Comparison of Two-Temperature Homogenized Model and Conventional Volumetric-Average Thermal Conductivity Model in Fully Ceramic Microencapsulated Fuel

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1. Introduction

As an accident tolerant fuel (ATF) concept, fully ceramic microencapsulated (FCM) fuel concept has been proposed by Oak Ridge National Laboratory [1].

The FCM fuel has a similar configuration to a fuel in the VHTRs, i.e., it consists of TRISO particles randomly dispersed in SiC matrix. For thermal analysis of fuel elements in VHTRs, volumetric-average thermal conductivity model was used [2]. However, it is not conservative in that thus obtained temperature profiles are lower than real values. Moreover, this model is unable to provide fuel-kernel and graphite matrix temperatures separately.

Recently, the authors applied a two-temperature homogenized model to the thermal analysis of the FCM fuel element [3, 4]. This model provides more realistic temperatures, e.g., providing fuel-kernels and SiC matrix temperature separately.

In this paper, we compare the two-temperature homogenized model, conventional volumetric-average thermal conductivity model, and harmonic-average thermal conductivity model in neutronic and thermal analysis of FCM fuel element, e.g., comparing eigenvalues and power distributions due to different thermal analysis model, and temperature profiles in the hottest single-channel.

2. Volumetric-Average Thermal Conductivity and Two-Temperature Homogenized Model for FCM Fuel Element

2.1 Harmonic- and volumetric-Average Thermal Conductivity

For thermal analysis of composites, the effective thermal conductivity is used. The Wiener bounds confine the effective thermal conductivity of a composite [5]. The following harmonic- and volumetric-average thermal conductivities serve as lower and upper bounds, respectively :

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

$$\text{Volumetric-average}: \bar{k} = \frac{\sum V_i k_i}{V}, \tag{2}$$

where i is material index in the composite.

In the thermal analysis of VHTRs, volumetric-average thermal conductivity is usually used [2]. In the FCM fuel element with packing fraction of 0.388, the harmonic- and volumetric-average thermal conductivities would be :

$$\underline{k} = \frac{V}{\sum V_i k_i} = 0.034\,\text{W/cmK}, \tag{3}$$

$$\bar{k} = \frac{\sum V_i k_i}{V} = 0.075\,\text{W/cmK}, \tag{4}$$

where thermal conductivities of the constituent materials in the FCM fuel pellet and their configurations are listed in Table I.

Table I. FCM fuel pellet configuration

Layer	Radius (cm)	Thermal conductivity (W/cmK)
Kernel	0.0425	0.02
Buffer	0.0475	0.005
Inner PyC	0.0510	0.04
SiC	0.0545	0.1
Outer PyC	0.0580	0.04
SiC matrix	0.0580	0.1

2.2 Two-Temperature Homogenized Model

Fig. 1 shows a heterogeneous FCM fuel as manufactured, in comparison with a homogenized FCM fuel that we would like to construct as a model.

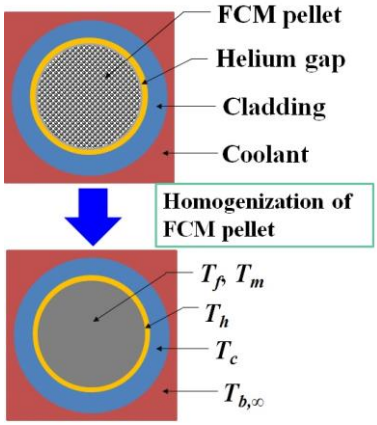

Fig. 1. Two-temperature homogenized model for FCM fuel element

In the homogenized model, FCM pellet region of the fuel element is represented by an imaginary homogeneous media characterized by two temperatures. The

medium representing fuel-kernels is to be characterized with thermal conductivity k_f and temperature T_f. Similarly, the medium representing SiC matrix is to be characterized with thermal conductivity k_m and temperature T_m. In order to consider the heat conduction from fuel-kernels to SiC matrix, we introduce a new parameter, μ. We call k_f, k_m, μ as homogenized parameters.

In the homogenized FCM pellet region, we write heat conduction equations for steady-state with homogenized parameters :

$$k_f \nabla^2 T_f - \mu\left(T_f - T_m\right) + q''' = 0, \quad (5)$$

$$k_m \nabla^2 T_m + \mu\left(T_f - T_m\right) = 0, \quad (6)$$

where q''' is homogenized power density determined as :

$$q''' = \frac{\sum_i q'''_{fi} V_{fi}}{V_{pellet}}, \quad (7)$$

q'''_{fi} is power density of i-th fuel kernel and V_{fi} is volume of i-th fuel-kernel and V_{pellet} is volume of pellets and the homogenized parameters are obtained by matching analytic solutions of Eqs. (5) and (6) with the results from Monte Carlo method [3, 6].

