method was developed based on a spherical unit cell model with explicit coated layers and a matrix layer, which is consistent MOC calculation region with PSM-DH for the DH resonance treatment. It also adopted the conventional collision probability solution method which has been well defined for general spherical cell model. Then, the performance of the proposed method is examined using VHTR mini block problems with burnable poison. The calculation results are presented in latter part of this paper. It should be noted that this work focuses the spatial self-shielding effect for non-resonant DH region and non-resonance energy range. The treatment of the self-shielding effect of resonant DH region was addressed by the PSM-DH which was described in detail in our previous work [5].

## 2. Methods

Commonly, the effective homogenized cross section method for DH is based on the assumption that first collision probabilities should be preserved. Starting with the rule, the previous studies [6–8] established various models with DH and proposed proper solution methods for them.

In this section, the general definitions and relations for the effective homogenized cross section method are presented first and a spherical unit cell model for the method and its solution method are described.

### 2.1. Review of effective homogenized cross section methods for double heterogeneity

Fig. 1 shows a typical compact unit cell model which consists of

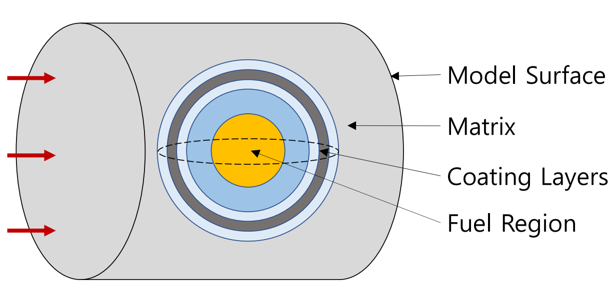



**Fig. 1.** A compact unit model with a matrix region and a multiple layered particle.

a matrix region and a multiple layered particle. It is assumed that the model boundary is conventionally a cylinder [6,8]. The effective homogenized cross section for the compact model can be derived by preserving the total reaction rate as follows:

$$\tilde{\Sigma}\overline{\phi}V = \sum_i \Sigma_i \phi_i V_i, \tag{1}$$

where $i$: sub-region index for matrix and particle layers, $\tilde{\Sigma}$: effective homogenized macroscopic total cross section, $\overline{\phi}$: homogenized flux for a compact, $V$: volume of a compact, $\Sigma_i$: macroscopic total cross section at sub-region $i$, $\phi_i$: flux at sub-region $i$, $V_i$: volume of sub-region $i$.

Eq. (1) can be rewritten with the self-shielding factor and volume fraction as follows:

$$\tilde{\Sigma} = \sum_i \Sigma_i \frac{\phi_i}{\overline{\phi}} \frac{V_i}{V} = \sum_i \Sigma_i f_i p_i, \tag{2}$$

where $f_i = \frac{\phi_i}{\overline{\phi}}$: self-shielding factor for sub-region $i$, $p_i = \frac{V_i}{V}$: volume fraction for sub-region $i$.

Approaching this model within the framework of first collision probability, the relation between the transmission probability and the first collision probability at sub-region is obviously given as:

$$T + \sum_i P_i = 1, \tag{3}$$

where $T$ is transmission probability for a neutron entering through the model boundary to exit through the same boundary without suffering any collisions and $P_i$ is first collision probability at sub-region $i$ for a neutron entering the boundary.

Considering the relation between the collision probability and the reaction rate, the ratio of the collision probability in a sub-region and the collision probability in all sub-region should be equal to the ratio of the effective cross sections in the same regions. This relation can be expressed as follow:

$$\frac{P_i}{\sum_i P_i} = \frac{p_i \tilde{\Sigma}_i}{\tilde{\Sigma}} = \frac{p_i f_i \Sigma_i}{\tilde{\Sigma}}, \tag{4}$$

where $\tilde{\Sigma}_i$ is the effective cross section in the sub-region $i$.

