MONTE CARLO METHOD EXTENDED TO HEAT TRANSFER PROBLEMS WITH NON-CONSTANT TEMPERATURE AND CONVECTION BOUNDARY CONDITIONS

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The Monte Carlo method for solving heat conduction problems [1-3] is extended for non-constant temperature boundary conditions in this study. The new method can treat problems with any given non-constant boundary temperatures, including heat convection problems with non-constant fluid bulk temperature. A set of problems, particularly the heat transfer problem in a pebble fuel, is analyzed by this new method. In addition, a new method to reduce the statistical errors in kernel fuel regions is introduced when the Monte Carlo method is applied to a pebble fuel.

KEYWORDS : Monte Carlo, Heat Transfer, MCNP, VHTR, Non-Constant Boundary Temperature, Hybrid Method

1. INTRODUCTION

The Monte Carlo method [1-3] that was developed to solve heat conduction problems is "meshless" and thus can treat problems with very complicated geometries. However, the usual numerical methods in heat transfer problems, such as the finite difference or finite element, are based on discretized mesh systems, thus they are inherently limited in the geometry treatment. The Monte Carlo method is based on the observation that heat conduction is a diffusion process whose governing equation is analogous to the neutron diffusion equation under no absorption, no fission and one speed condition, which is a special form of the particle transport equation. The method was applied to a pebble fuel to be used in very high temperature gas-cooled reactors (VHTGRs). Typically, a single pebble houses ~10,000 particle fuels randomly dispersed in graphite–matrix. Each particle fuel is in turn comprised of a fuel kernel and four layers of coatings. Such a level of geometric complexity and material heterogeneity defies the conventional mesh–based computational methods for heat conduction analysis.

Currently, the Monte Carlo method deals only with constant temperature boundary condition [1-3]. This paper extends the method to deal with, i) non-constant temperature boundary condition, ii) convection boundary condition, and, in addition, iii) provides a hybrid method of Monte Carlo and analytic solutions usefully applied to the pebble fuel problem.

2. METHOD DESCRIPTION

2.1 Non-constant Temperature Boundary Condition

The steady state heat conduction equation for a stationary and isotropic solid is given by [4]

$$\nabla \cdot k(\vec{r})\nabla T(\vec{r}) + q'''(\vec{r}) = 0, \tag{1}$$

where $k(\vec{r})$ is the thermal conductivity, $q'''(\vec{r})$ is the internal heat source.

The first kind of the boundary conditions is the prescribed surface temperature:

$$T(\vec{r}_s) = f(\vec{r}_s), \tag{2}$$

where $\vec{r}_s$ is on a boundary surface. Since the current Monte Carlo method can treat only zero temperature boundary condition (or equivalently constant temperature boundary condition), let T be decomposed into T^* and $\tilde{T}$:

$$T(\vec{r}) = T^*(\vec{r}) + \tilde{T}(\vec{r}), \tag{3}$$

where T^* satisfies the zero boundary condition, and $\tilde{T}$ is chosen such that it satisfies the given boundary condition (2). Eq. (1) can then be rewritten as :

$$-\nabla \cdot (k(\vec{r})\nabla T) = -\nabla \cdot (k(\vec{r})\nabla(T^* + \tilde{T})) = q'''(\vec{r}), \tag{4a}$$

or

$$-\nabla \cdot (k(\vec{r})\nabla T^*) = q^{*'''}(\vec{r}), \tag{4b}$$

where the new source $q^{*'''}(\vec{r})$ is defined by

$$q^{*'''}(\vec{r}) = \nabla \cdot k(\vec{r})\nabla \tilde{T}(\vec{r}) + q'''(\vec{r}). \tag{4c}$$

Eq. (4b) is to be solved for T^* by the Monte Carlo method [1-3]. The Monte Carlo method cannot deal easily with the gradient term, $\nabla\cdot(k(\vec{r})\nabla\tilde{T}(\vec{r}))$, in Eq. (4c) when the boundary condition temperature is not a constant and $k(\vec{r})$ is not smooth enough. In order to evaluate the new source term as simply as possible, let $\tilde{T}$ be zero in internally complicated thermal conductivity region as shown in Figure 1. In addition, $\tilde{T}$ and $\nabla\tilde{T}$ must be continuous in the whole problem domain to render the $\nabla\cdot(k(\vec{r})\ \nabla\tilde{T}(\vec{r}))$ term treatable.

