Two-temperature method for heat transfer process in a pebble fuel

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Abstract: The highly multi-scale heterogeneous configuration in a pebble bed type reactor makes a significant challenge and complexity for theoretical analysis. In a typical pebble fuel, the fueled region that consists of a graphite matrix and numerous dispersed fuel particles is surrounded by a thin non-fueled graphite shell. Moreover, an individual fuel particle named tristructural-isotropic (TRISO) particle typically consists of five distinct regions. These high heterogeneities lead to difficulty in explicit thermal calculation of a pebble fuel. Currently, a simple volumetric-average thermal conductivity approach and a harmonic-average thermal conductivity approach are used. However, the volumetric-average approach is non-conservative as well as underestimates both the fuel temperature and the graphite matrix temperature, and the harmonic-average approach is excessively conservative that overvalues temperatures too much. In this paper, we propose a two-temperature method (TTM) to do the temperature distribution calculation in a pebble fuel. The method is not only convenient to perform but also gives more realistic results due to particles and graphite matrix are considered separately.

Keyword: two-temperature method; pebble fuel; heat transfer

1 Introduction

The neutron transport and thermal hydraulics process in modular pebble bed reactors (MPBRs) take place in a highly multi-scale heterogeneous configuration, thus makes pebble bed type core design for MPBR[1] a significant challenge for geometric modeling. The complexity can be understood when the MPBR core scaling is established and divided into three parts. Figure 1a shows the first scale (scale a) which contains a set of randomly located pebble fuel elements immersed in a gas coolant. Heat is generated in these fuel pebbles and absorbed by the gas. Figure 1b shows the second scale (scale b), a fuel pebble, consists of a fueled region surrounded by a thin non-fueled graphite shell. The fueled region has a radius of approximately 25mm and consists of a graphite matrix and 10,000-15,000 dispersed fuel particles. The third scale (scale c) shown in Fig. 1c is the tristructural-isotropic (TRISO) particle. TRISO particles typically consist of five distinct regions. At the center of the particle is the fuel kernel, typically an oxide, carbide or oxycarbide, which contains the nuclear fuel. A porous carbon buffer surrounds the kernel, to weaken recoiling fission fragments and to accommodate particle dimensional variation and internal gas buildup. The outer layers consist of an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer.

Currently, a simple volumetric-average thermal conductivity approach and a harmonic-average thermal conductivity approach are used. Both of these two methods and two-temperature method (TTM) utilize a homogenized pebble model that shown in Fig. 2 and the structure of the manufactured heterogeneous pebble is plot in Fig. 3. However, the volumetric-average approach is non-conservative and underestimates the fuel temperature, and the harmonic-average approach overvalues the effect of fuel particles' low thermal conductivity. These two average thermal conductivities serve as lower and upper bounds respectively, named Wiener bounds[2]. To obtain the realistic temperature profile in a pebble fuel element, the fuel particles and graphite matrix should be considered respectively. Moreover, in case of the approximately 200 K temperature difference in an individual pebble, the material's thermal conductivity varies with the temperature.

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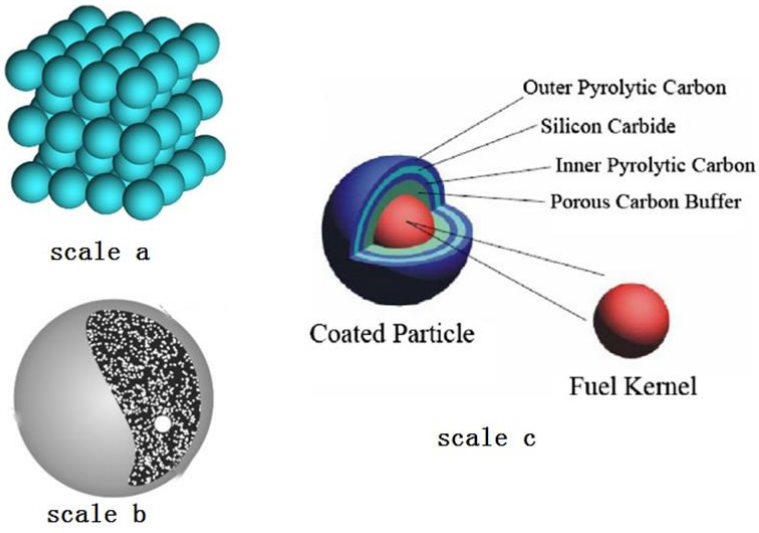

