An Innovative High Thermal Conductivity Fuel Design
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Summary of Project Status

During the program period reported above the computational model was modified to clarify some issues related to the validity of the model. Specific questions being looked at by Dr. Wei Jiang, a post doctoral research associate working part time on this project has been to incorporate the effect of temperature dependent properties. The outcome is a comprehensive study which has been accepted for publication in the *Journal of Nuclear Technology*.

It has been demonstrated that the effective thermal conductivity of this proposed advanced nuclear fuel, a mixture of SiC with enriched UO_2, is higher than the conventional UO_2 fuel. Predicted maximum temperatures at the center-line of the fuel rods have numerically been shown to be lower than what would be encountered in the conventional fuel rod.

The higher thermal conductivity of SiC along with its other prominent reactor-grade properties makes it a potential material to address some of the related issues when used in UO_2 [97% TD]. This ongoing research, in collaboration with the University of Florida, aims to investigate the feasibility and develop a formal methodology of producing the resultant composite oxide fuel. Calculations of effective thermal conductivity of the new fuel as a function of %SiC for certain percentages are presented as a preliminary approach. Heat transfer mechanism in this fuel is explained using a finite volume approach and validated against existing numerical models. FLUENT 6.1.22 was used for thermal conductivity calculations and to estimate reduction in centerline temperatures achievable within such a fuel rod. Later, computer codes COMBINE-PC and VENTURE-PC were deployed to estimate the fuel enrichment required, to maintain the same burnup levels, corresponding to a volume percent addition of SiC.

ACOMPLISHMENTS:

- *The result of the research work was published as a* ***MS thesis*** *of one of my students. "Enhanced Thermal Conductivity for Light Water Reactor Fuel The Composite Oxide Fuel Approach." By Sujan Pakala, University of South Carolina.*
- *S. Pakala is now Employed by Vogtle Nuclear Power Plant, GA, as an Engineer*
- *One Post Doctoral Research Assistant, Dr. Wei Jiang worked as part time researcher on this project.*
- ***Papers resulting from the grant****:*
    - Jamil A. Khan, Sujan B. Pakala, Wei Jiang, Knight W. Travis, James S. Tulenko, "*Enhanced Thermal Conductivity for LWR Fuel*", *Nuclear Technology*, in press, to appear in January 2010
    - Khan, J., S. Pakala, T. W. Knight, J. Tulenko, "Enhanced Thermal Conductivity for LWR Fuel," *Transactions Of The American Nuclear Society 2005 Winter Meeting*, Washington, DC November 13-17, 2005

Update on the last report:

The microstructure of fuel rod is assumed in three geometries: a best case, an average case and a poor case. Thermal conductivity is calculated numerically with the FLUENT under above assumptions. Then the effective thermal conductivity values obtained are used in the FLUENT to calculate temperature profiles considering in-pile conditions.

There were some problems reported in the last report, these have now been taken care of. Firstly, the calculation of effective thermal conductivity with the FLUENT is performed under the assumptions that calculating units of all three geometries are independent in the rod and that there is no heat transfer among the units. However, units do not meet the necessary symmetry requirements for the average case and poor case. In addition, the effective thermal conductivity should have been calculated over the entire relevant temperature range, and not only with average values of the thermal conductivity of the constituents.

Secondly, it is inadequate to conduct some comparisons with analytical models from the literature, which are not applicable to this material containing more than 90 volume percentage of inclusions. For example, the models of Maxwell, Meredith and Tobias should only be used for low volume fraction of inclusions. Realistically, it is also difficult to have this volume fraction of spheres in the material.

To solve the first problem, we remodeled the calculation units of average case and poor case, which were built in symmetry manners in the new models. In an effort to improve the average case, though the coating on UO_2 is still incomplete, the SiC layers cover two opposite faces rather than two adjacent faces against an edge in the original case. The poor case model is remodeled in a manner that SiC layers are separated by UO_2 blocks in the radial direction to satisfy the symmetry requirements. For the calculation in the entire temperature range, we now calculated thermal conductivity at several typical temperature points to satisfy range applicability requirement at reasonable simulation time cost.

For the second problem, two new volume percentages below 90%, such as 85% and 89%, were introduced into the simulations. Based on the FLUENT results in the new volume percentages, comparisons weree made with some analytical models from the literature to validate the models.

Below we describe the already completed work (complete work)

ABSTRACT

Thermal conductivity of the fuel in today's Light Water Reactors, Uranium dioxide, can be improved by incorporating a uniformly distributed heat conducting network of a higher conductivity material, Silicon Carbide. The higher thermal conductivity of SiC along with its other prominent reactor-grade properties makes it a potential material to address some of the related issues when used in UO_2 [97% TD]. This ongoing research, in collaboration with the University of Florida, aims to investigate the feasibility and develop a formal methodology of producing the resultant composite oxide fuel. Calculations of effective thermal conductivity of the new fuel as a function of %SiC for certain percentages and as a function of temperature are presented as a preliminary approach. The effective thermal conductivities are obtained at different temperatures from 600K to 1600K. The corresponding polynomial equations for the temperature-dependent thermal conductivities are given based on the simulation results. Heat transfer mechanism in this fuel is explained using a finite volume approach and validated against existing empirical models. FLUENT 6.1.22 was used for thermal conductivity calculations and to estimate reduction in centerline temperatures achievable within such a fuel rod. Later, computer codes COMBINE-PC and VENTURE-PC were deployed to estimate the fuel enrichment required, to maintain the same burnup levels, corresponding to a volume percent addition of SiC.

1. INTRODUCTION

Energy consumption in America is projected to grow by about 30% toward the end of the next decade [1]. Nuclear power plants, bearing about 20% of the current energy demand, will therefore have a much bigger role to play in the near future. The Light Water Reactor (LWR) is the primary source of nuclear power with one hundred and four currently operational commercial power reactors.

The maximum power of a nuclear power plant (NPP) is determined by the amount of heat that is removed from the reactor core [2]. Uranium dioxide is notorious for its poor conductivity with a range from 7 to 2.5 W/m-K corresponding to temperatures of 200˚C to 1200˚C [3], limits the energy removal rates. Although the chemical and irradiation tolerances [4] that UO_2 displays obscure the disadvantages.

