

Development of a two-regime heat conduction model for TRISO-based nuclear fuels

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HIGHLIGHTS

- Demonstrated a methodology for randomly distributed heat source calculation in a fuel pebble.
- Developed an advanced two-regime model for TRISO fuel temperature calculation.
- Peak temperature and average temperature used to validate the two-regime model.
- The proposed model shows improved agreement comparing to the homogeneous model.

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ABSTRACT

Several advanced nuclear reactors use Tristructural-isotropic (TRISO) fuel particles randomly distributed in a matrix to allow for aggressive operating conditions. Since those fuels are composites with randomly distributed fuel particles in a matrix, suitable smearing methods are needed to obtain fuel temperature fields for reactor design and safety analysis. By developing three-dimensional finite-element heat conduction models for randomly distributed heat generating particles in a matrix, this study evaluated the impact of the randomly distributed heat sources on the temperature fields of the fuel pebble. In addition, a two-regime heat conduction model was proposed in this study by assuming that all fuel particles are densely packed at the center of the fuel element. The present model provides a practical methodology to predict peak and average fuel temperatures of nuclear fuel elements with heat generating particles because, among the possible distribution patterns of the TRISO fuel particles, the peak fuel temperature is highest when all the fuel particles are densely packed at the center of the fuel element. Comparing to other models, the present model predicts more conservative temperature fields and shows improved agreement with both peak and average fuel temperatures of the simulated compacts and pebbles.

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1. Introduction

The Tristructural-isotropic (TRISO) fuels dispersed in a matrix are considered promising nuclear fuel candidates for several advanced reactors due to their unmatched high-temperature tolerance and suitability for high burnup operations [1]. Today, both Fluoride-salt-cooled High-temperature Reactors (FHRs) and Very High-Temperature Reactor (VHTR) are adopting pebbles with randomly distributed TRISO fuel particles to allow for aggressive

operating conditions, economic benefits, and improved safety [2].

Despite the aforementioned advantages, the modeling challenges uniquely arising from the random distribution of fuel particles introduce uncertainties in predicting neutronic, thermal, and mechanical behavior, which limit the use of the fuel concepts from the detailed reactor design and licensing standpoint [3]. In particular, prediction of fuel temperature is of paramount importance for reactor design, and safety analysis. The conventional approach treats a fuel element as a homogeneous domain with a uniform heat generation, q'' , and evaluates the temperature distribution of the fuel element using Eq. (1) with an effective thermal conductivity, k_e .

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$$\nabla \cdot (k_e \nabla T) + q''' = 0 \quad (1)$$

Numerous models have been proposed in the literature to predict effective thermal conductivities of the fuel elements. The Chiew and Glandt [4] model and the Maxwell model are considered as the most accurate among all those effective thermal conductivity models [5,6]. As Eq. (1) can only be used to predict average energy transport and temperature fields, a multi-layer fuel particle was modeled at the center of a fuel element to estimate the peak temperature [7–9]. It has been found that the temperature fields calculated using Eq. (1) are not conservative since local temperature fields in a given particle are not fully accounted for [10]. Instead, Cho, Yu and Kim [10] proposed a practical two-temperature homogenized model for the thermal calculation of a fuel pebble. Wang and Wang [11] proposed a two-level boundary element model for the large-scale thermal analysis of a fuel pebble.

This paper is a companion paper to Liu, Lee and Rao [6], which investigates the impact of randomly distributed TRISO fuel particles on the effective thermal conductivities of compacts, including Fully Ceramic Microencapsulated (FCM) and Ceramic metallic (cermet) fuel. This paper describes the thermal conductivities of fuel pebbles with randomly distributed TRISO fuel particles and a new two-regime heat conduction model for TRISO-based nuclear fuels. The objective of this study is to (1) investigate the temperature distribution of the pebble with random heat source distribution in matrix, (2) compare this temperature distribution with one obtained by existing correlations, and (3) develop a new heat conduction model for the peak temperature of the compact/pebble that is accurate and simple enough for nuclear reactor application.

2. Numerical simulation

This study used three-dimensional finite-element method (FEM) heat conduction models to examine the temperature distribution of reference fuel pebbles within a matrix. The temperature fields are used to support the two-regime heat conduction model developments and quantify uncertainties of the model due to the random packing of heat sources.

2.1. Reference fuel designs

This section presents information for the reference fuel pebble design used in the numerical simulation. A sub-scaled pebble based on Pebble Bed Modular Reactor (PBMR) 400 [12] is simulated in this study as illustrated in Fig. 1. Each randomly distributed TRISO fuel particle consists of a spherical kernel of uranium dioxide (UO_2) surrounded by four coating layers. The innermost coating layer is a porous carbon buffer layer and is followed in sequence by an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer [13]. The dimensions and thermal conductivity of the reference fuel particle and the graphite matrix used in the simulation are included in Table 1. The thermophysical properties of the TRISO fuel particle and the matrix were obtained from multiple sources [14–17]. The design parameters of the fuel pebble and the range of packing fractions are summarized in Table 2.

2.2. Numerical approach

Steady-state heat conduction simulations of a fuel pebble were performed using ANSYS 18.0. Each layer of the TRISO fuel particles was explicitly modeled in this study. A separate computer code was developed for random particle generation and was linked to ANSYS 18.0 for geometry import, property assignments, and mesh