Fig.1 Scales of the modular pebble bed reactor. 1) scale a, represents the scale of the pebble bed contains a set of randomly located pebble fuel elements, 2) scale b represents the structure of a pebble, 3) scale c is a show of a fuel particle composed by five regions.

A Monte Carlo method[3] was developed for the heat conduction analysis with complicated geometry. The method is based on the theoretical results of asymptotic analysis of neutron transport equation due to that heat conduction is a diffusion process that is analogous to neutron diffusion characterized by no absorption, a fixed source and one speed condition. For seeking the deterministic techniques to obtain the realistic temperature distribution, a two-temperature homogenized model[7] was proposed. However, the model doesn't consider the high temperature gradation in a pebble due to the homogenized conductivity is used. What's more, the two-temperature homogenized model uses three parameters $\boldsymbol{k_f, k_m, \mu}$ that determined by an optimization process relates to the Monte Carlo method calculation results. Consequentially, these parameters may cause the model to lose the realistic diffusion characteristics though it works well in the specific steady-state conditions, but may make a mistake in the transient process when time is involved.

In section 2, we briefly describe the methods introduced above for the thermal analysis of an individual pebble fuel. The two-temperature method is proposed and the dealt with three parameters $\boldsymbol{k_f, k_m, \mu}$ are described in section 3. The calculation results of several steady-state conditions are shown in section 4, with results comparisons included.

2 Methods description

2.1 Average thermal conductivity methods

In the literature, Wiener bounds serve as lower and upper bounds respectively for the thermal analysis of composites. Because the pebble fuel region contains coated fuel particles and graphite matrix material in between them, the average thermal conductivities of the fueled region of the pebble are estimated as follows,

volumetric-average

$$k_{fz} = \frac{1}{V_{fz}}(V_U k_U + V_b k_b + V_g k_g + V_I k_I + V_{Si} k_{Si} + V_O k_O + V_{fzm} k_{fzm}) \quad (1)$$

harmonic-average

$$k_{fz} = V_{fz}/(V_U/k_U + V_b/k_b + V_g/k_g + V_I/k_I + V_{Si}/k_{Si} + V_O/k_O + V_{fzm}/k_{fzm}) \quad (2)$$

In the thermal analysis of an individual pebble fuel, the volumetric-average method[5] is always used to calculate the pebble temperature distribution. For an individual fuel particle, the temperatures within individual particle layers can be determined by knowing the particle surface temperature obtained from the pebble temperature at the location of the particle in the pebble, and the volumetric heat generation in the fuel region of the particle.

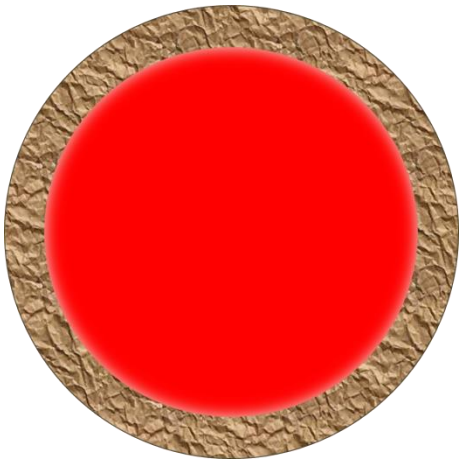

Fig.2 homogenized pebble model.

