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UO_2-BeO Composite Fuel Thermal Property and Performance Modeling

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Abstract: An enhanced thermal conductivity UO_2-BeO composite nuclear fuel was studied. A methodology to generate ANSYS (an engineering simulation software) FEM (finite element method) thermal models of enhanced thermal conductivity oxide nuclear fuels was developed. The results showed significant increase in the fuel thermal conductivities and have good agreement with the measured ones. Thus BeO is one of the promising candidates for fabricating two-phase high thermal conductivity ceramic nuclear fuels with UO_2. The reactor performance analysis showed that the decrease in centerline temperature was 250-350 K depending on different fabrication methods for the UO_2-BeO composite fuel, and thus we can improve nuclear reactors' performance and safety, and high-level radioactive waste generation for the existing and next generation nuclear reactors.

Key words: UO_2-BeO, composite fuel, thermal conductivity, FEM, ANSYS, temperature difference profiles.

1. Introduction

Commercial light-water reactors currently use UO_2 as a nuclear fuel, which has demonstrated several desirable characteristics. However, UO_2 has a low thermal conductivity that leads to the development of a large temperature gradient across the fuel pellet. This temperature gradient contributes to limits in the operational performance of the reactor due to effects that include thermal stresses causing pellet cladding interaction and the release of fission product gases [1-4].

These high fuel temperatures can be decreased and reactor performance improved by developing an enhanced thermal conductivity nuclear fuel. A high thermal conductivity nuclear fuel would decrease fuel temperatures and facilitate a reduction in pellet cladding interaction through lessening thermal stresses that result in fuel cracking, relocation, and swelling [1, 2]. Additionally, fission gas release would be decreased allowing for higher fuel burn-up, and the safety of the reactor would be improved with a faster thermal response and less stored energy in the fuel pins.

The development of high thermal conductivity ceramic-metallic fuels has been explored in the past. These efforts examined nuclear fuels where UO_2, UO_2-ThO_2 or UO_2-PuO_2 ceramic particles are dispersed in a stainless steel or zirconium alloy metal matrix [2, 5-7]. Other fuels forms include aligned metal fibers dispersed in a ceramic fuel matrix [8]. These fuel designs have mainly focused on cermets, but other options include the development of ceramic-ceramic composites.

A ceramic-ceramic composite nuclear fuel has an increased effective thermal conductivity due to adding a second compatible and high thermal conductivity ceramic to UO_2. SiC and BeO are two materials that demonstrate compatibility with UO_2 and have a high thermal conductivity [9, 10]. The UO_2-BeO phase diagram shows that these two components exist as solid

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equilibrium phases below the temperature of 2,100 °C [11]. Also, UO_2 has been shown to react with SiC to release CO and SiO gases above 1,650 K [12, 13]. These two components are thus excellent candidates for fabricating two-phase ceramic nuclear fuel with UO_2, resulting in high thermal conductivity UO_2-SiC and UO_2-BeO fuels.

The development of ceramic-ceramic composite nuclear fuels benefits from thermal modeling by providing an understanding on how fabrication variables, such as phase fractions, densities, geometry, and effective thermal conductivity. The FEM (finite element method) has been employed in the past [14-16] to determine the thermal conductivities of complex composites. This method can be applied to oxide nuclear fuels to determine their thermal conductivities through the characterization of their microstructures and compositions.

Boey et al. [14] examined the thermal conductivity of AlN (aluminum nitride) when a sintering aid, Y_2O_3, reacted to form Y3AL5O12 (YAG) at the AIN grain boundaries and triple points. The microstructure of the material was studied, along with its composition, in order to generate a model geometry and to choose the thermal conductivity curves of the materials. Then the thermal conductivity was calculated from the FEM thermal model. Ramani and Vaidyanathan [15], and Xu and Yagi [16] developed FEM models which where similar to that of Boey et al. [14], but for the composites with known thermal conductivity. These FEM thermal models thus demonstrate an ability to accurately model the thermal conductivity of composite materials.

