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Effects of Particle Size and Shape on U-Mo/Al Thermal Conductivity

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1. Introduction

The thermal conductivity of U-Mo/Al dispersion fuels is one of the most important material properties in determining the performances of the fuels. However, there is no enough measured data for it. The thermal conductivity of atomized U-Mo/Al dispersion fuels was measured only by Lee et al. [1] by laser-flash and differential scanning calorimetry (DSC) methods. As a result, an analytical model instead of an empirical model was developed from the Commissariat à l'Énergie Atomique (CEA) [2] by modifying the Hasin and Shtrikman model [3].

This model assumes that dispersed particles are spherical. Actually, however, dispersed particles are not perfect sphere. For the U-Mo particles, they are deformed during manufacturing process such as hot rolling and during irradiation by the creep deformation. Fricke [4] developed a model for the effective thermal conductivity of a dilute suspension of randomly oriented spheroidal particles. In general, the thermal conductivity of composite increase when the particle shape is not sphere.

This model is also based on continuum theory which assumes both temperature and heat flux are continuous across the interface. Kapitza [5], however, showed that there is a discontinuity in temperature across the interface at metal/liquid helium interface. In general, the discontinuity is from the thermal resistance at the interface. If the thermal resistance has a significant impact on the thermal conductivity, particle size is one of the essential parameter for determining the effective thermal conductivity of composite materials. Every, et al modified Bruggeman model to consider the interfacial thermal resistance. [6]. The U-Mo/Al dispersion fuel thermal conductivity calculation can be improved by considering the anisotropic effects and interface thermal resistances.

There have been various works to analyze the thermal conductivity through Finite Element Method (FEM). Coulson [7] developed a realistic FEM model to calculate the effective thermal conductivity of the fuel meat. This FEM model does not consider the anisotropic effects and interface thermal resistances. Therefore, these effects can be evaluated by comparing the FEM calculated effective thermal conductivity with measured data. In this work, the FEM analysis was done and the anisotropic effects and interface thermal resistances was estimated. From this results, the particle shape and size effects will be discussed.

2. Models and Methods

In this section, some mathematical models which are widely used for calculating the effective thermal conductivity, will be reviewed and the descriptions for the FEM model will be introduced.

2.1 Mathematical Models

Some theoretical models based on the electrostatic theory were developed and proposed by many researchers. Maxwell [8] developed a model in which a spherical particle is embedded in infinite discontinuous phase. He assumed that the spherical discontinuous phase was in small quantity so that the mutual interactions between particles were negligibly small and obtained a following formula:

$$k_{eff} = k_m \left[\frac{2k_m + k_p - 2V_p\left(k_m - k_p\right)}{2k_m + k_p + V_p\left(k_m - k_p\right)} \right] \quad (1)$$

where k_{eff} is the effective thermal conductivity of the composite material, and k_p and k_m are the thermal conductivity of particle and matrix respectively, and V_p is the volume fraction of particle.

Because of the assumptions made in the derivation of this model, however, Equation (1) is limited for dilute dispersions where the particle concentration is less than 10 to 15 volume percent [9]. Bruggeman [10] developed a more general equation applicable for any concentration by first differentiating the Maxwell equation and then integrating between the appropriate limits. The equation was suggested as follows:

$$k_{eff} = k_p + \left(1 - V_p\right)\left(k_m - k_p\right)\left(\frac{k_{eff}}{k_m}\right)^{1/3} \quad (2)$$

The applicable range of this model is where the particle volume fraction is no more than 74.05 volume percent which is the maximum packing density for spheres [9].

Some works were done on the anisotropic effects of particles considering the particle shape is spheroid. Fricke [4] developed a model for the effective thermal conductivity of a dilute suspension of randomly oriented spheroidal particles [11, 12]:

$$k_{eff} = k_m \left(\frac{Xk_m + k_p - XV_p\left(k_m - k_p\right)}{Xk_m + k_p + V_p\left(k_m - k_p\right)} \right) \quad (3)$$

where X is the dimensionless shape factor given by:

$$X = \frac{k_m + k_p(\beta - 1)}{k_p - k_m(\beta + 1)} \quad (4)$$

and β is a function of particle shape and orientation:

$$\beta = \frac{\delta - 1}{3}\left[\frac{2}{1+(\delta-1)f^{(x)}} + \frac{1}{1+(\delta-1)f^{(z)}}\right] \quad (5)$$

where δ is a dimensionless parameter, defined as ratio of thermal conductivities of particle and medium:

$$\delta = k_p / k_m \quad (6)$$

and $f^{(x)}$ and $f^{(z)}$ are defined as depolarization factors and expressed as follows:

$$f^{(z)} = \frac{1-e^2}{e^3}\left(\tanh^{-1}(e) - e\right) \quad (7)$$

$$f^{(x)} = \left(1 - f^{(z)}\right)/2 \quad (8)$$

which depend on the geometry of the particle through its eccentricity *e*, which is always less than 1:

$$e = \sqrt{1 - \left(\frac{b}{c}\right)^2} \quad (9)$$

where b and c are spheroidal polar and equatorial radii respectively.
The Fricke models, however, are assuming constant particle size and aspect ratio. It is clear that there exist distributions of particle size and aspect ratio in dispersed particles. Cherkasova [12] showed that the volume-weighted aspect ratio for randomly distributed particles give most consistent results. For N random particles dispersed, β can be defined as follows:

$$\beta = \frac{1}{3}(\delta - 1)\frac{\sum_1^N V_i\left(\frac{2}{1+(\delta-1)f^{(x)}} + \frac{1}{1+(\delta-1)f^{(z)}}\right)}{\sum_1^N V_i} \quad (10)$$

Anisotropic Correction Factor (ACF) was suggested as the ratio of the effective conductivity predicted by the Fricke model to that predicted by the dilute dispersion model:

$$\text{ACF} = \frac{\text{Equation (3)}}{\text{Equation (1)}} \quad (11)$$

The previous models do not consider the thermal resistance which cause a discontinuity in temperature or heat flux at interface. Every et al. [6] modified the Bruggeman model by taking the interfacial thermal barrier resistance into consideration:

$$\left(1 - V_p\right)^3 = \left(\frac{k_m}{k_{eff}}\right)^{\frac{1+2\alpha}{1-\alpha}}\left(\frac{k_{eff} - k_p(1-\alpha)}{k_m - k_p(1-\alpha)}\right)^{\frac{3}{1-\alpha}} \quad (12)$$

where the dimensionless parameter α is given by:

$$\alpha = \frac{R_b k_m}{a} \quad (13)$$

where *a* is the radius of the particles and R_b is a thermal boundary resistance.

Interfacial Resistance Correction Factor (IRCF) can be suggested as follows:

$$\text{IRCF} = \frac{\text{Equation (12): } \alpha \neq 0}{\text{Equation (12): } \alpha = 0} \quad (14)$$

2.2 FEM Model Description

A Python module described in the work of Coulson [7] was used to generate a random distribution of particles based on the particle distribution data used in KOMO-2 experiments at KAERI [13]. Randomly distributed particles were placed in a region of 600×300×600μm with various fuel volume fractions: 10%, 20%, 30%, and 40%. ABAQUS then generated this random particles and then cut it as a 300×300×300μm section as shown in Fig. 1.

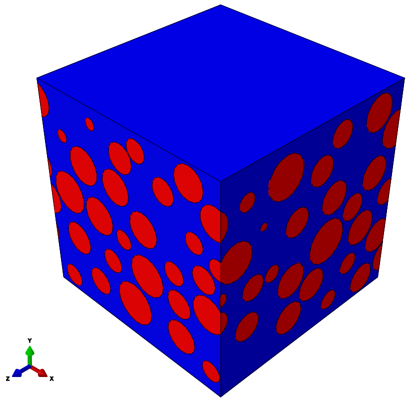

Fig. 1 FEM model for a volume fraction of 40 vol%.

The thermal conductivity of U-Mo fuel, and Al matrix were implemented into ABAQUS as a function of temperature. The fuel and matrix for the simulation were assumed to be U-10Mo and Al1060, respectively.

For the boundary conditions and loads, the top surface in the y-axis is held at a constant temperature of 400K, while a constant surface heat flux of 1.22×10^{-6} W·μm^{-2} was applied to the opposite surface. All the other sides were adiabatic and did not allow heat to escape. This allowed heat flow through y-direction which was consistent with heat transfer of real plate.

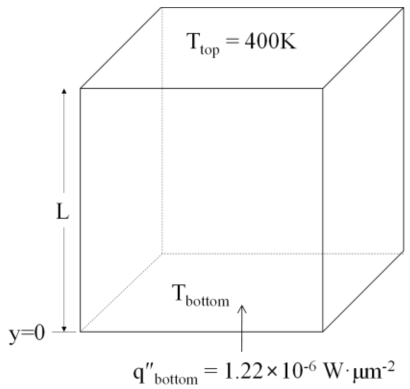

Fig. 2 Boundary condition and load for FEM model.

3. Results and Discussion

The FEM results obtained from this study and from Coulson [7] were compared with the measured data from Lee et al. [1]. Fig. 3 shows that as the volume fractions of the U-Mo fuel increase, the differences between FEM results and measured data increase. It was assumed that the differences may be mainly from the thermal resistance at interfaces. This is because as the volume fraction increases, the interface between particles and matrix increase, thus, the thermal resistance increases.