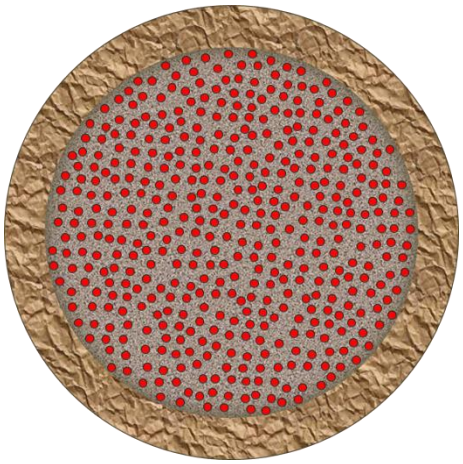

Fig.3 heterogeneous pebble model.

2.2 Monte Carlo method

The heat conduction process in an individual pebble is analogous to neutron diffusion process characterized by no absorption, a fixed source and one speed condition. The steady state diffusion equation of heat conduction for a stationary, isotropic solid is described by the following relationship,

$$\nabla k(\mathrm{r})\nabla T(\mathrm{r}) + q'''(\mathrm{r}) = 0 \tag{3}$$

Besides, the steady state, one-speed neutron diffusion process under isotropic scattering, no absorption, and a fixed source condition is calculated by the following equation,

$$\nabla \frac{1}{3\Sigma_{\mathrm{s}}} \nabla \Phi(\mathrm{r}) + \mathrm{S}(\mathrm{r}) = 0 \tag{4}$$

Therefore, the heat conduction analysis problem can be solved by solving the transport equation through MCNP5 code. The improved Monte Carlo method[4] uses an appropriate boundary layer correction to calculate the realistic temperature distributions that the kernel and graphite-matrix temperatures are shown distinctly.

2.3 Two-temperature homogenized model

In the two-temperature homogenized model, the inner fuel region of the pebble consists of a uniformly mixed composite of two homogeneous materials, graphite matrix and average fuel particle material. The heat diffusions within the two materials are calculated by the following relationships,

$$k_f \nabla^2 T_f(r,t) - \mu\left[T_f(r,t) - T_m(r,t)\right] + q'''(t) = (\rho c)_f \frac{\partial T_f(r,t)}{\partial t} \tag{5}$$

$$k_m \nabla^2 T_m(r,t) + \mu\left[T_f(r,t) - T_m(r,t)\right] = (\rho c)_m \frac{\partial T_m(r,t)}{\partial t} \tag{6}$$

In the outer non-fuel graphite shell, which is also homogeneous, the relationship is,

$$k_g \nabla^2 T_g(r,t) = (\rho c)_g \frac{\partial T_g(r,t)}{\partial t} \tag{7}$$

The homogenized parameters k_f, k_m, μ are determined by a procedure that best minimizing the following target function,

$$F\left(k_f, k_m, \mu\right) = \sum_i \left[T_f(r_i) - T_f^{MC}(r_i)\right]^2 + \sum_j \left[T_m(r_j) - T_m^{MC}(r_j)\right]^2 \tag{8}$$

where *i* and *j* are the Monte Carlo tally region indices. These homogenized parameters have undesirable properties that they are dependent on important operating conditions, *e.g.*, the volumetric heat generation and gas coolant temperature, since these conditions would greatly change the thermal conductivities, k_f and k_m, and the parameter μ is determined both by parameters k_f, k_m and the structural parameters of the pebble and particle, and this would be detailed in the next section.

3 Two-temperature method

The two-temperature method is based on the fundamental governing differential equation that the

increased heat in the control region equals the sum of the heat across the region's surfaces and the heat transferred from the region to the adjacent other material. As equations 5, 6 describe, the heat conduction process in a pebble fuel is analogous to the two-group neutron diffusion process characterized by no absorption, no fission, and a fixed source. T_f is considered as the fast neutron flux and T_m is the thermal neutron flux. The transfer between the two groups is supposed only to execute in the direction from higher temperature region to the lower parts, and this is similar to the principle in the transfer between the fast neutrons and the thermal neutrons. In case of the heat transfer item is driven by the temperature difference, the heat transferred from the region to the adjacent other material is calculated by the relationship, $\mu\left[T_f(r,t) - T_m(r,t)\right]$. The diffusion item expresses the difference of the heat migrating across the region's surfaces. When to divide the fuel region into two parts, the graphite matrix part and the fuel particles, the diffusion surface should be considered as a ratio of the sum, due to the equation control regions are arranged in the whole ball.

