Verification of two-temperature method for heat transfer process within a pebble fuel

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Abstract – A typical pebble fuel that used in high temperature reactor (HTR), mainly consists of a graphite matrix with numerous dispersed tristructural-isotropic (TRISO) fuel particles and a surrounding thin non-fueled graphite shell. These high heterogeneities lead to difficulty in explicit thermal calculation of a pebble fuel. We proposed a two-temperature method (TTM) to calculate the temperature distribution within a pebble fuel. The method is not only convenient to perform but also gives more realistic results since particles and graphite matrix are considered separately while the traditional ways are considering the fuel zone as average heat generation source. The method is validated both by Computational Fluid Dynamics (CFD) method and Wiener bounds. Results show that TTM has a stable performance and high accuracy.

Keyword: two-temperature method; pebble fuel; heat transfer; CFD

I. INTRODUCTION

A typical fuel pebble consists of a fueled region and a surrounding thin non-fueled graphite shell. The fueled region has a radius of approximately 25mm, including a graphite matrix and 10,000-15,000 dispersed tristructural-isotropic (TRISO) particles as shown in Fig. 1. TRISO particles typically consist of five distinct regions. At the center of the particle is the fuel kernel, typically an oxide, carbide or oxycarbide, which contains the nuclear fuel. A porous carbon buffer surrounds the kernel, to weaken recoiling fission fragments and to accommodate particle dimensional variation and internal gas buildup. The outer layers consist of an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer. These complexities of geometry make a significant challenge for thermal calculation of a pebble fuel. Currently, this type of structure is always considered as isotropic, two-component, heterogeneous, macro-scale porous material for a significant number of effective thermal conductivity models have been proposed [1-2] on this topic. Most of the models that have been proposed either empirically or theoretically are highly specific to a given material and modifications are need to be combined while accounting for variations in composition and structure.

The two-temperature method (TTM) was proposed [3] to calculate the temperature distribution within a pebble fuel. The method is not only convenient to perform but also gives more realistic results since particles and graphite matrix are considered separately. The following constrains are made to define the thermal calculation with TTM in this work,

Fig. 1: Schematic diagram of pebble fuel
1. There are only two components, fuel particles and graphite matrix.
2. Structure is isotropic and particles are dispersed regularly within the matrix.
3. No particles contact with each other, means particles could never form continuous conduction pathways.
4. The packing fraction of the fuel particle is low enough to avoid a significant temperature distribution exiting on the particle surface.
5. Graphite matrix is continuous everywhere.

Generically, the averaging volume method (AVM) is adopted for the homogenization treatment of the pebble fuel [4]. The volumetric-average approach is non-conservative and would underestimate the fuel temperature, while the harmonic-average approach overvalues the effect of the low thermal conductivity of fuel particles that would derive a much lower average thermal conductivity. These two average thermal conductivities serve as upper and lower bounds respectively, referred as Wiener bounds [5]:

- **Volumetric-average:**
  \[ k_v = \left( V_p k_p + V_m k_m \right) / V_s \]  
  (eq. 1)
- **Harmonic-average:**
  \[ k_h = V_s / \left( V_p / k_p + V_m / k_m \right) \]  
  (eq. 2)

Where, \( k_v \) is predicted effective thermal conductivity, \( k_p \) is thermal conductivity of fuel particle, \( k_m \) is thermal conductivity of graphite matrix. \( V_s \) is the total volume, while \( V_p \) is the total volume of all particles and \( V_m \) is the matrix occupied volume. Herein, Simplifications are made for convenience to regard particle as the UO\(_2\) type kernel and remain layers of particle are divided into graphite matrix, likewise in the establishment of the numerical CFD model of pebble fuel, since TRISO particle has a complex structure. Moreover, the graphite shell is removed for it is not the focus in this work. Above simplifications would not influence the verification of TTM.

Though some other models (such as Hashin-Shtrikman bounds [6] and the well-known Maxwell-Eucken model [7]) are may the best models for predicting thermal conductivity of macroscopically homogeneous, isotropic, two-component materials [8], we choose Wiener bounds to provide wider bounds to make sure both TTM calculated results and CFD calculated results are within the bounds.