In this work, the following $\tilde{T}$ is chosen for a three-dimensional spherical model :

$$\tilde{T} = U(r) f(r_s, \theta, \varphi)\frac{(r - r_0)^2}{(r_s - r_0)^2},$$
$$U(r) = \begin{cases} 1, & r_s - r_0 < r < r_s, \\ 0, & otherwise \end{cases}, \tag{5}$$

where $f(r_s,\theta,\varphi)$ is the given boundary condition (2), θ and φ indicate polar and azimuthal angle, respectively. r_s is radius to the boundary surface, and there may be internally complicated thermal conductivity region inside r_0.

2.2 Convection Boundary Condition

A convection boundary condition is usually given by

$$k_1 \frac{\partial T(\vec{r}_s)}{\partial n} = h(T_b - T(\vec{r}_s)), \tag{6}$$

where k_1 is the thermal conductivity of medium 1 (solid),

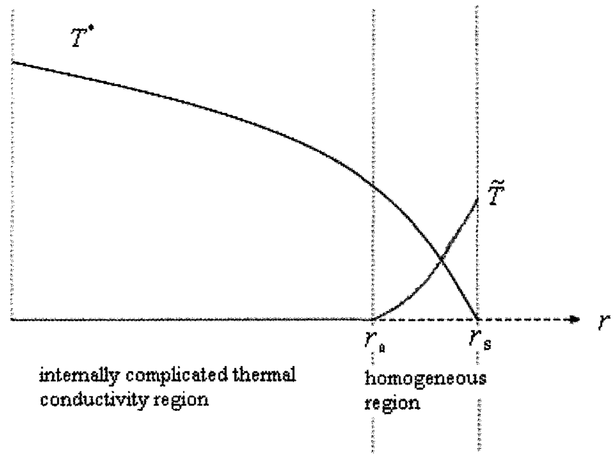

Fig. 1. Solution Decomposition $T=T^*+\tilde{T}$

Table 1. k_2 for Several Geometries

Geometry	k_2
Slab	$h(x_b - x_s)$
Cylinder	$hr_s \ln(\frac{r_b}{r_s})$
Sphere	$h(r_b - r_s)\left(\frac{r_s}{r_b}\right)$

h and T_b are the convective heat transfer coefficient and the bulk temperature of the convective medium, respectively. This condition can be equivalently transformed to a given temperature (T_b) boundary condition of a related problem, in which the convective medium is replaced by a conduction medium with thermal conductivity

$$k_2 = h\Delta n(\frac{r_s}{r_b}), \tag{7}$$

where Δn is additional thickness beyond $r_s(\Delta n = r_b - r_s)$ in a spherical geometry. Here, r_b is the radius where T_b occurs. k_2 involves a geometry factor and k_2's for several geometries are shown in Table 1 (see Appendix for the derivation). There is no approximation in the k_2 expressions for given h if there is no heat source in the fluid. The transformed problem can then be solved by the Monte Carlo method in Section 2.1 with replacement of r_0 by r_s and r_s by r_b.