Then, the calculation equations are constructed as following,

In the inner fueled region,

$$A_f k_f \nabla^2 T_f(r,t) - \mu\left[T_f(r,t) - T_m(r,t)\right] + q'''(t) = (\rho c)_f \frac{\partial T_f(r,t)}{\partial t} \quad (9)$$

$$A_m k_m \nabla^2 T_m(r,t) + \mu\left[T_f(r,t) - T_m(r,t)\right] = (\rho c)_m \frac{\partial T_m(r,t)}{\partial t} \quad (10)$$

In the outer non-fueled graphite shell,

$$k_g \nabla^2 T_g(r,t) = (\rho c)_g \frac{\partial T_g(r,t)}{\partial t} \quad (11)$$

Where, k_f is the harmonic average thermal conductivity of the particle, k_m is the thermal conductivity of the graphite matrix. T_f is the particle fuel kernel center temperature, T_m is the graphite matrix temperature.

3.1 Process to determine μ

To determine the theoretic value of μ, the heat transfer item can be treated to calculate the heat generation rate in a spherical solid region with fixed temperature boundaries as shown in Fig. 4. The inmost region is the fuel kernel.

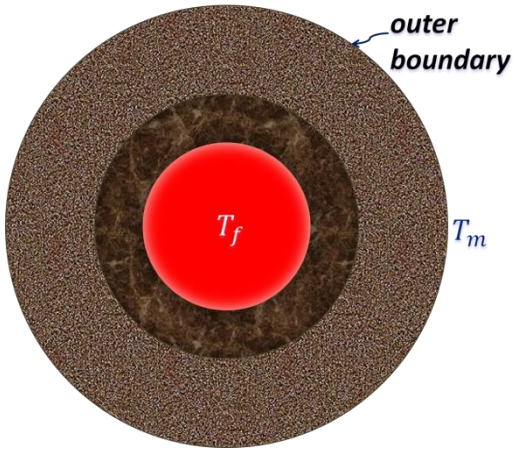

Fig.4 spherical solid region.

The secondary layer is simplified as an average of the four outer layers of a typical fuel particle. The outmost region is an equivalent spherical graphite matrix region that a single particle occupies in a pebble. The temperature in the fuel kernel center is supposed be constant T_f, while the outmost surface temperature is considered as constant T_m. The value of μ can be calculated by the following relationships,

$$\int_0^{r_U} \frac{rq}{3} dr = \int_0^{r_U} -k_U \frac{\partial T}{\partial r} dr \quad (12)$$

$$\int_{r_U}^{r_O} \frac{q}{4\pi r^2} dr = \int_{r_U}^{r_O} -k_f' \frac{\partial T}{\partial r} dr \quad (13)$$

$$\int_{r_O}^{r_{ms}} \frac{q}{4\pi r^2} dr = \int_{r_O}^{r_{ms}} -k_m \frac{\partial T}{\partial r} dr \quad (14)$$

$$\mu\left(T_f - T_m\right) = \frac{q}{V_{ms}} \quad (15)$$

$$V_{ms} = \frac{P_f V_{fz}}{num};\ r_{ms} = \left(\frac{3V_{ms}}{4\pi}\right)^{1/3} \quad (16)$$

Where, k_f' is the harmonic average thermal conductivity of the particle's four outer layers to make the calculation results conservative. The equivalent graphite matrix layer radius r_{ms} is processed in the way to find out the maximum radius to full fill all particles in the fueled region, while the