Thermal conductivity of the fuel can be improved by incorporating a material with higher conductivity into it in such a way that, a heat conducting network (percolation pathway) is obtained, resulting in a *composite oxide fuel* (COF). The higher thermal conductivity of Silicon Carbide [5], [6] along with its other prominent reactor-grade properties makes it a potential material to address some of the related issues when used in UO_2.

The broad objective of this research is to investigate the feasibility of achieving enhanced performance of the composite oxide fuel with the addition of SiC, and to develop a formal methodology of producing the fuel. Computational methods were employed to calculate the effective thermal conductivity (ETC) and then those results were validated with existing empirical models, available experimental data, and some current research. This provides an estimate of the empirical values of such the COF pellets that will be produced at the University of Florida (UF). The other objective of the study, which is a future research direction, is the estimation of in-reactor performance of the fuel, ranging from required U-235 enrichment to reactor transient behavior involving the new fuel.

The study is organized as follows. Firstly, a simple heat transfer model to determine effective conductivities is established and validated. The model was solved using a commercial CFD package [7],

FLUENT 6.1.22. In the subsequent sections, results are presented and validated against those from literature based on empirical models like the Effective Medium approach [8] or the well accepted Rayleigh's equation [9]. Then, a portion of fuel pin is simulated to determine the reduction in centerline temperatures achievable with such a composite oxide fuel. A brief description of the formal methodology to produce such composite oxide fuel, currently underway at the University of Florida [10], is then described. Finally the study is concluded by discussing present research in addressing some of the issues related to the implications of the composite form of fuel like estimating thermal conductivity in transient conditions, accounting for various factors that affect the conductivity in those conditions. Neutronic calculations to estimate the required U-235 enrichment to maintain the cycle length will be discussed.

2. LITERATURE SURVEY

Effective Thermal Conductivity of Composite Materials

Effective thermal conductivity was first formulated by Maxwell well over a century ago in his work on composites [8], where he proposed the effective medium approach. The approach was changed a little by Rayleigh [9], who assumed that the spherical inclusions form a cubical array rather than the random distribution employed by Maxwell. Landauer [11] provides a review of the related work which serves as a very important base.

The theories of composites can be broadly divided into two groups, where one group assumes inclusions are randomly distributed in a homogeneous matrix. The other group is essentially based on the work of Rayleigh [9] where the particles are assumed distributing in a regular manner within the matrix. Many researchers [12] ~ [16] later attempted to improve the Rayleigh's identity.

Much research has been done to understand the effects of thermal boundary resistance, known as *Kapitza resistance* [17] after the discovery by Kapitza in 1941. It can be seen that the boundary resistance will increase with a decrease in the size of the filler material, when the volume fraction is held constant, and this was shown experimentally in the 1990s [18], [19], [20]. Swartz and Pohl [21] in 1989 have compiled the most exhaustive literature on *Thermal Boundary Resistance*, which marked the culmination of significant research into the concept.

The Rayleigh's method was extended to accommodate boundary resistance by many researchers [12], [13], [14], [22], [23]. Richter, Viljoen, and Rensburg [24] have developed a theory, based on the Rayleigh's identity, to determine the expected contact area between different species. More recently, Mercier et al [25] and Verrall et al [26] have reported through their investigations that all these relations developed to accommodate the complex arrangement of inclusions and the boundary resistance, reduce to the original Rayleigh's equation for the simple case of ideal contact between surfaces i.e. with no boundary resistance.

For a more detailed review of the thermodynamic and transport properties of UO_2, the readers are directed to the works of J.K Fink [3], Minato et al [27], and Matzke et al [28], [29]

Properties of UO_2 and SiC

The thermal conductivity of UO_2 decreases due to phonon-defects from 7 W/m-K at 200˚C to 2.5 W/m-K at 1200˚C [4] and due to phonon-phonon scattering until about 1900K. These values, used throughout this study, have been calculated for a UO_2 density of 97% theoretical density [3].

Attractive properties of SiC for enhancing fuel conductivity are as follows: Very high thermal conductivity (78 W/m-K at 1000K); high melting point (2800C)[4]; mostly corrosion-resistant even at high temperatures; low neutron absorption; dimensional stability; non porous.

Solomon et al [30] attempted to employ a polymer impregnation and pyrolysis method to enhance the thermal conductivity of LWR fuels. But, their model fails because it resulted in a phase of silicon carbide that in itself blocks further impregnation deeper into the pellet. However, the idea being pursued [10] at the University of Florida, a CVD process, looks more promising.

3. EFFECTIVE THERMAL CONDUCTIVITY CALCULATIONS

3.1 Effective Thermal Conductivity from FLUENT

A typical Pressurized Water Reactor (PWR) fuel rod is 4m in length and 9.5 mm in diameter. The rod consists of a large number of uranium dioxide pellets stacked up inside a clad, made of Zircaloy-4. The pellets have a diameter of 8.2 mm, and the clad is 0.57 mm thick [2], [31]. The remaining gap between the pellet and clad, 0.08 mm, is filled with Helium which is an inert gas. The rods are arrayed in 17 X 17 bundles.

The resultant fuel material will be composed of a SiC phase which is rather uniformly distributed within UO_2. Thus the material of concern is a homogeneous composite solid with homogeneous heat generation rate. Based on these assumptions, it follows that there will be no significant temperature gradients within the fuel pellet azimuthally. The other key assumption is about axial heat transfer in the fuel rod. In the case of a fuel rod the ratio of the length of the rod to its diameter is greater than 10, therefore, the axial heat transfer is negligible.

For the purpose of estimating the conductivity of the fuel material, the above assumptions are applied to a pellet made of the composite oxide material, UO_2-SiC. Since there is no heat transferred axially or azimuthally, it therefore follows that the heat transferred in the radial direction, which is the equivalent of a one-dimensional steady state heat transfer, is a measure of the conductivity of the material. Thus,

temperature gradient measured along the radius of the fuel pellet will give a measure of the effective thermal conductivity of the composite fuel.