2.3 Hybrid Method

When the Monte Carlo method is applied to a pebble fuel problem, the fuel kernel temperatures have large standard deviations (or would require exorbitant computer

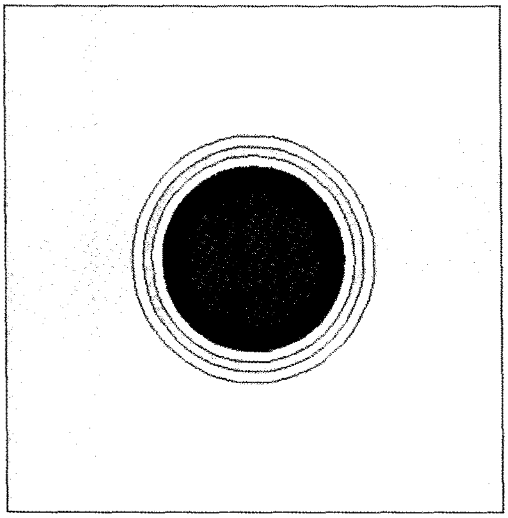

Fig. 2. A Fuel Particle in Graphite-matrix

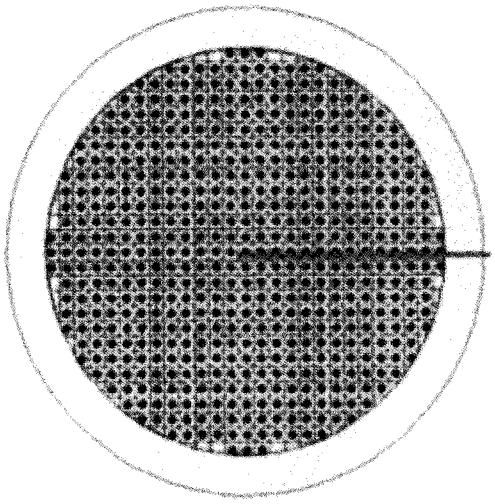

Fig. 3. CLCS Distribution

Table 2. Problem Description

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)	0.04000	0.2500	0.2500	
Radius (cm)	0.04576	2.5000	3.000	
Number of triso particles	9315			
Power/pebble	1893.94 W			

time) due to their very small tally volumes. Typically, one standard deviation in the fuel kernel temperatures is around 5 K, while that of graphite-matrix regions is around 0.6 K. We note that a particle fuel consists of several spherical shell layers with a fuel kernel at the center (see Figure 2), in which geometry analytical solutions to the heat conduction equation are available. Therefore, we propose a hybrid method, in which the graphite-matrix temperature is calculated by the Monte Carlo method but the fuel kernel and layers temperatures are calculated analytically using the temperature of the graphite-matrix surrounding the fuel particle as the boundary condition. This is justified, because the thermal conductivity of the graphite-matrix is high and the radius of a typical fuel particle is small.

3. APPLICATIONS

The method is applied to a pebble fuel with Coarse Lattice with Centered Sphere (CLCS) distribution of fuel particles [5]. The description of a pebble fuel is shown in Figure 3 and Table 2. The pebble fuel is surrounded by helium at given bulk temperature with convective heat transfer coefficient $h=0.1006(W/cm^2{\cdot}K)$. To apply the method, HEATON [6] based on MCNP was slightly modified. The number of histories used in the Monte Carlo calculation was 10^7.

3.1 Results of Non-constant Bulk Temperature Problems

Test Problem 1 is defined by the following bulk temperature of the helium coolant :

$$1173+10(1+\cos\theta)\ K, \tag{8a}$$

where θ is the polar angle, or equivalently

$$1173+10\left(1+\frac{z}{\sqrt{x^2+y^2+z^2}}\right), \tag{8b}$$

where

$$x^2 + y^2 + z^2 = r_b^2,$$

with r_b=3.1, x, y and z in centimeters.

The results are shown in Figures 4, 5, and 6.

