Nuclear Engineering and Technology 48 (2016) 650–659

Available online at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original Article

Steady- and Transient-State Analyses of Fully Ceramic Microencapsulated Fuel with Randomly Dispersed Tristructural Isotropic Particles via Two-Temperature Homogenized Model—I: Theory and Method

Yoonhee Lee [1], *Bumhee Cho* [2], *and Nam Zin Cho* [*]

Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

ARTICLE INFO

Article history:
Received 28 December 2015
Received in revised form
27 January 2016
Accepted 9 February 2016
Available online 27 February 2016

Keywords:
Doppler Temperature Feedback
Fine Lattice Stochastic Structure
Fully Ceramic Harmonic- and Volumetric-Average Thermal Conductivities
Microencapsulated Fuel
Reactor Physics Asia 2015
Two-Temperature Homogenized Model

ABSTRACT

As a type of accident-tolerant fuel, fully ceramic microencapsulated (FCM) fuel was proposed after the Fukushima accident in Japan. The FCM fuel consists of tristructural isotropic particles randomly dispersed in a silicon carbide (SiC) matrix. For a fuel element with such high heterogeneity, we have proposed a two-temperature homogenized model using the particle transport Monte Carlo method for the heat conduction problem. This model distinguishes between fuel-kernel and SiC matrix temperatures. Moreover, the obtained temperature profiles are more realistic than those of other models. In Part I of the paper, homogenized parameters for the FCM fuel in which tristructural isotropic particles are randomly dispersed in the fine lattice stochastic structure are obtained by (1) matching steady-state analytic solutions of the model with the results of particle transport Monte Carlo method for heat conduction problems, and (2) preserving total enthalpies in fuel kernels and SiC matrix. The homogenized parameters have two desirable properties: (1) they are insensitive to boundary conditions such as coolant bulk temperatures and thickness of cladding, and (2) they are independent of operating power density. By performing the Monte Carlo calculations with the temperature-dependent thermal properties of the constituent materials of the FCM fuel, temperature-dependent homogenized parameters are obtained.

* *Corresponding author.*
E-mail address: nzcho@kaist.ac.kr (N.Z. Cho).
[1] Present address: Korea Institute of Nuclear Safety, 62 Gwahak-ro, Yuseong-gu, Daejeon 34142, Republic of Korea.
[2] Present address: Standard Energy, 32-16 Techno 7-ro, Yuseong-gu, Daejeon 34029, Republic of Korea.

http://dx.doi.org/10.1016/j.net.2016.02.007

1. Introduction

The recent events at three of the Japanese Fukushima Daiichi reactors have sparked renewed interest in improving the safety of light water reactors. Accordingly, the events have called for research on nuclear fuels that increase safety margins with enhanced tolerance. To achieve such enhanced tolerance, the development of new fuels focuses on aspects such as lowering operating temperatures, slowing hydrogen generation rate, enhancing the retention of the fission product, etc. [1].

Recently, a fully ceramic microencapsulated (FCM) fuel has been proposed as a fuel with enhanced accident tolerance—a so-called accident-tolerant fuel [2,3]. The concept of FCM fuel is based on a proven safety philosophy that has been utilized operationally in high-temperature gas-cooled reactors (HTGRs). As shown in Figs. 1 and 2, nuclear fuel is contained within several layers of ceramic coating in a tristructural isotropic (TRISO) particle and the FCM fuel consists of TRISO particles randomly dispersed in a silicon carbide (SiC) matrix. This high heterogeneity in composition provides advantages in terms of safety features of the fuel, such as good thermal conductivity, radiation damage resistance, environmental stability, and proliferation resistance [2,3]. However, the heterogeneous composition also leads to difficulty in geometrical modeling for explicit thermal analyses of the FCM fuel. Therefore, an appropriate homogenization model is necessary.

For a fuel element of HTGRs with a similar configuration to the FCM fuel element, volumetric-average thermal conductivity was used [4,5]. However, this volumetric-average thermal conductivity model is not conservative in which the obtained temperature profiles are lower than the real values. Moreover, this model is unable to distinguish between fuel-kernel and matrix temperatures.

For the thermal analysis of research reactor fuels, where nuclear fuel particles are randomly dispersed in the matrix, a modified Hashin and Shtrikman correlation [6,7] is used. It is based on the effective medium theory (within Wiener bounds) [8] that pertains to analytical modeling to describe the macroscopic properties of the constituent materials. Since the model was developed for composite materials consisting of just two constituent materials, it is difficult to apply it to fuels with TRISO particles. This model is also unable to distinguish between fuel-kernel and matrix temperatures.

Recently, a method for homogenization of thermal conductivities in compact and block-type fuels in HTGRs was proposed [9]. This work is based on a two-scale asymptotic expansion method. It gives more realistic temperature profiles than those from the volumetric-average thermal conductivity model. However, this model is applicable to fuels with a

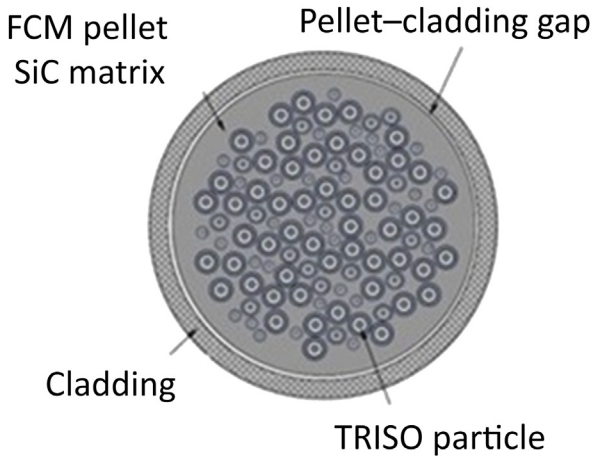

Fig. 2 – Configuration of the FCM fuel [2,18]. FCM, fully ceramic microencapsulated. Reproduced from K.A. Terrani, L.L. Snead, J.C. Gehin, Microencapsulated fuel technology for commercial light water and advanced reactor application, J. Nucl. Mater. 427 (2012) 209–224, copyright at Elsevier, 2012 and from Y. Lee, N.Z. Cho, Steady- and transient-state analyses of fully ceramic microencapsulated fuel loaded reactor core via twotemperature homogenized thermal-conductivity model, Ann. Nucl. Energy 76 (2015) 283–296, copyright at Elsevier, 2015.

