AN IMPROVED MONTE CARLO METHOD APPLIED TO THE HEAT CONDUCTION ANALYSIS OF A PEBBLE WITH DISPERSED FUEL PARTICLES

JAE HOON SONG and NAM ZIN CHO*
Korea Advanced Institute of Science and Technology
Daejeon, 305-701, Korea
*Corresponding author. E-mail : nzcho@kaist.ac.kr

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Improving over a previous study [1], this paper provides a Monte Carlo method for the heat conduction analysis of problems with complicated geometry (such as a pebble with dispersed fuel particles). The method is based on the theoretical results of asymptotic analysis of neutron transport equation. The improved method uses an appropriate boundary layer correction (with extrapolation thickness) and a scaling factor, rendering the problem more diffusive and thus obtaining a heat conduction solution. Monte Carlo results are obtained for the randomly distributed fuel particles of a pebble, providing realistic temperature distributions (showing the kernel and graphite-matrix temperatures distinctly). The volumetric analytic solution commonly used in the literature is shown to predict lower temperatures than those of the Monte Carlo results provided in this paper.

KEYWORDS : Monte Carlo, Extrapolation Thickness, Heat Conduction, MCNP, Scaling Factor, VHTR

1. INTRODUCTION

There are many deterministic techniques to solve heat transfer problems. However, they do not work well if complex geometry is involved. As the Monte Carlo method deals well with complicated geometries, it can be used to deal with heat transfer problems. Heat conduction is a diffusion process that is analogous to neutron diffusion characterized by no absorption, a fixed source and one speed condition [2,3]. The steady state differential equation of heat conduction for a stationary, isotropic solid is given by [2]

$$\nabla\cdot K(\mathrm{r})\nabla T(\mathrm{r})+q'''(\mathrm{r})=0, \qquad (1)$$

where $K(\mathrm{r})$ is the thermal conductivity and $q'''(\mathrm{r})$ is the internal heat source. On the other hand, the steady state, one-speed neutron diffusion equation under isotropic scattering, no absorption, and a fixed source condition is given by [3]

$$\nabla\cdot\frac{1}{3\Sigma_s}\nabla\phi(\mathrm{r})+S(\mathrm{r})=0, \qquad (2)$$

where ϕ represents the neutron flux, Σ_s is the scattering cross section, and S is the internal neutron source.

The neutron diffusion equation is an approximation to the neutron transport equation; therefore, it may be possible to solve diffusion problems using a transport method with

$$\Sigma_s=\frac{1}{3K(\mathrm{r})} \text{ and } S=q''' \qquad (3)$$

under isotropic scattering and boundary layer correction.

In heat conduction problems, three types of boundary conditions (B.C.s) are generally considered: i) the fixed boundary temperature $T(\mathrm{r}_s)=T_s$ given, ii) the convection heat transfer boundary condition

$$-K\frac{\partial T}{\partial n}\bigg|_{r_s}=h(T_s-T_\infty)$$

with a given value of T_∞, and iii) adiabatic (or reflective) boundary condition

$$\frac{\partial T}{\partial n}\bigg|_{r_s}=0\,.$$

For B.C. ii, the convection medium can be replaced by a conduction medium with a thickness that reflects the heat transfer coefficient h [1]. The given T_s or T_∞ can be rebaselined as $T_s=T_\infty=0$. Therefore, for B.C. i and ii, $T(r_s)=0$ or $T_\infty=0$ is considered without loss of generality.

Based on this idea, a Monte Carlo method for solving heat conduction problems was developed using MCNP [4] as the major engine and applied to the pebble fuel problem in high temperature gas-cooled reactors (HTGRs) [5, 6]. This paper provides a detailed description of the method and its rational with specific application results.

2. IMPROVED MONTE CARLO METHOD FOR HEAT CONDUCTION PROBLEMS

2.1 Method Description

It is known that between the two solutions from transport theory and from diffusion theory, a discrepancy appears near the boundary. Thus, the problem domain is extended using an extrapolated thickness for boundary layer correction, as shown in Fig. 2. This is in contrast to the tangential extrapolation from an internal position in Ref. 1, as shown in Fig. 1. It is then possible to determine the solution at the original problem boundary, through which amount the solution distribution is then translated.