Test Problem 2 is defined by the following bulk temperature of the helium coolant :

$$1173 + 10 + (x + y + z)\,K, \tag{9}$$

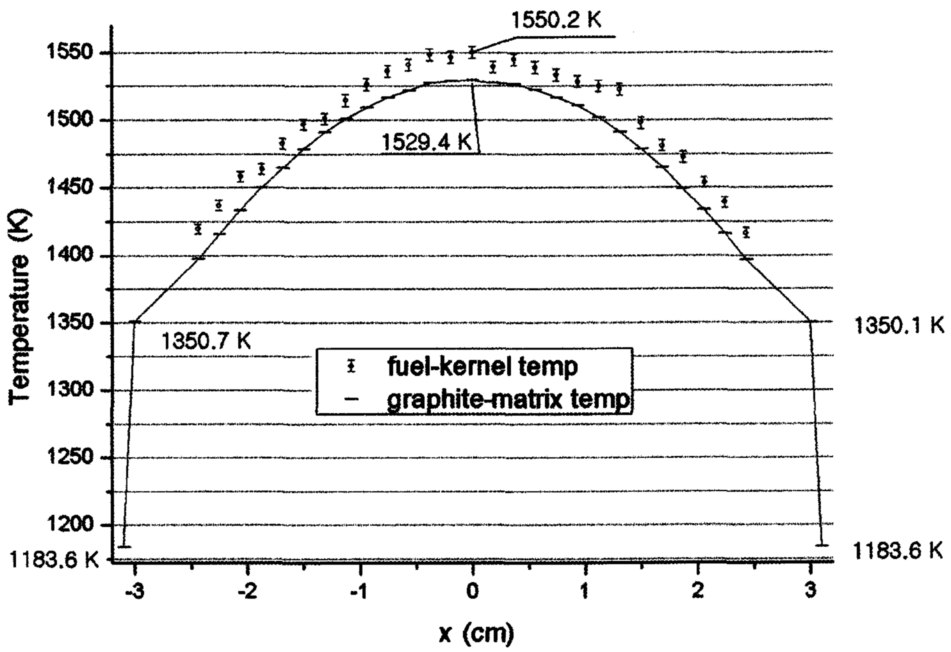

Fig. 4. Temperature Distribution along x-direction with y=z=0 in Test Problem 1

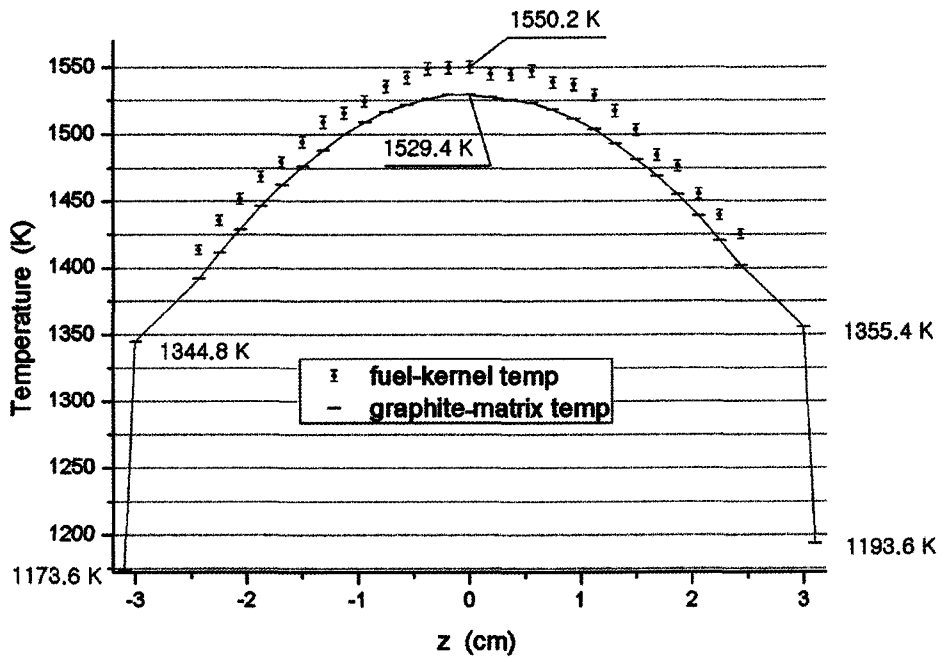

Fig. 5. Temperature Distribution along z-direction with x=y=0 in Test Problem 1