Katti et al. [17] and Chawla et al. [18] developed models to solve 3D (three dimensional).FEM problems, respectively. Katti et al. [17] constructed 3D finite element models of nacre based on reported microstructural studies on the “brick and mortar” micro-architecture of nacre. 3D eight noded isoparametric brick elements were used to design the microarchitecture of nacre. Tensile tests were simulated using this model. The results were comparable with the experimental data. Chawla et al. [18] used a serial sectioning process to develop a 3D representation of the microstructure of a SiC particle reinforced Al composite, for visualization and FEM. The Young’s modulus and stress-strain behavior of the composite predicted by the 3D model of microstructure correlated very well with experimental results.

2. ANSYS Thermal Modeling Methodology

ANSYS is an engineering simulation software with main module of multiphysics/structure mechanics. This code is based on the FEM and is capable of performing static (stress) analysis, thermal analysis, modal analysis, frequency response analysis, transient simulation and also coupled field analysis. The methodology to create an ANSYS FEM thermal model of a system was outlined by Moaveni [19]. The basic procedure was to generate a geometry, define the material properties, choose elements, mesh, and solve the model. These steps were universal in each thermal model, with the main differences being the assigned material properties and geometries.

The Fourier heat conduction equation was used in the FEM thermal models and is given as:

$$q_x^{"} = -k\frac{\partial T}{\partial x} \qquad (1)$$

where, $q_x^{"}$ is the heat flux, k is the thermal conductivity, and $\frac{\partial T}{\partial x}$ is the temperature gradient [20]. This equation was located at the element nodes, as showed in Fig. 1. The exact form of the Fourier equation used for the thermal analysis between two nodes is given as:

$$q_x^{"} = k\cdot\frac{\left(T_{i+1}-T_i\right)}{l} \qquad (2)$$

where, $q_x^{"}$ is the heat flux, k is the thermal conductivity, T_{i+1} is the temperature at node $i + 1$, and T_i is the temperature at node i, and is the distance between nodes [19]. A diagram of this FEM thermal analysis system is shown in Fig. 1.

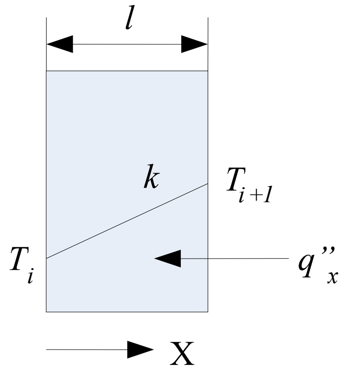

Fig. 1 FEM analysis for heat conduction in a solid between two nodes.

In the Fig. 1 system, the following variables would be known: the temperature at one boundary point, the thermal conductivity of the material, the applied heat flux, and the width of the material. Therefore, when solving the FEM model, a temperature gradient would be developed from heat traveling from one end of the material to the other until steady state temperatures were reached.

A composite material has multiple regions with different thermal conductivities, the effective thermal conductivity of a composite can be determined with FEM analysis of the composite by calculating the temperature gradient, when the heat flux, boundary temperatures, and material thickness are known. This solution requires a manipulation of the Fourier heat conduction equation, which appears as:

$$k_{effective} = q'' \cdot \frac{dx}{dT} \quad (3)$$

where, q'' is the known heat flux, dx is the known thickness, dT is the developed temperature difference, and $k_{effective}$ is the calculated effective thermal conductivity of a composite.

3. FEM Thermal Modeling of UO_2-BeO Nuclear Fuels

The ANSYS FEM thermal was used to predict the thermal conductivity of a nuclear fuel sample. This material was a UO_2-BeO nuclear fuel developed by Nippon Nuclear Fuel Development Co. Ltd. [21]. A comparison is made between the FEM thermal modeling predicted thermal conductivities and the experimentally measured thermal conductivities. The results would demonstrate the ability of the FEM thermal modeling to accurately predict the thermal conductivity of a fabricated fuel sample.

