

## A New Equivalence Theory Method for Doubly Heterogeneous Fuel

Sooyoung Choi, Deokjung Lee\*

Ulsan National Institute of Science and Technology, UNIST-gil 50, Eonyang-eup, Ulju-gun, Ulsan, 689-798, Korea

Mark L. Williams

Oak Ridge National Laboratory, 1 Bethel Valley Rd, Oak Ridge, TN 37830, United States

\*Corresponding author: deokjung@unist.ac.kr

### 1. Introduction

In VHTR and HTR systems, the microsphere fuel grains in the fuel compact represent point absorbers for neutrons in the resonance energy range, combining with the usual fuel compact and spherical fuel grains heterogeneity to yield double heterogeneity for the fuel grains. Special care must be taken into account to analyze doubly heterogeneous fuel in order to accurately predict spatial self-shielding of fuel in the resonance energy range. The unique characteristics cannot be handled easily by conventional computer code.

A new methodology is being developed to treat resonance self-shielding in a doubly heterogeneous system [1]. The method first homogenizes the material in the fuel compact region using an analytical approximation for the disadvantage factor based on equivalence theory [2]. The disadvantage factor accounts for spatial self-shielding of the resonance flux within the fuel grains. The doubly-heterogeneous effects are accounted by using a modified definition of background cross section, which includes geometry parameters and the cross sections of both the fuel grain and fuel compact regions.

For the verification, the new DH methodology was implemented in deterministic transport code TICTOC developed at UNIST which uses equivalence theory for resonance treatment and Method of Characteristics (MOC) for the ray tracing. In previous research [3], this new methodology was verified for several pin cell problems but further verification is required to confirm the validity of the methodology for various situations. Therefore, in this study, 9 cases for unit pin cell problems are designed and the accuracy of the new DH method is compared to the Monte Carlo code, McCARD [4].

### 2. Methodology

The Dancoff factor is defined as the reduction factor of the fuel escape probability compared to that of an isolated fuel lump [6]. The Dancoff factor for fuel grain can be written with a 2-region infinite medium assumption and Wigner's one term approximation as follows:

$$\Gamma_{grain} = (1-c) = \frac{\bar{l}_m \Sigma_m}{1 + \bar{l}_m \Sigma_m} \quad (1)$$

where  $\bar{l}_m$  and  $\Sigma_m$  are mean chord length and macroscopic total cross section of moderator in fuel compact, respectively.  $c$  is the Dancoff correction factor. The escape cross section for fuel grain is expressed by a function of the Dancoff factor as follows:

$$\Sigma_e = \frac{\Gamma_{grain}}{\bar{l}_f}, \quad (2)$$

where  $\bar{l}_f$  is mean chord length of a spherical fuel grain. The escape cross section in Eq. (2) accounts the neutron escape probability from fuel grains to fuel compact. The parameter  $\beta$  in Eq. (3) considers the heterogeneity of fuel grains.

$$\beta = \frac{\Sigma_e V_f}{\Sigma_m V_m}, \quad (3)$$

The flux disadvantage factor considers the spatial self-shielding of the fuel grain in the fuel compact. The flux disadvantage for the fuel grains is defined as follows:

$$d_f = \frac{\phi_f}{\phi_c} = \frac{V_c \phi_f}{V_f \phi_f + V_m \phi_m} = \frac{1}{1 + \omega \sigma_a^{(j)}} \quad (4)$$

where,

$$\omega = \frac{V_m(1-\beta)}{V_c \sigma_b^{(j)}} \quad (5)$$

$V_f$ ,  $V_m$ , and  $V_c$  are volume of fuel grain, moderator, and fuel compact, respectively. The sum of the volumes of fuel grain and moderator is identical with the volume of the fuel compact.  $\sigma_b^{(j)}$  and  $\sigma_a^{(j)}$  are the background cross section and absorption cross section for material  $j$  contained in the fuel grain. With intermediate resonance approximation, the background cross section of material  $j$  in a fuel grain is expressed as follows:

$$\sigma_b^{(j)} = \frac{\lambda \Sigma_p^{fuel} + \Sigma_e}{N^{(j)}} \quad (6)$$

Eq. (1) to (6) are described for the fuel grain in an infinite medium considering first heterogeneity between fuel grains and fuel compact.

The background cross section of the homogenized fuel compact is defined as follows:

$$\tilde{\sigma}_0^{(j)} = \frac{\lambda \tilde{\Sigma}_P^{Fuel} + \Sigma_E}{\tilde{N}^{(j)}}, \quad (7)$$

where  $\tilde{N}^{(j)}$  and  $\tilde{\Sigma}_P^{Fuel}$  are homogenized number density and potential cross section for material  $j$  in the fuel compact, respectively.  $\Sigma_E$  is the escape cross section of the homogenized fuel compact. The background cross section in Eq. (7) considers the second heterogeneity between the homogenized fuel compact and moderator. Similarly with Eq. (2), the escape cross section is corrected by the Dancoff factor for a cylindrical fuel compact. For simplicity, Wigner's one-term approximation is adopted in this description. The disadvantage factor in Eq. (4) modifies the background cross section in Eq. (7) by considering the spatial self-shielding effect in the first heterogeneity. With the disadvantage factor, the "double-het background cross section" can be expressed as follows:

$$\sigma_0^{*(j)} = \frac{\tilde{\sigma}_0^{(j)}}{1 + \omega \tilde{\sigma}_0^{(j)}} \quad (8)$$