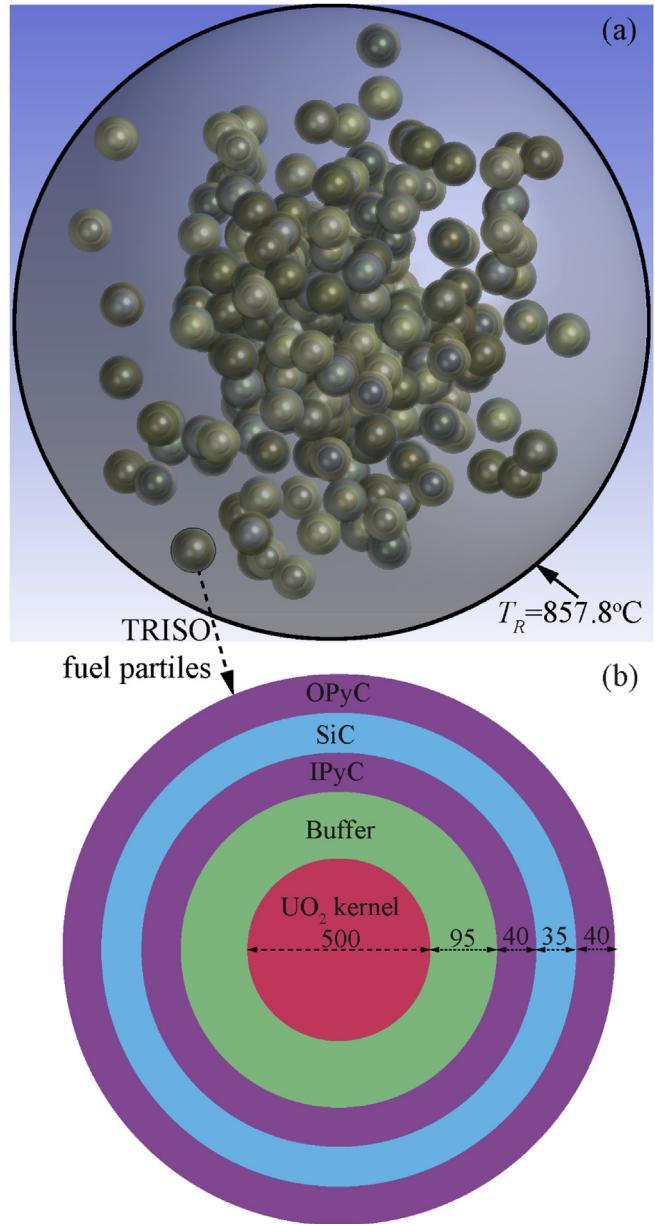


Fig. 1. Simulated fuel pebble with randomly distributed TRISO fuel particles (packing fraction $\phi = 0.09$): (a) fuel pebble, and (b) TRISO fuel particle (dimensions in μm).

Table 1

Reference parameters of the TRISO particle used in this study [12,18–20].

Layer	Outer radius (μm)	Thermal conductivity [$\text{W}/(\text{m} \cdot \text{K})$]
UO_2 kernel	250.0	3.86
Buffer	345.0	0.5
IPyC	385.0	4.0
SiC	420.0	10.0
OPyC	460.0	4.0
Matrix (graphite)	—	25.0

generation [6]. Mesh sensitivity studies were performed for all the presented cases to confirm mesh independence. Fig. 2 shows the mesh of the pebble and the TRISO fuel particles used in this study.

A sub-scaled fuel pebble with a packing fraction varying from 0.09 to 0.45 was simulated. Uniform heat generation was assumed in individual fuel kernels. For each packing fraction, 60 different

Table 2

Details of the fuel pebble used for this study.

Fuel pebble configuration	Value
Pebble radius (mm)	5.0–7.0
Packing fraction	0.09–0.45
Number of TRISO particles	254–1300
TRISO particle fuel kernel power generation rate	2.0 GW/m ³

random packing arrangements were simulated to investigate the random particle arrangement. **Table 3** summarizes each case simulated in the present study. As shown in Fig. 1 (a), a fixed temperature boundary condition of 857.8 °C was applied to the surface of the pebble. A constant volumetric power of 2.0 GW/m³ was applied to the fuel kernels in each case.

It is necessary to identify the limitations of this simulation due to assumptions and boundary conditions presented in this section. The simulation of fuel pebbles consisting of randomly distributed heat-generating particles was carried out based on the following two key assumptions: (1) uniform heat generation was assumed in

individual fuel kernels by ignoring the power distribution along the axial/radial direction of the compact and (2) the temperature dependence of the thermal conductivity of the fuel particle and the matrix was assumed constant. These assumptions simplified this study such that the simulation results were only influenced by the particle randomness.

3. Simulation of fuel pebbles with heat generating fuel particles

Contour plots for the temperature distributions of a pebble and kernels are shown in Fig. 3 (a)-(b). The contour plots show a spherical “hot zone” that exists at the center of the pebble where the fuel kernels have the highest temperature. Fig. 3 (c) presents a temperature distribution of the pebble that departs from the uniform heat generation temperature curve (solid line in the figure) caused by the random packing of the heat generating kernels.

The maximum temperature and average temperature of each pebble and fitted statistical distribution of 60 simulation cases are

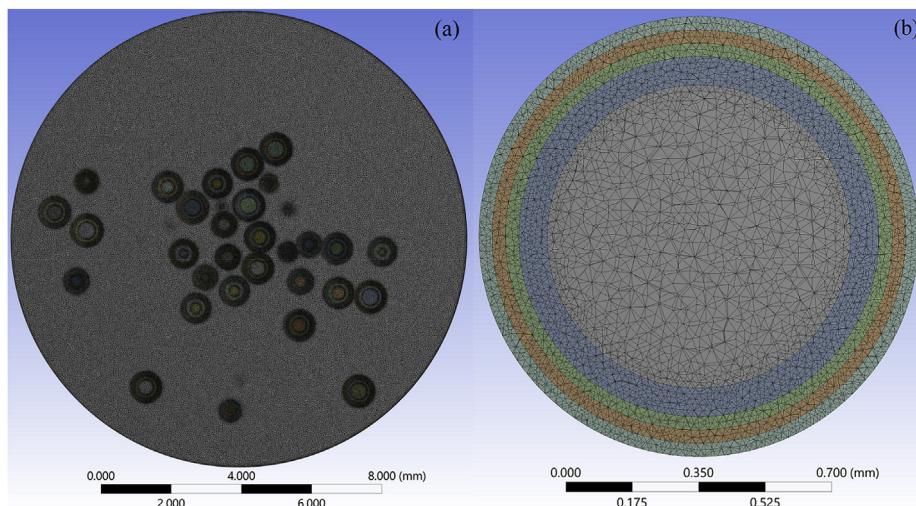


Fig. 2. Finite element mesh for the pebble with a total of 12296690 triangle elements and 22786256 nodes (packing fraction $\phi = 0.17$): (a) cross-section of the pebble, and (b) cross-section of a TRISO fuel particle.

Table 3

Fuel particle number and volumetric power of fuel pebble.