- UO_2-BeO nuclear fuel

The UO_2-BeO nuclear fuel fabrication processed by Ishimoto et al. [21] involved mixing UO_2 and BeO powders together in varying weighted mixtures, which included 0.6, 0.9, 1.2, and 13.6 wt% of BeO in UO_2. These powders were pressed into a pellet and sintered above the eutectic temperature of 2,423 K for an hour. The microstructures of BeO segregated at the UO_2 grain boundaries was formed from this process, as shown in Figs. 2 and 3. The legends of 50 microns and 100 microns are shown in Figs. 2 and 3, respectively.

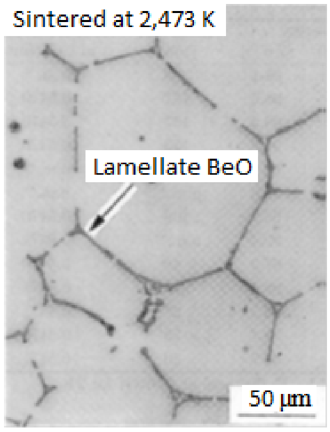

Fig. 2 The micrograph shows that the BeO phase being 0.9 wt% of the fuel and segregated at the UO_2 grain boundaries [21].

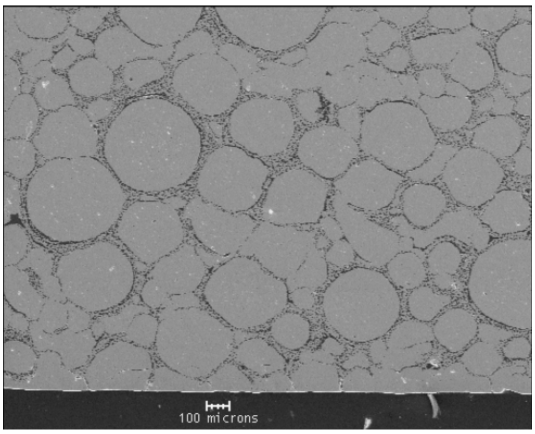

Fig. 3 Micrograph of BeO phase segregated by UO_2 grain boundaries (Kuchibhotla 2004) [9].

Therefore, the low thermal conductivity UO_2 grains were surrounded by a high thermal conductivity almost continuous BeO phase. This high thermal conductivity BeO phase should thus increase the effective thermal conductivity of the nuclear fuel. FEM thermal models were set up to replicate these fuels and the results were compared to the measured thermal conductivities of UO_2/BeO fuels.

- FEM thermal modeling

The FEM thermal models for the UO_2-BeO fuels were set up using a 2D (2 dimensional) grid pattern geometry. This geometric configuration represents the microstructure of the fuel, where BeO was segregated at the UO_2 grain boundaries. This analysis was performed in 2D given that fuel pellet heat flow is primarily directed in the radial direction.

The grid pattern geometry was produced from an automated program developed in Microsoft Excel to calculate the geometric inputs for ANSYS. This automated program calculated the sum of a square area and a thin surrounding perimeter to coincide with the given volume percentages of the two components of the fuel. Ishimoto et al. [21] reported data for grain sizes, which would correspond to the edge length of the square. These values were used as inputs into the geometry generating program, the BeO was assumed to be fully dense with the porosity assigned to the UO_2 phase, as given in Table 1.

Since the UO_2-BeO microstructure has BeO segregated at the UO_2 grain boundaries, the perimeter must have a corresponding thickness based on the grain size to meet a volume percentage ratio. Cells are set up to iterate to a grid pattern geometry that had the correct volume percentage ratio based on the edge length of the square and the thickness of the outside perimeter. The calculation converged in order that the total area of a single square in the grid met these set conditions.

Table 1 UO_2-BeO nuclear fuel sample characteristic data [21].

BeO			UO_2	
wt%	vol%	Width (μm)	Grain size (μm)	Density (%TD)
0.6	2.1	0.84	157	99.4
0.9	3.2	1.25	153	98.0
1.2	4.2	1.18	109	98.7
13.6	36.4	1.80	14.2	99.0

The FEM thermal models with grid pattern geometries were set up using this automated program. These thermal models were developed for UO_2-BeO fuels with 0.6, 0.9, 1.2 and 13.6 wt% of BeO in UO_2 using the data in Table 1. The subsequently calculated geometric values from the automated program were input into ANSYS to generate the fuel geometries, as shown in Fig. 4. Because the first three weight percentages of BeO, 0.6, 0.9 and 1.2 wt%, are very close, and are much smaller compared to the last one, 13.6 wt%, we cannot see the geometrical difference for the first three graphs in Fig. 4.