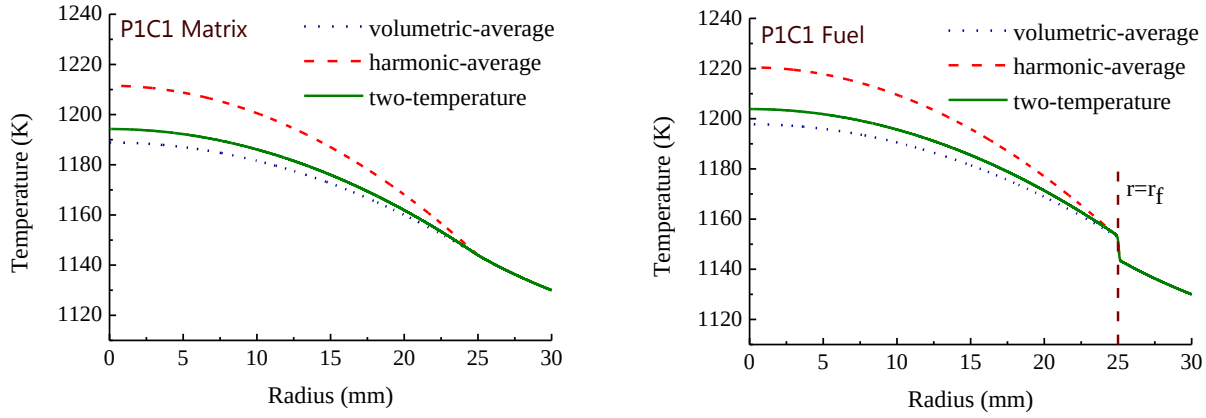

Fig.5 CASE P1C1 temperature distribution.

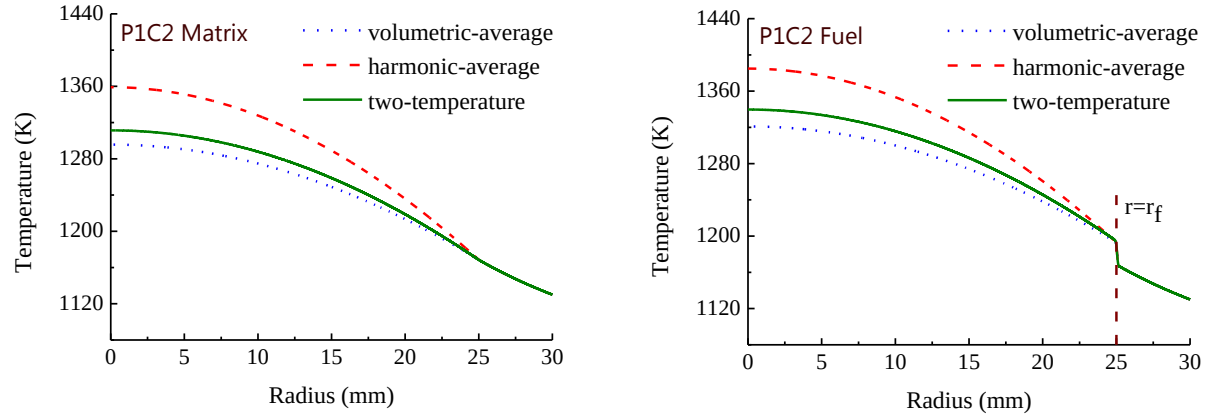

Fig.6 CASE P1C2 temperature distribution.

parameter P_f is similar to the packing factor in the fuel pebble bed, V_{ms} is the spherical volume that a single particle occupies. In this work, P_f is assigned 0.61 in case of the fuel particles are randomly located.

3.2 Process to determine A_f, A_m

A_f is the surface area ratio the fueled particle occupies, and A_m is the surface area ratio the non-fueled graphite occupies. Now that we know the ratio of one particle volume to the sum volume V_{ms}, we assume that the surface area ratio is 2.0/3.0 power of the volume ratio, calculation equations are shown as below,

$$A_f = \left(\frac{V_p}{V_{fz}}\right)^{2/3} \tag{17}$$

$$\mathrm{A_m} = 1 - \mathrm{A_f} \tag{18}$$

Where, V_p is the volume of all fuel particles in a pebble, and V_{fz} is the volume of fueled region.