Packing fraction	Pebble radius (mm)	Number of fuel particles in a pellet	Fuel particle volumetric power (GW/m ³)
0.09	6.5	254	2.0
0.11	6.5	310	2.0
0.13	6.5	367	2.0
0.15	6.5	423	2.0
0.17	6.5	480	2.0
0.20	5.5	342	2.0
0.20	6.0	444	2.0
0.20	6.5	564	2.0
0.20	7.0	705	2.0
0.20	7.5	867	2.0
0.20	8.0	1052	2.0
0.25	6.5	705	2.0
0.30	5.0	385	2.0
0.30	5.5	513	2.0
0.30	6.0	666	2.0
0.30	6.5	846	2.0
0.30	7.0	1057	2.0
0.30	7.5	1300	2.0
0.35	6.5	987	2.0
0.40	6.5	1129	2.0
0.45	6.5	1270	2.0

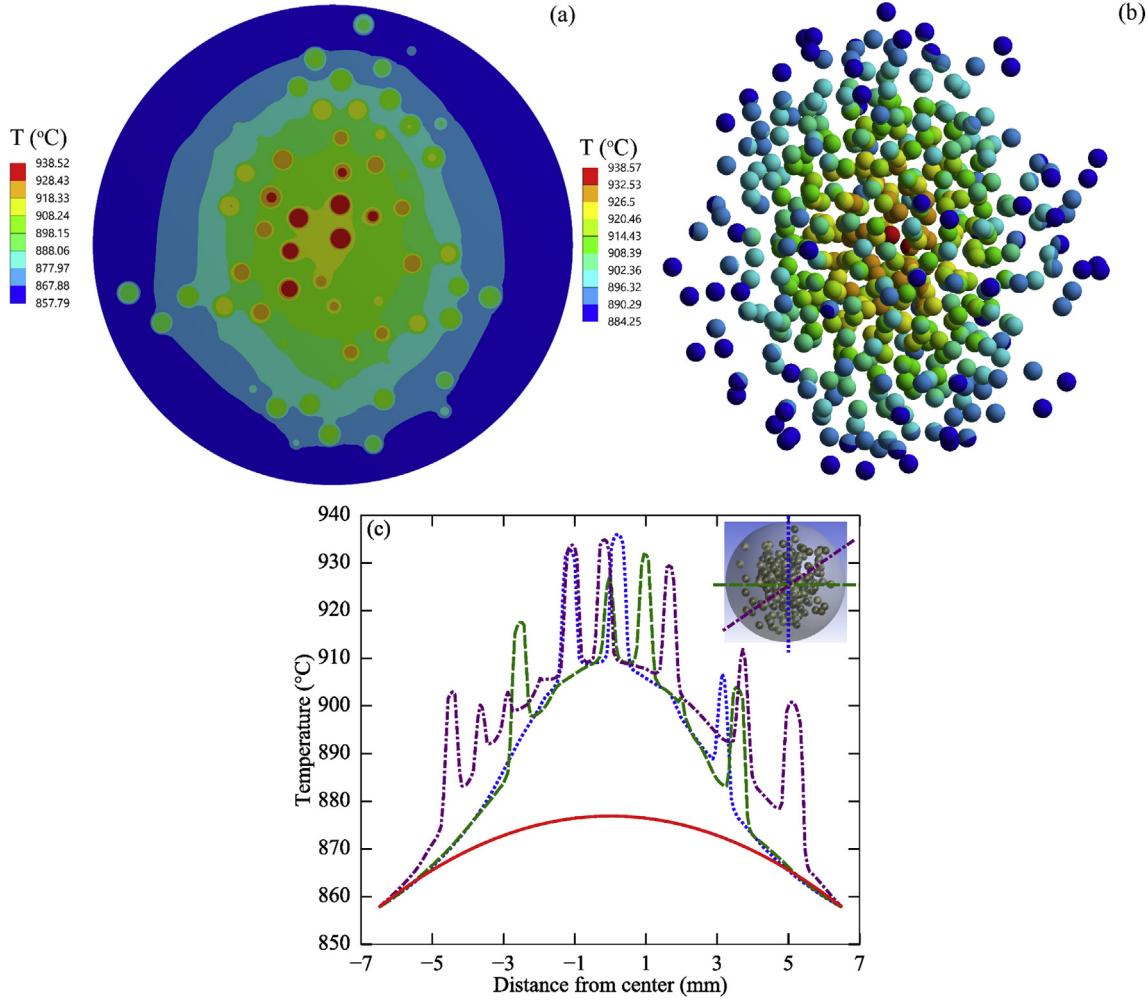


Fig. 3. Temperature contour of the pebble and the fuel kernels (packing fraction $\phi = 0.17$): (a) pebble; (b) fuel kernels; (c) Radial temperature distributions of the pebble.

illustrated in Fig. 4. As expected, the maximum temperature and average temperature with randomly distributed heat sources follow a normal distribution. As shown in Fig. 5 (a)-(b), the statistical distributions in peak particle temperature and pebble average temperature follow the normal distribution whose mean (μ) and standard deviation (σ) can be determined. At higher packing fractions, the degree of freedom in the particle arrangement decreases which leads to a more deterministic arrangement of fuel particles. This is reflected by the general decrease in the standard deviation of the peak kernel temperature distribution with increasing packing fraction. It was found that the standard deviation of the average temperature distribution increases with the higher packing fraction when the packing fraction $\phi < 0.25$. However, when the packing fraction $\phi > 0.25$, the degree of freedom in the particle arrangement decreases significantly which leads to a more deterministic arrangement of fuel particles. Thus, the standard deviation decreases with the increasing of packing fraction.

4. Two-region model

The conventional model assumes that the TRISO fuel can be modeled as a uniform media whose thermal conductivity can be estimated using the packing fraction and thermal conductivities of the fuel particles and matrix. This approach provides an effective temperature field but does not provide local temperature fields

resulting in peak temperatures in a particle. To improve the conventional model, Oh [7] calculated the fuel temperature using the conventional model (Eq. (1)) and a volumetric effective thermal conductivity (see Eq. (2)), and then models a fuel particle at the center of the fuel composite to calculate the maximum fuel particle temperature. However, likely due to usage of a volume-averaged effective thermal conductivity model (the theoretical maximum for effective thermal conductivity), Oh's approach under predicts the maximum fuel temperature [10]. The same material property values were used in the present model and Oh's model [7] to compare these two models, including thermal conductivity of the matrix (k_m) and the TRISO fuel particles (k_p). Oh uses the following equation to calculate the equivalent thermal conductivity of the TRISO fuel:

$$k_e = \frac{V_p k_p + V_m k_m}{V_p + V_m} \quad (2)$$

where V_p and k_p are the total volume and the volumetric effective thermal conductivity of the fuel particle, respectively, and V_m and k_m are the total volume and the thermal conductivity of the matrix, respectively.