In the helium gap and SiC cladding, we have :

$$k_h \nabla^2 T_h = 0, \quad (8)$$

$$k_c \nabla^2 T_c = 0, \quad (9)$$

where k_h and k_c are thermal conductivities of helium gap and SiC cladding, respectively.

The interface and boundary conditions are also written as :

i) at the interface between FCM pellet and helium gap,

$$-k_h \nabla T_h = -A_f k_f \nabla T_f - A_m k_m \nabla T_m, \quad (10)$$

where A_f and A_m are the fraction of effective interface areas associated with the fuel-kernel and the SiC matrix, respectively,

ii) at the interface between helium gap and SiC cladding,

$$-k_h \nabla T_h = -k_c \nabla T_c, \quad (11)$$

iii) at the boundary SiC cladding and adjacent to coolant,

$$-k_c \nabla T_c = h(T_{cb} - T_b). \quad (12)$$

2.3 Coupling of Thermal Analysis Model with Neutron Diffusion Nodal Method

Neutron diffusion model based on nodal expansion method (NEM) is coupled with thermal analysis models explained Sections 2.1 and 2.2. Temperature-dependent two-group cross sections are generated by lattice calculation using the Serpent code with temperature-dependent continuous cross section libraries processed by the NJOY code.

The assembly-averaged power distributions at each axial plain, calculated by NEM calculation, are divided by the number of fuel rods in the fuel assembly in order to obtain power distributions in the FCM fuel element. Then, single-channel thermal analysis is performed by one of the three thermal analysis models; two-temperature homogenized model, harmonic-, and volume-average thermal conductivity model. Average temperatures at each axial plane are then calculated to update two-group cross sections for NEM calculation. The iterations are performed until assembly-averaged power distributions converge. The calculational procedures are summarized in Fig. 2.

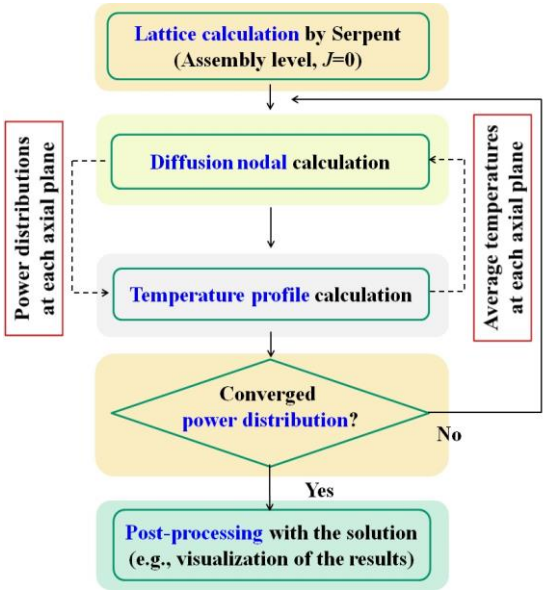

Fig. 2. Calculational procedures of neutronic and thermal analysis of FCM fuel

3. Numerical Results

Reactor configuration is shown in Tables II and III, and Fig. 4. Packing fraction of the pellet is 0.388. Boron concentration is set to 500 ppm. In the lattice calculation, the geometry of the assembly is derived from Westinghouse 17x17 assembly.

Table II. FCM fuel element configuration

Layer	Radius (cm)
Pellet	0.4095
Helium gap	0.4180
Cladding	0.4750
Pitch	1.26

Table III. Reactor configuration

Parameter		Value
Power [MW]		70.0
Enrichment of the fuel [w/o]		20
# of fuel assemblies		9
Assembly Type		Westinghouse 17x17
# of fuel rods per assembly		265
# of guide tubes per assembly		24
Active length [cm]		365.8
Guide tube	inner diameter [cm]	1.123
	outer diameter [cm]	1.204
Coolant inlet temperature [K]		555.8