3.3 process to determine T_f, at $r = r_f$

In the TTM method, continuity of heat flux and temperature at the interface within the pebble is applied. The graphite matrix temperature T_m at the fueled region surface is supposed to equal the adjacent graphite shell temperature. Knowing what T_m means we can get the fuel particle surface temperature. For an individual fuel particle, the temperature in the center of the fuel kernel can be determined by knowing the particle surface temperature and the volumetric heat generation rate in the fuel kernel. We assume that the temperature is symmetric about the particle center which is a simplification. In fact, there will be a gradient due to the temperature distribution in a pebble; indeed, this temperature distribution will also not be symmetric. However, the effect of this assumption will be minor, since the actual surface temperature difference from one side to another almost has no influence on the particle maximum temperature.

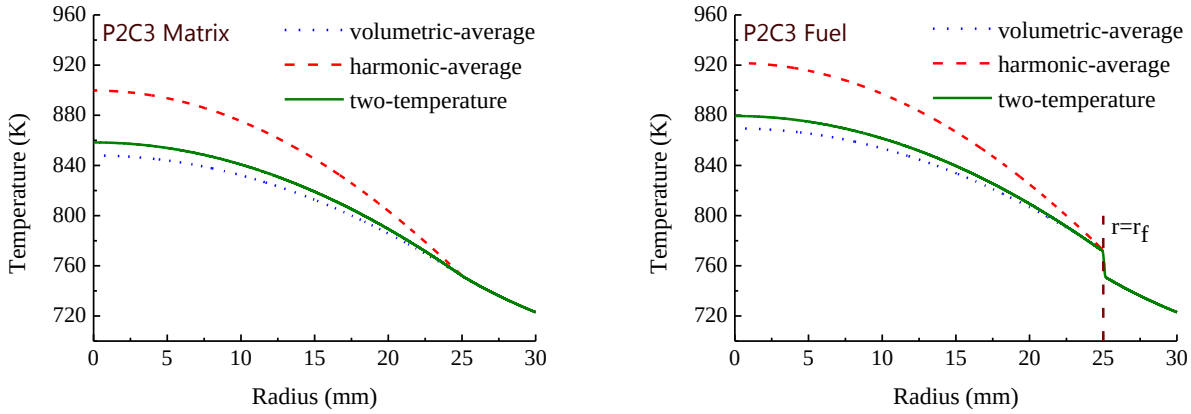

Fig.7 CASE P2C3 temperature distribution.

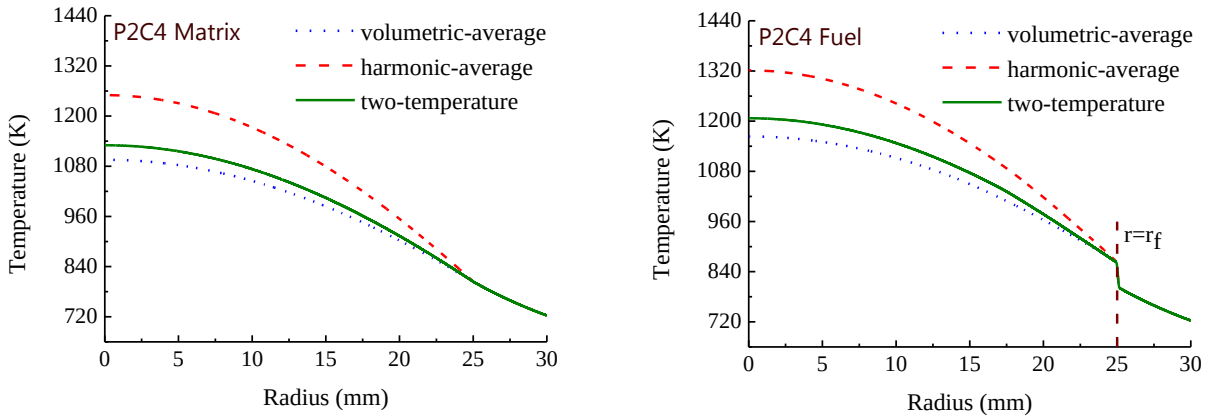

Fig.8 CASE P2C4 temperature distribution.