The UO_2-BeO thermal model geometries shown in Fig. 3 were assigned thermal conductivity curves for their respective UO_2 and BeO regions. The UO_2 thermal conductivity curves were corrected for density differences as reported by Ishimoto et al. [21] in all fuel samples [22]. A thermal conductivity curve as given by Touloukian [23] was used for BeO regions. The FEM thermal models were meshed with square PLANE55 elements over their entireties.

A heat flux of 5 kW/m^2 was applied to the geometries over the temperature range of 278 K to 1,860 K increments. The FEM thermal modeling was solved as a steady state problem, and consequently temperature distributions were developed across the geometries to determine the effective thermal conductivity of the nuclear fuel samples. The results of these calculations were compiled and graphed along with the experimentally measured thermal conductivities from Ishimoto et al. [21] of UO_2-BeO fuels.

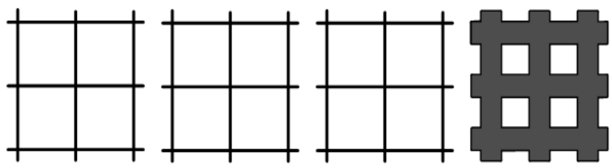

Fig. 4 The ANSYS FEM thermal model geometries of UO_2-BeO nuclear fuels with 0.6, 0.9, 1.2 and 13.6 wt% of BeO as generated by an automated program.

4. Modeling Results and Benchmarking

It was found there was no significant variation in the thermal conductivity of the system as the number of the elements increased. Therefore, in order to minimize the evaluation time needed, a mesh of 25 × 25 was used. Similarly, 3D models with hexagonal and octagonal elements were set up. The FEM thermal modeling calculated the effective thermal conductivity of the UO_2-BeO fuel both in 2D and 3D. These results were compared to the measured thermal conductivity values as reported by Ishimoto et al. [21] and are given in Figs. 5-8.

The comparisons show that the modeled and measured conductivities were relatively close in value, with only a few tenths of a W/(m·K) in difference between experimental and calculated data sets. The simulation results in 2D or 3D geometries are very close to each other. This also verified that FEM thermal modeling done by Boey [14], with similar geometries, concluded that little difference occurs between 2D and 3D modeling.

The UO_2-BeO composite nuclear fuels thermal conductivity can increase significantly as the BeO weight percentage increases in the temperature range of interest. The UO_2-BeO composite nuclear fuels at the same weight percentage show a decrease with the temperature increase. At the beginning, the decrease is rapid, and then is slow with the temperature decrease. FEM modeling method demonstrates the potential to predict effective thermal conductivity of an enhanced thermal conductivity oxide UO_2-BeO nuclear fuel.

The data set trends followed approximately the same thermal conductivity curves in Figs. 5-8. Figs. 9-12 compared measured and calculated thermal conductivities for different BeO weight percentages. The percent difference between the calculated and measured values was about 10% or lower for all the nuclear fuels. The percent difference was initially larger at low temperatures, then decreased as the temperature increased, and the modeling data and experimental data are almost the same at last. Also, the

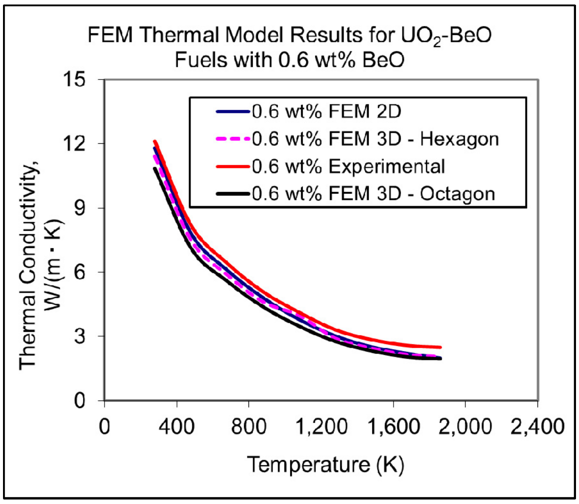

Fig. 5 FEM thermal modeling and measured thermal conductivities for UO_2-BeO fuels with 0.6 wt% BeO.