To be more rigorous, we note the following results of asymptotic theory that provides correspondence between the transport equation and diffusion equation (e.g. heat conduction equation). For a heat conduction problem,

$$-\nabla K(r)\nabla T(r) = q'''(r),\quad B.C.:\ T(r_s)=0, \tag{4}$$

we consider a transport equation

$$\Omega\cdot\nabla\psi(r,\Omega)+\beta\Sigma_s(r)\psi(r,\Omega)=\frac{1}{4\pi}\beta\Sigma_s(r)\phi(r)+\frac{1}{\beta}\frac{S(r)}{4\pi}, \tag{5}$$

$B.C.:\ \psi(r_s+d,\Omega)=0\ \ for\ \ n\cdot\Omega<0,\ d=$ extrapolation distance.

The notations are standard in neutron transport theory [7].

The asymptotic ($\beta\rightarrow\infty$) solution of Eq. (5) satisfies the following diffusion equation:

$$-\nabla\frac{1}{3\Sigma_s(r)}\nabla\phi(r)=S(r),\quad B.C.:\ \phi(r_s+d)=0. \tag{6}$$

Thus, we can use

$$\Sigma_s=\frac{1}{3K}$$

and $S=q'''$ in Eq. (5) with a large β and the problem domain extended by d. Then, Eq. (5) is solved by the transport (Monte Carlo) method [7] to obtain $\phi(r)$. The resulting $\phi(r)$ is then translated to provide $T(r)=\phi(r)-\phi(r_s)$ as the solution of Eq. (4).

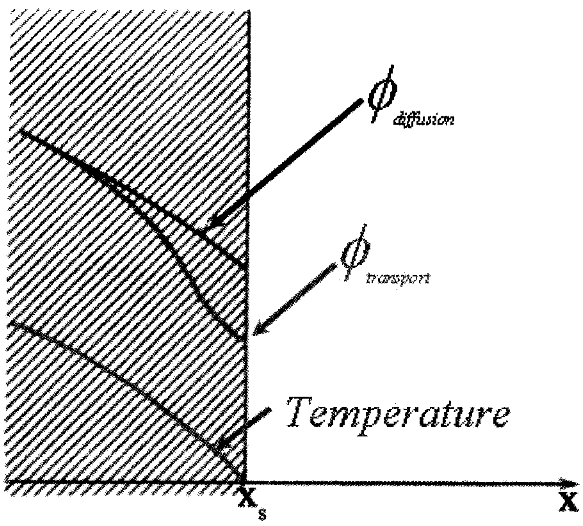

Fig. 1. Boundary Correction with Internal Extrapolation

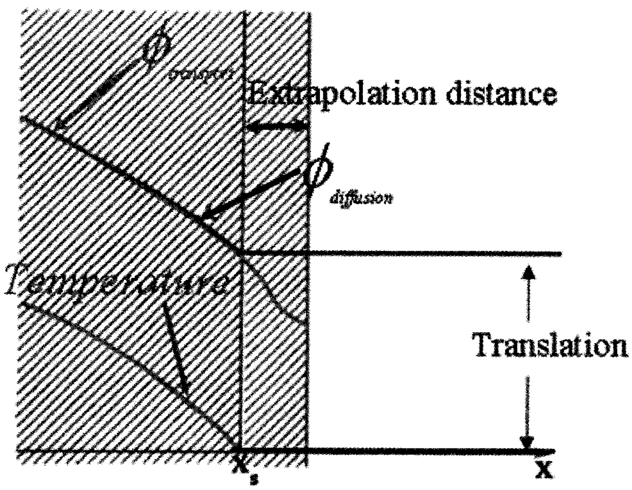

Fig. 2. Boundary Correction with an Extrapolated Layer

Here, $\beta>1$ is a scaling factor rendering the transport phenomena diffusion-like. A large scaling factor plays the additional role of reducing the extrapolation distance to a minimum, since the extrapolation distance is on the order of a mean free path.

To choose a proper value for β, we introduce an adjoint problem to perform sensitivity studies, specific results for a pebble problem provided in Section 3.2.