Inserting Eq. (3) to Eq. (4), the self-shielding factor can be derived as follow:

$$f_i = \frac{\tilde{\Sigma}}{p_i \Sigma_i} \frac{P_i}{1 - T}. \tag{5}$$

If $\tilde{\Sigma}$ for the compact model and $P_i$ at all sub-regions are known, the self-shielding factors for all sub-regions can be calculated. Then, the effective macroscopic cross section at sub-region $i$ can be obtained as follow:

$$\tilde{\Sigma}_{xi} = f_i \Sigma_{xi}, \tag{6}$$

where $\tilde{\Sigma}_{xi}$: effective macroscopic cross section for type $x$ at sub-region $i$, $\Sigma_{xi}$: macroscopic cross section for type $x$ at sub-region $i$. Finally, the effective macroscopic cross section with type $x$ for a compact can be readily calculated using $\tilde{\Sigma}_{xi}$.

### 2.2. Spherical compact model with explicit particle layers and its collision probabilities

When the model boundary is a cylinder as shown in Fig. 1, obtaining $P_i$, the collision probabilities for the layers of the particle, needs considerably complicated formula derivations due to the different geometry between the cylindrical matrix and the spherical particle.

In order to consider the explicit particle layers without a mathematical complexity, the spherical unit cell model as shown in Fig. 2 is adopted in this work. The model is identical to the two-step homogenization model widely used in the resonance treatment of DH [5,9]. Also, this model is similar to the that for PSM-DH [4]. However, the unit cell model for the new method just includes multi-layered particle and the matrix layer whereas that of PSM-DH includes an additional layer for the moderator region to reflect the moderation effect in the region. The simplicity of the model for the new method allows a simple derivation of the solution method. The radius of the matrix layer in the model can be easily determined from the particle packing fraction. The collision probabilities for the multi-layered spherical geometry can be obtained using well-defined solution methods such as Kavenoky technique [10].

Applying the technique to the spherical model, the collision probability,$P_{ij}$, can be readily obtained, which is defined as the probability that a neutron born in sub-region $i$ has its first collision at sub-region $j$. Then, the $P_i$ and $T$ can be obtained using the following relations [2]:

$$P_{ei} = 1 - \sum_j P_{ij}, \tag{7}$$

$$P_i = \bar{l} p_i \Sigma_i P_{ei}, \tag{8}$$

$$T = 1 - \sum_i P_i, \tag{9}$$

where $\bar{l}$ is the average chord length through the model boundary and $P_{ei}$ is the escape probability that a neutron born in sub-region $i$ crosses the boundary without undergoing any collision.

To evaluate the self-shielding factor using Eq. (5), the effective homogenized macro total cross-section ($\tilde{\Sigma}$), the remaining unknown in the right-hand side of Eq. (5), should be determined. It should be noted that the transmission probability in the homogenized spherical compact shown in Fig. 3 is determined by the effective homogenized macro total cross-section and also that the transmission probability for the homogeneous sphere model is identical to that for the heterogeneous sphere model according to the preservation rule of the collision probability.

Assuming that a neutron travels the homogenized sphere with a chord, $l$, the transmission probability without any collisions in the path can be defined as follows:

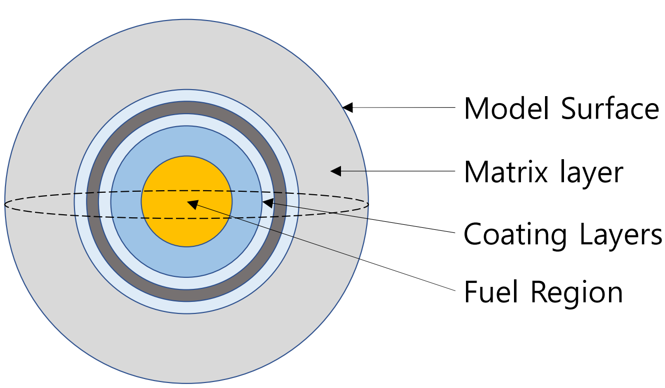



**Fig. 2.** Spherical unit cell model with a matrix layer and a multiple layered particle.

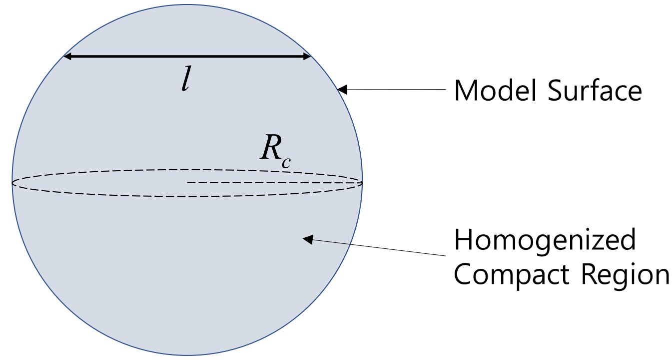



**Fig. 3.** Homogenized spherical compact model.

$$t(l) = e^{-\tilde{\Sigma} l}. \tag{10}$$

In addition, the probability density function for the chord length in the sphere [11] is defined as:

$$f(l) = \frac{l}{2R_c^2}, \tag{11}$$

where $R_c$ is the radius of the homogenized spherical compact unit cell as shown in Fig. 3. It can be calculated using the relation, $R_c = R_T / \sqrt{F3}$, and $R_T$ is the radius of the TRISO particle and $F$ is the packing fraction of the particles in the compact.

From Eqs. (10) and (11), the transmission probability for the whole spherical compact can be expressed as:

$$T = \int_0^{2R_c} t(l) f(l) dl = \int_0^{2R_c} e^{-\tilde{\Sigma} l} \frac{l}{2R_c^2} dl. \tag{12}$$

After integrating Eq. (12), the transmission probability for the homogenized sphere can be obtained as:

$$T = \frac{1}{2R_c^2 \tilde{\Sigma}^2} \left(1 - e^{-2R_c\tilde{\Sigma}}(1 + 2R_c\tilde{\Sigma})\right). \tag{13}$$

However, $\tilde{\Sigma}$ cannot be expressed as an explicit function of $T$ from Eq. (13), because the equation includes exponential and polynomial forms for $\tilde{\Sigma}$. Instead, if applying fourth order Taylor expansion for the exponential function, $e^{-2R_c\tilde{\Sigma}}$, the effective cross section can be approximated as:

$$\tilde{\Sigma} \cong \frac{1}{2R_c}\left(1 - \frac{5}{3\sqrt{3}\,\widehat{T}} + \frac{\widehat{T}}{3\sqrt{9}}\right), \tag{14}$$

where $\widehat{T} - \sqrt{27 - 54T + 2\sqrt{3}\sqrt{92 - 243T + 243T^2}3}$

For verifying the accuracy of the approximation, Eq. (14), the reference solution for Eq. (13) was obtained using the Newton-Raphson method [12] with an error of $1.0 \times 10^{-10}$. It was confirmed that the relative differences between the approximation, Eq. (14), and the reference are less than 0.01% in the three conventional VHTR problems used in section 3. However, the approximation has the limitation originated from the fourth order Taylor expansion of the exponential function, which has an error of less than 0.012% for $R_c\tilde{\Sigma}$ less than 0.2. Direct use of the Newton-Raphson method instead of the approximation can avoid this limitation in application.

Therefore, $\tilde{\Sigma}$ can be calculated using $T$ which is obtained from Eq. (8).

Finally, the self-shielding factor, Eq. (5), can be calculated from Eqs. (8), (9) and (14).

## 3. Verification calculations

For evaluating the performance of the proposed method, three problems were analyzed in this work. Table 1 shows the material information for the three problems. The first case is a single fuel pin problem with the TRISO fuel particles which is taken from OECD/NEA MHTGR-350 benchmark exercise III [13]. Fig. 4 shows the configuration of the DH fuel pin. This problem was intended to evaluate the DH effect of the fuel compact in the thermal energy range. As already described, the DH effect of the resonant nuclides in the resonance energy range was addressed by the PSM-DH and is beyond the scope of this work. The second case, as shown in Fig. 5, is a single mini fuel block which consists of the DH fuel pins of the first case and a BP pin with a homogeneous mixture of 1.6 wt% $B_4C$ and 98.4 wt % graphite. This case was intended to evaluate the DH effect of the fuel compact near BP in the thermal range. The last case is a single mini fuel block with the DH fuel pins and a BP pin with $B_4C$ BISO particles. This case was intended to evaluate the DH effect of the $B_4C$ BISO BP compact itself.