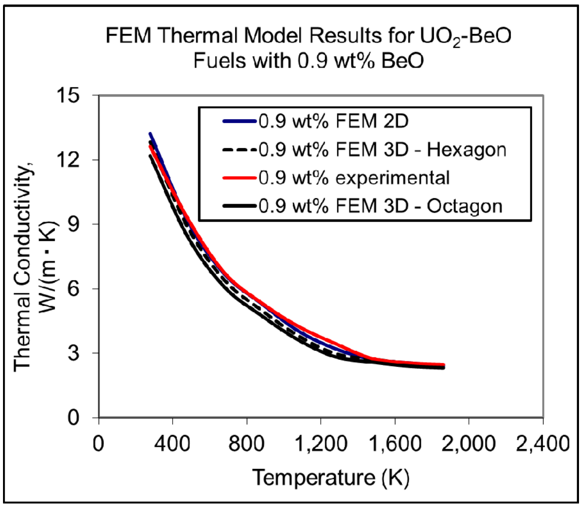

Fig. 6 FEM thermal modeling and measured thermal conductivities for UO_2-BeO fuels with 0.9 wt% BeO.

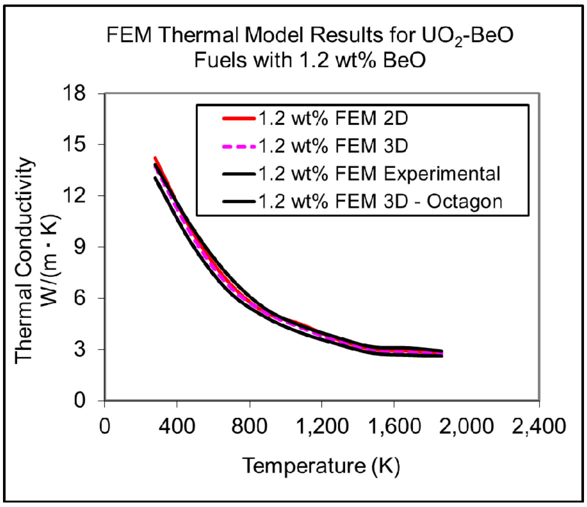

Fig. 7 FEM thermal modeling and measured thermal conductivities for UO_2-BeO fuels with 1.2 wt% BeO.

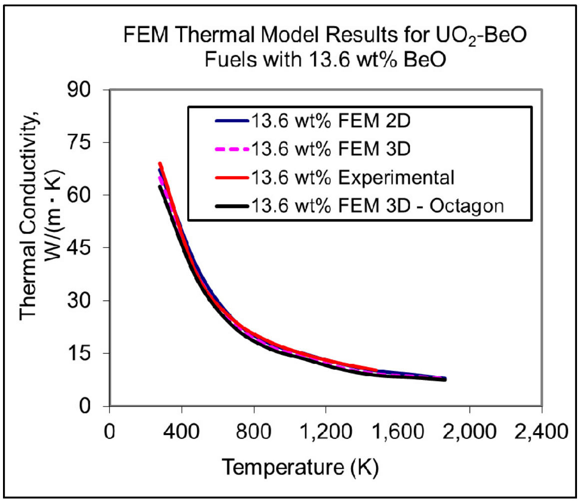

Fig. 8 FEM thermal modeling and measured thermal conductivities for UO_2-BeO fuels with 13.6 wt% BeO.