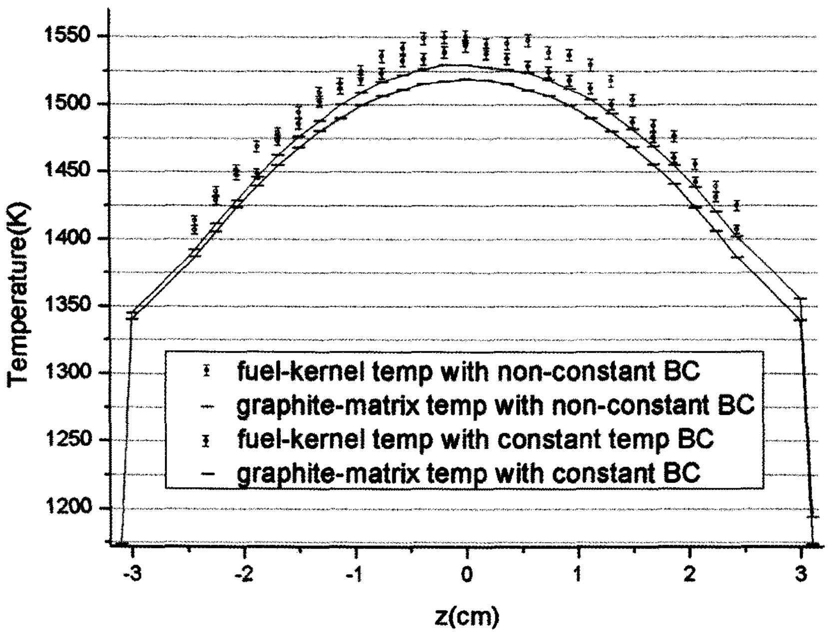

Fig. 6. Comparison of Test Problem 1 and a Problem with Constant Helium Bulk Temperature (1173 K)

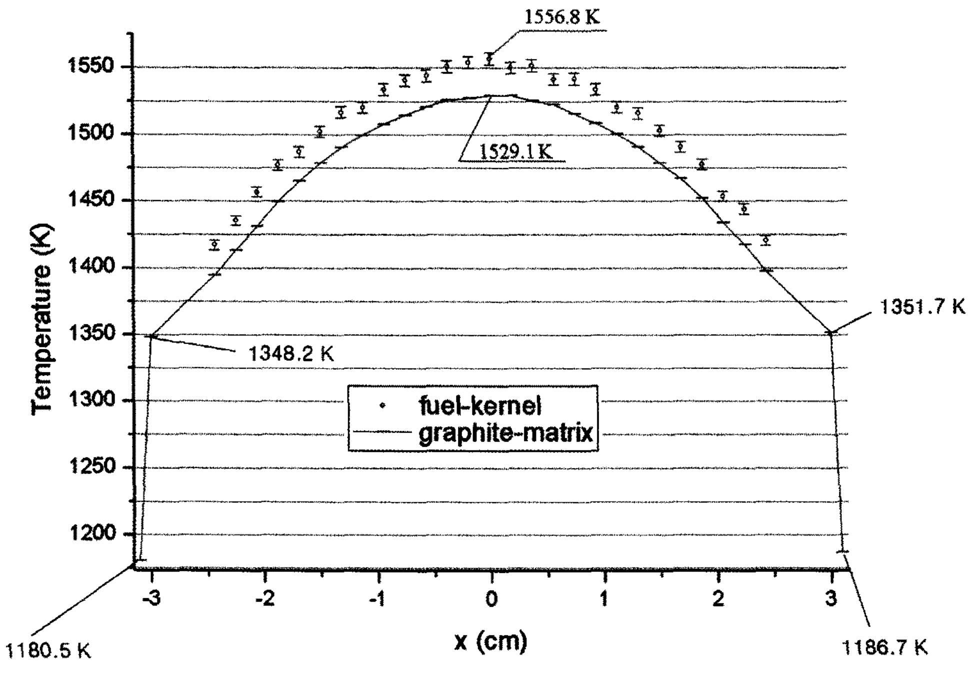

Fig. 7. Temperature Distribution along x-direction with y=z=0 in Test Problem 2

where

$$x^2 + y^2 + z^2 = r_b^2,$$

with r_b=3.1, x, y and z in centimeters.