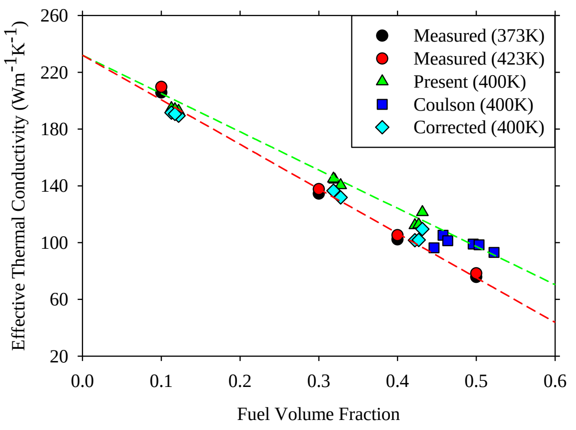

Fig. 3 Comparison of effective thermal conductivity between measured data and FEM results.

The ACF and IRCF were calculated by using the Eq. (11) and Eq. (14) when the particle size is 50 μm and α is 10, 50, and 100. Fig. 4 shows that both ACF and IRCF decrease as the volume fractions of fuel increase. However, ACF shows an extremely small amount of decreases. This is mainly due to the very small aspect ratio of U-Mo particle. IRCF, on the other hand, shows a considerable change compared to ACF. From this results, we can consider interfacial thermal resistances will be the main factor for the differences.

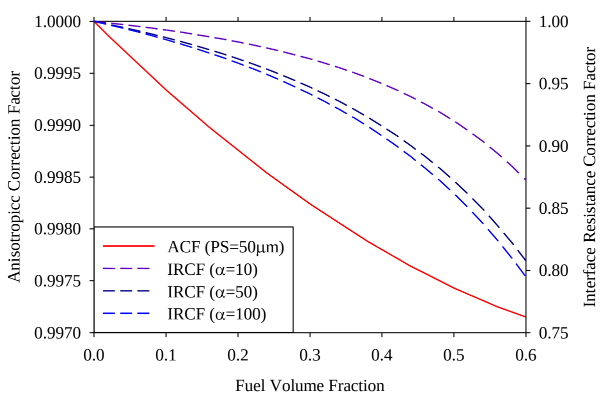

Fig. 4 ACF and IRCF as a function of the fuel volume fraction when particle size is 50 μm and α is 10, 50, and 100, respectively.

The FEM results were corrected considering ACF and IRCF. Fig. 3 shows the corrected values when the IRCF is 50 are close to the measured data. It seems that dimensionless parameter α is a range of 10 to 100 and the thermal boundary resistance, R_b can be calculated by using Eq. (13). As a result, R_b is in a range of 2.156×10^{-6} to 2.156×10^{-5}. With this result, the effective thermal conductivity can be calculated by using the following equation:

$$k_{eff} = \text{ACF} \times \text{IRCF} \times \text{Eq. (2)} \tag{15}$$

Fig. 5 shows the effective thermal conductivity as a function of particle size when the volume fraction of fuel is 40%. When the particle size is less than 200 μm, a sharp increase of thermal conductivity is observed.

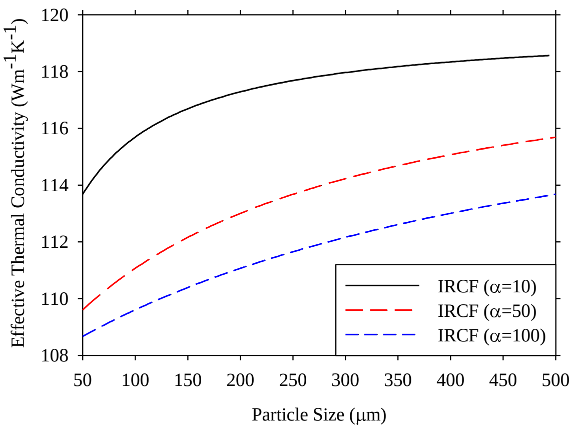

Fig. 5 The effective thermal conductivity as a function of the particle size when the volume fraction is 40%.

4. Conclusions

Many thermal conductivity models for the particle dispersed composites have been developed by many researchers. However, no rigorous basis to determine an effective thermal conductivity for these composites until now. For U-Mo/Al, a modified Hasin and Shtrikman model have been used to calculate the thermal conductivity. This model, however, does not consider particle anisotropic and particle size effects. Fricke [4] and Every et al. [6] developed a thermal conductivity model considering particle shape and interfacial thermal resistance, respectively. We considered this two factors for the calculations by defining ACF and IRCF and the following conclusions can be drawn about U-Mo/Al:

1. The particle anisotropic effects are negligible due to the small aspect ratio.
2. The thermal boundary resistance, R_b is in a range of 2.156×10^{-6} to 2.156×10^{-5} and the thermal conductivity increases as the particle size increases.

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