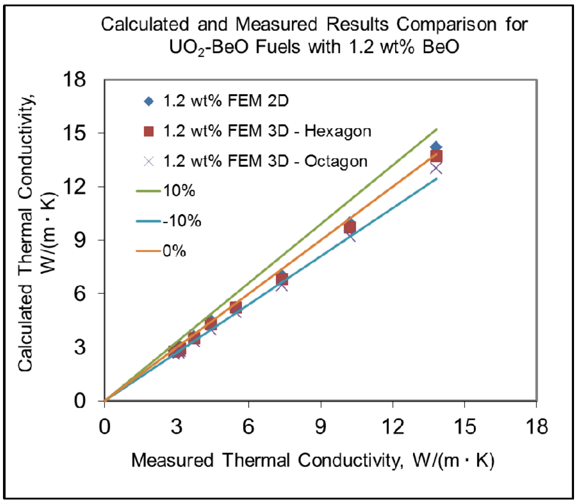

Fig. 11 Calculated and measured results comparison for UO_2-BeO fuels with 1.2 wt% BeO.

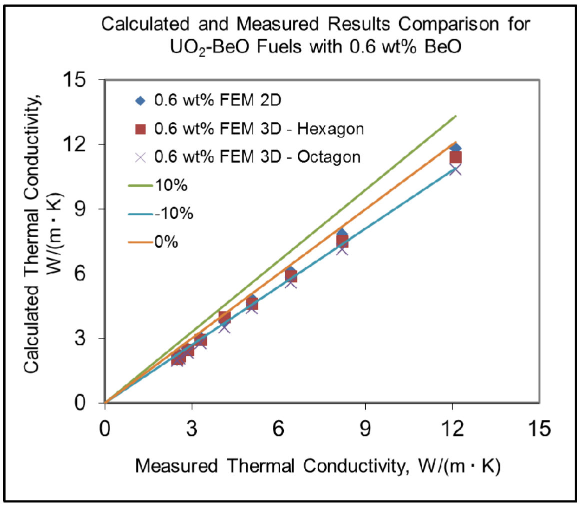

Fig. 9 Calculated and measured results comparison for UO_2-BeO fuels with 0.6 wt% BeO.

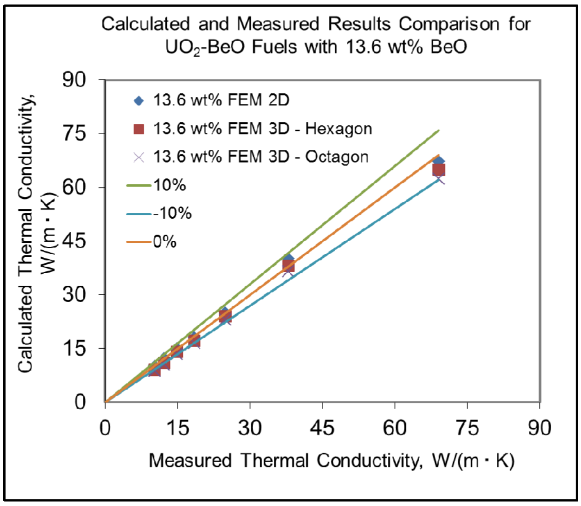

Fig. 12 Calculated and measured results comparison for UO_2-BeO fuels with 13.6 wt% BeO.

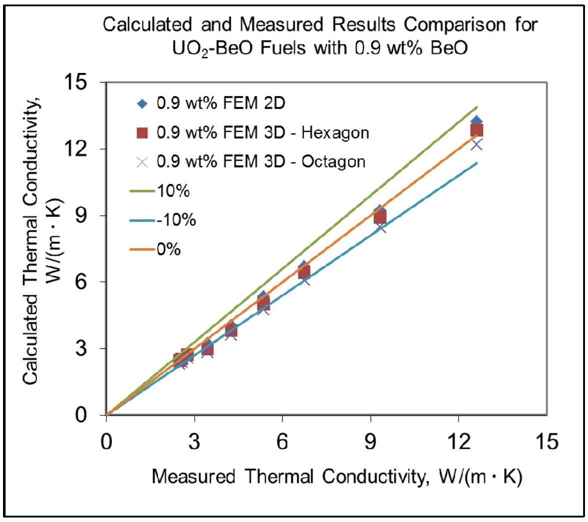

Fig. 10 Calculated and measured results comparison for UO_2-BeO fuels with 0.9 wt% BeO.

percent difference between the two data sets decreased as the concentration of BeO in UO_2 increased. This shows further analysis is needed for the high temperature and lower thermal conductivity part, which may invove more complex phenomena of chemical composition, microstructure evolution and so on, to have better physical understanding and better thermal conductivity prediction for UO_2-BeO nuclear fuels under very high temperature.