Then the governing equations for a particle are,
For the kernel,

$$\frac{d}{dr}(r^2 q'') = q''' r^2 \tag{19}$$

For all layers in a particle,

$$\frac{d}{dr}(r^2 q'') = 0 \tag{20}$$

For the kernel and all layers,

$$q'' = -k\,\frac{dT}{dr} \tag{21}$$

3.4 Accuracy check for parameters calculation

The parameter μ is dependent on both the parameters k_f, k_m and the structural parameters of the pebble and particle. To check the accuracy of the μ, A_f and A_m calculation methods, two temperature homogenized model calculation results provided by Cho and Yu[7] are used as reference. Cho gave two methods to determine the boundary conditions and hypothesis to make the calculation able to implement.

Method I: (i) the convection boundary condition at the pebble surface, (ii) continuity of heat flux from $T_f(r)$ and $T_m(r)$ to $T_g(r)$ at $\mathrm{r} = r_f$, (iii) conservation of heat generation rate q''' within r_f to $T_g(r)$ at $\mathrm{r} = r_f$, and (iv) continuity of $T_m(r)$ and $T_g(r)$ at $\mathrm{r} = r_f$. Where r_f is the fueled region radius.

Method II: The conditions (i), (ii) and (iii) above are applied. However, condition (iv) is not chosen instead of considering a temperature discontinuity that defined as $df = [T_m(r_f) - T_\infty]/[T_g(r_f) - T_\infty]$, where T_∞ is the pebble surface temperature.

Table 1 Comparison results between TTM and previous methods

method	A_f $(W/cm\,K)$	A_m (W/cm K)	μ (W/cm^3 K)	df	T_{f_max} (K)	T_{m_max} (K)
volumetric-average	-	-	-	-	1537.28	1508.58
harmonic-average	-	-	-	-	1585.44	1556.75
Method I	0.010	0.21	1.18	-	1540.49	1517.08
Method II	0.012	0.20	1.18	0.9825	1541.56	1518.42
TTM I	0.004	0.21	0.99	-	1552.88	1523.43

Table 2 Typical pebble bed reactor core parameters

Parameter	Core height (m)	Thermal power (MW)	Coolant inlet temperature (K)	Coolant outlet temperature (K)	Coolant mass flow rate (kg/s)	No. pebbles in core	Pebble fuel region radius (mm)	Pebble radius (mm)
Value	10.0	250	723	1130	118	360,000	25	30

Table 3 Dimensions of two particles used in thermal calculations

Parameter	fuel type	No. particles per pebble	kernel radius (μm)	buffer radius (μm)	IPyC radius (μm)	SiC radius (μm)	OPyC radius (μm)
Type 1 (P1)	UO_2	11,000	250	350	390	425	465
Type 2 (P2)	UO_2	10,000	255	345	385	420	460

Table 4 Case matrix for thermal calculations

Particle Type	Condition 1 (C1)	Condition 1 (C2)	Condition 1 (C3)	Condition 1 (C4)
Type 1 (P1)	average power at outlet, PF = 1	high power at outlet, PF = 2.74	average power at inlet, PF = 1	high power at inlet, PF = 2.74
Type 2 (P2)	average power at outlet, PF = 1	high power at outlet, PF = 2.74	average power at inlet, PF = 1	high power at inlet, PF = 2.74

Table 5 Thermal calculation results comparison.

	volumetric-average method			harmonic-average method			two-temperature method		
CASES	T_∞ (K)	T_{fuel_max} (K)	T_{matrix_max} (K)	T_∞ (K)	T_{fuel_max} (K)	T_{matrix_max} (K)	T_∞ (K)	T_{fuel_max} (K)	T_{matrix_max} (K)
P1C1	1130	1197.80	1188.86	1130	1220.49	1211.49	1130	1203.87	1194.26
P1C2	1130	1321.01	1295.66	1130	1384.87	1359.01	1130	1339.67	1311.39
P1C3	723	775.04	767.69	723	796.61	789.15	723	778.29	771.56
P1C4	723	870.37	849.26	723	932.23	910.67	723	880.57	860.64
P2C1	1130	1320.10	1293.96	1130	1374.52	1347.92	1130	1338.38	1308.34
P2C2	1130	1688.60	1608.95	1130	1843.46	1763.8	1130	1750.17	1653.82
P2C3	723	869.51	847.92	723	921.69	899.71	723	879.41	858.35
P2C4	723	1163.39	1095.44	723	1321.43	1250.25	723	1206.93	1130.22