The results are shown in Figures 7, 8, and 9.

3.2 Results of Hybrid Method

Test Problem 3 is defined by constant bulk temperature of the helium coolant at 1173K. Recall that the particle consists of fuel kernel, buffer, inner PyC, SiC and outer PyC layers. Material properties of a triso particle are shown in Table 2. The fuel kernel generates heat at the

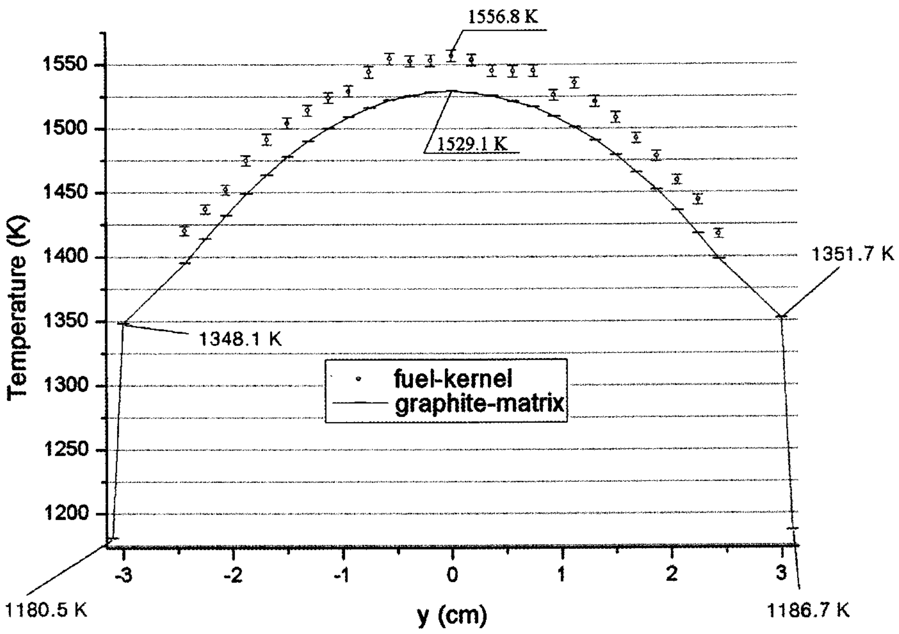

Fig. 8. Temperature Distribution along z-direction with x=y=0 in Test Problem 2

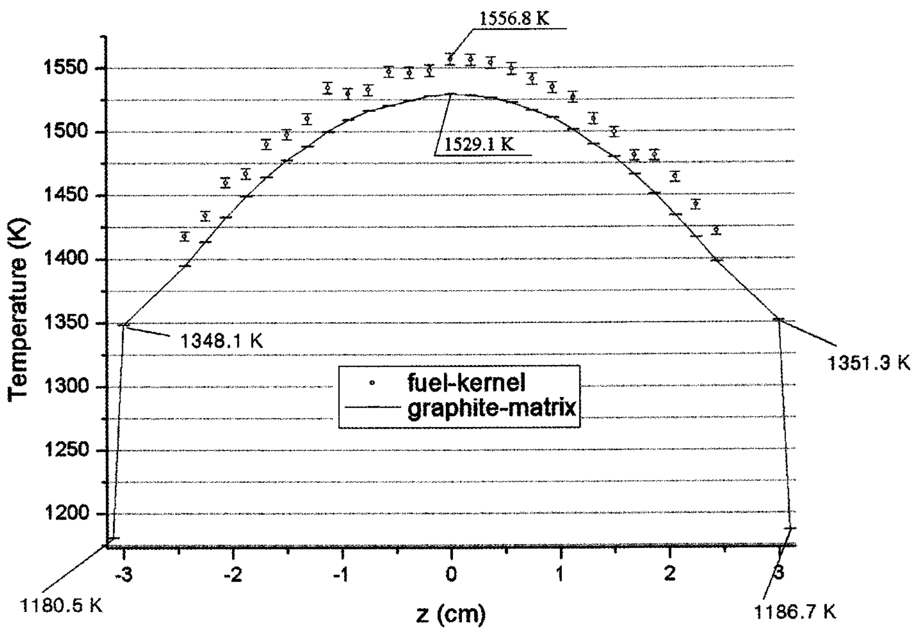

Fig. 9. Temperature Distribution along y-direction with x=z=0 in Test Problem 2

rate, q'''=3069.51 W/cm^3. The analytical solutions are shown in Figure 10 with the outer surface temperature of the particle set equal to zero.

In the hybrid method, the volume-average fuel kernel temperatures from analytical solutions are superposed on the graphite-matrix temperatures that are obtained by the Monte Carlo method. The volume-average fuel kernel temperatures are calculated by :

$$\frac{\int_{kernel} T(r)4\pi r^2 dr}{\int_{kernel} 4\pi r^2 dr}. \tag{10}$$

The results are shown in Figure 11.