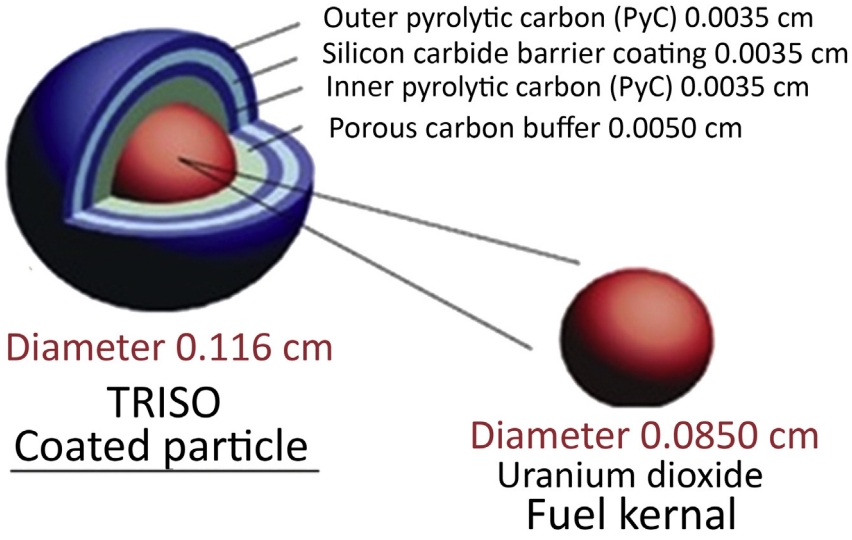

Fig. 1 – Configuration of the TRISO particle [18]. Reproduced from Y. Lee, N.Z. Cho, Steady- and transient-state analyses of fully ceramic microencapsulated fuel loaded reactor core via twotemperature homogenized thermalconductivity model, Ann. Nucl. Energy 76 (2015) 283–296, copyright at Elsevier, 2015.

periodic structure and may not be applicable to fuels in which TRISO particles are randomly distributed.

We have proposed a two-temperature homogenized model for randomly distributed TRISO fuels using the particle transport Monte Carlo method devised for heat conduction problems [10–14]. With explicit modeling of a fuel element, a particle transport Monte Carlo calculation is performed via the HEATON program [15], which is a Monte Carlo heat conduction calculation program based on MCNP 5 as the major computation engine. The homogenized parameters are obtained by "matching" steady-state analytic solutions of a two-temperature homogenized model for the fuel element with the results of the HEATON calculation. Using the parameters thus obtained and solving the heat conduction equations of the model, we can distinguish between fuel-kernel and SiC matrix temperatures. Moreover, the temperature profiles obtained are more realistic than those of the volumetric-average model. The authors have applied the model to the thermal analysis of the HTGR fuel element [16] and the FCM fuel element [17,18]. In this model, we can distinguish between fuel-kernel and matrix temperatures. In previous works [17,18], the authors applied this model to FCM fuels in which TRISO particles are distributed in a coarse lattice with a centered sphere structure [19]. In addition, in the works of Lee and Cho [17,18], the model was applied to FCM fuels with UO_2 kernels.

Recently, we have applied the two-temperature homogenized model to the FCM fuel element in which TRISO particles are randomly distributed in a fine lattice stochastic (FLS) structure [20], which is more random than the coarse lattice with a centered sphere structure. At the Reactor Physics Asia 2015 Conference, we presented preliminary results comparing this model with harmonic- and volumetric-average thermal conductivity models, in terms of temperature profiles.

In this paper, first, the two-temperature homogenized model is applied to the FCM fuel with uranium nitride (UN) kernels, which is currently considered as the kernel material due to its high density. The UN kernels lead to a fuel cycle length that is comparable with that of conventional UO_2 fuel. In addition, temperature-dependent homogenized parameters are obtained with temperature-dependent thermal conductivities of the SiC matrix, which is the major heat conduction medium in the FCM fuel. The data are now available from Terrani et al. [21] study. In a previous work [18], we considered the thermal conductivity of the SiC matrix to be temperature independent. This model is also coupled with a reactor analysis module in COREDAX based on the analytic function expansion nodal method for the neutron diffusion model [22], in order to analyze the FCM fuel-loaded reactor in which TRISO particles are distributed in the FLS structure. The results are compared with those from the harmonic- and volumetric-average thermal conductivity models.

This paper is composed of two parts. Part I consists of a description of the two-temperature homogenized model for the FLS structure and conventional models for thermal analysis of composite materials that are used to compare the results of analysis of the FCM fuel-loaded reactor in Part II [23]. Part II deals with coupling of the two-temperature homogenized model with a reactor analysis module in COREDAX based on the analytic function expansion nodal method for the neutron diffusion model.

Part I of the paper is organized as follows: Section 2 provides a brief description of the harmonic- and volumetric-average thermal conductivity models; Section 3 describes the two-temperature homogenized model for the FCM fuel elements in which TRISO particles are distributed in the FLS structure; and finally, discussions and conclusions are provided in Section 4.

2. Harmonic- and volumetric-average thermal conductivity models for the FCM fuel element

Harmonic- and volumetric-average thermal conductivity models are based on the effective thermal conductivity. The Wiener bounds confine the effective thermal conductivity of a composite [8]. The following harmonic- and volumetric-average thermal conductivities serve as lower and upper bounds, respectively:

$$\text{Harmonic average}: \underline{k} = \frac{V}{\sum V_i/k_i} \tag{1}$$

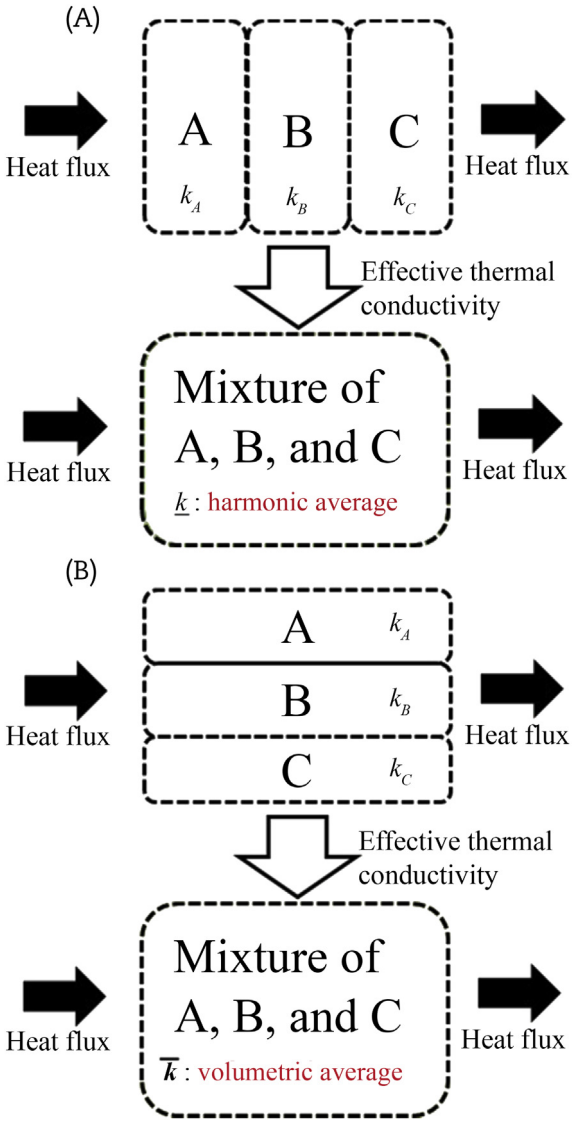

Fig. 3 – Concept of harmonic- and volumetric-average thermal conductivities. (A) Harmonic average. (B) Volumetric average.

$$\text{Volumetric average}: \bar{k} = \frac{\sum V_i k_i}{V} \quad (2)$$

where i is the material index of the composite.