All the calculations were performed using DeCART with ENDF/B-VII.1 cross-section library. In this work, the DH effect for the resonant nuclides in the resonance energy range was calculated using the PSM-DH module [4] of DeCART. On the contrary, the self-shielding factors for the fuel compact in the thermal energy range and those for the BISO BP compact in entire energy range were obtained using the effective homogenization method proposed above.

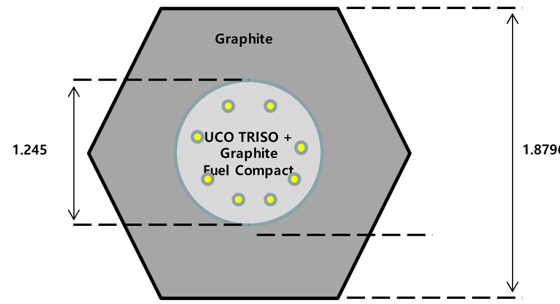
The additional time for this method is negligible because the module calculates the self-shielding factors using the total cross sections for 190 group used in DeCART.

For accuracy comparison, reference self-shielding factors were obtained using the McCARD code [14] based on the Monte Carlo method.

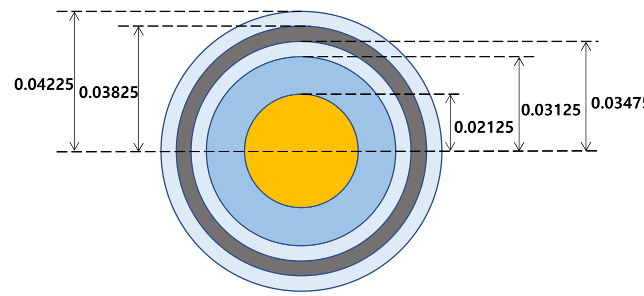
### 3.1. Double heterogeneity effect of TRISO particles in thermal energy range

This case is for evaluating the DH effect of single fuel pin in thermal energy range which was ignored due to relatively small effect in our previous work.

Fig. 6 shows the self-shielding factors of the MHTGR single fuel pin problem with a packing fraction of 35% at 1100K. Because the homogenized spherical model represents the homogenized compact, self-shielding factors for a fuel sub-region in the spherical model corresponds with those for all fuel sub-region in the compact. It is observed that the maximum errors of the self-shielding factor by the effective homogenization method (denoted as Ehom. in Fig. 6) proposed in this work with respect to the reference result by McCARD are about 1.48% for the fuel layer and 0.19% for the matrix layer at the lowest energy, where the reaction rate is very small.




(a) Single fuel pin cell

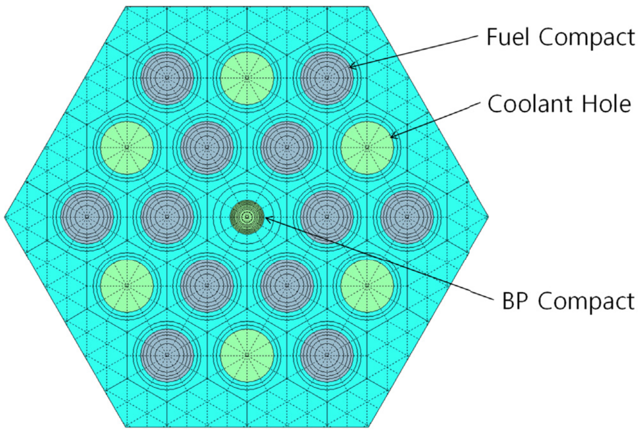



(b) TRISO fuel particle

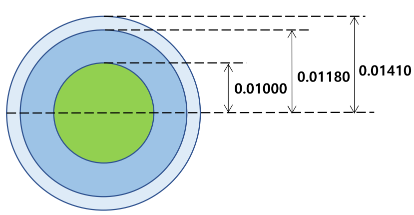
**Fig. 4.** Configuration of the MHTGR single fuel pin cell.