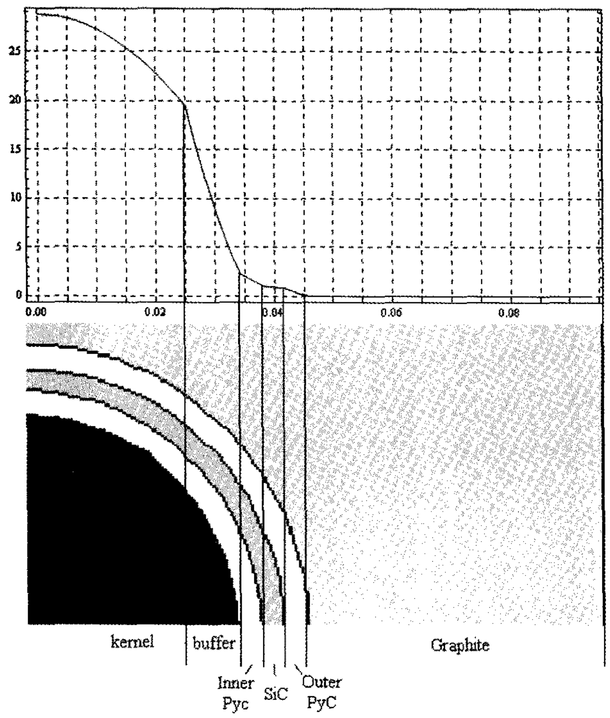

Fig. 10. Analytic Solution of a Triso Particle

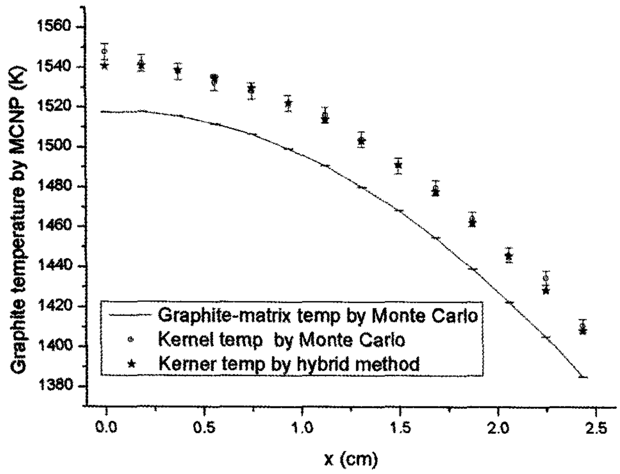

Fig. 11. Solutions by Hybrid Method

4. CONCLUSIONS

The Monte Carlo method for the heat conduction problems was extended to treat i) non-constant temperature boundary condition, ii) heat convection boundary condition, and iii) provide a hybrid method, and application results on three test problems were presented in the paper. For the fuel pebble problem, the Monte Carlo method provides fuel kernel temperatures with large standard deviations due to their very small tally volumes (unless exorbitant computer times are used), therefore a hybrid method based on Monte Carlo and analytic solutions was proposed to reduce the computing time without sacrificing accuracy. This was borne out by an example problem in the paper, where the fuel-kernel temperatures were calculated analytically (without statistical errors) and superposed on the graphite-matrix temperatures that were calculated by the Monte Carlo method with small statistical errors. The results of these heterogeneous calculations are to be used to construct the two-temperature homogenized model [7], as an example.

APPENDIX

The expressions of k_2 (equivalent thermal conductivity) for the convective medium are derived in this Appendix for three (sphere, cylinder, slab) geometries.

A. Sphere Geometry

The heat conduction equation in spherical coordinates is, in a region free of heat source,

$$\frac{k_2}{r^2}\frac{d}{dr}r^2\frac{dT}{dr}=0. \tag{A1}$$

Thus,

$$r^2\frac{dT}{dr}=c_1, \tag{A2}$$

$$\frac{dT}{dr}=\frac{c_1}{r^2}, \tag{A3}$$

$$T=-\frac{c_1}{r}+c_2. \tag{A4}$$

From Eq. (A4),