The TRISO fuel particles are randomly distributed in the matrix. Among the possible distribution patterns of the fuel particles, the peak fuel temperature is the highest when all the fuel particles happen to be densely packed at the center of the matrix. To

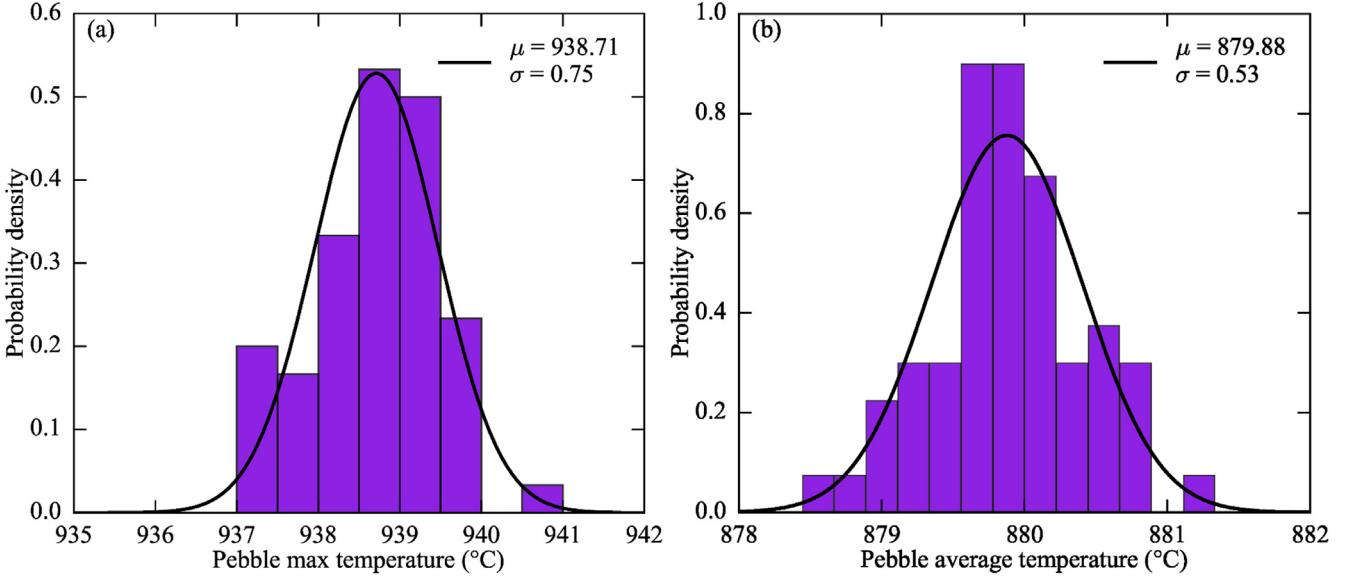


Fig. 4. Simulated temperature of 60 simulation cases and fitted statistical distribution (packing fraction $\phi = 0.17$): (a) Pebble maximum temperature, and (b) Pebble average temperature.

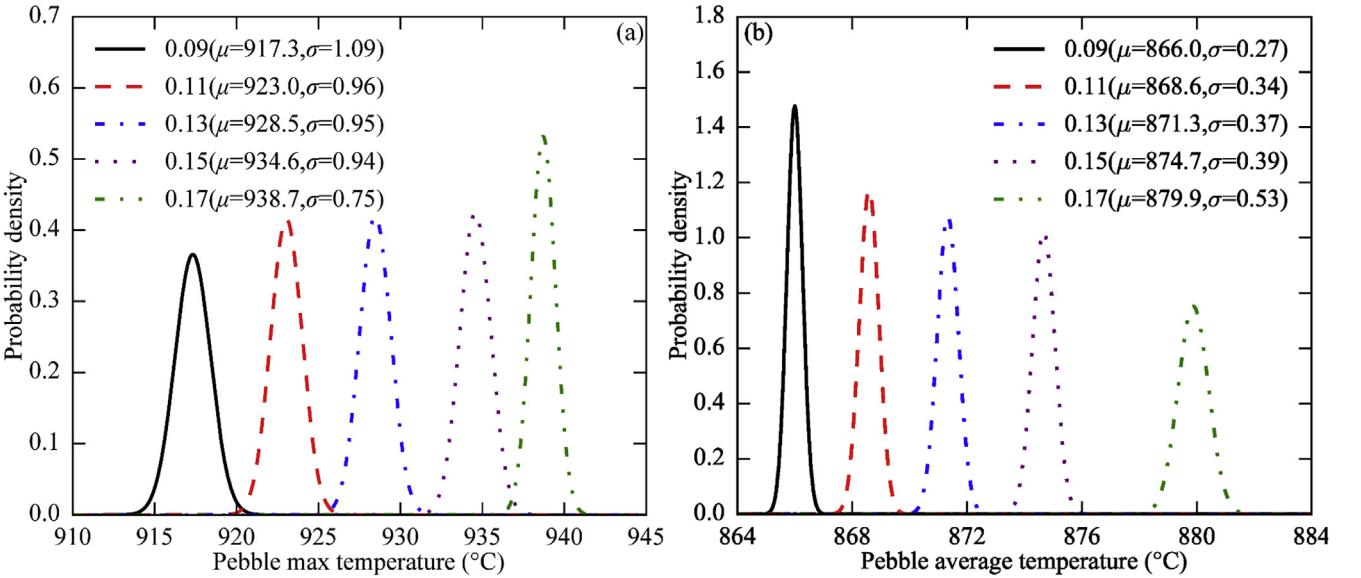


Fig. 5. Calculated temperature distribution for cases with different packing fractions ($\phi = 0.09 – 0.17$): (a) Pebble maximum temperature, (b) Pebble average temperature.

estimate the peak fuel temperature, a two-regime model was proposed by assuming a distribution pattern that all randomly distributed fuel particles are densely packed at the center of the fuel element. Thus, in this model, as shown in Fig. 6 (a)-(d), the compact/pebble is divided into two homogenized regions in which region I represents a mixture of TRISO particles and the matrix at the state of dense packing with the packing fraction ϕ_{max} ; and region II models only the matrix. Thus, the volume of region I, V_I , can be calculated using Eq. (3) based on the definition of the packing fraction of the compact/pebble $\phi_p = \frac{NV_{TRISO}}{V_p}$ and the packing fraction of region I $\phi_{max} = \frac{NV_{TRISO}}{V_I}$.

$$\frac{V_I}{V_p} = \frac{\phi_p}{\phi_{max}} \quad (3)$$

where N is the total number of TRISO particles in the fuel element,

V_{TRISO} is the volume of each TRISO fuel particle, and V_p is the volume of the fuel element. The maximum packing fraction, ϕ_{max} , is determined by the compact/pebble size and the fuel particle diameter [21]. For the present study, ϕ_{max} was set to 0.56 and 0.64 for the compact and pebble, respectively [21,22]. By further assuming region I as a uniform media with uniform heat generation as shown in Fig. 6 (b) and (d), the steady-state heat conduction equation for both regions can be written as:

$$\nabla \cdot (k_I \nabla T) + q''_I = 0, \quad R \leq r \leq R_I \text{ (Region I)} \quad (4)$$

$$\nabla \cdot (k_m \nabla T) = 0, \quad r < R_I \text{ (Region II)} \quad (5)$$

where T is fuel temperature, k_m is the thermal conductivity of the matrix, $q''_I = \frac{NV_{kernel} q''_{kernel}}{V_I}$ represents the power density within region

