A Synergistic Combination of the Deterministic and Monte Carlo Methods for Double-Heterogeneous Problems

Y. Kim[*1], H. J. Shim[2] and T. Noh[3]
[1]*Korea Atomic Energy Research Institute, 150, Deokjin-dong, Yuseong-gu, Daejeon 305-353, Korea*
[2]*Nuclear Engineering Department, Seoul National University, San 56-1, Shinlim-dong, Kwanak-gu, Seoul, Korea*
[3]*Department of Applied Mathematics, Hongik University, 72-1 Sangsu-dong, Mapo-gu, Seoul 121-791, Korea*

Abstract

To resolve the double-heterogeneity (DH) problem resulting from the TRISO fuel of high-temperature gas-cooled reactors (HTGRs), a synergistic combination of a deterministic method and the Monte Carlo method has been proposed. As the deterministic approach, the RPT (Reactivity-equivalent Physical Transformation) method is adopted. In the combined methodology, a reference k-infinite value is obtained by the Monte Carlo method for an initial state of a problem and it is used by the RPT method to transform the original DH problem into a conventional single-heterogeneous one, and the transformed problem is analyzed by the conventional deterministic methods. The combined methodology has been applied to the depletion analysis of typical HTGR fuels including both prismatic block and pebble. The reference solution is obtained using a Monte Carlo code MCCARD and the accuracy of the deterministic-only and the combined methods is evaluated. For the deterministic solution, the DRAGON and HELIOS codes were used. It has been shown that the combined method provides an accurate solution although the deterministic-only solution shows noticeable errors. For the pebble, the two deterministic codes cannot handle the DH problem. Nevertheless, we have shown that the solution of the DRAGON-MCCARD combined approach agrees well with the reference.

KEYWORDS: HTGR, Double-Heterogeneity, RPT, Compact, Pebble, Hybrid Monte Carlo and Deterministic, MCCARD, DRAGON

1. Introduction

High Temperature Gas-cooled Reactors (HTGRs) are under development as a Gen-IV reactor concept in the world. In HTGRs, a particulate fuel with multi-coating layers, which is called TRISO, is employed to achieve a high fuel performance in terms of the burnup and fission gas confinement. Typically, the TRISO fuels are utilized in two fuel types, either a cylindrical compact or a spherical pebble, depending on the reactor type. In both fuel types, TRISO particles

[*] Corresponding author: Tel. 82-42-868-2067, Fax. 82-42-868-4717, E-mail: yhkim@kaeri.re.kr

are randomly dispersed in a graphite matrix with a relatively low volume fraction. This special fuel configuration leads to the so-called double-heterogeneity (DH) problem, which requires special computational methodologies.[1,2] Currently, most conventional lattice codes cannot handle the double-heterogeneity media and only a few computer code systems such as WIMS[3], APOLLO[4], and DRAGON[5] are applicable to the problem, with a limited accuracy.

In order to use the conventional lattice code systems for the TRISO fuels, the double-heterogeneous region needs to be transformed to a homogeneous one. It is known that a simple volume-weighted homogenization (VWH) of a double-heterogeneous fuel zone results in a highly under-estimated reactivity.[6] This is mainly because the resonance self-shielding of the fuel is substantially reduced in a homogeneous case. In the double-heterogeneous case, the resonance self-shielding is quite significant since fuel is lumped into small particles and the fuel volume fraction is relatively low. The self-shielding effect is also enhanced by the small scattering cross section of the graphite moderator in the resonance region. If the VWH is used, the fuel density is usually very low in the homogenized fuel zone and both spatial and resonance self-shielding effects are greatly reduced, resulting in a substantial under-estimation of the reactivity. The self-shielding effect should be appropriately corrected in the homogeneous model.

Recently, a fundamentally different method has been proposed to deal with the double heterogeneity of the HTGR fuels, which is called RPT (Reactivity-equivalent Physical Transformation).[7,8] In the RPT method, a double-heterogeneous problem is transformed into a conventional single-heterogeneous one. Thereby, the conventional methods can be effectively used for the double-heterogeneous fuels. For the RPT method, the reference reactivity of a double-heterogeneous problem should be known a priori.

Based on the RPT method, in this paper, a synergistic combination of the Monte Carlo and deterministic methods are proposed for accurate analysis of double-heterogeneous HTGR fuel elements. In the hybrid method, the reference reactivity for RPT is obtained with a continuous energy Monte Carlo code, MCCARD[9], and the resulting single-heterogeneous problem is analyzed by deterministic codes such as DRAGON and HELIOS[10].