The concept of the harmonic- and the volumetric-average thermal conductivities is illustrated in Fig. 3.

The physical meaning of the harmonic-average thermal conductivity is that heat flux is parallel to the direction of the constituent materials mixed, as shown in Fig. 3A. In order to transfer heat to the right from the left in Fig. 3A, heat flux should flow through all constituent materials. Therefore, the harmonic-average thermal conductivity is the lowest thermal conductivity among all models.

By contrast, the physical meaning of the volumetric-average thermal conductivity is that heat flux is perpendicular to the direction of the constituent materials mixed, as shown in Fig. 3B. In this case, the heat flux can choose one of the constituent materials to flow from left to right. This means that the thermal resistivity is the lowest among all cases of the materials. Therefore, the volumetric-average thermal conductivity is the highest thermal conductivity among all models.

In a real composite, the constituent materials are combined in various directions, i.e., a mixture of parallel and perpendicular directions to the heat flux. Therefore, the value of the real effective thermal conductivity for a composite material lies between the values of the harmonic average and the volumetric average.

For the FCM fuel element, with a typical packing fraction of 0.361, the temperature-dependent, harmonic- and volumetric-average thermal conductivities are shown in Fig. 4. Density × specific heat (ρc) for the FCM fuel is calculated by the volume-weighted average of the (ρc) of the constituent materials of the FCM fuel, and the results are shown in Fig. 5. The detailed geometry [27,28], thermal conductivities, and (ρc) of the constituent materials are listed in Table 1 [21,24,25,29–31]. For calculating the harmonic- and volumetric-average thermal conductivities, thermal conductivities of UN, shown in Fig. 6, are considered to be temperature dependent. In addition, the thermal conductivities of the SiC matrix, shown in Fig. 7, are considered to be irradiated, since they are saturated to the irradiated case for short time operation of the reactor [21].

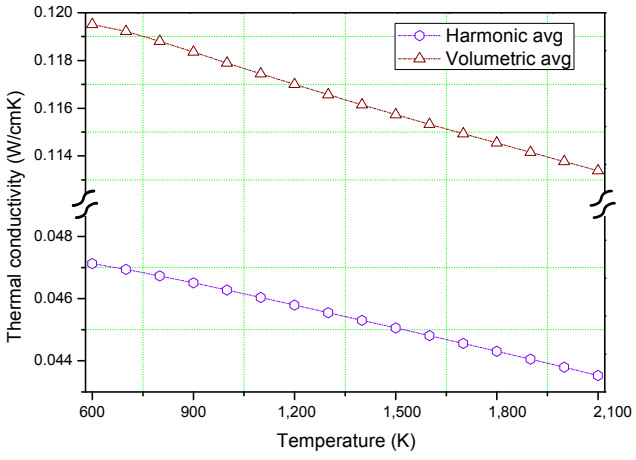

Fig. 4 – Temperature-dependent harmonic- and volumetric-average thermal conductivities for the FCM fuel. FCM, fully ceramic microencapsulated.

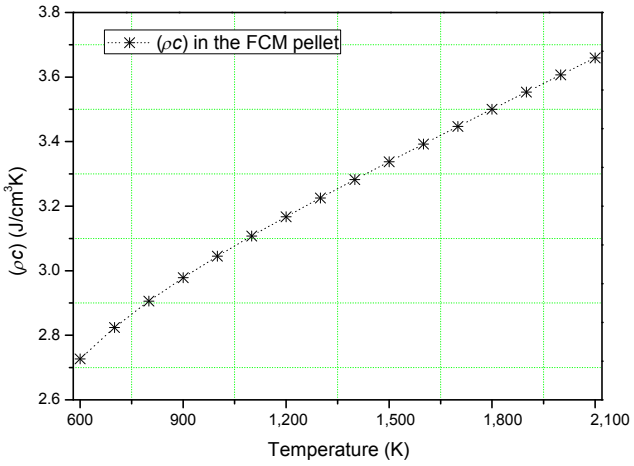

Fig. 5 – Temperature dependence (ρc) of the FCM fuel element. FCM, fully ceramic microencapsulated.

In Fig. 6, the thermal conductivity of UN is compared to that of UO_2. The thermal conductivity of materials involves two primary mechanisms: atomic vibration and electronic transport. For a typical ceramic fuel, e.g., UO_2, atomic vibration is the dominant mechanism of thermal conductivity. Hence, thermal conductivity decreases with temperatures owing to increasing vibration of the crystal lattice. In contrast to UO_2, thermal conductivity of UN increases with temperature owing to the transport of a large number of electrons [32].

Thermal conductivity of the UN kernel [25], International Atomic Energy Agency (IAEA) model for (ρc) of the UN kernel [25], and Snead's model for (ρc) of SiC [26] are expressed in Eqs. (3)–(5), respectively:

$$k_{\text{kernel}}(T) = \frac{1}{100}\left(1.37\varsigma^{0.41}\right) \quad (3)$$

$$(\rho c)_{\text{kernel}}(T) = 3.766 \times 10^{-5}\cdot T + \frac{3.766 \times 10^{9}}{T^2}\exp(-18081/T) + 0.2029\left(\frac{365.7}{T}\right)^2 \frac{\exp(365.7/T)}{[\exp(365.7/T) - 1]^2} \quad (4)$$

$$(\rho c)_{\text{SiC}}(T) = 2.9621 + 0.0012\cdot T - 2.5363 \times 10^{-7}\cdot T^2 - \frac{1.0223 \times 10^{5}}{T^2} \quad (5)$$

where T: temperature in K; $\varsigma = T - 273.15$, temperature in °C; and $\tau = T/1{,}000$.

Table 1 – FCM fuel pellet configurations.

Layers	Radius (cm)	k_i (W/cm K)	$(\rho c)_i$ (J/cm^3 K)
Kernel (uranium nitride)	0.0425	Fig. 6	Eq. (4)
Buffer	0.0475	0.005	0.00165
Inner PyC	0.0510	0.04	0.00255
SiC	0.0545	0.1	Eq. (5)
Outer PyC	0.0580	0.04	0.00255
SiC matrix	0.05801	Fig. 7 (irradiated case)	Eq. (5)

FCM, fully ceramic microencapsulated; PyC, pyrolytic carbon; SiC, silicon carbide.