2.2 Proof of Principles of the Method

In order to confirm or provide proof of principles of the Monte Carlo method described in Section 2.1, we consider a simple heat conduction problem which allows analytic solution. The problem consists of one-dimensional

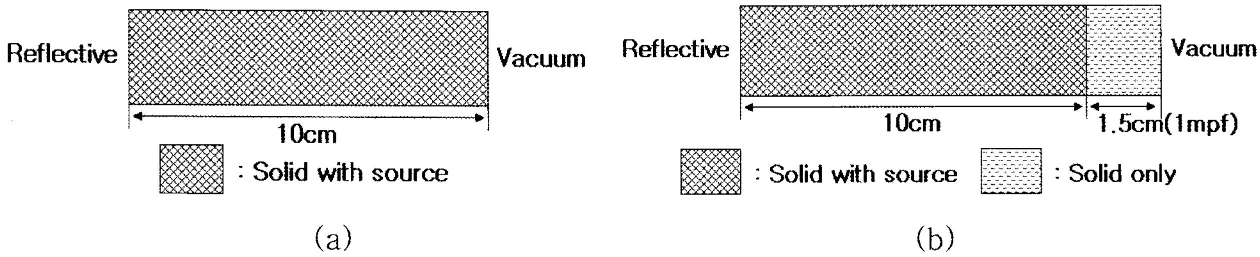

Fig. 3. A One-Dimensional Slab Test Problem

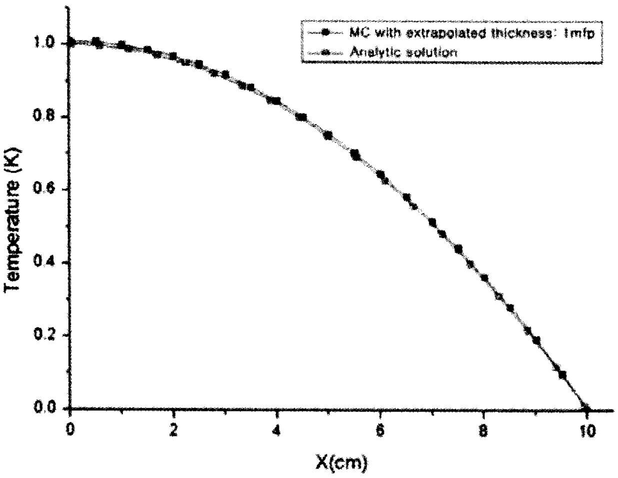

Fig. 4. Monte Carlo Heat Conduction Solution for Figure 3 with Added Layer

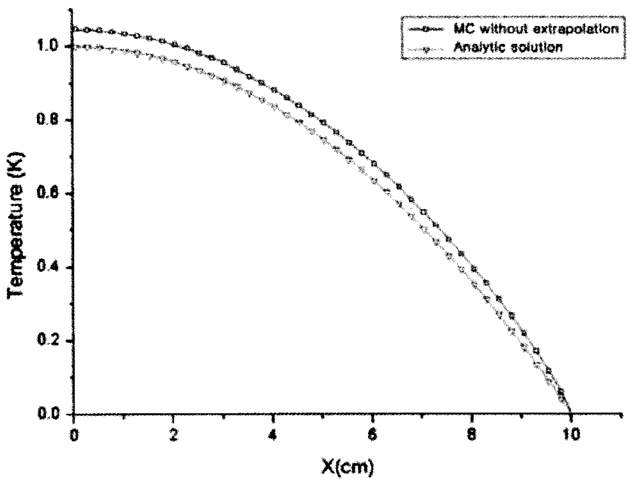

Fig. 5. Monte Carlo Heat Conduction Solution without Added Layer

Table 1. Calculation Conditions for Simple Problem

Thermal Conductivity (*W/cm·K*)	Internal heat source (*W/cm*^{3})	Extrapolation thickness (*mfp)*	Scaling factor
0.5	0.01	1	1

slab geometry, isotropic solid, and uniformly distributed internal heat source under steady state. The left side has reflective boundary condition and the right side has zero temperature boundary condition. Fig. 3(a) shows the original problem and Fig. 3(b) shows the extended problem to be solved by the Monte Carlo method, incorporating the boundary layer correction. Table 1 provides the calculational conditions.