For the validation of the hybrid method, two types of HTGR fuel elements (a prismatic fuel compact and a pebble fuel), are considered. Depletion calculations have been performed for the fuel elements and the hybrid results are compared with those of the MCCARD depletion calculations.

2. Hybrid Monte Carlo and Deterministic Method

Unlike the conventional homogenization methods, in the RPT method, the group constants are not modified, instead the physical configuration of the original problem is geometrically transformed into a single-heterogeneous one such that the transformed problem have the same reactivity as the reference case.

The RPT method is based on two features of the self-shielding effects of VHTR fuel elements: 1) a simple smearing of the double-heterogeneous fuel zone results in a reduced self-shielding and a lower resonance escape probability, 2) increasing the TRISO packing fraction (PF) leads to a higher self-shielding and a higher resonance escape probability. In a HTGR fuel element, either compact or pebble, with a given number of TRISO particles, the neutron multiplication factor is highly dependent on the packing fraction of the TRISO particles. The reactivity increases with

the fuel packing fraction since the mutual shadowing effect is enhanced: the Dancoff factor is higher for more closely packed TRISO particles.

The concept of the RPT method is depicted in Fig. 1 for either a cylindrical or a spherical geometry: first, the fuel particles are moved into a smaller volume to achieve a higher fuel packing fraction and then the inner double-heterogeneous fuel zone is simply homogenized in a volume-weighted sense. When increasing the packing fraction, it is important to reduce the surface area of the new fuel zone. In the RPT method, the only one unknown variable, the radius of the homogeneous fuel zone, is determined such that the corresponding neutron multiplication factor (k) should be equal to the reference value. Hereafter, the reduced fuel radius is called the RPT radius. It is worthwhile to note that the inner radius of the annular fuel is not changed in the RPT transformation.

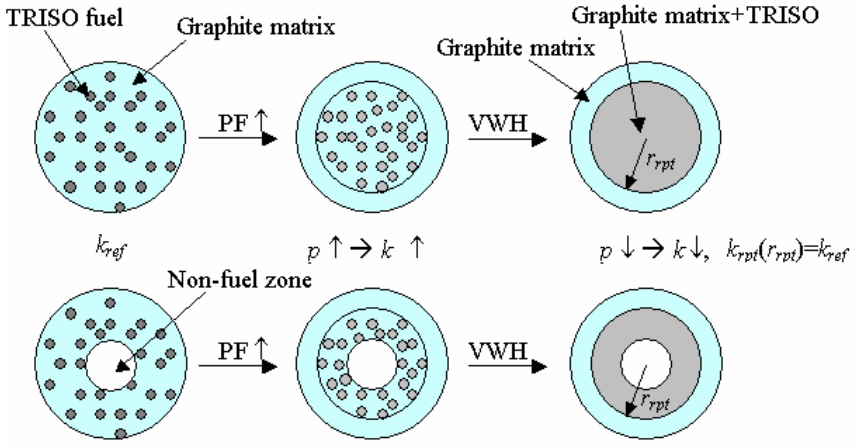

Fig. 1. The RPT concepts (p=resonance escape probability).

It has been shown that the RPT radius is very insensitive to fuel burnup and the fuel temperature. Therefore, a RPT radius for the initial fuel condition can be used over a whole burnup period.[7] In addition, the original double-heterogeneous problem is very similar to the RPT model in terms of the microscopic fuel characteristics.[8]

Only three steps are involved in the hybrid Monte Carlo and deterministic method. Step 1) Calculation of the reference reactivity for an initial fuel composition. Step 2) Determination of the RPT radius. Step 3) Conventional deterministic analysis.

In general, the Monte Carlo method can provide most reliable reference reactivity. However, treatment of the randomness of the TRISO particle is still a pending issue. It is known that the fuel reactivity weakly depends on the random distribution of TRISOs. A simple way is to use an average reactivity of multiple random distributions as the reference reactivity. In this work, we have obtained the reference reactivity for a random distribution, since the effect of the randomness is very small and the objective of this study is only to characterize the hybrid method. However, the multiple sampling scheme should be utilized in the actual design or analysis of the HTGR core.