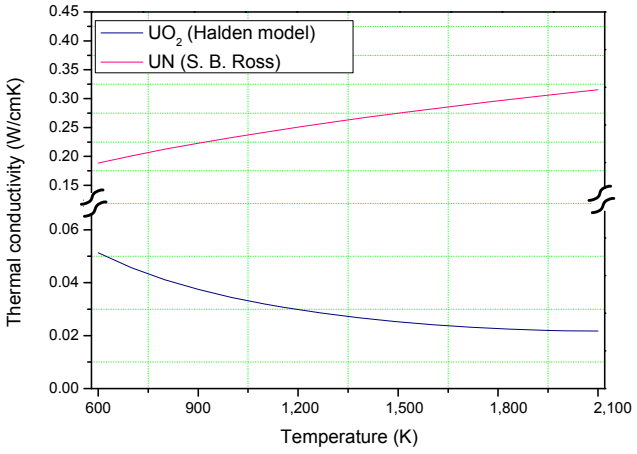

Fig. 6 – Comparison of thermal conductivities of uranium nitride and UO_2. UN, uranium nitride.

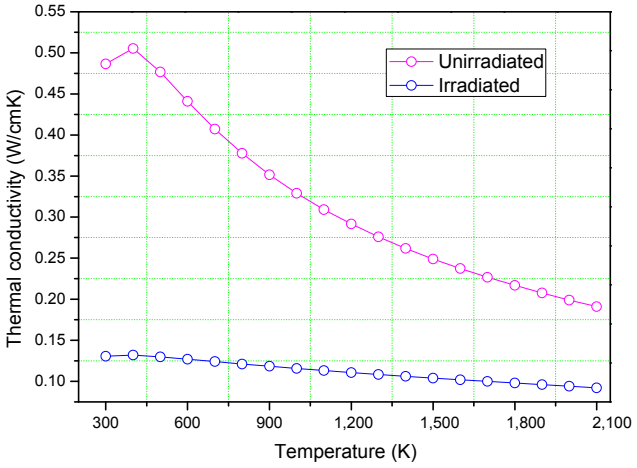

Fig. 7 – Comparison of thermal conductivities of the unirradiated and irradiated SiC matrix.

3. Two-temperature homogenized model for the FCM fuel element

3.1. *Description of the model for the FCM fuel element with randomly distributed TRISO particles*

Fig. 8 shows a heterogeneous FCM fuel element in which TRISO particles are distributed in the FLS structure. In the FLS, the fuel pellet is divided into small cubes of particle size, and randomly choose this fine cube and place a particle there as many as allowed by packing fraction. Rather than the heterogeneous configuration, we wish to construct a homogenized FCM fuel as a model.

In the homogenized model, the FCM pellet region of the fuel element is represented by an imaginary homogeneous medium characterized by two temperatures. The medium representing fuel kernels is characterized by thermal conductivity k_f, temperature T_f, and density × specific heat in the fuel kernels $(\rho c)_f$. Similarly, the medium representing the coating layers of the TRISO particles and the SiC matrix surrounding

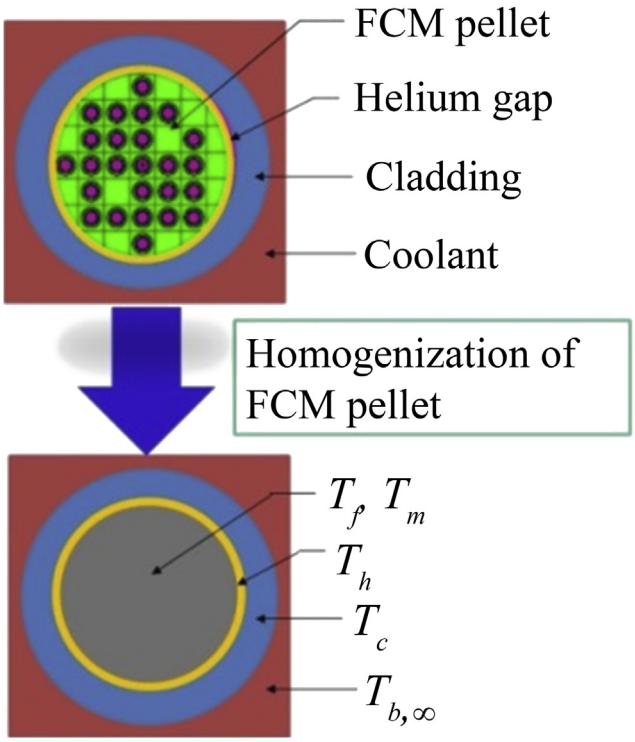

Fig. 8 – Two-temperature homogenized model for the FCM fuel element. FCM, fully ceramic microencapsulated.

the particles (which is denoted as SiC matrix in the remainder of this paper) is characterized by thermal conductivity k_m, temperature T_m, and density × specific heat in the SiC matrix $(\rho c)_m$. To consider the heat conduction from the fuel kernels to the SiC matrix, we introduce a new parameter μ. We refer to k_f, k_m, μ, $(\rho c)_f$, and $(\rho c)_m$ as homogenized parameters.

In the homogenized FCM pellet region, using the five homogenized parameters (k_f, k_m, μ, $(\rho c)_f$, and $(\rho c)_m$), we write heat-conduction equations for the fuel kernels and SiC matrix, respectively, as follows:

$$\nabla k_f \nabla T_f - \mu(T_f - T_m) + q'''(t) = (\rho c)_f \frac{\partial T_f}{\partial t} \tag{6}$$

$$\nabla k_m \nabla T_m + \mu(T_f - T_m) = (\rho c)_m \frac{\partial T_m}{\partial t} \tag{7}$$

where $q'''(t)$ is the power density in the homogenized FCM pellet, obtained by a process of homogenization as follows:

$$q'''(t) = \frac{\sum_i q'''_{fi}(t) V_{fi}}{V_{f-m}} \tag{8}$$

and $q'''_{fi}(t)$: power density of the i^{th} fuel kernel in the heterogeneous FCM pellet; V_{fi}: volume of the i^{th} fuel kernel; and $V_{f\text{-}m}$: volume of the FCM pellet.

It is assumed that heat transfer between the two imaginary media is caused by the temperature difference. In order to assess the effect of such heat transfer, Eqs. (6) and (7) include an additional term, $\mu(T_f - T_m)$, in the general heat conduction equation.

In the helium gap and cladding, which are already homogeneous, thermal conductivities are then retained as k_h, and

k_c, respectively, while temperatures are represented by T_h and T_c, respectively:

$$\nabla k_h \nabla T_h = (\rho c)_h \frac{\partial T_h}{\partial t} \tag{9}$$

$$\nabla k_c \nabla T_c = (\rho c)_c \frac{\partial T_c}{\partial t} \tag{10}$$

where $(\rho c)_h$ and $(\rho c)_c$ are density × specific heat in the helium gap and cladding, respectively.