Figs. (4) and (5) show the Monte Carlo method results with and without the extension by extrapolation thickness in comparison with the analytic solution. Note that the result of the Monte Carlo method with boundary layer correction described in Section 2.1 is in excellent agreement with the analytic solution.

3. APPLICATIONS

3.1 Pebble Problem Description

In this paper, the FLS (Fine Lattice Stochastic) model and CLCS (Coarse Lattice with Centered Sphere) model [8] for the random distribution of fuel particles in a pebble are used to obtain the heat conduction solution by the improved method described in Section 2. Details of this process are described in Table 2 and Fig. 6. The power distribution generated in a pebble is assumed uniform within a kernel and across the particle fuels. The pebble is surrounded by helium at 1173K with the convective heat transfer coefficient h=0.1006($W/cm^2{\cdot}K$). A Monte Carlo program HEATON [5] was written to solve heat

Table 2. Problem Description for a Pebble

Material	kernel	buffer	Inner PyC	SiC
Thermal Conductivity (*W/cm·K*)	0.0346	0.0100	0.0400	0.1830
Radius (cm)	0.02510	0.03425	0.03824	0.04177

Material	Outer PyC	Graphite-matrix	Graphite-shell
Thermal Conductivity (*W/cm·K*)	0.0400	0.2500	0.2500
Radius (cm)	0.04576	2.5000	3.0000

Number of triso particles	9394
Power/pebble	1893.95W

Table 3. Results of Fig. 6 Problem

Scaling Factor	Maximum Temp.(K)	Relative Error[a] (%)	Graphite Temp. Near Center(K)	Relative Error[a] (%)	Computing Time(sec)	Translation Temp. (K)
1	1674.21	1.59	1587.33	0.71	534	27.08
10	1556.96	1.14	1533.53	0.34	6,692	2.72
20	1558.54	1.12	1531.67	0.30	20,297	1.36
50	1553.22	1.11	1527.07	0.28	99,454	0.54

[a] One standard deviation in temperature / mean estimate of temperature by Monte Carlo × 100%

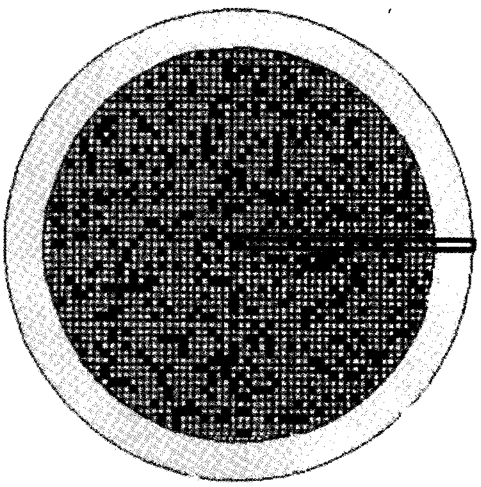

Fig. 6. A Planar View of a Particle Random Distribution for a Pebble Problem with the FLS Model

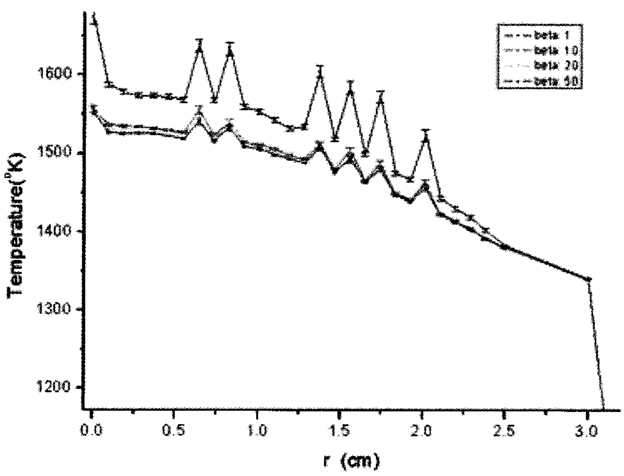

Fig. 7. Results along the Red Line of Fig. 6 vs. the Scaling Factor

conduction problems using the MCNP5 code as the major computational engine.