3. Application of the Hybrid Method to HTGR Fuels

3.1 Prismatic Fuel Compact

In order to apply the hybrid Monte Card and deterministic method to a prismatic fuel, a model problem is considered, which is depicted in Fig. 2. The hexagonal unit cell is derived from the US NGNP design study.[11] The TRISO kernel is a UO_2 fuel with a10% uranium enrichment. In the actual analysis, a helium gap of 0.0125 is also modeled between the fuel compact and graphite block.

The UO_2 kernel diameter of the TRISO particle is 350μm and the fuel density is 10.41 g/cm^3. Typical coating thicknesses are adopted here: buffer=100μm, inner PyC=35μm, SiC=35μm, outer PyC=35μm. Density of each coating layer is as follows: 1.05 g/cm^3 for buffer, 1.90 g/cm^3 for both inner and outer PyC, and 3.18 g/cm^3 for SiC. The fuel packing fraction is 28.916%. The material temperature is assumed to be constant, 300 °K, in this work. Density of the graphite block is 1.74 g/cm^3 and the density of the compact matrix is assumed to be 1.2 g/cm^3.

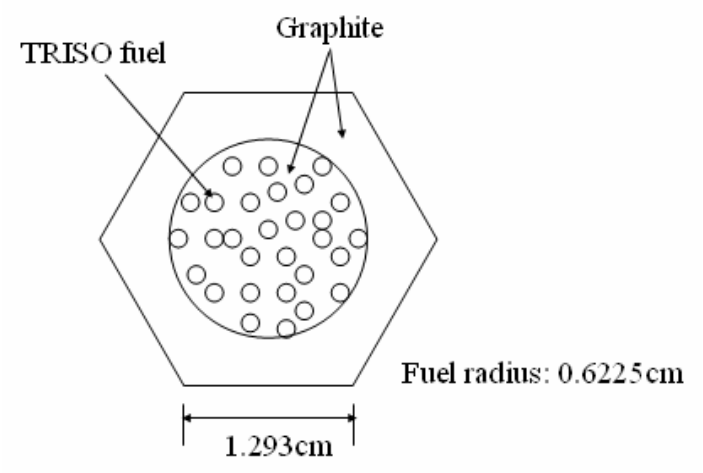

Fig. 2. Model problem for prismatic fuel compact.

In Table I, various results for initial composition of the model problem are provided. In the MCCARD calculation, a total of 3,000 cycles with 60 inactive ones was used and 5,000 neutrons were simulated in each Monte Carlo cycle. In the DRAGON calculation, a 170-group cross section library was used and a 190-group library in HELIOS. All the libraries are based on the ENDF/B-VI. It is shown that the DH effect is large and DRAGON's solution for the original problem shows a noticeable error with respect to the MCCARD double-heterogeneous model.

The RPT radii in Table I were all determined with the reference reactivity from the MCCARD-DH solution. As expected, the RPT radius is slightly different according to the method used in the single-heterogeneous problem. The difference in the RPT radius can be ascribed mainly to the cross section libraries of the codes and partly to the neutron transport methods. The RPT radius by HELIOS is close to the value by MCCARD.

Table II compares microscopic cross sections of U-235 and U-238 for various approaches. It is clear that the MCCARD RPT model well preserves the fuel characteristics of the original

problem. One can see that the DRAGON-DH model shows a relatively large difference in the capture cross section of U-238. It is interesting to see that determination of the RPT radius by DRAGON shows a better agreement than using the RPT radius from MCCARD. This is because the RPT radius by MCCARD is independent of the DRGAGON methodology. In principle, both Monte Carlo and deterministic RPT radii can be used in the hybrid method, if the deterministic method is highly reliable. The RPT radius by HELIOS is very similar to that by MCCARD. This implies that HELIOS provides an accurate solution for the initial state. Nevertheless, it should be noted that the capture cross section of U-238 is slightly improved by determining the RPT radius by HELIOS.