Therefore a unit radial element is considered as the base model. SiC is taken to form a matrix around UO_2 blocks, arranged as shown in Figure 1 and its dimensions are specified in Table 1. This approach clearly simplifies the actual structure of the composite fuel material.

Fig. 1 – Unit Radial fuel element

Table 1: Radial unit of fuel rod; Dimensions

In order to calculate effective thermal conductivity for a specific temperature, we set the temperature at the right end of the rod as T1, while the temperature at the left end of the rod as T1+1. Then heat flux in the cell can be obtained from the Fluent simulation. The conductivity of the material can be calculated by the following equation:

$$\mathbf{k = (q*L)/ \Delta T \quad - Eqn.1}$$

where,

k = Effective thermal Conductivity of the composite fuel material;

q = Heat flux between the left end of rod and the right end of rod;

L = Length of the model over which the temperature difference is calculated;

ΔT = temperature difference observed between the center of fuel (left end of rod) and the fuel outer face (right end of rod).

Six temperatures are selected from 600K to 1600K to investigate how temperature affects effective thermal conductivity

With ΔT fixed, the amount of SiC and the way this high conductivity phase is distributed within the fuel has a definite impact on the q. Thickness of the SiC coating developed on UO_2 particles can be anywhere between a complete encapsulation to an absolute no coating. The thickness of the coating is a direct measure of the percentage of SiC employed or the resulting density of UO_2 in the fuel material. So to determine an acceptable value for the effective thermal conductivity, we discuss two models based on the coating patterns. One pattern where all the UO_2 particles are completely encapsulated in SiC and another, where there is partial coating on few faces of UO_2 particles.

A worst case possible is that we have a layer of SiC on just one face of each block of UO_2 which may be arranged rather irregularly along the length of the model (i.e., radius of the pellet). This model does not really figure in the simulation as the actual fuel produced according to the procedure being employed at UF will have a structure in between the case 1 and the case 2. However, the conductivity of such a fuel element is also obtained to get a conservative estimate of the effective thermal conductivity. All the models simulated have three separate cases each, which account for three different percentages of SiC in the total radial unit; 12%, 8% and 0% rendering the UO_2 content to 85%, 89 % and 97 % respectively by volume. 0% SiC model is a UO_2 block with no SiC coating and simply serves as a reference model. In modeling the geometry, the gap between fuel and clad has been avoided because the final required result was the temperature difference between the centerline and surface of the fuel, which can be observed to be equivalent without the gap in the two cases of:

- fuel with a % of SiC; and
- fuel of 97% TD UO_2 , i.e. no SiC

The case 1 model where all the UO_2 particles are completely encapsulated within a layer of SiC is shown in Figure2 . The effective thermal conductivity values obtained from this model are later compared to the results predicted by empirical models in literature. Alongside providing the continuous

path for heat transfer from the center of fuel to the outer face, the model in such a configuration may also act partially as the first line of containment for fission products.

Fig. 2 – Radial unit, showing the UO2 blocks within SiC matrix – Case 1

In the second model, the coating on UO_2 is not complete (Fig 3). Throughout the length of the radial unit, we would see either UO_2 or SiC or both on any of the faces. To arrive at a model that averages this distribution we consider eight UO_2 blocks placed on two opposite faces along the length of the model, which make up the percentage of volume under consideration. SiC layers are also present between the UO_2 blocks. Thus, the case 2 model is represented by Figure 3.

Fig. 3 – Case 2 model

The worst case model, referred to as the case 3 model, is modeled as shown in Figure 4. Eight UO_2 blocks which have a coat of SiC are arranged so that all the SiC coatings are disconnected.

Fig. 4 – Case 3 model

Modeling and meshing the geometry was carried out using Gambit 2.4.6 and then imported into FLUENT solver for a computational solution. The solution values have been verified for different sizes of the elements in the discretized geometry. It was observed that for a hexahedral mesh size of 0.05 and 0.04 mm the temperature distribution varied to a considerable extent. The mesh was then refined for smaller sizes. A size of 0.035 mm also showed changes, but from a mesh size of 65% the length of the

least edge the values were very much stable, i.e. values obtained for mesh sizes of 0.03 mm and below did not show any significant difference. The values presented in all the above tables and plots which are to follow are for mesh sizes of 0.02 mm. Structured hexahedral mesh with about 145896 elements in all geometries were obtained for the various zones in the geometries.

3.2 Material Conditions

The thermal conductivities of UO2 and SiC are temperature-dependent variables. In this work, six temperatures 600K, 800K, 1000K, 1200K, 1400K and 1600K are chosen to investigate the effective thermal conductivity at different temperatures. The corresponding thermal conductivities of UO2 and SiC are shown in table (2).

Table 2: Thermal conductivities [W/K*M] of UO2 and SiC at different temperatures [32] [36]

3.3 Boundary Conditions

Wall boundary conditions with zero heat flux were applied on the four faces over the length of the model and also the centre face. These conditions are based on the assumptions, which basically govern the model, with zero heat transfer axially and azimuthally. The other constraint applied is to the temperature on the outer face of the clad. In all the simulations, the fixed temperature at the right end of the rod is selected from table (2) while the temperature at the left side of the rod is one degree higher than that of the right end.

3.4 Results and Discussion

Fig 5 and 6 show the temperature distribution and temperature profile of the rod for the case 1, 85% UO2. Similar figures are obtained for the other cases.

Case 1 Model: with 12% SiC (85% UO_2) at 600K

Fig. 5 – Temperature distribution within the radial unit composite fuel, 85% UO_2

Case 1 Model: with 12% SiC (85% UO_2) 600K

Fig. 6 – Temperature profile from centerline (face) to clad outer surface, 85% UO_2

We now present the results of thermal conductivities measured in all the above cases. The effective thermal conductivity K-eff calculated by Eqn. 1 is shown in fig 7.

Fig. 7 – Effective thermal conductivity for all cases under six temperatures

It is important to note that the difference observed between the case 1 model and case 2 model is small although the arrangement of the SiC matrix around the UO_2 blocks is evidently quite different. This small difference was an expected result based on the fact that the continuous SiC layer holds the key to providing that percolation path way. The big difference between case 3 and case 1/case2 shows that the disconnecting SiC blocks has little improvement on the fuel conductivities.