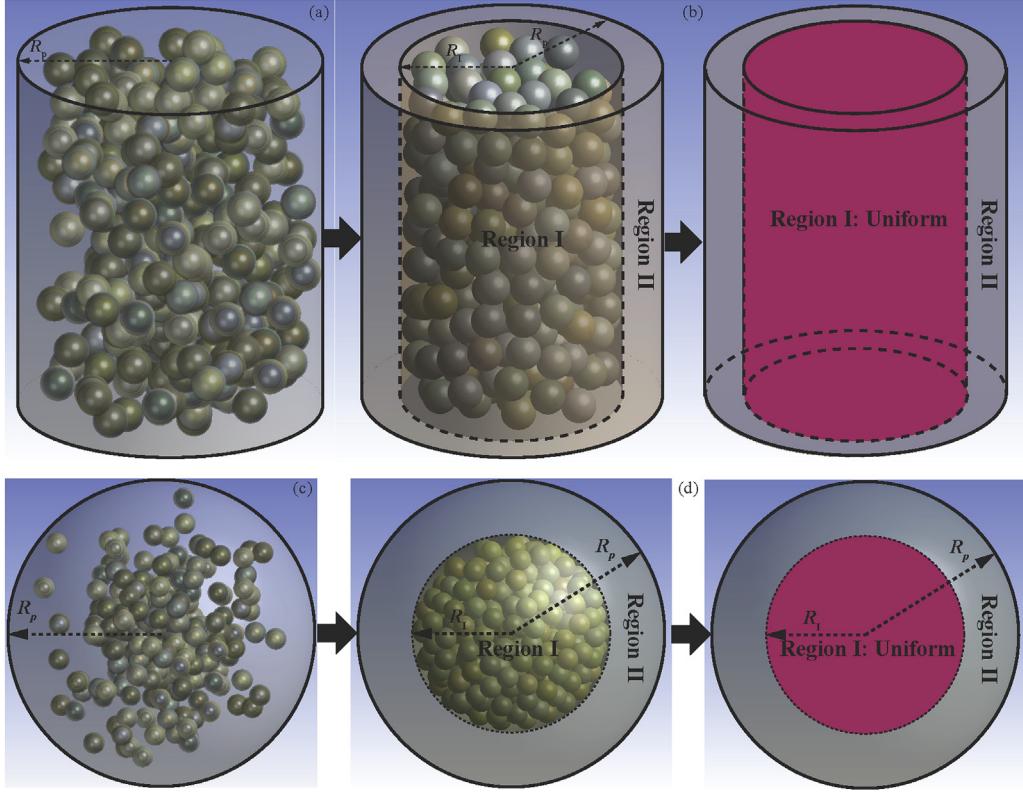


Fig. 6. Two-region model: (a) compact; (b) compact two-region model; (c) pebble; (d) pebble two-region model.

I , and k_I is the effective heat conductivity of region I, which can be calculated using the Maxwell model (Eq. (6)) [5,6]:

$$\frac{k_e}{k_m} = \frac{1 + 2\beta\phi}{1 - \beta\phi} \quad (6)$$

where ϕ is the packing fraction, and k_p is the equivalent heat conductivity of the fuel particle, which can be calculated using the method proposed by Stainsby et al. [23].

The temperature distribution for this two-region cylindrical compact can be found by

$$T(r) = \begin{cases} T_R + \frac{q'''' R_I^2}{2k_m} \ln \frac{R_p}{r}, & R_p \leq r \leq R_I \\ T_R + \frac{q'''' R_I^2}{2k_m} \ln \frac{R_p}{R_I} + \frac{q''''}{4k_I} (R_I^2 - r^2), & r < R_I \end{cases} \quad (7)$$

And for the spherical pebble,

$$T(r) = \begin{cases} T_R + \frac{q'''' R_I^3}{3k_m} \left(\frac{1}{r} - \frac{1}{R_p} \right), & R_p \leq r \leq R_I \\ T_R + \frac{q'''' R_I^3}{3k_m} \left(\frac{1}{R_I} - \frac{1}{R_p} \right) + \frac{q''''}{6k_I} (R_I^2 - r^2), & r < R_I \end{cases} \quad (8)$$

where the radius of region I can be written as

$$R_I = \begin{cases} R_p \sqrt{\frac{\phi_p}{\phi_{max}}}, & \text{for compact} \\ R_p \sqrt[3]{\frac{\phi_p}{\phi_{max}}}, & \text{for pebble} \end{cases} \quad (9)$$

The simulation results of the compact [5] and pebble with randomly distributed TRISOs are used to validate the present model. Fig. 7 (a) and (b) compare the simulated temperature of the compact and pebble with temperature predicted by the present two-regime model, Oh's model [7] and conventional model using two different effective thermal conductivity correlations (Maxwell [24] and Bruggeman [25]), along with the indicated radial direction. The conventional model predicted a much lower temperature distribution than the simulation results. Oh [7] proposed a widely used method that first calculate the fuel temperature using the conventional model and then models a fuel particle at the center of the fuel to estimate the maximum fuel temperature, whose outer surface temperature is equal to the temperature at the center of the fuel calculated using the conventional model. The differential volume average temperatures of the compact and pebble at different radial positions are shown in Fig. 8 (a) and (b). As can be inferred in Figs. 7 and 8, although Oh's work [7] modeled a fuel particle at the center of a fuel element to estimate the peak fuel temperature, it still significantly underestimated the peak temperature because it assumes the fuel element as a homogeneous media and does not account for the randomly packed heat generating fuel particles. On the other hand, the two-region model proposed in the present study gives conservative temperature distributions (see Figs. 7 and 8) and shows improved agreement with both peak fuel temperature and the average temperature of