Table I Double heterogeneity effect and the RPT radius of the fuel compact

Model	k-infinite	Error ($\Delta\rho$)*, pcm
MCCARD-DH	1.53624±0.00017	---
MCCARD-VWH	1.47650±0.00018	-2,634
DRAGON-DH	1.54688	+448
DRAGON-VWH	1.47944	-2,499
	RPT radius, cm	k-infinite
MCCARD-RPT	0.4062	1.53635±0.00018
DRAGON-RPT	0.4062	1.53969
	0.4164 [1]	1.53630
HELIOS-RPT	0.4062	1.53495
	0.4021 [2]	1.53629

* Relative to MCCARD-DH, [1]RPT radius by DRAGON, [2]RPT radius by HELIOS

Table II Impacts of the hybrid method on the principle cross sections

Model	U-235, σ_f (barn)	U-235, σ_g (barn)	U-238, σ_f (barn)	U-238, σ_g (barn)
MCCARD-DH	98.4	20.5	0.030	3.73
MCCARD-RPT	98.4	20.5	0.030	3.73
DRAGON-DH	99.0	20.6	0.030	3.62
DRAGON-RPT(M) [1]	98.7	20.6	0.029	3.70
DRAGON-RPT(D) [2]	98.6	20.5	0.029	3.73
HELIOS-RPT(M) [3]	98.6	20.5	0.031	3.77
HELIOS-RPT(H) [4]	98.6	20.5	0.031	3.75

[1]RPT radius by MCCARD, [2]RPT radius by DRAGON, [3]RPT radius by MCCARD, [4]RPT radius by HELIOS

Figures 3 and 4 show results of various depletion calculations. In Fig. 4, the reactivity

difference is relative to the double-heterogeneous MCCARD model. Standard deviation of the MCCARD results is less than 0.00050 for the k-infinite value.

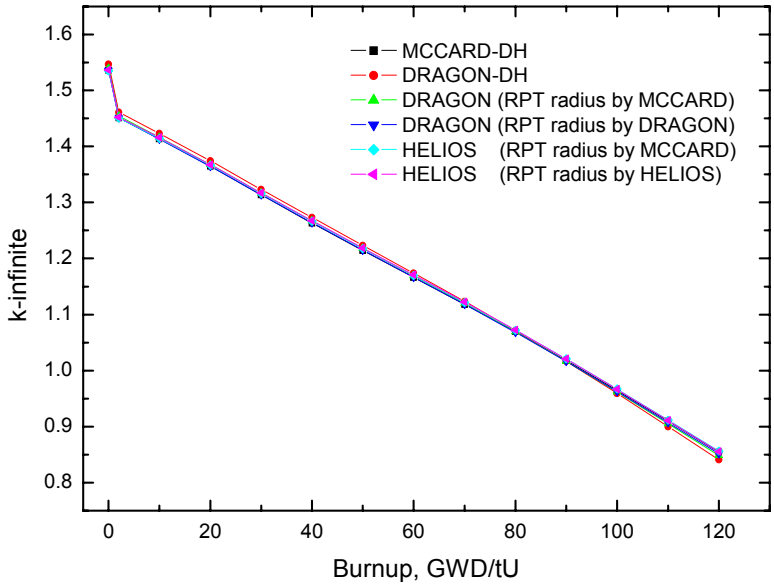

Fig. 3. Reactivity v.s. fuel burnup in the prismatic compact.

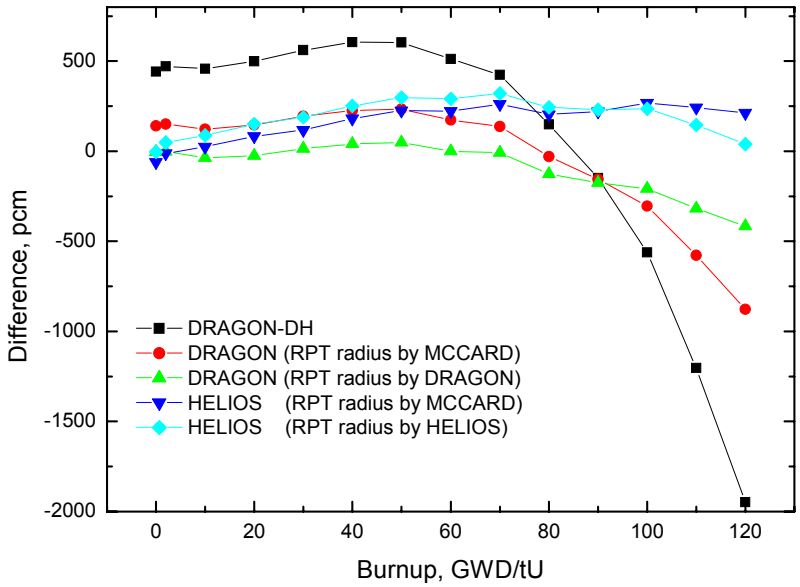

Fig. 4. Reactivity difference between Monte Carlo and various hybrid methods.