Table 3: Case 1 model – results

The polynomial equations for effective thermal conductivity can be obtained as:

85% UO2: $K\text{-eff} = -9.59E\text{-}09T^3 + 4.29E\text{-}05T^2 - 6.87E\text{-}02T + 4.68E+01$ **- Eqn.2**

89% UO2: $K\text{-eff} = -1.16E\text{-}08T^3 + 5.03E\text{-}05T^2 - 7.76E\text{-}02T + 4.91E+01$ **- Eqn.3**

Table 4: Case 2 – Results

85% UO2: $K\text{-eff} = -8.59E\text{-}09T^3 + 3.81E\text{-}05T^2 - 6.05E\text{-}02T + 4.07E+01$ **- Eqn.4**

89% UO2: $K\text{-eff} = -9.74E\text{-}09T^3 + 4.33E\text{-}05T^2 - 6.91E\text{-}02T + 4.73E+01$ **- Eqn.5**

Table 5: Case 3 – Results

85% UO2: $K\text{-eff} = -4.28E\text{-}09T^3 + 1.92E\text{-}05T^2 - 2.98E\text{-}02T + 1.99E+01$ **- Eqn.6**

89% UO2: $K\text{-eff} = -3.00E\text{-}09T^3 + 1.47E\text{-}05T^2 - 2.48E\text{-}02T + 1.77E+01$ **- Eqn.7**

The values obtained for all the above models will be compared to those predicted by literature. For simplicity, we only compare them at temperature 600K. The three equations Rayleigh's, Meredith & Tobias, and Maxwell's [11], [15], [8] give effective thermal conductivity values as tabulated below:

Rayleigh's Equation:

$$Keff\_R(\psi) := Ksic\left[1 + 3\frac{\psi}{\left[\frac{(Kuo2 + 2.Ksic)}{Kuo2 - Ksic}\right] - \psi + 1.569\left[\frac{(Kuo2 - Ksic)}{3Kuo2 - 4Ksic}\right]\cdot\psi^{\frac{10}{3}}}\right] \qquad \text{Eqn - 8}$$

Table 6: Rayleigh's equation results

Meredith and Tobias':

$$\lambda_C = \lambda_m \frac{A - 2f + 0.409Bf^{7/3} - 2.133cf^{10/3}}{A + f + 0.409Bf^{7/3} - 0.906cf^{10/3}} \qquad \text{Eqn – 9}$$

where,

$$A = \frac{2 + k}{1 - k}, \quad B = \frac{6 + 3k}{4 + 3k},$$
$$C = \frac{3 - 3k}{4 + 3k}, \quad \text{and } k = \frac{\lambda_f}{\lambda_m},$$

Table 7: Meredtih & Tobias' equation results

Maxwell's:

$$k_{Maxwell} = \frac{k_p + 2k_l + 2(k_p - k_l)\phi}{k_p + 2k_l - (k_p - k_l)\phi} k_l \qquad \text{Eqn - 10}$$

Table 8: Maxwell's equation results

These values are plotted in the following graph (Fig. 8) with the values from the models:

Fig. 8 – Validating Finite Volume results against numerical models

This figure shows that case 1 and case 2 well match the results from The Rayleigh's and Maxwell's approaches. The results obtained from the Meredith & Tobias' [15] relation show the difference at 85% UO2. Thus the lattice model would provide a near exact solution for a whole composite system which accounts for the effects of interaction between the numerous dispersions. In other words, the lattice model is a good tool to approximate the effective thermal conductivity tensor while a finite volume approach would be more case specific. Thus our approach is governed by the boundary conditions that are very much valid for the models employed and the results can be realized in the situation where these boundary conditions can be applied. While thermal conductivity measurement of a fuel pellet made of the composite material may show values around those predicted by the Rayleigh's relation, those values are bound to be off by about the same difference when the pellets are operational within a fuel rod in a reactor.

4. COMPOSITE OXIDE FUEL PRODUCTION

The model described in the first section assumes the SiC matrix has uniform thickness around all the UO_2 particles, which is similar to the case 1 desirable. A worst case, a radial block of UO_2 with SiC coat only on one of its radial faces, and a case 2 on two opposite faces along the length of the model, have shown little difference in the temperatures achievable. It was also shown [23] that an uneven distribution of SiC around UO_2 particles also has an equivalent effect of high effective thermal conductivity.

The latter model is tantamount to achieving a thin coat of SiC over the UO_2 particles. This unique concept is currently being developed by researchers at the University of Florida. They are employing a Chemical Vapor Deposition process [10] to achieve a thin coated layer of silicon carbide on UO_2 particles. The CVD process involves chemical reactions of gaseous reactants in an activated (heat, light, plasma) environment, followed by the formation of a stable solid product. The coated particles are then passed through a 100-mesh sieve, producing uniform agglomerates of about 50 μm.

They have selected three main precursors for the CVD SiC process, namely: Trimethylsilane (TMS), Methyltrichlorosilane (MTS), and Silacryclobutane (SCB). TMS was initially selected to understand the sintering process between SiC and UO_2 and they have confirmed the formation of SiC film on UO_2 powder. UO_2 powder coated by SiC was pressed into pellets and later sintered at high temperatures in an inert gas atmosphere aiming to achieve smooth coatings of the deposited SiC. They are currently investigating the effects of the Hydrogen-Argon gas mixture used during sintering of pellets and also the percentage of carbon necessary to prevent thermal decomposition of SiC. They are also attempting to review the fabrication process and establish the best precursor for the composite fuel.

5 - CENTERLINE TEMPERATURE FROM CFD ANALYSIS

To arrive at an estimate of the reduction in centerline temperatures achievable with an improved thermal conductivity, our next step was to simulate temperature distributions within a portion of the fuel rod. A fuel pin 9.5-mm in diameter and 100-mm long is considered. It should be noted that, the first part of the research involved only arriving at an estimate for the effective thermal conductivity of the system, which was established to be consistent with the estimates of existing theory. In this part of the research, the higher thermal conductivity is used as property of the fuel material as a whole, i.e. the fuel material is given a name UO_2-SiC and material properties assigned to this solid as a whole, with no distinction

made between the inert matrix or the fuel itself. Results are compared with varying percentage by volumes of UO_2 in SiC. This is done by using the corresponding thermal conductivity.