3.2 Effective Scaling Factor for a Pebble Problem

Thermal conduction solutions for the pebble problem with the data in Table 2 using the Monte Carlo method are shown in Table 3 and Fig. 7. The number of histories used was 10^7. Parallel computation with 60 CPUs (3.2GHz) was used. When the scaling factor increases, the solution of the pebble problem approaches its asymptotic solution (diffusion solution). However, the computational time increases rapidly as the scaling factor increases. In Table

Table 4. Maximum Temperature and Computing Time for Fig. 8

Scaling factor	Maximum Temp. (°K)	Standard deviation(°K)	Computing time (sec)
1	1685.131	0.409	47
20	1558.817	0.308	1,427
50	1553.931	0.304	7,298
80	1553.586	0.304	17,976
100	1552.995	0.303	27,240
120	1552.713	0.303	39,435

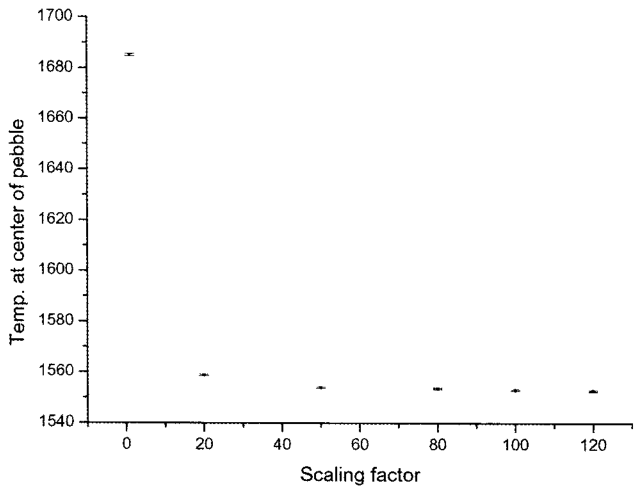

Fig. 8. Center Temperature by the Adjoint Calculation

3 and Fig. 7, it is shown that a scaling factor of 10 used in Ref. 1 is not large enough.

Therefore, it is necessary to determine an effective scaling factor that renders the problem more diffusive. This was done in this work using an adjoint calculation. Using an adjoint calculation, the computing time is reduced as the calculation transports particles backward from the detector region (at the center of the pebble) to the source region. Additionally, it is possible that the changed tally regions used in the adjoint calculation allow effective particle tallies.

In order to confirm the effective scaling factor, the problem with the data of Table 2 and in Fig. 6 was again tested with a smaller number (10^6) of histories compared to the number used in the forward calculation. The results depending on the scaling factor are shown in Fig. 8 and Table 4.

Fig. 8 shows that the center temperature of a fuel pebble approaches its asymptotic solution (diffusion solution) as the scaling factor increases. Therefore, to obtain a diffusion solution, a scaling factor of > 30 (e.g. 50) is required.

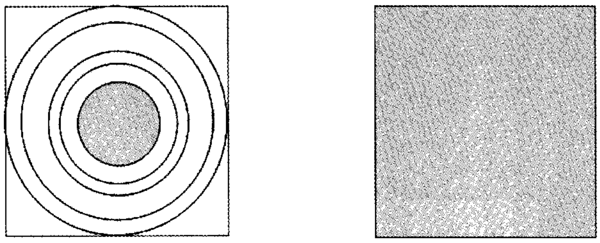
Fig. 9. Tally Regions with and without a Heat Source

4. RESULTS ON PEBBLE PROBLEMS

4.1 Comparisons between the FLS (Fine Lattice Stochastic) Model and Analytic Bound Solutions

In this section, the data of the geometry information and thermal conductivity are identical to those in Table 2. Based on the results in the previous section, temperature distributions were calculated using a scaling factor of 50. Three triso particle configurations obtained by randomly distributed fuels in a pebble were considered (using the FLS model in Ref. 8). In contrast to the runs in Ref. 1 in which a tally region consists of several cubical lattices, the tally regions as shown in Fig. 9 were chosen. If a (fine) lattice has a heat source, the tally is done over the kernel volume. If the lattice consists of only graphite, tally is done over the lattice cubical volume.

Fig. 10 shows the temperature distributions obtained from the Monte Carlo method compared to the two analytic bound solutions superimposed with a particle located at the center of the pebble based on commonly quoted homogenized models [9]. It is important to note that the volumetric analytic solution usually presented in the literature [10] predicts lower temperatures than those of (thus underestimates) the Monte Carlo results. In our Monte Carlo results, the fuel-kernel temperature and graphite-matrix temperature are distinctly calculated. The results are summarized in Table 5.