The interface and boundary conditions are also written as follows:

(1) At the interface between the FCM pellet and the helium gap, we require a heat flux continuity condition expressed as follows:

$$-k_h \nabla T_h = -A_f k_f \nabla T_f - A_m k_m \nabla T_m \tag{11}$$

where A_f and A_m refer to the fractions of the effective interface areas of the fuel kernels and SiC matrix, respectively, interfacing with the helium gap inner surface.

The area fractions in Eq. (11) involve an elusive concept other than their summation being unity. In this study, we assume that the effective interface areas for the fuel kernels and SiC matrix are proportional to volume of the fuel-kernels to two-third and that of SiC matrix in the pellet.

Sensitivity studies were performed for various values of A_f. Temperature profiles and the maximum temperatures of the fuel kernel, SiC matrix, helium gap, and cladding are shown in Fig. 9 and Table 2.

As shown in Fig. 9 and Table 2, for a typical packing fraction that is in the range of 0.3–0.5, the temperature profiles in the pellet and other regions of the fuel elements are not affected significantly by the values of A_f (a reasonable value is 0.05).

(2) At the interface between the helium gap and SiC cladding, a conventional heat flux continuity condition is used as follows:

$$-k_h \nabla T_h = -k_c \nabla T_c \tag{12}$$

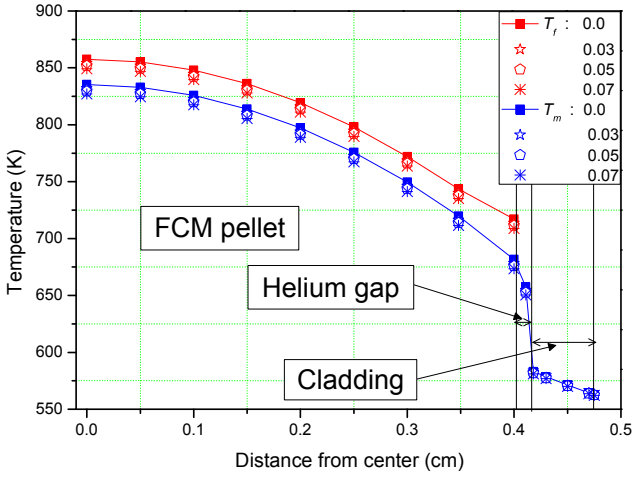

Fig. 9 – Comparison of the temperature profiles for various values of A_f. FCM, fully ceramic microencapsulated.

Table 2 – Maximum temperature in the fuel kernel, SiC matrix, helium gap, and cladding for various values of A_f.

A_f	Maximum temperature (K)			
	Fuel kernel	SiC matrix	Helium gap	Cladding
0	857.6	835.4	657.6	583.0
0.03	854.1	831.8	654.5	582.2
0.05	851.7	829.4	652.4	581.6
0.07	849.3	827.0	650.4	581.0

SiC, silicon carbide.

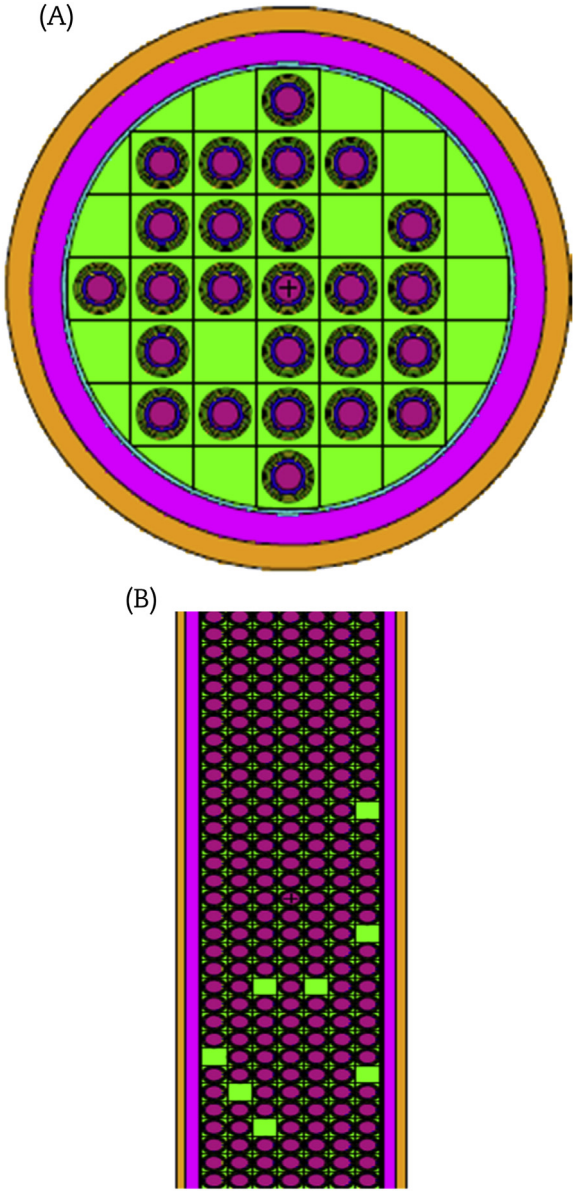

Fig. 10 – HEATON modeling for the FCM fuel element with an FLS configuration. (A) Radial view. (B) Axial view. FCM, fully ceramic microencapsulated; FLS, fine lattice stochastic.

(3) At the boundary between the SiC cladding and the coolant, a convective boundary condition is used as follows:

$$-k_c \nabla T_c = h(T_{cb} - T_\infty) \tag{13}$$

where h is the heat transfer coefficient of the coolant and T_∞ is the coolant bulk temperature.

3.2. Calculation of temperature-dependent homogenized parameters

To obtain the parameters of k_f, k_m, and μ, we perform a steady-state Monte Carlo heat conduction calculation using the HEATON program with explicit modeling of the heterogeneous FCM fuel pellet configuration, to obtain the reference solutions [10–15]. In this calculation, TRISO particles in the pellet are explicitly modeled and distributed in an FLS structure, as shown in Fig. 10. The detailed geometry [27,28] and material properties [29–31] used in this study, and the computational conditions of the HEATON calculations are listed in Table 3. In the HEATON calculations, boundary conditions in the radial and axial directions are set to be insulated.