5.1 The model

The arrangement shown in Fig. 9 below, illustrates a section of the fuel pin – UO_2-SiC fuel enclosed within Zr-4 cladding, all within a channel to simulate the flow of coolant. The channel [2] is unit cell averaged to a radius of 7.11mm

Fig. 9 – Finite volume model for centerline temperature

Thermal performance of the reactor is dictated by bounds on the maximum allowable primary coolant inlet temperature which is usually fixed. Therefore, improved thermodynamic performance requires increased coolant outlet temperatures. The high coolant outlet temperatures necessitate higher pressures. The sub-cooled state of coolant is maintained by applying a pressure of 15.5 MPa over the system. The coolant is given an inlet velocity of 8.1 m/s and an inlet temperature of 560K. The flow in our case was considered laminar, with no cross sectional variation in flow region along its length. This was primarily because the section of fuel rod simulated falls well within the distance between two spacer grids, where the flow is mostly smooth and does not see any significant cross fluxes. The pressure losses that would otherwise be prominent have also not been considered for the same reason. A heat generation rate of 251.12 MW/m^3 is applied to the fuel material.

Results of the simulation are shown next. Two sets of figures are shown for each case. The first illustrates the temperature distribution within the fuel material, while the second is just a plot of the temperature values at specific locations on the cross section of the material.

5.2 Results and Discussion

Fig. 10 – Temperature contours within fuel material – 12% SiC

Fig. 11 – Temperature contours within fuel material – 8% SiC

Fig. 12 – Temperature contours within fuel material –0% SiC

The figures illustrate centerline temperatures achieved for various thermal conductivities of the fuel material. The varying volume percent of UO_2 in SiC is therefore tantamount to the different effective thermal conductivity of the composite fuel.

- Simulation results with 97% UO_2, Figure 12 shows a centerline temperature of about 882K.
- Simulation results with 89% by volume UO_2, Figure 11 shows a centerline temperature of about 732K
- Simulation results with 85% by volume UO_2, Figure 10 shows a centerline temperature of only 724K.

A reduction in the typical fuel centerline temperatures by a clear margin of 150K was therefore observed with a 8% inclusion of SiC by volume, which is arranged in any form as good as the case 3 model within the pellet. The results have been checked for any variation in the values of centerline temperature by changing the size of the elements in the mesh. No significant variations were observed for grid sizes of up to 0.02mm. Thus, we believe that the results are independent of grid size.

6 - NEUTRONIC CALCULATIONS

Typical enrichment levels specified for LWRs are [33] about 3.5% to 4.5% U-235 by weight in UO_2. Now with the addition of SiC, the volume of UO_2 is reduced and so does the volume of U-235, the fissile material. The reactors may operate at the same power levels with composite oxide fuel in place without any further enrichment to compensate for reduced fissile material. But the length of the fuel cycle in this case gets shortened because there is now a decrease in the installed excess reactivity at the beginning of cycle that corresponds to the amount of fissile content, for an expected specific burnup. i.e., the energy released per unit mass of the fuel will be lesser with lesser fissile content.

To maintain length of the fuel cycle, it is therefore necessary to increase the enrichment by a certain amount corresponding to the volume percent addition of SiC. To arrive at an estimate for the required enrichment, computer codes COMBINE-PC [34] and VENTURE-PC [35] have been used. The results have not been validated against any empirical results or benchmarked against other computer codes. However, the enrichment calculations obtained from the multi-group calculations of COMBINE, gives a decent estimate of the required U-235 content for a 5% by volume inclusion of silicon carbide with uranium dioxide. Future work includes usage of computer codes like MCNP5 and CASMO-3 to arrive at more accurate results. The following section illustrates the procedure undertaken.

6.1 Procedure

A Pressurized Water Reactor is considered, based mostly on the design of Westinghouse Sequoyah reactor. The core was presented into COMBINE input as a three region problem; Fuel, Core-barrel, Reflector.

Fig. 13 – Three region problem for Combine

Table 9 – Reactor dimensions

Geometric buckling was calculated using the following equation for a right circular cylinder:

$$B_g^2 = (2.405/R_{ex})^2 + (\pi/H_{ex})^2 \qquad \text{- Eqn.11}$$

Where, the radius and height are extrapolated dimensions. An initial enrichment of 4 weight percent U-235 was assigned for the fuel region, without any silicon carbide. A chemical shim was used to bring down the installed excess reactivity. Boron concentration was adjusted so that a near critical value of effective multiplication constant was obtained. Then with the composite fuel, 5% SiC included, the enrichment of U-235 was adjusted to arrive at the same effective multiplication factor.

To calculate the multi group constants and the neutron spectra, the input deck for COMBINE was prepared based on the number densities calculated as per the following tables. First, for the case of 4 weight percent U-235 in the fuel, without any SiC, number densities of the elements constituting the fuel lump were calculated based on a UO_2 theoretical density of 97%.

6.3 Results and Discussion

The COMBINE and VENTURE runs, adjusting the enrichment of U-235, were repeated until almost same values were obtained for the effective multiplication factor. It was observed that with 5% SiC by volume, U-235 has to be increased by a weight percent of about 0.8.

Table 10: Enrichment calculations; Effective multiplication factor

To see the effects of carbon and silicon separately, two more runs were made. In the input for COMBINE, silicon was removed to see the effects of carbon in the fuel. Although higher values were expected for the effective multiplication factor due to the higher moderating capabilities of carbon, the values observed in the runs were a tad higher than the expected. This effect is still to be explained and constitutes part of future work with more runs and other computer codes. The runs for silicon however, were well along the expected lines, given its low absorption cross section (higher than carbon) and low scattering cross section (lower than carbon).

