Heat Generation Effects on U-Mo/Al through Abaqus FEM Simulation

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1. Introduction

U-Mo/Al dispersion fuels have been considered a most promising candidate for a replacement of Highly Enriched Uranium (HEU) fuel in many research reactors. The thermal conductivity of U-Mo/Al dispersion fuels is one of the most important material properties in determining the performances of the fuels. There are considerable decreases in thermal conductivity during reactor operation due to the chemical interaction between U-Mo particles and Al matrix.

For the thermal conductivity of U-Mo dispersion fuel, there are no enough measured data because measuring it is both difficult and expensive. As a result, an analytical model instead of an empirical model was developed from the Commissariat à l'Énergie Atomique (CEA) by modifying the Hasin and Shtrikman model. This model has been used to calculate the thermal conductivity of the dispersion fuel meat. However this model is assuming the homogenization of fuel meat, thus there have been various works to analysis the thermal conductivity through Finite Element Method (FEM).

Coulson [1] developed a FEM model which show the fuel meat realistically and compared the thermal conductivity results of two and three dimensional model. Williams [2] also developed a FEM model which are different from the former in that it use regularly meshed unit cells. He showed a heat generation effects through FEM simulation and the effective thermal conductivity of the fuel with heat generated in the fuel particles is a little lower than that of the fuel with no heat generated.

There are no ways to see the heat generation effect through experiments. This can be analyzed through the finite element method. In the current work, the heat generation effects are analyzed and discussed in a wider range of volume fraction with more realistic models by using ABAQUS finite element package.

2. Model Description

2.1 Model Geometry

A Python module described in the work of Coulson [1] is used to generate a random distribution of particles based on the particle distribution data used in KOMO-2 experiments at KAERI [3]. Random distributed particles with uniform interaction layers (ILs) are placed in a region of $600\times(300+2\cdot\text{IL})\times600\mu\text{m}$ with various fuel volume fractions: 10%, 20%, 30%, and 40%. ABAQUS CAE then generate this random particles and then cuts it as a $300\times(300+2\cdot\text{IL})\times300\mu\text{m}$ section as shown in Fig. 1.

By leaving the original section through y-axis, the edge effects associated with the packing of the fuel particles are minimized and uniform loads and boundary conditions are applied.



Fig. 1. Model of $300 \times 310 \times 300$ µm with a Volume Fraction of 40 vol% and an Interaction Layer Thickness of 5 µm

2.2 Material Properties

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

The thermal conductivity of U-10Mo is from the U-Mo Fuels Handbook [4]. The thermal conductivity of Al1060 was measured by Lee [5] and a fitting equation from it was used. The interaction layer was assumed to be UAl_{3.5} considering most interaction layer observed are in a composition of UAl₃ and UAl₄. There is no measured thermal conductivity data for the ILs until now. Lee et al. [6] measured the thermal conductivity of the heat treated dispersion fuel. This result makes it possible to estimate the thermal conductivity of the ILs in the similar manner of William [2] by choosing a value which best matched the observed degradation as a function of the volume fraction of the ILs. The thermal conductivity of ILs is chosen as 3 W/m/K. Fig. 2 shows the thermal conductivity degradation of U-10wt%Mo dispersion fuel with the IL volume fraction through this simulation. The thermal conductivity decreases almost linearly with the IL volume fraction.



Fig. 2. Thermal Conductivity Comparison with Measured Data on U-10wt%Mo Dispersion Fuel Reported by Lee [6].

2.3 Boundary Conditions and Loads

To evaluate heat generation effects, two different boundary conditions and Loads are applied to the model.

For the no heat generation case, the top surface in the y-axis is held at a constant temperature of 400K, while a constant surface heat flux of $1.22 \times 10^{-6} \text{ W} \cdot \mu \text{m}^{-2}$ is applied to the opposite surface. All the other sides are adiabatic and do not allow heat to escape. This allows heat flow through y-direction which are consistent with heat transfer of real plate.

For the heat generation case, both top and bottom surface are held at a constant temperature of 400K, while a body heat flux is applied to the fuel particles and to interaction layers to simulate the volumetric heat generation caused by fissions in the similar way of Coulson [1]. The internal heat generation in the fuel and in the interaction layer is assumed to be proportional to the amount of uranium in each and thus, the applied body heat flux are as follows:

$$q_{Fuel}^{\prime\prime\prime} = \frac{q^{\prime\prime}xz}{V_{r_{e},l} + \Gamma \cdot V_{r_{e}}} \tag{1}$$

$$q_{IL}^{\prime\prime\prime} = q_{Fuel}^{\prime\prime\prime} \Gamma \tag{2}$$

where Γ is the uranium ratio between Fuel and ILs and expressed as follows:

$$\Gamma = \frac{N_{U,IL}}{N_{U,Fuel}} = \frac{\rho_{IL}A_{235U}}{\rho_{Fuel}A_{235UAI_3} \left(1 - wt\%Mo\right)}$$
(3)

For this model, Γ of U-10Mo with a UAl_{3.5} as ILs is 0.2809. The applied loads to fuels and ILs are set based on the desired total plate heat flux of $4.88 \times 10^{-6} \text{ W} \cdot \mu \text{m}^{-2}$, which comes from results seen during irradiation of plate R6R018 in the Advanced Test reactor at Idaho National Laboratory [7].