Finally, the effective "double-het cross section" for fuel in a double heterogeneous system is expressed as follows:

$$\tilde{\sigma}_{X,g}^{(j)} = \frac{\sigma_{X,g}^{(j)}(\sigma_0^{*(j)})}{1 + \sigma_{a,g}^{(j)}(\sigma_0^{*(j)})}, \quad (9)$$

where,

$$\sigma_{X,g}^{(j)}(\sigma_0^{*(j)}) = \frac{\left\langle \frac{\sigma_X^{(j)}(E)}{\sigma_a^{(j)}(E) + \sigma_0^{*(j)}} \frac{\Phi_\infty}{E} \right\rangle}{\left\langle \frac{1}{\sigma_a^{(j)}(E) + \sigma_0^{*(j)}} \frac{\Phi_\infty}{E} \right\rangle} \quad (10)$$

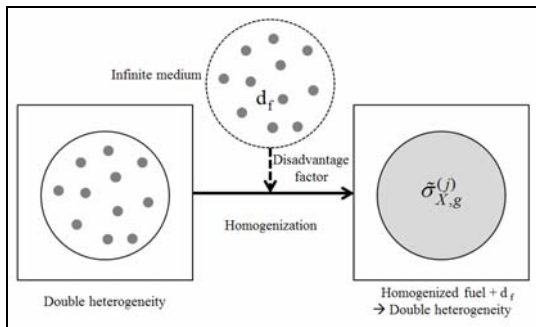


Fig. 1. Scheme of DH methodology

Fig. 1. presents the scheme of the new methodology.

In addition to the above methodology, a DH bell factor was introduced to increase the accuracy. The DH bell factor is multiplied to  $\beta$  as follows:

$$\beta' = a_{DH} \beta = \frac{a_{DH} \Sigma_e V_f}{\Sigma_m V_m} \quad (11)$$

The DH bell factor was determined to minimize the error of  $k_{eff}$  compared to the results of Monte Carlo code.

### 3. Verification

9 test problems were designed for the verification of the doubly-heterogeneous method. The VHTR pincell problem is designed as shown in Fig. 2. Table I and II present the fuel enrichment, grain radius and description of material composition for each test case.

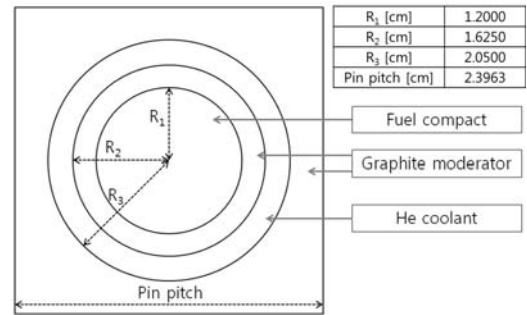


Fig. 2. Model geometry

Table I. Material composition

| Density [g/cc] |                     |            |                    |
|----------------|---------------------|------------|--------------------|
| Fuel grain     | Graphite in compact | He coolant | Graphite moderator |
| 10.41          | 1.7                 | 7.55E-05   | 1.75               |

Table II. Descriptions for model problems

| Case         | Fuel enrichment [wt%] | Grain radius [cm] | Fuel volume fraction[%] |
|--------------|-----------------------|-------------------|-------------------------|
| 1(base case) | 3                     | 0.030             | 9.33%                   |
| 2(base case) | 6                     |                   |                         |
| 3(base case) | 10                    |                   |                         |
| 4            | 3                     | 0.035             | 14.82%                  |
| 5            | 6                     |                   |                         |
| 6            | 10                    |                   |                         |
| 7            | 3                     | 0.040             | 22.13%                  |
| 8            | 6                     |                   |                         |
| 9            | 10                    |                   |                         |

In the Table II, cases 1~3 are base cases which are similar to a conventional VHTR pin-cell. Cases 4~9 have the same number of fuel grains in the compact but have different radii of fuel grains. Material composition is fixed for these cases except enrichment.

The verification tests for 9 pin problems were done and compared with results from McCARD. Tables III

and IV present the verification results for the 9 pin cases described in Table II. Double Heterogeneity (DH) means the eigenvalue test results for the problem. Single Heterogeneity (SH) means the test results for homogenized problems with the fuel volume fraction. The standard deviation of McCARD results are 10~15pcm. DH effect is the difference between DH and SH cases.

For the SH test cases in Table III, TICTOC shows good agreement for  $k_{eff}$  within about 100pcm of errors compared to McCARD. This means that pincell-wise resonance treatment is implemented well. High accuracy of pincell-wise resonance treatment is important for analysis of doubly-heterogeneous systems because the bias in pincell-wise treatment would be included in the final results.