7. CONCLUSION

The enhanced thermal performance of light water reactor fuel has been established by demonstrating the reduction achievable in centerline temperatures. Thermal conductivity of the oxide fuel is shown to increase by the introduction of silicon carbide and an estimate of the effective thermal conductivity is provided for the composite oxide fuel, benchmarked against well accepted numerical methods. Centerline fuel temperatures of as low as 724K were calculated as achievable with a uranium dioxide of 85% TD. Effective thermal conductivity was observed to improve significantly as predicted by the well accepted Rayleigh's identity and centerline temperatures lowered by about 150K compared to normal fuel configuration were achieved accordingly. The results achieved are in good agreement with theory, and with the conservative assumptions made; the model can be readily extended to simulation of the heat transfer within a fuel rod bundle. The results obtained serve to provide a finite volume analysis of the thermal performance of the composite oxide fuel, and will be corroborated by experimental result in the near future. Nuclide concentration analysis provided an estimate of the required U-235 enrichment to maintain the cycle length of fuel. With current research on production of

the composite fuel pellets, we are now setting about to perform neutronic calculations on the reactivity transients due to the new fuel inside the reactor core.

Some of the key issues we are working to address in our future work are the measurement of effective thermal conductivity of the composite oxide fuel during reactor operation, subject to change due to burn up and fission products [19] along with fission gas release. Thermal behavior under transient conditions should be explained so that a proper estimate of limits of operability may be established for various accident situations and normal reactor modes.

The novel CVD method to achieve the proposed composite oxide fuel can be readily incorporated into the procedure currently in use for the production of UO_2 fuel. However, processing of silicon carbide usually requires very high temperatures and pressures and will be key criteria in the production method being formalized.

8. ACKNOWLEDGEMENTS

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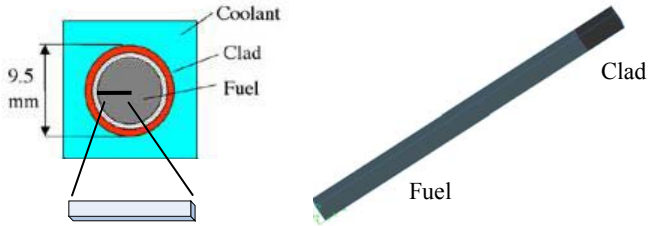

Fig. 1 – Unit Radial fuel element

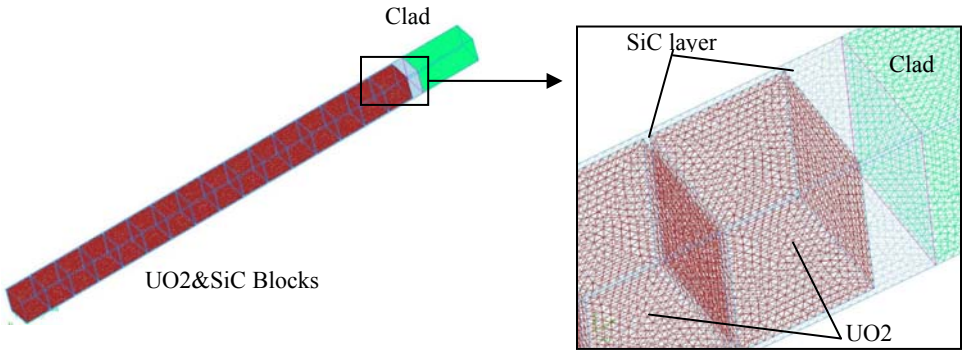

Fig. 2b – Radial unit, showing the UO2 blocks within SiC matrix – Case 1

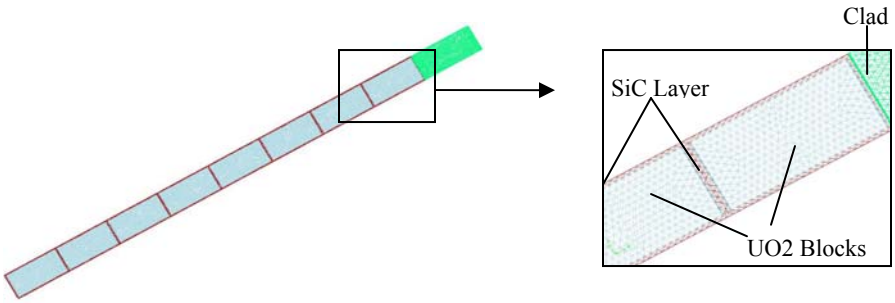

Fig. 3 – Case 2 model

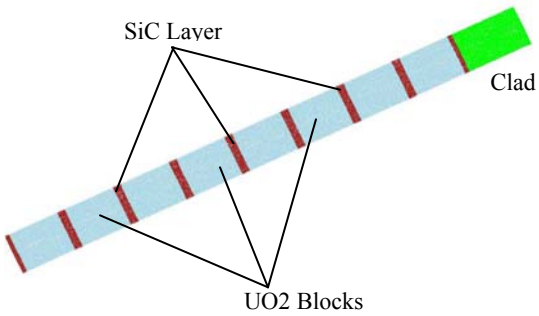

Fig. 4 – Case 3 model

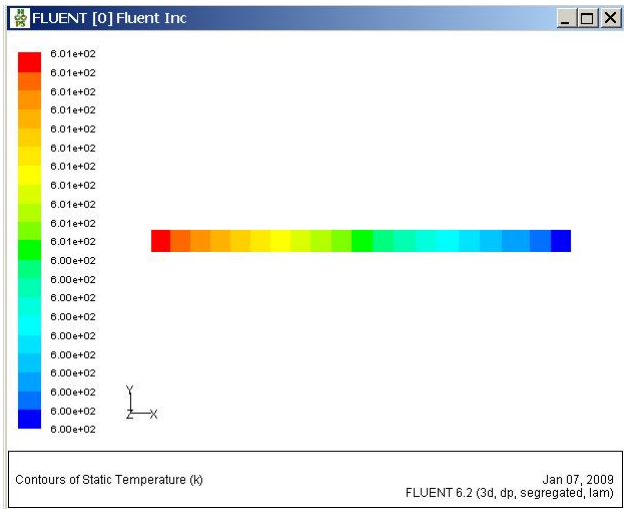

Fig. 5 – Temperature distribution within the radial unit composite fuel, 85% UO_2