5. Temperature Profiles of UO_2-BeO Fuels in a LWR (Light Water Reactor)

The thermal conductivity curves of the fuels were used to calculate temperature difference profiles using the following assumptions. The fuel pellet was assigned a linear heat generation rate, LHGR (linear heat generation rate), of 17.52 kW/m, for a channel in a PWR (pressurized water reactor). This LHGR was then multiplied by a 1.7 peaking factor, a thermal power limit, to examine the fuel temperature difference profile in a hot channel of a PWR. The outer radius of the fuel pellet in the hot channel was calculated to be 849 , and was kept constant to demonstrate the effect of the high conductivity phase under equal power generation and external temperature conditions.

The thermal conductivity curves for a SB-UO$_2$-BeO fuel and a green granule UO$_2$-BeO nuclear fuel were determined from FEM thermal modeling and used in the reactor performance analysis (SB and green granule are two methods to fabricate UO$_2$-BeO composite fuels). Fig. 13 shows the axial temperature profile along the nuclear fuel assembly from bottom to top. The temperature profiles are for the coolant, cladding outer and inner temperatures, nuclear fuel outer surface temperature, and nuclear fuel centerline temperatures with different fuels of UO$_2$, SB-UO$_2$-BeO, and GG-UO$_2$-BeO. Figs. 14-17 show the radial temperature profiles at different axial positions of the nuclear fuel.

As shown in Figs. 13-17, due to the green granule UO$_2$-BeO thermal conductivity is greater than the SB-UO$_2$-BeO fuel, and both composite fuels' thermal conductivities are greater than UO$_2$, the results

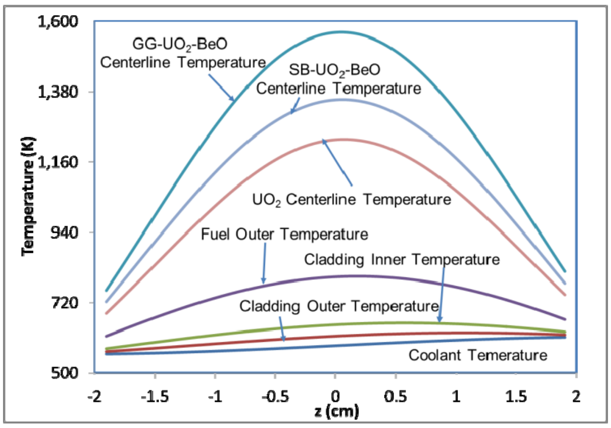

Fig. 13 Steady state axial temperature profiles.

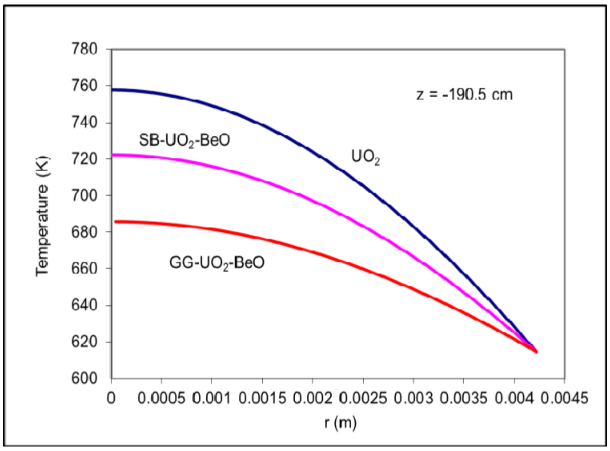

Fig. 14 Steady state radial temperature profiles at z = -190.5 cm.