**II. TTM DESCRIPTION**

The proposed two-temperature method is based on the fundamental governing differential equation that the increasing heat in the control region equals the sum of the heat across all the surfaces of the region and the heat transferred from the region to the adjacent other material. As equations 3, 4 describe, the heat transfer process in a pebble fuel is analogous to the two-group neutron diffusion process characterized by no absorption, no fission, and a fixed source. \( T_f \) is regarded as the fast neutron flux and \( T_m \) is the thermal neutron flux. Heat transfer between the two groups is assumed only to execute in the direction from higher temperature region to the lower region, and this is similar to the principle in the transfer between the fast neutrons and the thermal neutrons. Accounting for the region heat transfer term is driven by the temperature difference, the heat transferred from local region to the adjacent other material can be calculated by the relationship, \( \mu [T_f(r, t) - T_m(r, t)] \). The diffusion term expresses the heat migrating across all surfaces of the region. The fuel region is divided into two regions, the graphite matrix region and the fuel particles region. The diffusion surfaces of these two regions should be considered as a ratio of the sum respectively. Calculation equations are constructed as following.

In the inner fueled region,

\[ A_f k_f \nabla^2 T_f(r, t) - \mu [T_f(r, t) - T_m(r, t)] + q'''(t) \]

\[ = (\rho c)_f \frac{\partial T_f(r, t)}{\partial t} \]  
  (eq. 3)

\[ A_m k_m \nabla^2 T_m(r, t) + \mu [T_f(r, t) - T_m(r, t)] \]

\[ = (\rho c)_m \frac{\partial T_m(r, t)}{\partial t} \]  
  (eq. 4)

In the outer non-fueled graphite shell,

\[ k_g \nabla^2 T_g(r, t) = (\rho c)_g \frac{\partial T_g(r, t)}{\partial t} \]  
  (eq. 5)

Where, \( k_f \) is the thermal conductivity of fuel kernel, \( k_m \) is the thermal conductivity of graphite matrix, \( k_g \) is the thermal conductivity of graphite shell. \( T_f \) is the temperature at the center of fuel kernel, \( T_m \) is the temperature of graphite matrix, \( T_g \) is the temperature of graphite shell. \( A_f \) is the ratio of fuel kernel diffusion surface area to the complete surface area, \( A_m \) is the ratio of graphite matrix diffusion surface area to the complete surface area. \( \mu \) is the region heat transfer coefficient. \( q''' \) is homogenized volumetric heat generation rate in fuel kernel. \( c \) is specific heat, and \( \rho \) is mass density.

**II.A. Process to determine \( \mu \)**

As described in chapter I, the model of an individual pebble is simplified as a continuous graphite matrix with numerous UO\(_2\) kernels regularly dispersed inside. To this situation, the region heat transfer term \( \mu [T_f(r, t) - T_m(r, t)] \)
indicates the heat transferred from the fuel kernel to adjacent graphite matrix while the temperature at center of the fuel kernel is $T_f$ and temperature of the matrix is $T_m$. To determine the theoretic value of $\mu$, the region heat transfer term can be treated to calculate the volumetric heat generation rate in the total region while temperatures are constant both at the center of fuel kernel and boundary.

As shown in Fig. 2, the inner region of red color is fuel kernel, and the outer layer is graphite matrix that a single fuel kernel occupies in a pebble. The radius of the occupied matrix region $r_{mo}$ is determined by following equation,

$$V_{mo} = \frac{P_f V_s}{num}, \quad r_{mo} = \left(\frac{3V_{mo}}{4\pi}\right)^{1/3} \quad (eq. 6)$$

Where, $V_{mo}$ is the volume that occupied by a single fuel kernel, num is the number of fuel kernel in a pebble. $P_f$ is a coefficient linked to the fuel arrangement of fuel kernel.