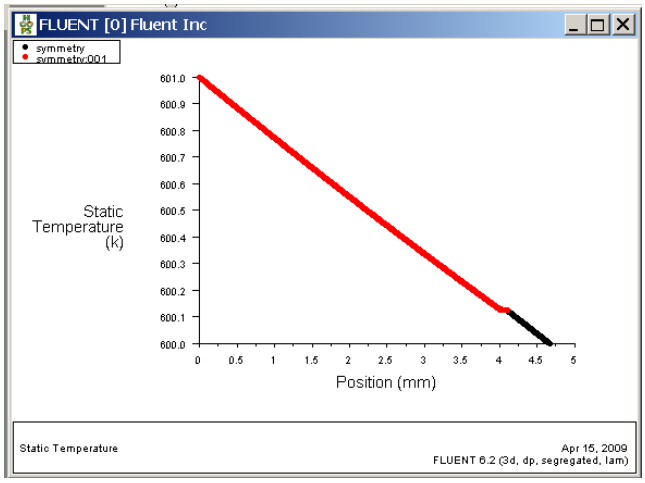

Fig. 6 – Temperature profile from centerline (face) to clad outer surface, 85% UO_2

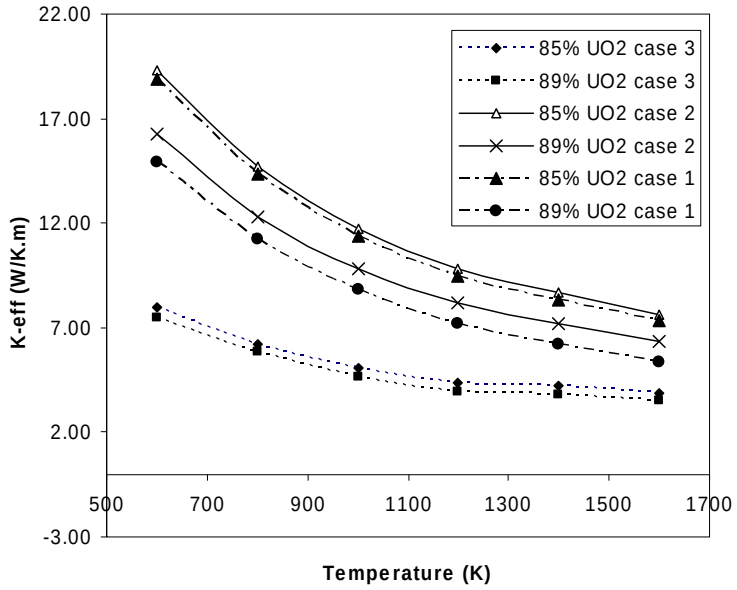

Fig. 7 – Effective thermal conductivity for all cases under six temperatures

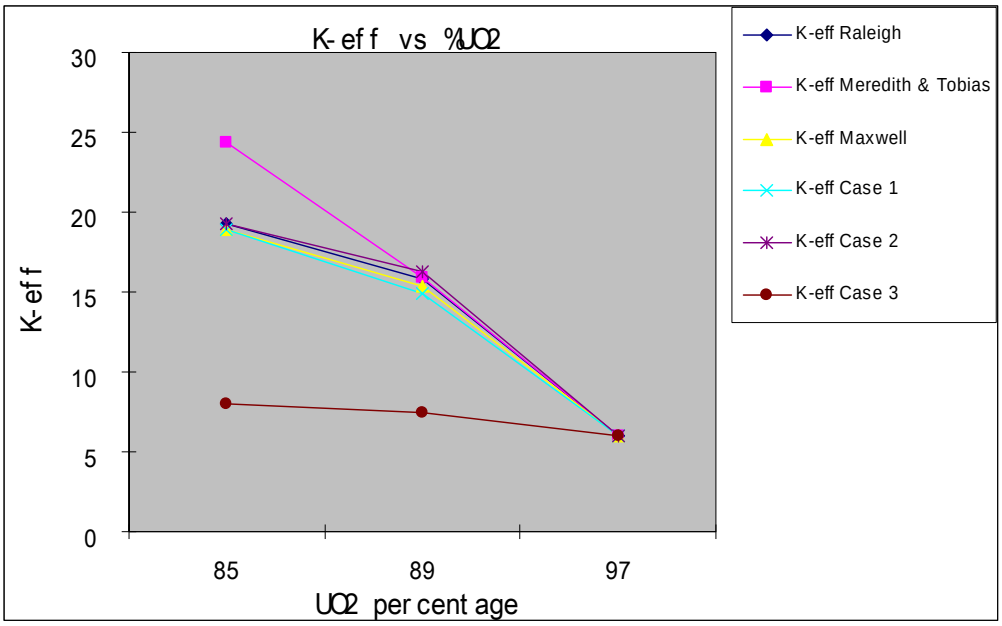

Fig. 8 – Validating Finite Volume results against numerical models

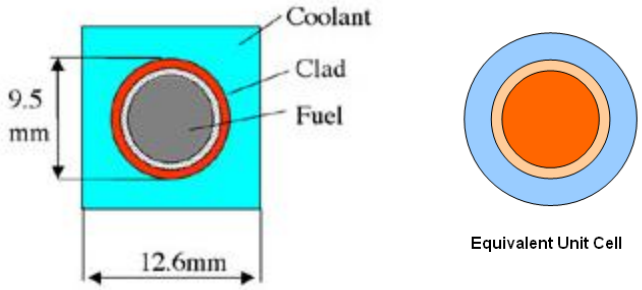

Fig. 9 – Finite volume model for centerline temperature

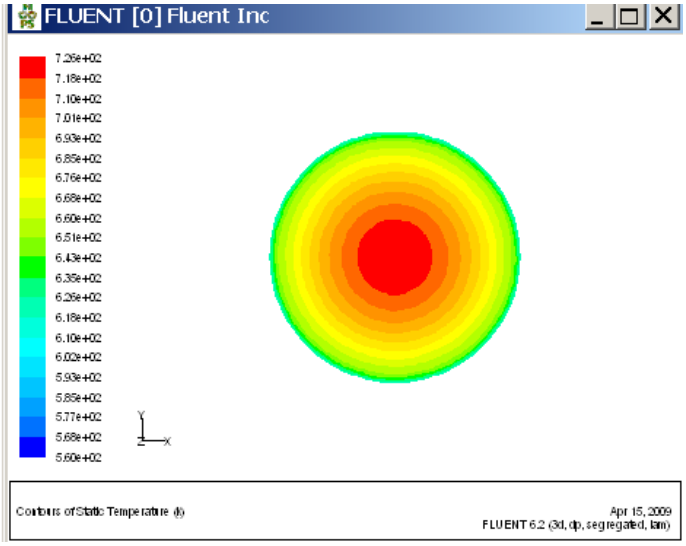

Fig. 10 – Temperature contours within fuel material – 12% SiC

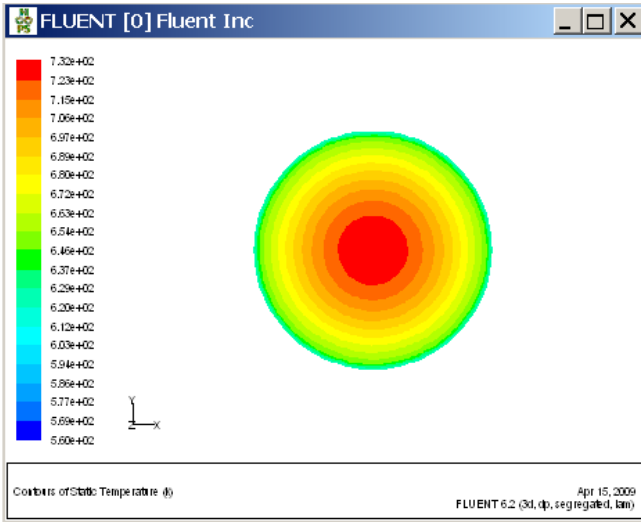

Fig. 11 – Temperature contours within fuel material – 8% SiC

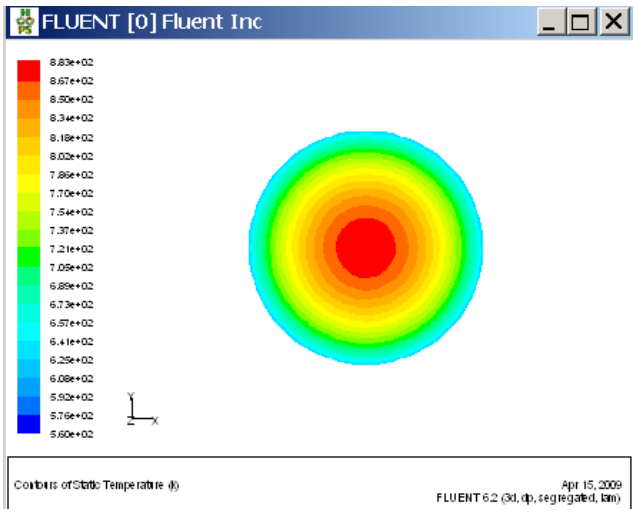

Fig. 12 – Temperature contours within fuel material –0% SiC

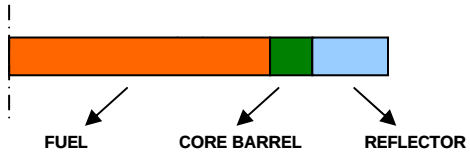

Fig. 13 – Three region problem for Combine

Table 1: Radial unit of fuel rod; Dimensions

Radial unit of Fuel rod:

length (radius)	4.1	mm
Height	0.25	mm
Width	0.25	mm
total volume	0.25625	mm3

Table 2: Thermal conductivities of UO2 and SiC under different temperature[][]

Temperature	600K	800K	1000K	1200K	1400K	1600K
UO2	6	4.5	3.5	2.9	2.7	2.4
SiC	126	89.2	69	56.3	47.6	41.1

Table 3: Case 1 model – results

Case 1 Model - (4.1 x 0.25 x 0.25)mm3 - 16 blocks

	600K	800K	1000K	1200K	1400K	1600K
K-eff(85% UO2)	18.89	14.34	11.35	9.48	8.34	7.35