Table III. Eigenvalue calculation results (SH)

| Case    | Single Heterogeneity |         |             |
|---------|----------------------|---------|-------------|
|         | McCARD               | TICTOC  | Error [pcm] |
| 1(base) | 1.20783              | 1.20717 | -66         |
| 2(base) | 1.29929              | 1.29913 | -16         |
| 3(base) | 1.34390              | 1.34404 | 14          |
| 4       | 1.10385              | 1.10310 | -75         |
| 5       | 1.19133              | 1.19104 | -29         |
| 6       | 1.24231              | 1.24267 | 36          |
| 7       | 1.00467              | 1.00413 | -54         |
| 8       | 1.09746              | 1.09727 | -19         |
| 9       | 1.16348              | 1.16386 | 38          |

\*Standard deviations of Monte Carlo results are 10~15 pcm.

In Table IV, the fuel volume fraction and radius of fuel grains are changed as indicated in Table II. The results of TICTOC for these cases have a slight bias when the radius of fuel grains is changed. TICTOC predicts smaller DH effects compared to McCARD for large sizes of fuel grain. The DH effects are slightly underestimated for cases which have large radius of fuel grain. From case 1 to 9, however, the overall results of TICTOC show good agreement in eigenvalue with about 200 pcm of error. Fig. 3 and 4 show the flux distribution calculated by McCARD and TICTOC for Case 1. In case of McCARD, the flux in the fuel compact is merged and normalized. TICTOC shows good results of flux distribution for both single and doubly heterogeneous system

Table IV. Eigenvalue calculation results (DH)

| Case    | Double Heterogeneity |         |             |
|---------|----------------------|---------|-------------|
|         | McCARD               | TICTOC  | Error [pcm] |
| 1(base) | 1.24427              | 1.24430 | 3           |
| 2(base) | 1.33679              | 1.33661 | -18         |
| 3(base) | 1.37959              | 1.37981 | 22          |
| 4       | 1.13247              | 1.13118 | -129        |
| 5       | 1.21980              | 1.21862 | -118        |
| 6       | 1.26920              | 1.26814 | -106        |
| 7       | 1.02591              | 1.02335 | -256        |
| 8       | 1.11773              | 1.11556 | -217        |
| 9       | 1.18220              | 1.18028 | -192        |

\*Standard deviations of Monte Carlo results are 10~15 pcm.

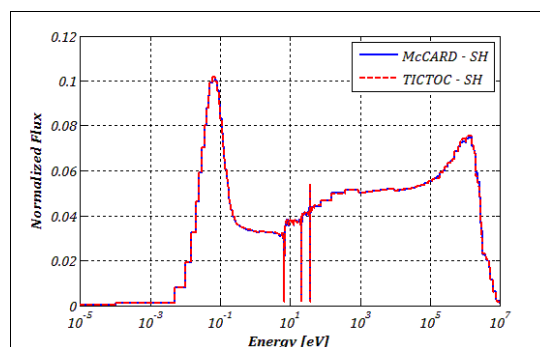


Fig. 3. Flux distribution (Case 1 - SH)

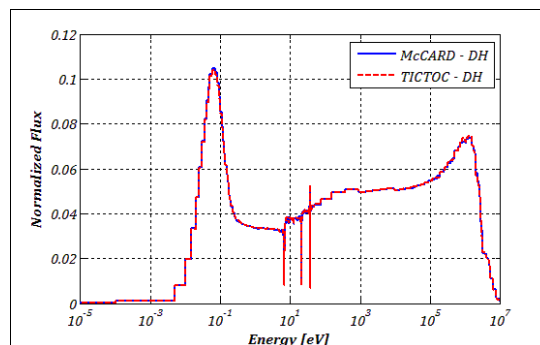


Fig. 4. Flux distribution (Case 1 - DH)

#### 4. Conclusions

The new method for doubly-heterogeneous self-shielding using equivalence theory was summarized and calculation procedure was presented. The new methods use analytical expression for the disadvantage factor therefore additional complicated module is not required. The new method was verified for 9 pin cell models. As a result, TICTOC with the new DH method predicts the eigenvalues within about 200 pcm error compared with Monte Carlo results for the most of problems. It is concluded that the new doubly-heterogeneous self-shielding method was verified because about 200 pcm of error is acceptable in view of resonance treatment for deterministic transport calculation.

#### ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (No. 2013M2B2A9A03051323 and 20120005839).

#### REFERENCES

- [1] M. L. Williams, Methodology for Doubly Heterogeneous Self-shielding Using the Intermediate Resonance Approximation, ORNL Technical Note RNSD-TN-11-008, Oak Ridge National Laboratory, Oak Ridge, TN
- [2] R.J.J. Stamm'ler, and M. J. Abbate, Methods of Steady-State Reactor Physics in Nuclear Design, London: Academic Press, Vol. 111, 1983.

[3] D. Lee and M. L. Williams, Verification of New Doubly-Heterogeneous Self-shielding Method in SCALE, Transactions of the American Nuclear Society 105 , pp. 849 - 850, 2011

[4] Shim, Hyung Jin, et al., McCARD: Monte Carlo code for advanced reactor design and analysis, Nuclear Engineering and Technology, 44.2, pp. 161-176, 2012