As shown in Fig. 3, the circular curve of red color represents the occupied matrix region when $P_f$ equals 1.0. Likewise in the body-centered cubic arrangement, the minimum value of $P_f$ is 0.68. In the process of calculation, $P_f$ is recommended the average of minimum and maximum.

Till radius of the occupied matrix region $r_{mo}$ is determined, we can derive $\mu$ through following equations,

$$\int_{0}^{r_f} \frac{r q''''(t)}{3} dr = \int_{0}^{r_f} -k_f \frac{\partial T(r,t)}{\partial r} dr \quad (eq. 7)$$

$$\int_{r_f}^{r_{mo}} \frac{q(t)}{4\pi r^2} dr = \int_{r_f}^{r_{mo}} -k_m \frac{\partial T(r,t)}{\partial r} dr \quad (eq. 8)$$

$$\mu(T_f(t) - T_m(t)) = \frac{q(t)}{V_{mo}} \quad (eq. 9)$$

Where, $r_f$ is the radius of the fuel kernel, $q''''$ is homogenized volumetric heat generation rate in fuel kernel, $q$ is the heat generation rate of a single fuel kernel.

**II.B. Process to determine $A_f$, $A_m$**

$A_f$ is the ratio of fuel kernel diffusion surface area to the complete surface area and $A_m$ is the ratio of non-fueled graphite surface area to the complete surface area. Now that we know the ratio of one fuel kernel volume to the sum volume $V_s$, we assume that the surface area ratio is 2.0/3.0 order of the volume ratio. Calculation equations are shown as below,

$$A_f = \left(\frac{V_f}{V_s}\right)^{2/3} \quad (eq. 10)$$

$$A_m = 1 - A_f \quad (eq. 11)$$

Where, $V_f$ is the volume of an individual fuel kernel.

**II.C. Process to determine $T_f$, $T_m$ at boundary**

In the TTM method, continuity of heat flux and temperature at the interface within the pebble is applied. Temperature of graphite matrix $T_m$ on the surface of fueled region is supposed to equal the temperature of adjacent graphite shell. Knowing what $T_m$ means we can obtain the temperature on the surface of the fuel kernel. For an individual fuel kernel, the temperature at the center of the fuel kernel can be derived by knowing the temperature of kernel surface and the volumetric heat generation rate in the fuel kernel. We assume that the temperature is symmetric about the center of fuel kernel which is a simplification herein.
Table 1: Case matrix for thermal calculations.

<table>
<thead>
<tr>
<th>CASES</th>
<th>Particle diameter (mm)</th>
<th>Particle numbers</th>
<th>Particle arrangement</th>
<th>Packing fraction (%)</th>
<th>Pebble diameter (mm)</th>
<th>Pebble thermal power (W)</th>
<th>Boundary temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.5</td>
<td>1411</td>
<td>BCC</td>
<td>11.597</td>
<td>11.5</td>
<td>100.0</td>
<td>500.0</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.5</td>
<td>1411</td>
<td>BCC</td>
<td>11.597</td>
<td>11.5</td>
<td>200.0</td>
<td>500.0</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.5</td>
<td>1411</td>
<td>BCC</td>
<td>3.590</td>
<td>17.0</td>
<td>100.0</td>
<td>500.0</td>
</tr>
<tr>
<td>Case 4</td>
<td>0.5</td>
<td>1411</td>
<td>BCC</td>
<td>3.590</td>
<td>17.0</td>
<td>200.0</td>
<td>500.0</td>
</tr>
</tbody>
</table>

Table 2: Thermal calculation results comparison.