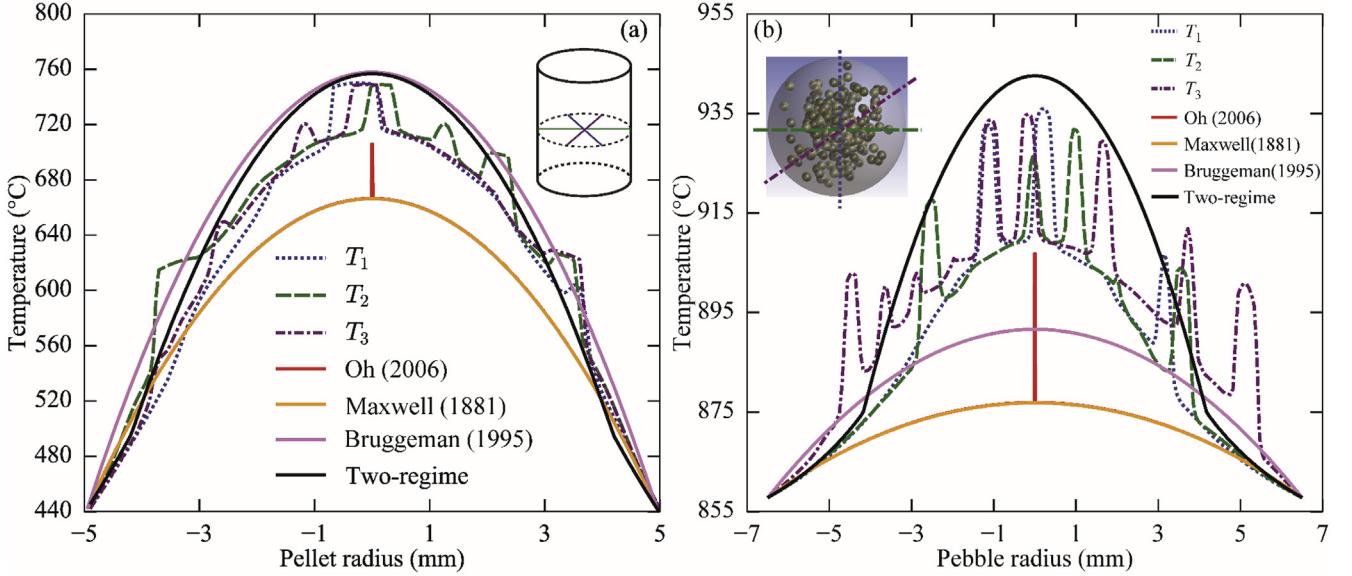


Fig. 7. Comparison of the model prediction with simulated fuel elements temperature distribution: (a) Compact ($\phi = 0.40$); (b) Pebble ($R_p = 6.5$ mm, $\phi = 0.17$).

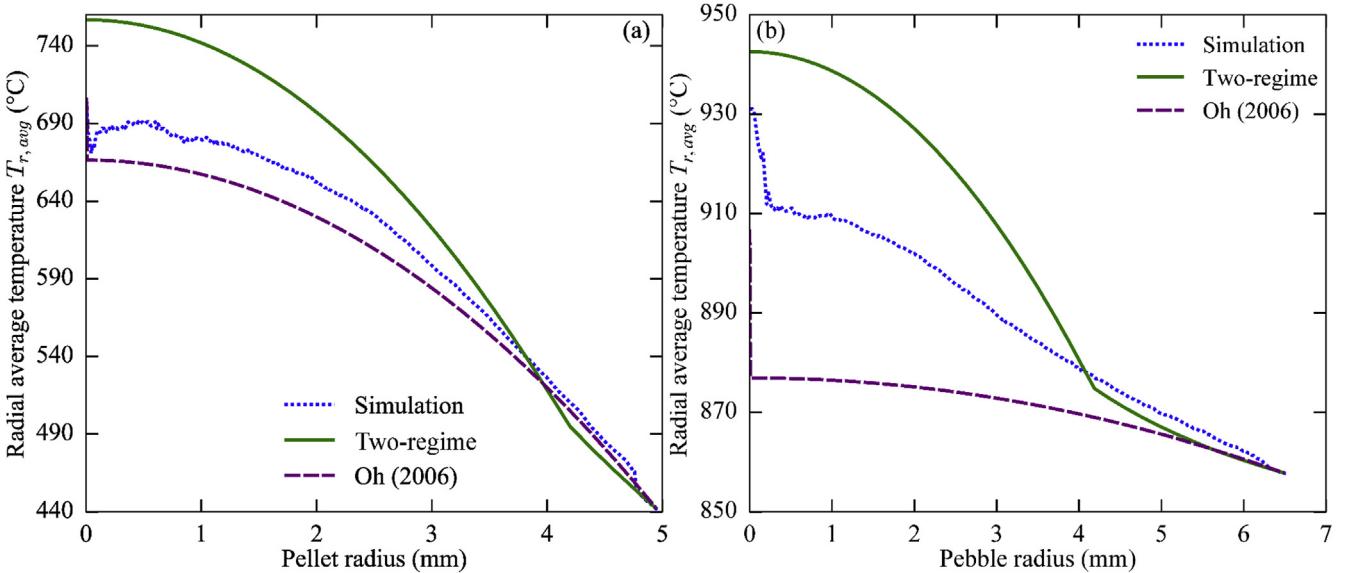


Fig. 8. Comparison of the model prediction with calculated fuel average radial temperature: (a) Compact ($\phi = 0.40$); (b) Pebble ($R_p = 6.5$ mm, $\phi = 0.17$).

the compact and pebble ($T_{\text{avg}} = \frac{\int T_{\text{dv}}}{V_p}$), as shown in Fig. 9 and Fig. 10, respectively. The maximum errors of the proposed two-regime model are 1.9% and 2.8% for peak fuel temperature and fuel average temperature, respectively. Comparison of the model prediction of fuel pebble peak temperature and pebble average temperature with different pebble radii was presented in Fig. 11 and Fig. 12. The maximum error of the present model is 1.2% and 1.4% for peak fuel temperature and fuel average temperature. In summary, the proposed two-regime model shows improved agreement on the temperature field prediction of compact and pebble including the peak and average temperature and radial temperature distribution comparing to the conventional homogeneous model. The two-regime model, in general, slightly over predicts peak kernel temperatures but slightly underpredicts pebble and compact averaged temperatures.