**Table 1**
Material compositions for the MHTGR problems.

| Material | | Nuclide | Number Density (#/barn-cm) |
|---|---|---|---|
| TRISO Fuel Particle | Kernel | U-235 | $3.70 \times 10^{-3}$ |
| | | U-238 | $1.99 \times 10^{-2}$ |
| | | O-16 | $3.55 \times 10^{-2}$ |
| | | Graphite | $1.18 \times 10^{-2}$ |
| | Porous Carbon | Graphite | $5.02 \times 10^{-2}$ |
| | IPyC | Graphite | $9.53 \times 10^{-2}$ |
| | SiC | Si-28 | $4.43 \times 10^{-2}$ |
| | | Si-29 | $2.25 \times 10^{-3}$ |
| | | Si-30 | $1.49 \times 10^{-3}$ |
| | | Graphite | $4.81 \times 10^{-2}$ |
| | OPyC | Graphite | $9.53 \times 10^{-2}$ |
| BISO BP Particle | BP Kernel | B-10 | $2.14 \times 10^{-2}$ |
| | | B-11 | $8.63 \times 10^{-2}$ |
| | | Graphite | $2.76 \times 10^{-2}$ |
| | Porous Carbon | Graphite | $5.02 \times 10^{-2}$ |
| | PyC | Graphite | $9.38 \times 10^{-2}$ |
| Compact Matrix | | Graphite | $8.27 \times 10^{-2}$ |
| Block Graphite | | Graphite | $9.28 \times 10^{-2}$ |




(a) Mini fuel block




(b) BISO BP particle

**Fig. 5.** Configuration of the mini fuel block with a burnable poison pin at the center.

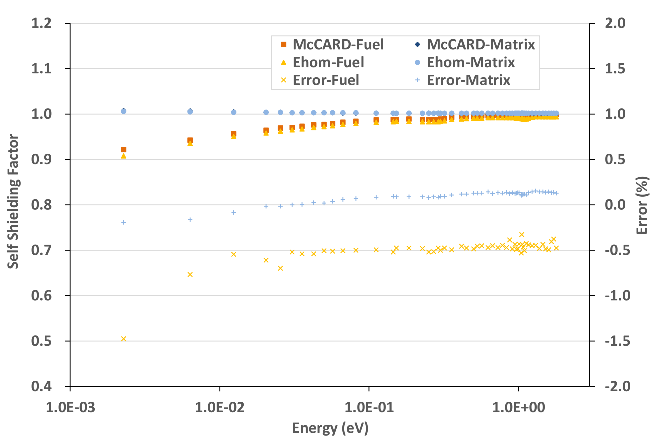



**Fig. 6.** Self-shielding factor for fuel and matrix layers in the single fuel pin problem.

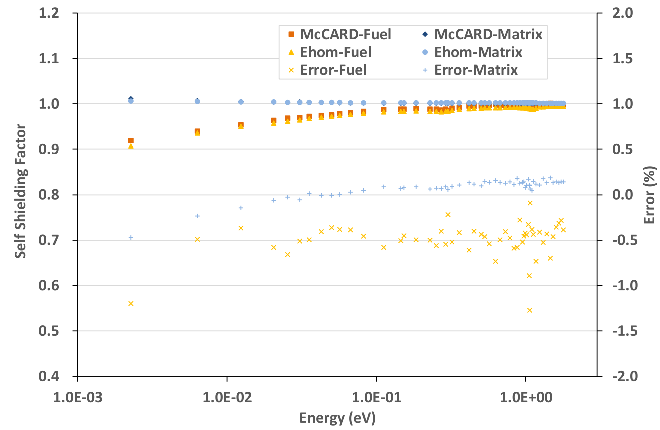



**Fig. 7.** Self-shielding factor for fuel and matrix layers in the mini fuel block with homogeneous BP.

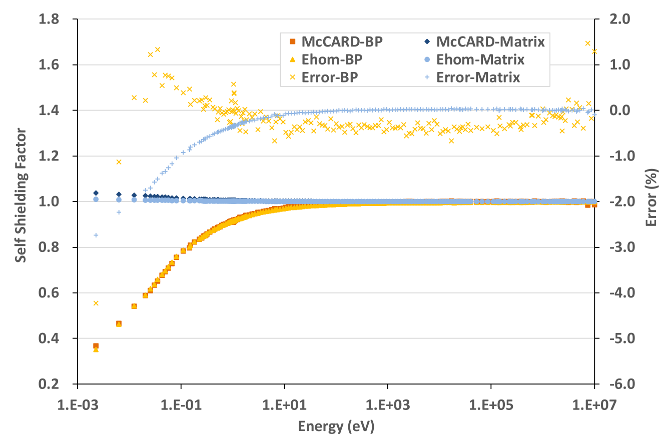



**Fig. 8.** Self-shielding factor for BP and matrix layer of the BISO BP compact in the mini fuel block.

Table 2 compares the $k_{inf}$ and DH effect of the single fuel pin problem with various TRISO packing fractions. It reveals that the DH effect in the thermal range is negligibly small (less than 35 pcm), compared with the DH effect (about 4500 pcm) in the resonance range [4].