In the steady state, the right-hand sides of Eqs. (6), (7), (9), and (10) become equal to zero. After some algebra, we can obtain analytic solutions of Eqs. (6), (7), (9), and (10) for an infinite cylindrical geometry, as follows:

$$T_m(r) = c_1 \frac{I_0(\sqrt{A}r)}{A} - \frac{B}{4A} r^2 + c_4 \tag{14}$$

$$T_f(r) = -\frac{k_m}{\mu}\left[c_1 I_0\left(\sqrt{A}r\right) - \frac{B}{A}\right] + T_m(r) \tag{15}$$

$$T_h(r) = c_5 \ln(r) + c_6 \tag{16}$$

$$T_c(r) = c_7 \ln(r) + c_8 \tag{17}$$

where I_0 = zeroth order modified Bessel function of the first kind

$$A = \frac{\mu(k_f + k_m)}{k_f k_m} > 0,\ B = \frac{\mu q'''}{k_f k_m} > 0 \tag{18}$$

There are unknown coefficients c_1, c_4, c_5, c_6, c_7, and c_8 in the solution forms of Eqs. (14–17). To determine the coefficients, we apply the following: (1) a convective boundary condition at the cladding surface; (2) the continuity of heat flux from the fuel kernel and SiC matrix, to the helium gap at the pellet surface, as expressed in Eq. (11); (3) the continuity of $T_m(r)$ and $T_h(r)$ at the pellet surface; and (4) the continuity of $T_h(r)$ and $T_c(r)$ at the cladding inner surface.

The next step is to determine the homogenized parameters k_f, k_m, and μ. The concept involved in determining the parameters is to "match" the analytic solutions for the homogenized FCM pellet obtained above with the results of the HEATON calculation. The two solutions are matched through the least squares of the differences between the two solutions in the FCM pellet. In other words, the procedure finds the parameters that minimize the following functional expression:

$$F(k_f, k_m, \mu) = \sum_i \left[T_{f,i} - T_{f,i}^{MC}\right]^2 + \sum_j \left[T_{m,j} - T_{m,j}^{MC}\right]^2 \tag{19}$$

where i and j are the Monte Carlo tally region indices. The calculation procedures are summarized in Fig. 11.

The homogenized parameters for the transient analysis, $(\rho c)_f$ and $(\rho c)_m$, are calculated using Eqs. (20) and (21) by preserving the total enthalpies in the fuel kernels and SiC matrix, respectively:

$$(\rho c)_f = \frac{\sum_i \int_{V_{f,i}} dV (\rho c)_{f,i}^{het} T_{f,i}^{het}}{\int_{V_{f-m}} dV T_f^{hom}} \tag{20}$$

Table 3 – Information on the unit FCM fuel element and computational condition for HEATON calculation.

Materials		Kernel/buffer/inner PyC/SiC/outer PyC/SiC matrix
Radius (cm)		0.0425/0.0475/0.0510
		0.0545/0.0580
Length of unit cell (cm)		0.11602
Pellet radius (cm)		0.4095
Gap	Material	He
	Radius (cm)	0.4180
	Heat transfer coefficient (W/cm^2 K)	1
Cladding	Material	SiC
	Radius (cm)	0.4750
	Thermal conductivity (W/cm K)	0.1
Coolant	Bulk temperature (K)	570
	Extrapolation length (cm)	0.045
	Heat transfer coefficient (W/cm^2 K)	4.223
Pitch (cm)		1.26
Packing fraction		0.361
Number of histories in HEATON calculation		10,000,000
Scaling factor		50

FCM, fully ceramic microencapsulated; PyC, pyrolytic carbon; SiC, silicon carbide.

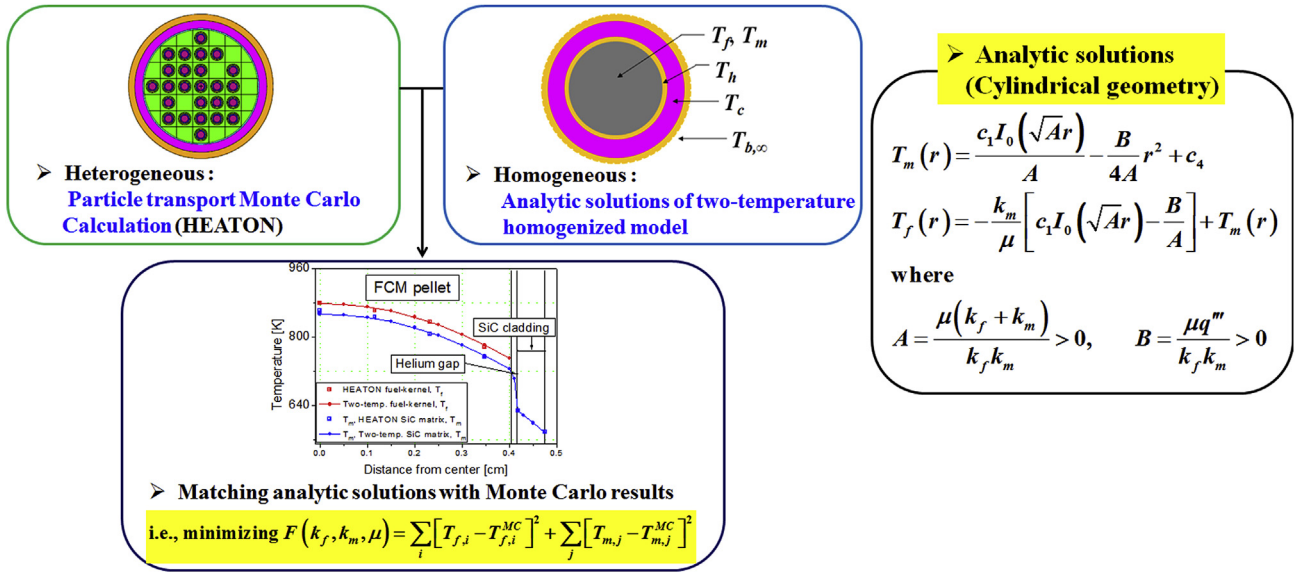

Fig. 11 – Calculational procedures to obtain homogenized parameters (k_f, k_m, μ).

$$(\rho c)_m = \frac{\sum_j \int_{V_{m,j}} dV(\rho c)_{m,j}^{het} T_{m,j}^{het}}{\int_{V_{f-m}} dV T_m^{hom}} \tag{21}$$

where $T_{f,i}^{het}$ and $T_{m,j}^{het}$ are the results from the HEATON calculations.

If we perform the procedures shown in Fig. 11 and Eqs. (20) and (21) with the temperature-dependent thermal properties of the constituent materials in the FCM fuel pellet, as shown in Table 1, we can obtain temperature-dependent homogenized parameters, as shown in Figs. 12 and 13. The modeling equations for the temperature-dependent homogenized parameters are expressed as follows:

$$k_f(T) = \alpha_0 + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \alpha_3 \cdot T^3 + \alpha_4 \cdot T^4 + \alpha_5 \cdot T^5 \tag{22}$$

$$k_m(T) = \alpha_0 + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \alpha_3 \cdot T^3 + \alpha_4 \cdot T^4 + \alpha_5 \cdot T^5 \tag{23}$$

$$\mu(T) = \alpha_0 + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \alpha_3 \cdot T^3 + \alpha_4 \cdot T^4 + \alpha_5 \cdot T^5 \tag{24}$$

$$(\rho c)_f(T) = \alpha_0 + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \alpha_3 \cdot T^3 + \alpha_4 \cdot T^4 + \alpha_5 \cdot T^5 \tag{25}$$

$$(\rho c)_m(T) = \alpha_0 + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \alpha_3 \cdot T^3 + \alpha_4 \cdot T^4 + \alpha_5 \cdot T^5 \tag{26}$$

where T is temperature in Kelvin in Eqs. (3–5), while the coefficients used in Eqs. (22–26) are listed in Table 4.