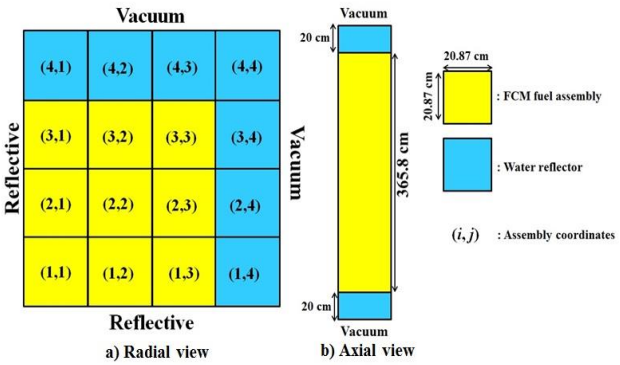

Fig. 4. Radial and axial views of the reactor

In contrast to the 2-D FEM/1-D FDM hybrid method in prismatic block type VHTR application [7], 2-D FDM in *R-Z* geometry is used in this study to calculate temperature profiles in the FCM fuel element. Computation conditions of the 2-D FDM are shown in Table IV. Also, computation conditions for NEM are shown in Table V. Homogenized parameters and thermophysical coefficients used in the two-temperature homogenized model (TTHM), harmonic-(HATC), and volumetric-average thermal conductivity model (VATC) are shown in Table VI.

Table IV. Computation conditions of 2-D FDM in *R-Z* geometry

Parameter		Value
Element type		Triangular
# of cells in axial direction		36 (Δz=10.16 cm)
# of cells in .radial direction	Pellet	30 (Δr_f=0.01365 cm),
	Gap	10 (Δr_h=8.5E-4 cm)
	Cladding	20 (Δr_c=0.00285 cm)
Matrix equation solver		BICGSTAB
Preconditioner		Symmetric Gauss-Seidel
Convergence criterion		1.0E-07

Table V. Computation conditions of NEM

Parameter		Value
Cell size (x,y,z) [cm]	Fuel	10.435, 10.435, 10.16
	Reflector	10.435, 10.435, 10
Matrix equation solver		Sweeping
Source convergence criterion		1.0E-06

Table VI. Homogenized parameters and thermophysical coefficients

Parameters	TTHM	HATC	VATC
k_f (W/cmK)	0.00412	N/A	N/A
k_m (W/cmK)	0.04032		
μ (W/cm^{3}K)	7.617		
A_f	0.18		
$\bar{k}$ (W/cmK)	N/A	N/A	0.075
$\underline{k}$ (W/cmK)	N/A	0.034	N/A
k_f (W/cmK)	0.0036		
k_c (W/cmK)	0.1		
h (W/cm^{2}K)	4.223		

Eigenvalues and power distributions from NEM calculations with two-temperature homogenized model, harmonic- and volumetric-average thermal conductivity model are shown in Table VII, Figs. 5 and 6. Differences in k_{eff} eigenvalues due to thermal analysis models are not negligible.

Table VII. Comparison of eigenvalues

	Thermal analysis model		
	TTHM	HATC	VATC
k_{eff}	1.147208	1.146568	1.147394
Difference[1] [pcm]	N/A	-63.99	+18.57

[1] Difference= HATC (or VATC)-TTHM

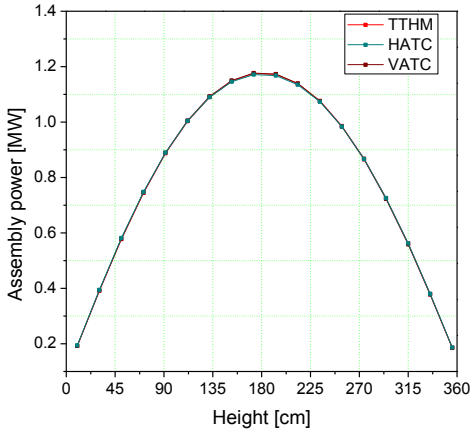

Fig. 5. Axial power distributions of the assembly (1,1)