From Fig. 4, it is noted that the original DRAGON-DH model shows a relatively big difference from the MCCARD-DH model. In particular, the difference is large in the high burnup range. On the other hand, the hybrid methods agree fairly well with the direct MCCARD calculation over

the whole burnup period. With the MCCARD RPT radius, the DRAGON shows relatively noticeable error when the burnup is high, while the DRAGON RPT radius results in a substantially better agreement. In the case of HELIOS, the two RPT radii produce comparable results since they are already very similar. The HELIOS code turns out to over-estimate the reactivity over the whole burnup, while DRAGON under-estimates the reactivity in the high burnup period. This might be due to the possible differences in the isotope depletion chain in each code and their cross section libraries. Basically, the current cross section libraries of DRAGON and HELIOS is mainly for a PWR application, which is not fully validated for the HTGR fuels. Results of DRAGON and HELIOS depletion should have some difference with respect to the continuous Monte Carlo depletion.

3.2 Pebble Fuel

The hybrid methodology is applied to a single pebble fuel in this section. The currently available DRAGON code cannot handle double heterogeneity of a pebble fuel. However, once the original DH problem is converted to a single-heterogeneous one by the RPT method, the DRAGON code can be efficiently used for the pebble analysis.

In pebble-bed reactors, a rather standardized pebble fuel is used. In the typical pebble fuel, the kernel diameter is usually 500μm and the TRISO packing fraction is ~9% and number of TRISO particles is ~15,000. A Monte Carlo analysis of a single pebble is quite challenging even on the modern parallel computers due to the large number of TRISO particles. In this work, a UO_2 fuel kernel with a 10% uranium enrichment is considered and the number of TRISOs was reduced to 3,600 and the kernel diameter was accordingly changed to keep the typical heavy metal loading per pebble, i.e., 9g. Figure 5 shows configuration of the model pebble problem.

The UO_2 kernel diameter of the TRISO particle is 800μm and the fuel density is 10.41 g/cm^3. Coating thickness and material density of each layer are the same as in the prismatic compact. The material temperature is assumed to be constant, 300 °K in this work. Density of the graphite block and graphite matrix is 1.74 g/cm^3.

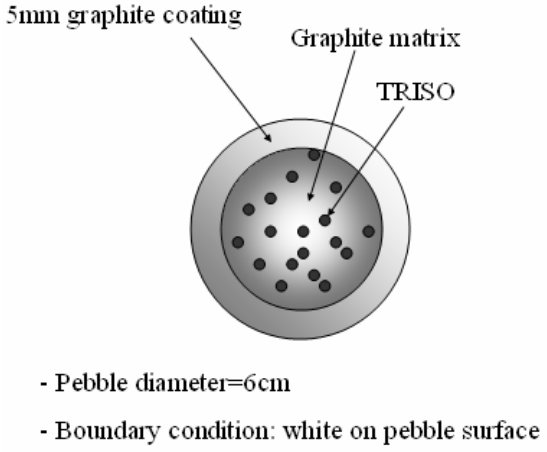

Fig. 5. Model problem for pebble fuel.

In the model problem, the initial fuel loading is ~8.85g and the kernel size (800μm) is much larger than in the usual case. The TRISO packing fraction is 5.2% in the problem. This results in an enhanced DH effect, mainly due to the enhanced self-shielding of the TRISO particle. Table III shows the MCCARD results for the initial state of the pebble. In the MCCARD calculations, a total of 3,000 cycles with 60 inactive ones were used and 5,000 neutrons were simulated in each cycle. The Monte Carlo calculations provide highly reliable solutions with a very small standard deviation less than 0.00020.

From Table III, one can see that the DH effect is huge and the RPT radius is much smaller than the original fuel radius, 2.5cm. The RPT radius corresponds to a packing fraction of 19.61%. The MCCARD-based RPT radius is very similar to the MCCARD-DRAGON RPT radius. This indicates that DRAGON provides an accurate solution for the initial single-heterogeneous problem. Table IV compares the one-group major cross sections of fuel. One can see that the hybrid model is very similar to the original problem in terms of the fuel cross sections. Furthermore, it is observed again that the DRAGON RPT radius slightly improves the U-238 capture reaction as in the prismatic compact case.