Homogenized parameters from the HEATON calculations and those fitted by Eqs. (22–26) show good agreements, i.e., the differences are less than ~0.5%, as indicated by the error bars in Figs. 12 and 13, since 10^7 histories are used in order to minimize the stochastic errors in the HEATON calculations.

Note that the homogenized parameters obtained in this study are insensitive to the random arrangements with the same packing fraction. Sensitivity studies show that

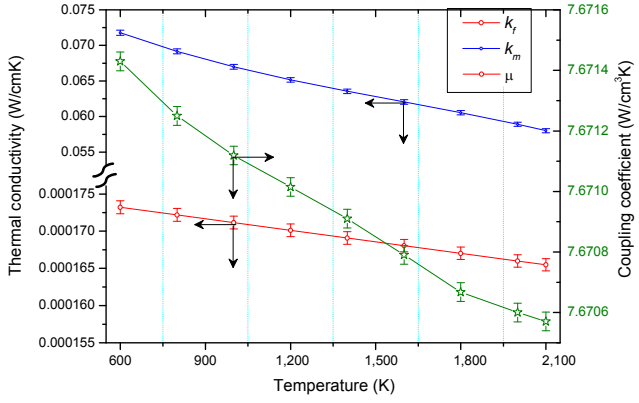

Fig. 12 – Temperature-dependent homogenized parameters (k_f, k_m, μ).

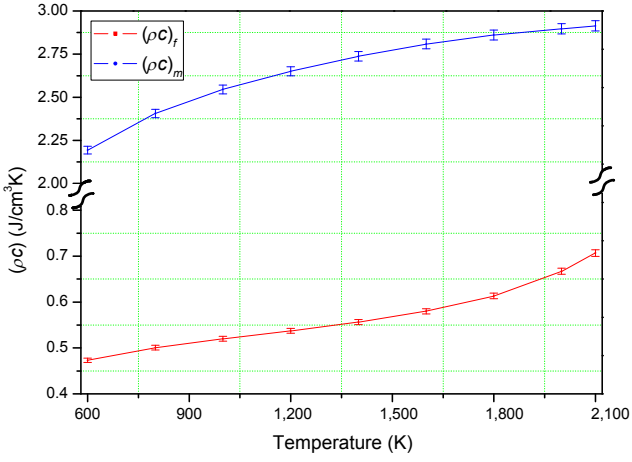

Fig. 13 – Temperature-dependent homogenized parameters [$(\rho c)_f$, $(\rho c)_m$].

Table 4 – List of coefficients in Eqs. (22–26).

Coefficient	Eq. (22)	Eq. (23)	Eq. (24)	Eq. (25)	Eq. (26)
α_0	1.7630E−04	8.3634E−02	7.6721E+00	1.5810E−01	1.7574E−01
α_1	−5.1550E−09	−2.5845E−05	−4.9082E−07	1.1300E−03	6.6300E−03
α_2	−4.5436E−23	1.1642E−08	−2.7521E−09	−1.5742E−06	−8.0928E−06
α_3	3.2616E-26	−2.4503E−12	4.0776E−12	1.1934E−09	5.4314E−09
α_4	−1.2136E−29	−2.3154E−30	−2.2298E−15	−4.6203E−13	−1.8469E−12
α_5	1.7119E−33	1.4213E−34	4.2362E−19	7.4705E−17	2.4785E−16

depending on the random arrangements, there is < 1% difference in the homogenized parameters, yielding ~5 K difference in terms of temperature profiles.

In Part I, we discussed the two-temperature homogenized model for the FCM fuel in which TRISO particles are randomly dispersed. The two-temperature homogenized model for the FCM fuel element was obtained by a particle transport Monte Carlo calculation applied to the pellet region consisting of TRISO particles randomly dispersed in a SiC matrix. Homogenized parameters in the model were obtained by (1) matching steady-state analytic solutions of the model with the results of particle transport Monte Carlo method for heat conduction problems and (2) preserving total enthalpies in the fuel kernels and SiC matrix, respectively. The homogenized parameters have two desirable properties: (1) they are insensitive to boundary conditions such as coolant bulk temperatures and the thickness of cladding, and (2) they are independent of operating power density. Thus, with one reference heterogeneous calculation, the parameters can be applied to various cases of the FCM fuel elements having different cladding thicknesses, coolant bulk temperatures, and operating power densities. By performing the Monte Carlo calculations with the temperature-dependent thermal properties of the constituent materials of the FCM fuel, temperature-dependent homogenized parameters were obtained.

The homogenized parameters obtained in this study are insensitive to random arrangements with the same packing fraction. There is < 1% difference in the homogenized parameters depending on the random arrangement, which yields ~5 K difference in terms of temperature profiles.

Since the two-temperature homogenized model is obtained by heterogeneous calculations of the FCM fuel element via the particle transport Monte Carlo calculation, this model can give more realistic temperature profiles in the pellet. Moreover, it can distinguish between fuel-kernel and SiC matrix temperatures. Especially, the availability of the fuel-kernel temperature profile will allow incorporation of Doppler temperature feedback more realistically in transient scenarios.

Part II describes a reactor core loaded by FCM fuels, in which TRISO particles are randomly distributed in FLS structures. This reactor core is analyzed via the two-temperature homogenized model at steady and transient states, coupling the two-temperature homogenized model with the COREDAX neutron diffusion model.

Conflicts of interest

All authors have no conflicts of interest to declare.

REFERENCES

[1] S.J. Zinkle, K.A. Terrani, J.C. Gehin, L.J. Ott, L.L. Snead, Accident tolerant fuels for LWRs: a perspective, J. Nucl. Mater. 448 (2013) 374–379.

[2] K.A. Terrani, L.L. Snead, J.C. Gehin, Microencapsulated fuel technology for commercial light water and advanced reactor application, J. Nucl. Mater. 427 (2012) 209–224.

[3] K.A. Terrani, L.L. Snead, J.C. Gehin, Fully ceramic microencapsulated fuels for LWRs, Trans. Am. Nucl. Soc. 106 (2012) 1106–1107.

[4] A.C. Kadak, R.G. Ballinger, M.J. Driscoll, S. Yip, D.G. Wilson, H.C. No, J. Wang, H. MacLean, T. Galen, C. Wang, J. Lebenhaft, T. Zhai, D.A. Petti, W.K. Terry, H.D. Gougar, A.M. Ougouag, C.H. Oh, R.L. Moore, G.K. Miller, J.T. Maki, G.R. Smolik, D.J. Varacalle, Modular Pebble Bed Reactor Project: University Research Consortium Annual Report, INEEL/EXT-2000–01034, Idaho National Engineering & Environmental Laboratory, Idaho, 2000.