5. Discussion

Accurate evaluation of the fuel peak temperature is essential for reactor design and safety analysis. The conventional approach treats a fuel element as a homogeneous domain with a uniform heat generation and evaluates the temperature distribution of the fuel element using an effective thermal conductivity. The previous studies have proved the limitation of the conventional homogeneous model on in the prediction of fuel peak temperature because the effective thermal conductivity defined for the TRISO fuel element should only be used to predict average temperature fields of the fuel element. Hence, the present study proposes a new two-regime model to overcome the limitation of the conventional homogeneous model. The two-regime model developed in this study assumes a unique distribution pattern that all fuel particles are

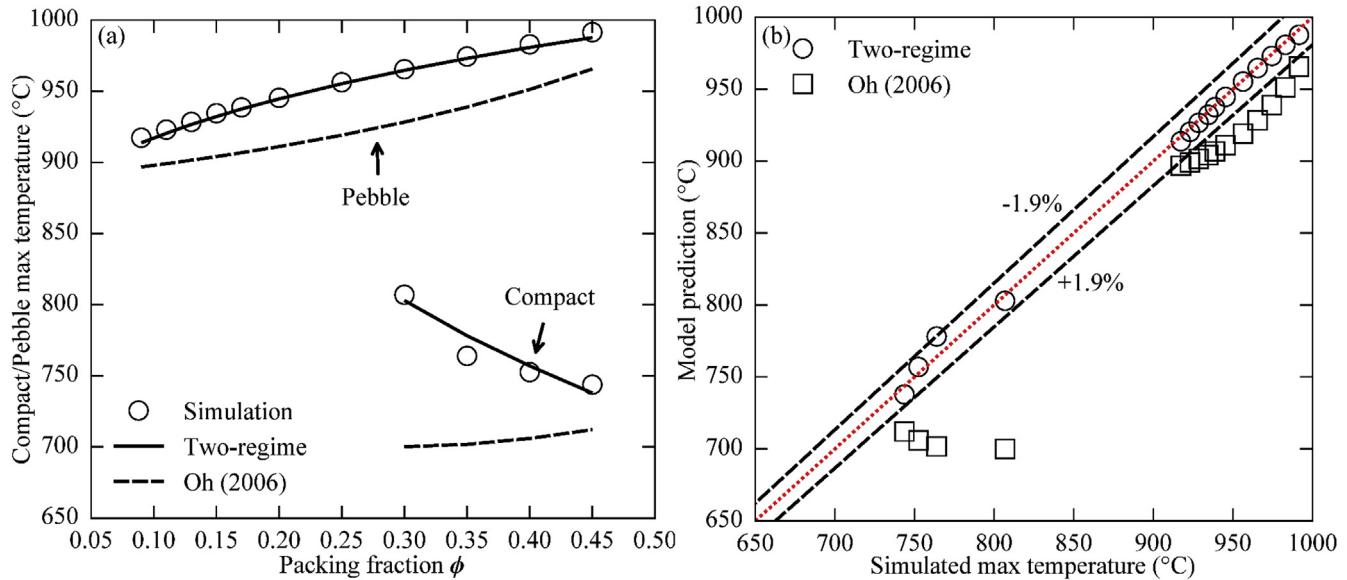


Fig. 9. Comparison of the model prediction of maximum temperature for compacts and pebbles with different packing fraction: (a) Maximum temperature; (b) Error of the prediction.

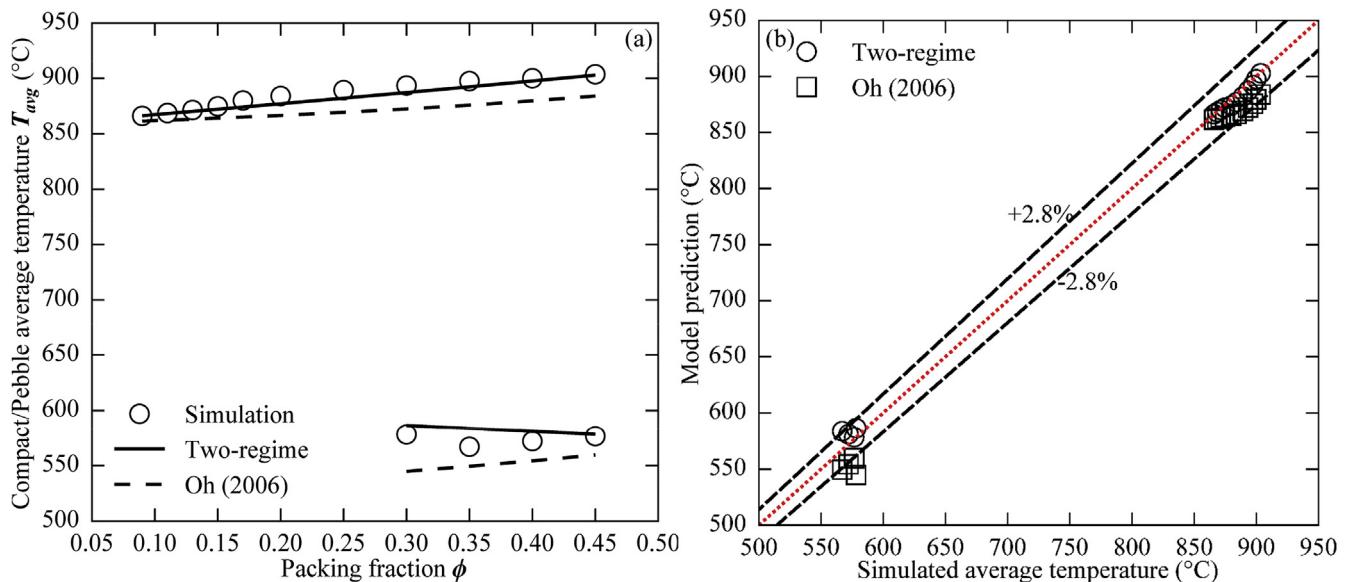


Fig. 10. Comparison of the model prediction of fuel average temperature for compacts and pebbles with different packing fraction: (a) Average temperature; (b) Error of the prediction.

densely packed at the center of the fuel element. Compared to the conventional homogeneous model, the proposed two-region model gives an improved prediction for both peak and average fuel temperature for the compact and pebble. It is important to point out that Oh's model gives a good result as well, but it just underestimated the peak fuel temperature slightly because it uses a volumetric average effective thermal conductivity. Hence, when a proper thermal conductivity is used, Oh's approach gives an acceptable temperature prediction.

6. Conclusion

In this study, numerical simulations were performed using an in-house developed code and ANSYS 18.0 to study the effective

thermal conductivity of composite fuels consisting of spherical particle type nuclear fuels, including compacts (previous paper [6]) and pebbles. This study quantitatively explores the impact of randomly distributed heat sources on the peak and the average temperature of the TRISO-embedded compact and pebble.

The practical value of using the effective thermal conductivity for temperature prediction is very much limited, as it inherently neglects the statistical nature of heat generating TRISO distribution associated with random packing. This study illuminates the practical limitation of effective thermal conductivity, and propose a practical way of predicting average and peak temperature, thereby directly supporting improved reactor design and safety analysis.