Table III Double heterogeneity effect and the RPT radius of the pebble fuel

Model	k-infinite	Error, pcm
Reference (MCCARD)	1.59185±0.00017	---
Homogeneous fuel zone (MCCARD)	1.43666±0.00019	-6,786 pcm
	RPT radius, cm	k-inf
MCCARD	1.6062	1.59164±0.00017
DRAGON	1.6092	1.59183

Table IV Comparison of the principle cross sections

Model	U-235, σ_f (barn)	U-235, σ_g (barn)	U-238, σ_f (barn)	U-238, σ_g (barn)
MCCARD-DH	97.9	20.4	0.031	3.22
MCCARD-RPT	97.7	20.3	0.031	3.21
DRAGON-RPT(M) [1]	97.6	20.3	0.031	3.19
DRAGON-RPT(D) [2]	97.6	20.3	0.031	3.20

[1]RPT radius by MCCARD, [2]RPT radius by DRAGON

For the model pebble problem, depletion calculations were performed by using both MCCARD and DRAGON codes and the results are compared in Fig. 6. In the Monte Carlo depletion for the original problem, TRISO particles are explicitly modeled and they are independently depleted. The standard deviation of the k-infinite values is less than 0.00050 in the MCCARD depletion calculation. The maximum time step was 25 days in the depletion calculations, although the comparison was done every 50 days in Fig. 6.

In Fig. 6, the MCCARD and DRAGON models agrees very well over the whole depletion period. It is observed that the three results almost coincide with each other and the error starts to increase after about 40 GWD/tU. Thus, the difference is mainly due to the plutonium buildup in the fuel.

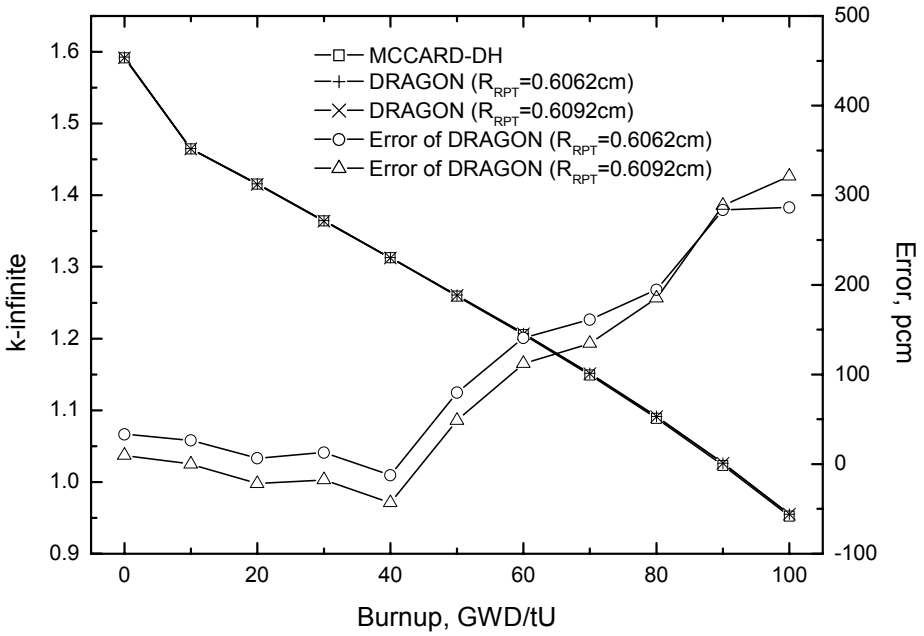

Fig. 6. Hybrid MCCARD-DRAGON depletion calculation for the pebble problem

4. Conclusions

A hybrid Monte Carlo and deterministic method, based on the RPT methodology, has been developed for an accurate and efficient analysis of the HTGR fuels. In the hybrid method, the original double-heterogeneous problem is transformed into a conventional single-heterogeneous one by the RPT method and the conventional problem is analyzed by the deterministic method. For the reference Monte Carlo solution, the MCCARD code has been used, and DRAGON and HELIOS codes are synergistically combined with MCCARD. The hybrid method has been applied to both a prismatic fuel compact and a pebble fuel element. We have shown that the RPT-based hybrid method successfully converts the double-heterogeneous problem into the conventional one and the HTGR fuels can be efficiently handled by the well-developed deterministic methods. If the deterministic method is highly accurate, both the Monte Carlo and the hybrid RPT parameter should provide very similar result. However, a hybrid RPT parameter may result in an improved accuracy, if the Monte Carlo and hybrid RPT radii are significantly different from each other.

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