3. Results and Discussion

The model was executed for various fuel conditions to determine the effects of fuel loading, IL volume fraction, and the heat generation. The results of the simulation are presented and discussed below.

3.1 Calculation of the effective thermal conductivity

The effective thermal conductivity is calculated by solving Poisson's equation for one-dimensional heat flow considering that the heat flows along y-direction.

For the no heat generation, the average temperature in the bottom surface are used to calculate the effective thermal conductivity as follows:

$$k_{eff} = \frac{q''L}{\left(T_{Bottom} - T_{Top}\right)} \tag{4}$$

where q'' is surface heat flux, L is the length of plate in the y-direction.

For the heat generation case, the average temperature in the center of the plate are used to calculate the effective thermal conductivity as follows:

$$k_{eff} = \frac{q'''L^2}{8(T_{CL} - T_c)} \tag{5}$$

where q''' is body heat flux, L is the length of plate in the y-direction.

3.2 Comparison to the analytical model

The thermal conductivity of dispersion type fuels have been estimated by using an analytical model developed from CEA [8]. This is compared with the simulation results in Fig. 3 as a function of volume fraction of fuel. It is seen that the CEA model slightly underestimates than present model and the differences increase as the volume fraction of fuel increases.



Fig. 3. Effective Thermal Conductivity Comparison between Present Model and CEA Equation.

3.3 Effect of Heat Generation within the Fuel

The traditional thermal conductivity models are based on the flux law assuming heat has a tendency to flow through more high conductivity regions, thus only a small portion of heat will be transferred through interaction layers if heat is applied to a surface. For U-Mo dispersion fuel surrounded with interaction layers, the heat is generated both in the fuel particle and interaction layers by fission. This is different from when the traditional heat transfer case in that most of heat should pass through interaction layers.

Fig. 4 and Fig. 5 show heat generation effects on thermal conductivity when the volume fraction of fuel is 10% and 20% each. There are considerable decreases in the thermal conductivity when heat is generated. This is because the fuel particles are insulated and the local temperature perturbations increases as seen in Fig. 6. However the heat generation effects begin to decrease



Fig. 4. The Effects of the Heat Generation on the Thermal Conductivity of Dispersion Fuel when the U-Mo is 10 vol%.



Fig. 5. The Effects of the Heat Generation on the Thermal Conductivity of Dispersion Fuel when the U-Mo is 20 vol%.



Fig. 6. The Temperature Distribution of the Dispersion Fuel with a Volume Fraction of 20 vol% and an Interaction Layer Thickness of 13 μm

after a point of volume fraction. This is because most heat have to pass through interaction layers. The results are consistent with that of Williams [2]. Fig. 7 and Fig. 8 also show heat generation effects when the volume fraction of fuel is 30% and 40% each. The observed heat generation effects are small compared with the small volume fraction cases. This is because the small volume fraction of interaction layers are enough to diminish the local temperature perturbation due to its large volume



Fig. 7. The Effects of the Heat Generation on the Thermal Conductivity of Dispersion Fuel when the U-Mo is 30 vol%.



Fig. 8. The Effects of the Heat Generation on the Thermal Conductivity of Dispersion Fuel when the U-Mo is 40 vol%.



Fig. 9. The Temperature Distribution of the Dispersion Fuel with a Volume Fraction of 40 vol% and an Interaction Layer Thickness of 9 μ m

fraction of the fuel as seen in Fig. 9. The above results indicate that when the sum of the volume fraction of fuels and interaction layers exceeds 40-50 vol%, the heat generation effects are diminished.

3.3 Particle size and distribution effects

In the present model, the particle size and distribution follow the case of KOMO-2. However, particle size and its distribution will affect the conduction of heat. First of all, the larger particle size is, the lower actual thermal conductivity will be. It is because there exists thermal resistance between particle and matrix. However, this was not simulated in this model because giving thermal resistance on the boundary of particles and matrix is limited in ABAQUS. Particle distribution itself does not give a remarkable effect in the model. Therefore, the particle size and distribution effects will be not significantly observed in the model when heat is not generated but transferred through the particles and matrix. However, when the heat is generated in the particles, this particle configurations are estimated to give a considerable effects on heat conduction. This will be further studied with other particle configuration data.

4. Conclusions

The FEM model is used to determine the effective thermal conductivity of U-Mo/Al and to simulate the heat generation effects in the study. This model reflected the microscopic morphology of the fuel very well by making random distribution particles although the particle shape is considered as sphere.

All simulation results show the heat generation effects although the effects are small when the volume fraction of fuels are high. When the particles are surrounded with interaction layers, the heat transfer from the particle to matrix is disturbed by interaction layers due to the low thermal conductivity of interaction layers. However this effects decreases when the sum of the volume fraction of fuels and interaction layers exceeds 40-50 vol% because a great portion of the heat must pass through fuels and interaction layers although the heat is applied on the surface. Therefore particle size and initial particle volume fractions will be the important factors for the heat generation effects when interaction layers grow during irradiations.

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