Specific comparison results are listed in Table 1. a_f and a_m are the diffusion factors. Method I means two-temperature homogenized model calculation results by using the Method I boundary conditions. TTM I means the TTM calculation results by using the Method I boundary conditions. The TTM calculation results show that μ greatly depends on k_f and k_m and it affects the temperature difference between fuel particles and graphite matrix, while the parameters k_f and k_m influence the magnitude of the temperature.

For implementing TTM, convection boundary at the pebble surface is given as follows,

$$h\left[T_g(r_s,t)-T_\infty(t)\right]=-k_g\frac{\partial T_g(r,t)}{\partial t};\ r=r_s \quad (22)$$

4 Thermal analysis

Several cases for a typical pebble bed reactor were analyzed. The specifications for these cases are listed in Table 2. The intention was to investigate the temperature profiles of different types of coated particles at different power levels and locations in the reactor core, as well as to show a comparison with two average methods mentioned above. We choose two types of fuel particles as given in Table 3 and several various conditions. The matrix for thermal calculation is constructed as listed in Table 4.

For example, P1C1 means a pebble fuel containing 11,000 type 1 particles is positioned at the outlet of the core where the gas coolant's temperature is 1130 K, and experiencing an average power 694 W per pebble. We want to know the graphite matrix temperature and the fuel particle center temperature at any position in the pebble. TTM and two average methods are used to make a comparison and some of the key resulting temperature values are listed in Table 5. Temperature profiles in a pebble fuel under all of these cases show the similar characteristics, and Fig. 5 through Fig. 8 are plot as a demonstration. Through this analysis, we have the following observations,

- Three methods are used to show that the temperature profiles are very similar for the two pebbles with two different types particles embedded in them, because the power and fuel materials are the same, but make a little difference about the particle dimensions and the number of particles.
- Both the fuel particle center temperature, graphite matrix center temperature and the temperature drop across the pebble are much higher for Type 1 particle than for Type 2 particle. It shows that the pebble maximum temperature has a significant relation with the particle structure due to the power and fuel materials are the same.
- In all cases, both the pebble surface temperature, the pebble power and particle type have a great variation. The best and worst thermal conditions for a typical pebble bed reactor are all considered. The calculated temperature profiles plot in the Figs. 5-8 show that the TTM has a good stability.

5 Conclusions

We have presented a two temperature method to calculate the temperature distribution in the pebble. The heat conduction process in a pebble fuel is analogous to the two-group neutron diffusion process characterized by no absorption, no fission, and a fixed source. The diffusion and transfer coefficients are determined in a convenient and conservative way with some reasonable assumptions.

Several cases for a typical pebble bed were analyzed based on TTM. Compared to the two average methods, this method gives more realistic temperature profile in the fuel pebble due to the fuel particles and graphite matrix are considered separately.

Further consideration for this work would be investigating whether the method is excessively conservative, and a neutronics code would be coupled to show whether the method is still working well in the analysis of the fuel pebble transient performance while Doppler temperature feedback is involved.

Nomenclature

k	thermal conductivity
A	surface area ratio
V	volume
T	temperature
Σ_s	scattering cross section
S	internal neutron source
Φ	neutron flux
q'''	volumetric heat generation rate
q''	heat flux
q	heat generation rate
r	radius
μ	transfer coefficients
c	specific heat
ρ	density
PF	power peaking factor
P	packing factor
Superscript	
MC	Monte Carlo
Subscript	
fz	fueled zone
f	fuel particle
num	number of particles in a pebble
ms	equivalent spherical graphite matrix region

m	graphite matrix
s	surface
g	graphite shell
U	UO_2
b	carbon buffer
I	IPyC
Si	SiC
O	OPyC
fzm	graphite matrix in fueled zone

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