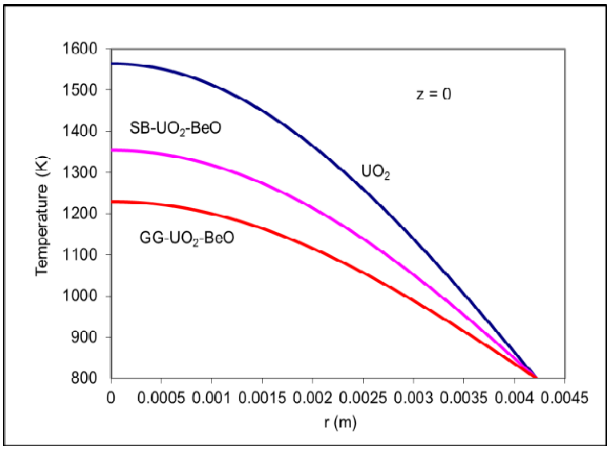

Fig. 15 Steady state radial temperature profiles at z = 0.

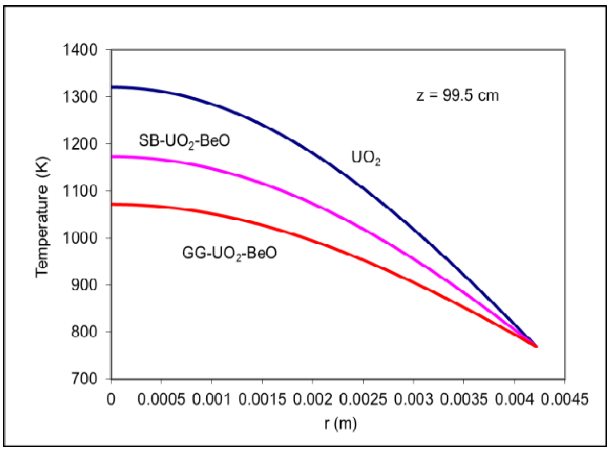

Fig. 16 Steady state radial temperature profiles at z = 99.5 cm.

showed that the minimum decrease in centerline temperature was 250 K for the SB-UO$_2$-BeO fuel and 350 K for the green granule UO$_2$-BeO fuel for steady state.

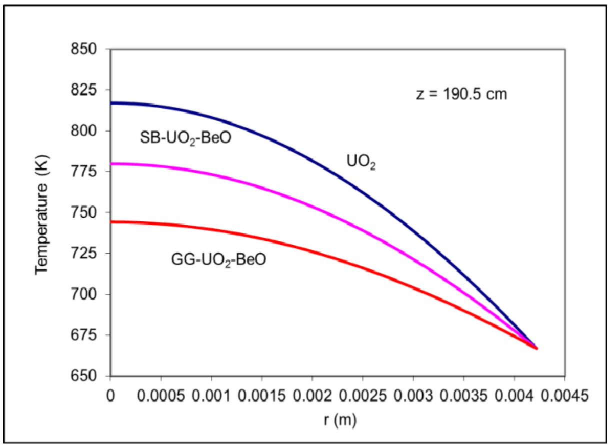

Fig. 17 Steady state radial temperature profiles at z = 190.5 cm.

6. Conclusions

The methodology to generate ANSYS FEM thermal models of enhanced thermal conductivity oxide nuclearfuels was developed. FEM thermal models were then generated and the results compared to the measured UO_2-BeO fuel sample thermal conductivities. A comparison showed that the thermal modeling was in agreement with the measured values, having a difference of about 10% or lower between the two. These benchmarking cases with the FEM thermal modeling method successfully demonstrated the potential of the models to accurately predict the effective thermal conductivity of an enhanced thermal conductivity oxide nuclear fuel.

The thermal conductivity curves for a SB-UO_2-BeO fuel and a green granule UO_2-BeO nuclear fuel were determined from FEM thermal modeling and used for reactor performance analysis. The temperature profiles of the oxide nuclear fuels were calculated for use in the hot channel of a PWR. The results showed that the minimum decrease in centerline temperature was 250 K for the SB-UO_2-BeO fuel. The green granule UO_2-BeO fuel had the maximum decrease in centerline temperature of 350 K.

Acknowledgments

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