For a fourth triso particle configuration (Case 4), the

Table 5. Maximum, Average Kernel and Graphite Temperatures from Fig. 10

	Max. Temp. (°K)	Average kernel Temp. (°K)	Average graphite Temp. (°K)
Case 1	1555.07	1497.84	1487.61
Case 2	1553.77	1499.63	1480.43
Case 3	1550.87	1501.89	1489.38
Average	1553.23	1499.79	1485.80

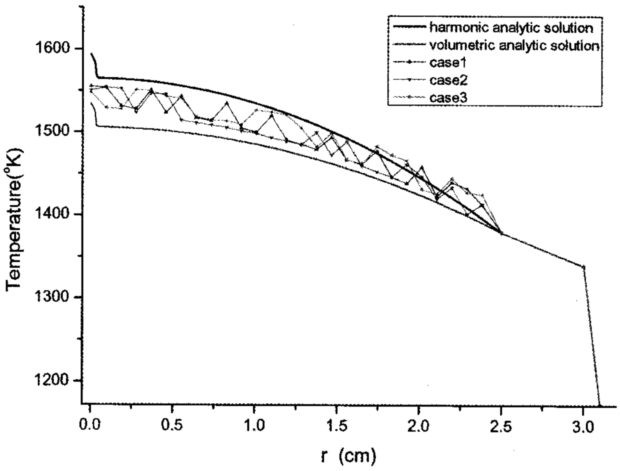

Fig. 10. Temperature Profiles Depending on the Triso Particle Distribution Configuration Compared to Two Homogenized Models

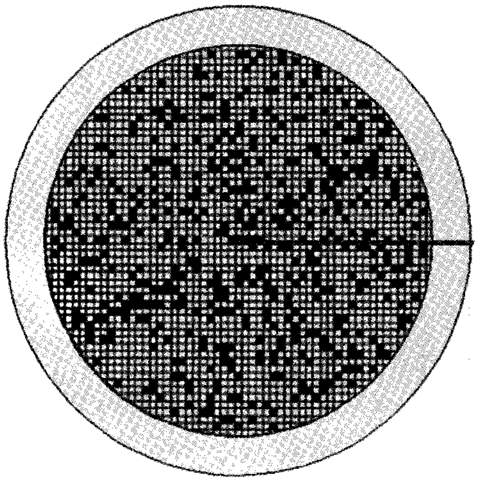

Fig. 12. A Planar View of a Fourth Particle Distribution Configuration with the FLS Model

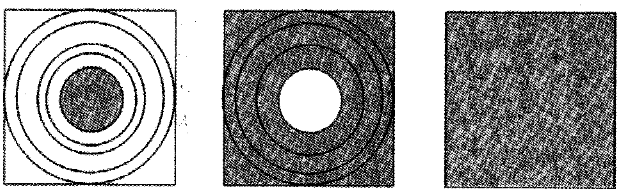

Fig. 11. Tally Regions Depending on the Geometries

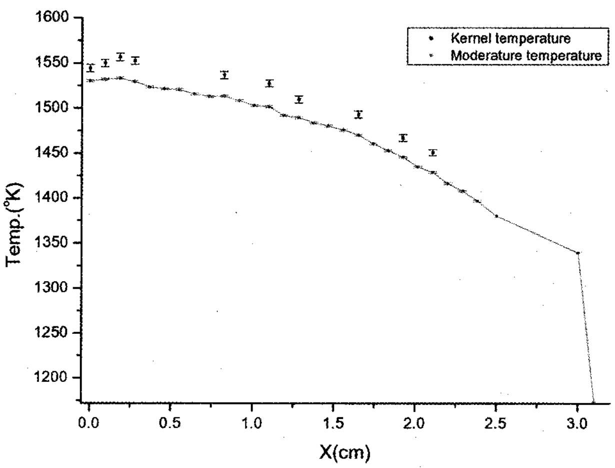

Fig. 13. Temperature Distribution along Red Line for Fig. 12

tally region was further refined as shown in Fig. 11 to provide more accurate graphite-moderator temperature. Essentially, if the lattice has a kernel (heat source), the tally is done over the kernel volume and over the moderator (graphite and layers) volume separately. Otherwise, if the lattice consists of only graphite, the tally is done over the cubical volume.