### 3.2. Double heterogeneity effect of TRISO particles near burnable poison

The mini fuel block problem with a homogeneous BP pin was used to evaluate the DH effect of fuel compact near BP pin.

Fig. 7 shows the self-shielding factors in the thermal energy

**Table 2**
DH effect of fuel compact with TRISO in thermal energy range.

| TRISO Packing Fraction | Multiplication Factor | | | | | DH Effect [c] in Thermal Energy Range |
|---|---|---|---|---|---|---|
| | McCARD (M) (σ ≈ 14pcm) | DeCART with Hom. [a] (H) | DeCART with Ehom [b] (E) | Δρ(H−M) (pcm) | Δρ(E−M) (pcm) | |
| 15% | 1.50021 | 1.50045 | 1.49968 | 11 | −24 | −34 |
| 25% | 1.35817 | 1.35729 | 1.35690 | −48 | −69 | −21 |
| 35% | 1.26244 | 1.26117 | 1.26093 | −80 | −95 | −15 |
| 40% | 1.22552 | 1.22497 | 1.22477 | −37 | −50 | −13 |

[a] vol weighted homogenization for thermal energy range, PSM-DH treatment for resonance energy range.
[b] Effective homogenization method for thermal energy range, PSM-DH treatment for resonance energy range.
[c] $\rho_{DH} - \rho_{HOM} \approx \frac{1}{k_H} - \frac{1}{k_E}$

**Table 3**
DH effect of TRISO fuel compact facing BP in thermal energy range (BP radius = 0.3 cm).

| TRISO Packing Fraction | Homogeneous BP Radius = 0.3 cm | | | | | |
|---|---|---|---|---|---|---|
| | Multiplication Factor | | | | | DH Effect in Thermal Energy Range |
| | McCARD (M) (σ ≈ 14pcm) | DeCART with Hom. (H) | DeCART with Ehom. (E) | Δρ(H-M) (pcm) | Δρ(E-M) (pcm) | |
| 15% | 1.16237 | 1.17002 | 1.16087 | 563 | −111 | −674 |
| 25% | 1.25841 | 1.26243 | 1.25650 | 253 | −121 | −374 |
| 35% | 1.28098 | 1.28404 | 1.27994 | 186 | −63 | −249 |
| 40% | 1.28186 | 1.28503 | 1.28156 | 192 | −18 | −211 |

**Table 4**
DH effect of TRISO fuel compact facing BP in thermal energy range (BP radius = 0.4 cm).

| TRISO Packing Fraction | Homogeneous BP Radius = 0.4 cm | | | | | |
|---|---|---|---|---|---|---|
| | Multiplication Factor | | | | | DH Effect in Thermal Energy Range |
| | McCARD (M) (σ ≈ 14pcm) | DeCART with Hom. (H) | DeCART with Ehom. (E) | Δρ(H-M) (pcm) | Δρ(E-M) (pcm) | |
| 15% | 0.96673 | 0.97510 | 0.96528 | 888 | −155 | −1043 |
| 25% | 1.10258 | 1.10795 | 1.10095 | 440 | −134 | −574 |
| 35% | 1.15557 | 1.15977 | 1.15468 | 313 | −67 | −380 |
| 40% | 1.16855 | 1.17248 | 1.16809 | 287 | −34 | −321 |