<table>
<thead>
<tr>
<th>CASES</th>
<th>$T_{\text{par, max}}$ (K)</th>
<th>$T_{\text{mat, max}}$ (K)</th>
<th>$T_{\text{par, max}}$ (K)</th>
<th>$T_{\text{mat, max}}$ (K)</th>
<th>$T_{\text{par, max}}$ (K)</th>
<th>$T_{\text{mat, max}}$ (K)</th>
<th>$T_{\text{par, max}}$ (K)</th>
<th>$T_{\text{mat, max}}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>546.332</td>
<td>542.805</td>
<td>546.588</td>
<td>543.571</td>
<td>542.142</td>
<td>538.382</td>
<td>561.096</td>
<td>557.336</td>
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<tr>
<td>Case 2</td>
<td>592.664</td>
<td>585.610</td>
<td>593.177</td>
<td>587.143</td>
<td>584.285</td>
<td>576.765</td>
<td>622.192</td>
<td>614.672</td>
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<td>529.363</td>
<td>525.851</td>
<td>529.007</td>
<td>525.906</td>
<td>527.902</td>
<td>524.142</td>
<td>531.926</td>
<td>528.166</td>
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<tr>
<td>Case 4</td>
<td>558.727</td>
<td>551.704</td>
<td>558.015</td>
<td>551.812</td>
<td>555.803</td>
<td>548.284</td>
<td>563.853</td>
<td>556.333</td>
</tr>
</tbody>
</table>

III. VERIFICATION OF METHOD

The CFD model is simplified as numerous UO$_2$ particles uniformly dispersed in graphite matrix without graphite shell. Four cases for validating TTM were analyzed by giving temperature profiles in different pebble structures and different power levels. Specifications for these cases are listed in table 1. Herein packing fraction means the volumetric ratio of all particles to the pebble. For all cases, the particle diameter is 0.5mm, particle numbers is 1411, and the arrangement applied for the particle distribution is BCC. Case 1 and case 2 adopt denser structure than in case 3 and case 4 to investigate the accuracy of TTM in the condition of high packing fraction since the method always has a better performance with lower packing fraction. Both two average methods and CFD method are used to provide comparisons with TTM. The CFD modeling is demonstrated in the Fig.4. The geometry is generated through reading rpl script file in ANSYS ICEM, more in over density boxes are applied in the domain of particles, and the thermal calculation are implemented by ANSYS CFX [9].

The intention of the calculation is to know the temperature of graphite matrix and the temperature in the center of the particle at every location within the pebble. Some of the key resulting temperature values are listed in Table 2. $T_{\text{par, max}}$ represents the maximum temperature in all of the particles. $T_{\text{mat, max}}$ represents the maximum temperature of the graphite matrix. Temperature profiles in a pebble fuel under all of these cases show the similar characteristics, and Fig. 5 is plot as a demonstration. Through this analysis, we have the following observations,

- Both the temperature in the center of fuel particle and graphite matrix and the temperature drop across the pebble are much higher in case 1 and case 2 than in case 3 and case 4. It shows that the pebble maximum temperature has a significant relation with the pebble structure and pebble thermal power while all cases adopt the same material and particle dimension.

- The widely used volumetric-average method is merely suitable for low packing fraction. With the structure becoming denser and denser, obvious calculation errors would appear. However, TTM perform well not only in low packing fraction but also in a relative high packing fraction.

- In all cases, predicted temperatures of particles by TTM match well with the CFD calculated results, which are considered as the reference values. However, TTM predicted matrix temperatures are slightly lower than the CFD results.
Fig. 5: Temperature distribution of four cases
IV. CONCLUSIONS

We have presented a two temperature method to calculate the temperature distribution in the pebble. The heat conduction process in a pebble fuel is analogous to the two-group neutron diffusion process characterized by no absorption, no fission, and a fixed source. The diffusion and transfer coefficients are determined in a convenient way with some reasonable assumptions.

CFD method is used to validate TTM. In this work, four cases were analyzed based on CFD, TTM, and two average methods. Compared to the two average methods, this method gives more realistic temperature profile in the fuel pebble due to the particles and graphite matrix are considered separately. Through the comparison with CFD calculated results, TTM is proved to be highly accurate in the large variation of both packing fraction and thermal power level. Since the parameters $\mu A_f$ and $A_m$ can be easily described as variations of location, this proposed method is prospect to be a candidate to calculate the temperature profile of heterogeneous structure.

Further consideration for this work would be investigating whether the method is still accurate in a higher packing fraction, especially in the condition of particles nearly contacting with each other.

REFERENCES