In this problem, geometry information is identical to those shown in Table 2. The distributed particle configuration is shown in Fig. 12. The kernel and graphite-moderator temperatures are shown in Fig. 13 and Table 6.

The temperature profile on the z=0 plane along red line is shown in Fig. 13 and Table 6. In this FLS model, the maximum fuel temperature appears not at the center point but near the central region, as the fuels are concentrated

Table 6. Results for the Fourth Configuration Shown in Fig. 13

Maximum temperature (°K)	1556.70
Averaged kernel temperature (°K)	1518.88
Averaged moderator temperature (°K)	1484.61
Surface temperature at 2.5cm (°K)	1379.82
Surface temperature at 3.0cm (°K)	1339.65
Computing time	43h 35m 9s

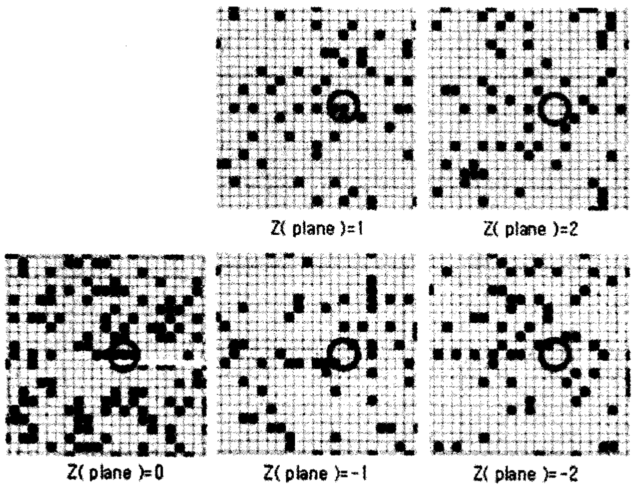

Fig. 14. Cross-sectional Views for Fig. 12

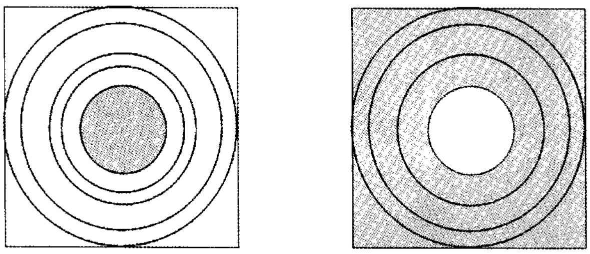

Fig. 15. Tally Regions for the CLCS Model

on the right side of the center point on the z=0 plane, as shown in Fig. 14. Note that the red circle in Fig. 14 denotes particles with the dominant effect of the temperature increase on the z=0 plane.

4.2 CLCS (Coarse Lattice with Centered Sphere) Model

The temperature distribution was obtained again for the CLCS (Coarse Lattice with Centered Sphere) model [8]. In this model, the tally regions used are shown in Fig. 15. The general geometry information is identical to