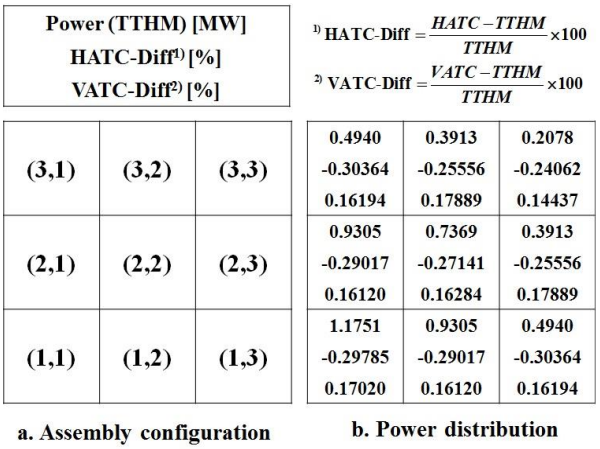

Fig. 6. Power distribution at the elevation of z=172.72 cm

Axial temperature profiles at the centerline of FCM fuel element in the assembly (1,1) and its radial temperature profiles at the elevation of 172.72 cm are shown in Figs. 7 and 8, respectively. Note that difference in maximum temperatures between two-temperature homogenized model and harmonic-average thermal conductivity model is 112.6 K. The difference between two-temperature homogenized model and volumetric-average thermal conductivity model is 162. 8 K.

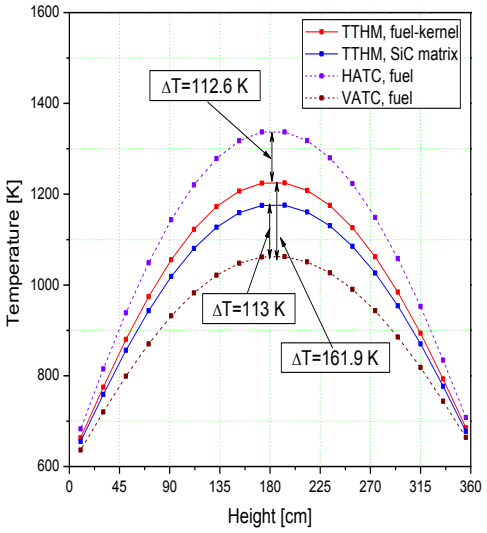

Fig. 7. Axial temperature profiles at the centerline of the FCM fuel element in assembly (1,1)

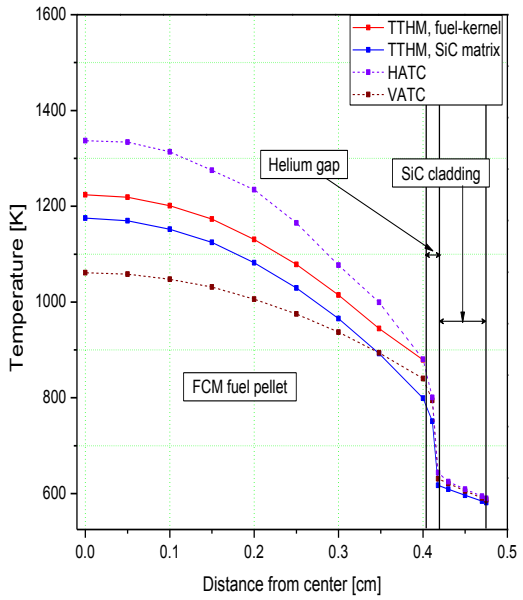

Fig. 8. Radial temperature profiles at the elevation of z=172.72 cm

4. Conclusions

Coupling with neutron diffusion nodal model based on nodal expansion method, we compared the two-temperature homogenized model, harmonic-, and volumetric-average thermal conductivity model on the neutronic and thermal analysis of the FCM fuel. In terms of neutronics results, Differences in eigenvalues due to the three thermal analysis models are not negligible i.e., showing several tens of pcm differences in eigenvalues.

Meanwhile, the three thermal analysis models show significant differences in temperature profiles. The two-temperature homogenized model gives ~110 K lower maximum temperature than that from harmonic-average thermal conductivity model, and ~160 K higher maximum temperature than that from volumetric-average thermal conductivity model. Since the two-temperature homogenized model is developed using heterogeneous calculations of the FCM fuel element, we can obtain more realistic temperature profiles by the two-temperature homogenized model.

In this study, we assumed that homogenized parameters are independent of temperatures, burnup, etc. Since the parameters are equivalent to thermal conductivities in general heat conduction equations, temperature and burnup dependence of the homogenized parameters are actually not negligible. Therefore, as a future work, we will study temperature and burnup dependence of the homogenized parameters. With the temperature and burnup dependent homogenized parameters, comparison of the two-temperature homogenized model and volumetric-average thermal conductivity model in transient scenarios is also an important future work, in particular for the Doppler temperature feedback, since the two-temperature homogenized model can provide fuel-kernel temperatures while volumetric-average thermal conductivity model cannot.

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