K-eff(89% UO2)	18.16	13.25	10.21	8.52	7.21	6.35

Table 4: Case 2 – Results

Case 2 Model - (4.1 x 0.25 x 0.25)mm3 - 8 blocks

	600K	800K	1000K	1200K	1400K	1600K
K-eff(85% UO2)	19.29	14.68	11.75	9.83	8.68	7.65
K-eff(89% UO2)	16.27	12.3	9.79	8.16	7.22	6.37

Table 5: Case 3 – Results

Case 3 Model - (4.1 x 0.25 x 0.25)mm3 - 8 blocks

	600K	800K	1000K	1200K	1400K	1600K

K-eff(85% UO2)	8	6.23	5.04	4.34	4.23	3.89
K-eff(89% UO2)	7.5	5.84	4.68	3.96	3.76	3.51

Table 6: Rayleigh's equation results

Results from Rayleigh's Equation	
K-UO2 (97% TD) W/m-K	6
K-SiC (W/m-K)	60

% UO2 (ψ)	K-eff - Rayleigh
85	12.3070
89	10.739
97	6

Table 7: Meredtih & Tobias' equation results

K-UO2 (97% TD)	6 (W/m-K)

K-SiC	126 (W/m-K)
k (Ksic/Kuo2)	10
	-
A	1.333333333
B	1.058823529
	-
C	0.794117647

% UO2	**K-eff M&T**
85	24.48
89	16
97	6

Table 8: Maxwell's equation results

K-eff Maxwell	
K-UO2 (97% TD)	6
W/m-K	
K-SiC (W/m-K)	60

% UO2 (Φ)	K-eff Maxwell
85	6.068
89	6.136

97 6

Table 9 – Reactor dimensions

Reactor dimensions (m)	
vessel radius	2.415
vessel height	13.4
core radius	1.685
core height	3.66
core barrel outer radius	1.758
Reflector outer radius	2.012
Buckling (cm2)	0.000277

Table 10: Enrichment calculations; Effective multiplication factor

CASE	**% UO2**	**w/o U-235**	**K-eff**
No SiC	97	4	0.9924074
5% SiC	92	4.88	0.9990293
5% C	92	4	1.2456532
		4.88	1.2986671
5% Si	92	4	0.9170006

	4.88	0.998598