[5] R. Stainsby, M. Worsley, A. Grief, F. Dawson, M. Davies, P. Coddington, J. Baker, A. Dennier, Development of local heat transfer models for safety assessment of high temperature gas-cooled reactor cores—Part I: pebble bed reactors, J. Eng. Gas Turbines Power 132 (2010) 01296.

[6] J. Hashin, S. Shtrikman, A variational approach to the theory of the effective magnetic permeability of multiphase materials,, J. Appl. Phys. 33 (1962) 127–140.

[7] V. Marelle, F. Huet, P. Lemoine, Thermo-mechanical modeling of U-Mo fuels with MAIA, 8th International Topical Meeting on Research Reactor Fuel Management, Munich (Germany), March 21–24, 2004.

[8] R.C. Progelhof, J.L. Throne, Method for predicting the thermal conductivity of composite systems: a review, Ploym. Eng. Sci. 16 (1976) 615–625.

[9] J. Chang, Homogenization of thermal conductivity in a periodic structure, Korean Nuclear Society Spring Meeting, Jeju (Korea), May 5–7, 2015.

[10] N.Z. Cho, Particle transport Monte Carlo method for heat conduction problems, in: V.S. Vikhrenko (Ed.), Heat Conduction—Basic Research, chapter 13, InTech, Rijeka (Croatia), 2011.

[11] B.H. Cho, N.Z. Cho, Monte Carlo method extended to heat transfer problems with non-constant temperature and convection boundary conditions, Nucl. Eng. Technol. 40 (2010) 65–72.

[12] J. Shentu, S. Yun, N.Z. Cho, A Monte Carlo method for solving heat conduction problems with complicated geometry, Nucl. Eng. Technol. 39 (2007) 207–214.

[13] J.H. Song, N.Z. Cho, Temperature distributions in a pebble with dispersed fuel particles calculated by Monte Carlo method, Trans. Am. Nucl. Soc. 98 (2008) 443–445.

[14] J.H. Song, N.Z. Cho, An improved Monte Carlo method applied to the heat conduction analysis of a pebble with dispersed fuel particles, Nucl. Eng. Technol. 41 (2009) 279–286.

[15] Y. Lee, N.Z. Cho, HEATON—a Monte Carlo code for thermal analysis of fuel element with randomly dispersed TRISO

particles, NURAPT-15–01 [Internet]. Korea Advanced Institute of Science and Technology, 2015. Available from: http://nurapt.kaist.ac./kr/NurapT-Archives/NurapT-15-01.pdf.
[16] N.Z. Cho, H. Yu, J.W. Kim, Two-temperature homogenized model for steady-state and transient thermal analyses of a pebble with distributed fuel particles, Ann. Nucl. Energy 36 (2009) 448–457 see also Corrigendum, Ann. Nucl. Energy 37 (2010) 1793.
[17] Y. Lee, N.Z. Cho, Three-dimensional single-channel thermal analysis of fully ceramic microencapsulated fuel via two-temperature homogenized model, Ann. Nucl. Energy 71 (2014) 254–271.
[18] Y. Lee, N.Z. Cho, Steady- and transient-state analyses of fully ceramic microencapsulated fuel loaded reactor core via two-temperature homogenized thermal-conductivity model, Ann. Nucl. Energy 76 (2015) 283–296.
[19] H. Yu, N.Z. Cho, Comparison of Monte Carlo simulation models for randomly distributed particle fuels in VHTR fuel element, Trans. Am. Nucl. Soc. 95 (2006) 719–721.
[20] Y. Lee, N.Z. Cho, Nuclear–thermal analysis of fully ceramic microencapsulated fuel with randomly dispersed TRISO particles via two-temperature homogenized model, Presented in Reactor Physics Asia 2015 (RPHA15) Conference, Jeju (Korea), September 16–18, 2015.
[21] K.A. Terrani, J.O. Kiggans, C.M. Silva, C. Shih, Y. Katoh, L.L. Snead, Progress on matrix SiC processing and properties for fully ceramic microencapsulated fuel form, J. Nucl. Mater. 457 (2015) 9–17.
[22] B. Cho, N.Z. Cho, Theory Manual for the Rectangular Three-Dimensional Diffusion Nodal Code COREDAX-2, Version 1.0, NURAPT-2014-01, Korea Advanced Institute of Science and Technology, 2014.
[23] Y. Lee, B. Cho, N.Z. Cho, Steady- and transient-state analyses of fully ceramic microencapsulated fuel with randomly dispersed TRISO particles via two-temperature homogenized model—II: applications by coupling with COREDAX, Nucl. Eng. Technol. 48 (2016) 660–672.
[24] S.B. Ross, M.S. El-Genk, Thermal conductivity correlation for uranium nitride fuel between 10 and 1923 K, J. Nucl. Mater. 151 (1988) 313–317.
[25] International Atomic Energy Agency (IAEA), Thermophysical properties database of materials for light water reactor and heavy water reactors, IAEA-TECDOC-1496, Vienna (Austria), 2006.
[26] L.L. Snead, T. Nozawa, Y. Katoh, T.S. Byun, S. Kondo, D.A. Petti, Handbook of SiC properties for fuel performance modeling, J. Nucl. Mater. 371 (2007) 329–377.
[27] N.R. Brown, H. Ludewig, A. Aronson, G. Raitses, M. Todosow, Neutronic evaluation of a PWR with fully ceramic microencapsulated fuel. Part I: lattice benchmarking, cycle length, and reactivity coefficient, Ann. Nucl. Energy 62 (2013) 538–547.
[28] N.R. Brown, H. Ludewig, A. Aronson, G. Raitses, M. Todosow, Neutronic evaluation of a PWR with fully ceramic microencapsulated fuel. Part II: nodal core calculations and preliminary study of thermal hydraulic feedback, Ann. Nucl. Energy 62 (2013) 548–557.
[29] B.P. Collin, Modeling and analysis of UN TRISO fuel for LWR application using the PARFUME code, J. Nucl. Mater. 451 (2014) 65–77.
[30] D. Petti, P. Martin, M. Pélip, R. Ballinger, Development of Improved Models and Designs For Coated-Particle Gas Reactor Fuels: Final Report under the International Nuclear Energy Research Initiative (I-NERI), INEEL/EXT-05–02615, Idaho National Engineering & Environmental Laboratory, Idaho, 2004.
[31] L.L. Snead, K.A. Terrani, Y. Katoh, C. Silva, K.J. Leonard, A.G. Perez-Bergquist, Stability of SiC-matrix microencapsulated fuel constituents at relevant LWR conditions, J. Nucl. Mater. 448 (2013) 389–398.
[32] B. Szpunar, J.A. Szpunar, Thermal conductivity of uranium nitride and carbide, Int. J. Nucl. Energy 2014 (2014) 178360.