**Table 5**
DH effect for BISO BP compact with a radius of 0.3 cm

| BISO Packing Fraction | Double Het. BP Compact Radius = 0.3 cm | | | | | |
|---|---|---|---|---|---|---|
| | Multiplication Factor | | | Double Het. Effect for BP Compact | | |
| | McCARD (M) (σ ≈ 14pcm) | DeCART with Ehom. (E) | Δρ(E-M) (pcm) | McCARD (σ ≈ 14pcm) (pcm) | DeCART with Ehom. (pcm) | Error (pcm) |
| 7% | 1.24209 | 1.24077 | −132 | 2511 | 2483 | −28 |
| 10% | 1.17180 | 1.17025 | −155 | 2792 | 2729 | −63 |
| 12% | 1.13387 | 1.13232 | −155 | 2875 | 2790 | −84 |
| 15% | 1.08677 | 1.08519 | −158 | 2911 | 2789 | −122 |

**Table 6**
DH effect for BISO BP compact with a radius of 0.4 cm

| BISO Packing Fraction | Double Het. BP Compact Radius = 0.4 cm | | | | | |
|---|---|---|---|---|---|---|
| | Multiplication Factor | | | Double Het. Effect for BP Compact | | |
| | McCARD (M) (σ ≈ 14pcm) | DeCART with Ehom. (E) | Δρ(E-M) (pcm) | McCARD (σ ≈ 14pcm) (pcm) | DeCART with Ehom. (pcm) | Error (pcm) |
| 7% | 1.10344 | 1.10234 | −110 | 3626 | 3599 | −26 |
| 10% | 1.01924 | 1.01765 | −159 | 3867 | 3767 | −100 |
| 12% | 0.97609 | 0.97447 | −162 | 3867 | 3748 | −118 |
| 15% | 0.92471 | 0.92288 | −183 | 3818 | 3622 | −196 |

range for the fuel compact facing the BP. The packing fraction of TRISO fuel was 35%. It shows that the maximum errors are about 1.27% for the fuel layer and 0.47% for the matrix layer and the trend is similar to the previous single fuel pin problem.

Tables 3 and 4 compare the $k_{inf}$ and DH effect for the fuel block problems with various TRISO packing fractions and two BP pin radii. It is observed that the DH effect of the fuel pin in the thermal range are considerably larger than that in the single fuel pin problem. In addition, it is noted that the reactivity error in case of simple volume weighted homogenization for thermal energy region can be over 800 pcm. The difference of the DH effect between fuel compact only and fuel compact near BP is originated from the difference of the thermal utilization caused by the self-shielding effect in the thermal range [15]. Thus, it is clear that the DH effects in thermal range for fuel block with homogeneous BP must be taken into consideration and the effective homogenization method proposed in this work can reduce the reactivity error to a value of under 200 pcm.

### 3.3. *Double heterogeneity effect of BISO particles with burnable poison material*

The configuration of the mini fuel block in Fig. 5 was also used in this calculation to evaluate the DH effect of the BP with BISO particles. The homogeneous BP pin at the center of the block was replaced with a BP compact which consists of $B_4C$ BISO particles and a graphite matrix.

Fig. 8 presents the self-shielding factor for the central BP compact by McCARD and DeCART with the proposed method. The packing fractions for the TRISO fuel and the BISO BP were 35% and 10%, respectively. It reveals that the maximum errors are about 1.46% for the BP layer and 2.24% for the matrix layer except the minimum energy point in the range from 1E-3eV to 1E+7eV.

Tables 5 and 6 compare the $k_{inf}$ and DH effect for the mini fuel block problems with various BISO packing fractions and two compact radii. The DH effect by each code was obtained from the two calculations with a DH BP pin and with a homogenized BP pin by each code.

They show that the DH effects are about 2800 pcm for a radius of 0.3 cm and about 3800 pcm for a radius of 0.4 cm, respectively. In addition, it is observed that the error of the DeCART result with respect to the reference McCARD result in the multiplication factor and DH effect are less than 200 pcm, respectively. The DH effect for BISO compact is large and positive while the DH effect of fuel compact is small and negative. For DH BISO compact, compared to the homogeneous case, the absorption reaction rate is reduced due to the self-shielding effect, which results in a large positive DH effect. In contrast, in case of fuel compact, both the capture and fission reaction rates in thermal energy range are reduced due to the self-shielding effect, and a small positive DH effect or a small negative DH effect is possible depending on the reduction of the two reactions.