$$T_s-T_b=c_1\left(\frac{1}{r_b}-\frac{1}{r_s}\right)=c_1\frac{r_s-r_b}{r_sr_b}, \tag{A5}$$

and thus

$$c_1=\frac{r_sr_b}{r_s-r_b}(T_s-T_b). \tag{A6}$$

The convective boundary condition equation for spherical geometry is,

$$-k_2\left.\frac{dT}{dr}\right|_{r_s}=h(T_s-T_b). \tag{A7}$$

Substituting Eqs. (A3) and (A6) into (A7), we have

$$k_2 = h(r_b - r_s)\left(\frac{r_s}{r_b}\right). \tag{A8}$$

B. Cylinder Geometry

The heat conduction equation in cylindrical coordinates is, in a region free of heat source,

$$\frac{k_2}{r}\frac{d}{dr}r\frac{dT}{dr} = 0. \tag{B1}$$

Thus,

$$r\frac{dT}{dr} = c_1, \tag{B2}$$

$$\frac{dT}{dr} = \frac{c_1}{r}, \tag{B3}$$

$$T = c_1 \ln r + c_2. \tag{B4}$$

From Eq. (B4),

$$T_s - T_b = c_1(\ln r_s - \ln r_b) = c_1 \ln(\frac{r_s}{r_b}), \tag{B5}$$

and thus

$$c_1 = \frac{T_s - T_b}{\ln(r_s / r_b)}. \tag{B6}$$

The convective boundary condition equation for cylindrical geometry is,

$$-k_2 \frac{dT}{dr}\bigg|_{r_s} = h(T_s - T_b). \tag{B7}$$

Substituting Eqs. (B3) and (B6) into (B7), we have

$$k_2 = hr_s \ln(\frac{r_b}{r_s}). \tag{B8}$$

C. Slab Geometry

The heat conduction equation in slab geometry is, in a region free of heat source,

$$k_2 \frac{d^2T}{dx^2} = 0. \tag{C1}$$

Thus,

$$\frac{dT}{dx} = c_1, \tag{C2}$$

$$T = c_1 x + c_2. \tag{C3}$$

From Eq.

$$T_s - T_b = c_1(x_s - x_b), \tag{C4}$$

and thus

$$c_1 = \frac{T_s - T_b}{x_s - x_b}. \tag{C5}$$

The convection boundary condition equation for slab geometry is,

$$-k_2 \frac{dT}{dx}\bigg|_{x_s} = h(T_s - T_b). \tag{C6}$$

Substituting Eqs. (C2) and (C5) into (C6), we have

$$k_2 = h(x_b - x_s). \tag{C7}$$

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