A universal two-region model was developed for compacts and pebbles to overcome the limitation of the conventional

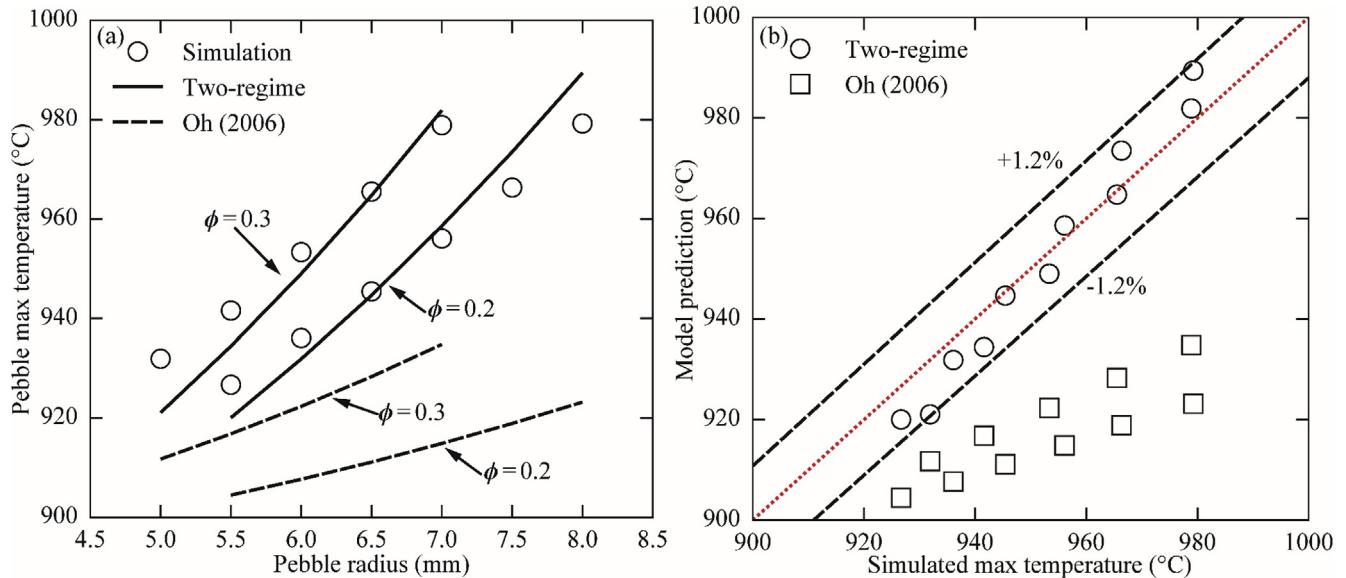


Fig. 11. Comparison of the model prediction of fuel pebble maximum temperature with different radii: (a) Maximum temperature; (b) Error of the prediction.

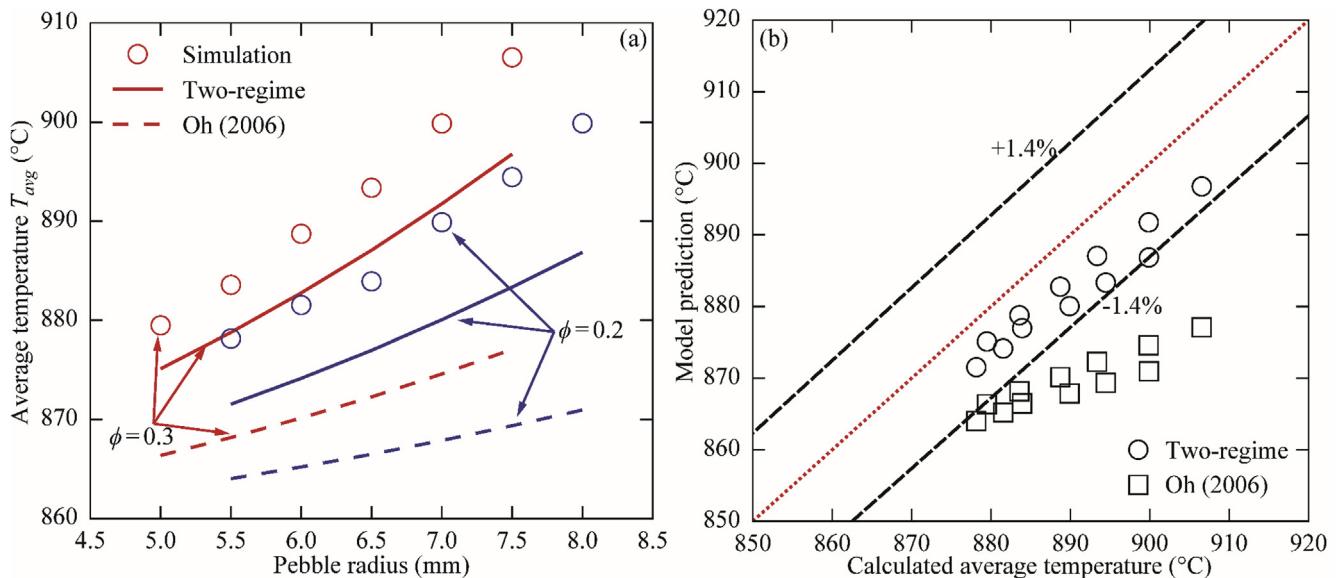


Fig. 12. Comparison of the model prediction of pebble averaged temperature with different radii: (a) Average temperature; (b) Error of the prediction.

homogeneous model on the prediction of fuel peak temperature. Comparing to the conventional homogeneous model, the present model assumes that the fuel particles are densely packed at the center of the fuel element. Thus, it predicts more conservative temperature distributions and shows improved agreement with both peak fuel temperature and the average temperature of compacts and pebbles. The presented methodology would improve nuclear fuel design and safety analysis for a wide range of TRISO-embedded nuclear fuels.

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Nomenclature

k	thermal conductivity, W/(m·K)
k_e	effective thermal conductivity, W/(m·K)
N	particle number
q'''	power density, W/m ³
r_1	outer radius of the fuel kernel, m
r_2	outer radius of the buffer layer, m
r_3	outer radius of the OPyC layer, m
r_4	outer radius of the SiC layer, m
r_5	outer radius of the OPyC layer, m
R_p	fuel pebble radius, m
T	temperature, °C
T_R	surface temperature, °C
V	volume, m ³

Greek Symbols

ϕ packing fraction

Subscripts

avg	average value
p	compact or pebble
kernel	TRISO fuel kernel
max	maximum value
r	radial
TRISO	TRISO particle
I, II	region I and II, respectively

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