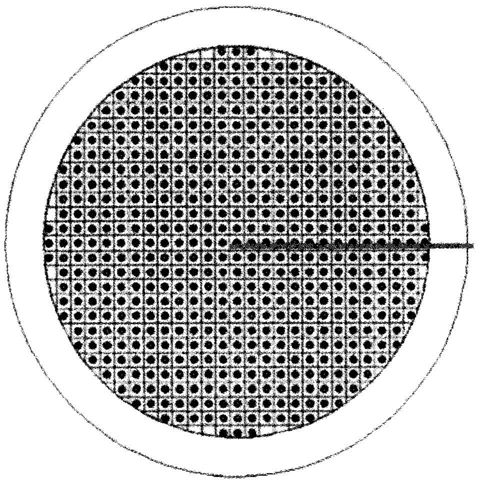

Fig. 16. Fuel Particle Configuration for the CLCS Model

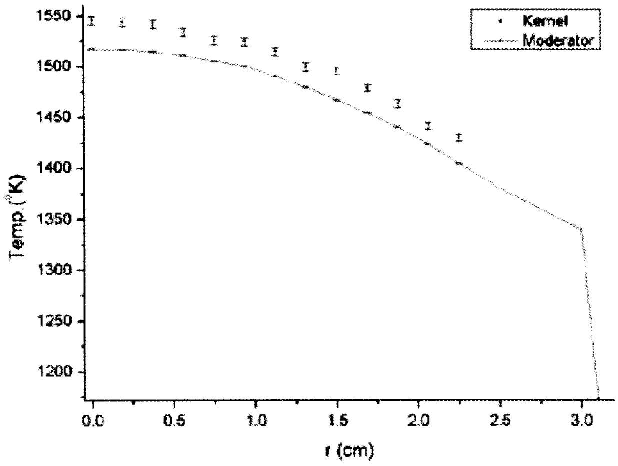

Fig. 17. Results of Cubes along Red Line for Fig. 16

that in Table 2, except that there are 9315 triso particles and each triso particle takes one lattice cube (and vice-versa), as shown in Fig. 16. The resulting temperature distribution for the CLCS model is shown in Fig. 17.

4.3 Comparison with the Previous Model

Fig. 18 shows the MCNP results calculated by the previous model [1]. The previous model has disadvantages in providing the accurate temperature distribution in a pebble. First, the tally region in the previous model consists of collection of several cubes containing fuel kernels and moderator (several layers and graphite) so that it does not provide fuel-kernel and graphite temperatures distinctly, as shown in Fig. 10 or in Fig. 17. Second, even though the model did not use any homogenization method to calculate the temperature distribution, the maximum temperature always appears at the center of the pebble,

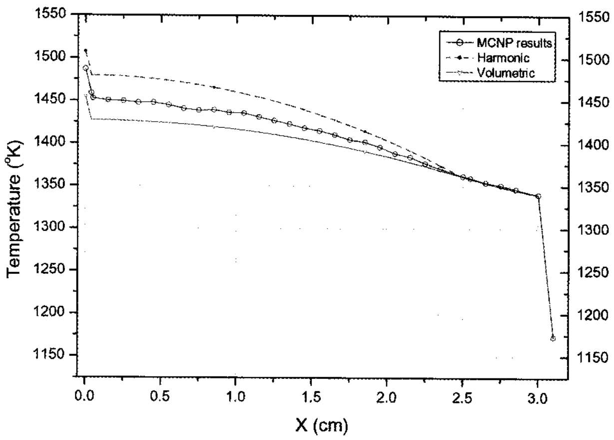

Fig. 18. Temperature Profile of the Previous Model

even with particle distributions generated by the FLS model. This is in contrast to the results in Fig. 13 in this paper. This is due to the fact that in the previous model the tally region is big, consisting of several cubes, resulting in temperatures averaged over larger volumes.

5. CONCLUSIONS

A Monte Carlo method for heat conduction analysis was presented in this paper. This is improvement over the previous study in that i) boundary layer correction is introduced in the extended problem domain, ii) scaling factor is put in perspective with diffusivity of the problem so that the asymptotic theory in transport equation is utilized, iii) proper scaling factor is determined on a more theoretical basis using the adjoint problem, and iv) more refined tally regions are used.

The Monte Carlo method can be used to solve heat conduction problems with complicated geometry (e.g. due to the extreme heterogeneity of a fuel pebble in a VHTR). The HEATON code was written using MCNP as the major engine to solve these types of heat conduction problems. A value of around 50 for a scaling factor is adequate for fuel pebbles in VHTRs. Monte Carlo results for randomly sampled configurations were presented (showing the fuel kernel temperatures and graphite matrix temperatures distinctly). The fuel kernel temperatures can be used for more accurate neutronics evaluations, such as incorporating the Doppler feedback. It was found that the volumetric analytic solution commonly used in the literature predicts lower temperatures than those of the Monte Carlo results provided in this paper. Therefore, it will lead to inaccurate prediction of the fuel temperature under Doppler feedback.

The Monte Carlo method described in this paper enables prediction of the temperature distributions within a complicated structure such as a pebble fuel element, in which thousands of coated fuel particles are randomly distributed in graphite matrix.

As future work, extensions of the method to variable temperature boundary condition problems and to the problem of multiple pebbles should be worthwhile to pursue.

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