## 4. Conclusions

In this work, for reflecting the DH effect of fuel compact in the thermal energy range and that of BP compact with BISO, a new approximation method to evaluate the spatial self-shielding factor was proposed and verification calculations were performed with conventional VHTR problems. The method was developed based on the effective homogenization method and a spherical unit cell model with explicit coated layers and a matrix layer. It has consistent MOC calculation region with PSM-DH for the DH resonance treatment.

The self-shielding factor can be derived from the relation between the collision probabilities for a DH compact and the effective cross section for the homogenized compact. First, the collision probabilities and transmission probabilities for all layers of the spherical unit cell representing a DH compact should be calculated using conventional collision probability solver. Then, the effective cross section for the homogenized sphere cell representing the homogenized compact can be obtained from the transmission probability which can be calculated by using the probability density function of a chord length.

The verification calculations revealed that the proposed method gives the self-shielding factor with a maximum error of 2.3% and the DH effect with a maximum error of 200 pcm for various packing fractions and BP compact sizes.

This method was successfully implemented into DeCART for the lattice calculation in VHTR problems. Thus, it is expected that the method can be used for the treatment of non-resonant spatial self-shielding effect of DH region of various type VHTRs in company with PSM-DH for the treatment of resonance shelf-shielding effect of DH region. In the future, this method will be improved so that it can be applied to multiple grain types such as compacts with mixed TRISO and BISO particles.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## References

[1] J.Y. Cho, T.Y. Han, H.J. Park, S.G. Hong, H.C. Lee, Improvement and verification of the DeCART code for HTGR core physics analysis, Nucl. Eng. Technol. 51 (2019) 13–30.
[2] R. Sanchez, G. Pomraning, A statistical analysis of the double heterogeneity problem, Ann. Nucl. Energy 18 (1991) 371–395.
[3] R. Sanchez, E. Masiello, Treatment of the Double Heterogeneity with the Method of Characteristics, Proc. PHYSOR2002, Seoul, Korea, 2002. Oct. 7-10.
[4] S.Y. Choi, D.J. Lee, Resonance treatment using pin-based pointwise energy slowing-down method, J. Comput. Phys. 330 (2017) 134–155.
[5] T.Y. Han, J.Y. Cho, C.K. Jo, H.C. Lee, Extension of pin-based point-wise energy slowing-down method for VHTR Fuel with double heterogeneity, Energies 14 (2021) 2179.
[6] V.M. Shmakov, Effective Cross Sections for Calculations of Criticality of Dispersed Media, Proc. PHYSOR2000, Pittsburgh, PA, USA, 2000. May 7–11.
[7] T. Yamamoto, Extension of effective cross section calculation method for neutron transport calculations in particle-dispersed media, J. Nucl. Sci. Technol. 43 (2006) 77–87.
[8] D. She, An equivalent homogenization method for treating the stochastic media, Nucl. Sci. Eng. 185 (2017) 351–360.
[9] M.L. Williams, Resonance self-shielding methodologies in SCALE 6, Nucl. Technol. 174 (2011) 149–168.
[10] G. Marleau, DRAGON theory manual, Part 1: collision probability calculations, in: *Tech. Rep*. IGE-236 Revision 1, Department de genie mecanique, Ecole Polytechnique de Montreal, 2001.
[11] K.M. Case, Introduction to the theory of neutron diffusion, Los Alamos (1953) 21.
[12] A. Gil, J. Segura, N.M. Temme, Numerical Methods for Special Functions, Society for Industrial and Applied Mathematics. SIAM., 2007.
[13] J. Ortensi, Prismatic Coupled Neutronics/Thermal Fluids Transient Benchmark of the MHTGR-350 MW Core Design: Benchmark Definition, OECD Nuclear Energy Agency, 2013. NEA/NSC/DOC(2013).
[14] H.J. Shim, B.S. Han, J.S. Jung, H.J. Park, C.H. Kim, McCARD, Monte Carlo code for advanced reactor design and analysis, Nucl. Eng. Technol. 44 (2012) 161–176.
[15] Y.H. Kim, Elimination of double-heterogeneity through a reactivity-equivalent physical transformation, Proc. GLOBAL Oct. 9–13 (2005). Tsukuba, Japan.