# Homogenization of thermal conductivity in a periodic structure

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## 1. Introduction

TRISO particle is used for a high temperature gas cooled reactor. There are few billions of TRISO particles in a reactor core. It is practically impossible to use a detailed model for diffusion calculations such as temperature or neutron flux analysis.

It is necessary to develop a homogenization model for compact level or block level calculation. It is widely accepted to obtain a (flux-) volume average of inverse of diffusion coefficient such as the neutron diffusion coefficient or the thermal conductivity as an analogy to the neutron transport cross section. However there are large difference in the averaged conductivity when the structure is highly heterogeneous. Effective conductivity model derived by Maxwell[1] for dispersed particles in a matrix is widely accepted for accurate conductivity calculation. Stainsby[2,3] and Folsom[4] used a detailed finite element model to find the effective conductivity. Cho et al. [5] have developed a two-temperature model based on empirical solution using the Monte Carlo simulations. Cho's method gives a quite reasonable result for practical application. However, Cho's method is not accurate in the sense that a Monte Carlo method is based on the Fredholm integral equation, and a diffusion equation cannot be converted into a Fredholm equation rigorously.

Two scale asymptotic expansion method for periodic problem was developed by Bensoussan et al [6]. This method converges to accurate solution when periodicity is great. Recently, Allaire applied the homogenization of the elliptic problem on periodic structures in various fields, such as the thermal conduction problem [7], and the neutron diffusion equation [8].

## 2. Two scale asymptotic expansion method

We have extended the original two scale asymptotic expansion method for periodic source problems such as TRISO particles in a pebble fuel or in a compact where heat source are present. The heat source is almost periodic considering that the neutron diffusion length is sufficiently large comparing the size of TRISO.

Thermal conduction equation in a periodic structure with periodic heat source is written as following.

$-\nabla\left(k\nabla\phi_\varepsilon\right)=f_\varepsilon$ , where $k$ is a conductivity tensor.

For a periodic structure, we can separate the variables in two independent variables, a slowly varying $x$ and a periodically varying $y$. $y$ can be written as $x/\varepsilon$ for convenience. Now, the heat source will be written as;

$f_\varepsilon = f_0\left(x\right)+\varepsilon f_1\left(x,x/\varepsilon\right)$.

Solution is approximated by an asymptotic series expansion;

$\phi_\varepsilon\left(x\right)=\phi_0\left(x\right)+\varepsilon\phi_1\left(x,x/\varepsilon\right)+\varepsilon^2\phi_2\left(x,x/\varepsilon\right)+\cdots$ .

We say $f_\varepsilon$ and $\phi_\varepsilon$ is Y-periodic.

Considering that the derivative can be expressed as sum of a slowly varying variable and a periodic variable as;

$$\frac{\partial}{\partial x_j}\Rightarrow\frac{\partial}{\partial x_j}+\frac{1}{\varepsilon}\frac{\partial}{\partial y_j}\ .$$

Using operator notation, we can expand the diffusion operator as:

$A^\varepsilon\equiv-\nabla k\nabla=\varepsilon^{-2}A_1+\varepsilon^{-1}A_2+\varepsilon^0A_3+\cdots$ ,

where,

$$A_1=-\frac{\partial}{\partial y_i}\left(k_{ij}\left(y\right)\frac{\partial}{\partial y_j}\right),$$

$$A_2=-\frac{\partial}{\partial y_i}\left(k_{ij}\left(y\right)\frac{\partial}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(k_{ij}\left(y\right)\frac{\partial}{\partial y_j}\right),$$

$$A_3=-\frac{\partial}{\partial x_i}\left(k_{ij}\left(y\right)\frac{\partial}{\partial x_j}\right).$$

We can write the original equation as

$A_1\phi_0=0$ ,

$A_1\phi_1+A_2\phi_0=f_1$ ,

$A_1\phi_2+A_2\phi_1+A_3\phi_0=f_0$ ,

etc.

First equation is trivial one where $\phi_0$ is only dependent on $x$ not $y$ .

The second equation reduces to

$$A_1\phi_1=\frac{\partial}{\partial y_j}k_{ij}\left(y\right)\frac{\partial\phi_0}{\partial x_j}+f_1\left(y\right).$$

Let us introduce auxiliary functions $\omega^j\left(y\right)$ and $\psi\left(y\right)$ which are Y-periodic, satisfying;

$$A_1\omega^j = -\frac{\partial k_{ij}}{\partial y_i} ,$$

and

$$A_1\psi = f_1(y).$$

Then the general solution is written as;

$$\phi_1 = -\omega^j \frac{\partial \phi_0}{\partial x_j} + \psi .$$

The last equation can be integrated over a periodic region Y.

$$\int_Y \left( A_2\phi_1 + A_3\phi_0 \right) dy = \int_Y f_0 dy = |Y| f_0 .$$

This can be explictly written as

$$-\frac{\partial}{\partial x_i}\left( k_{ij}^* \frac{\partial \phi_0}{\partial x_j} \right) = f_0$$

with the homogenized conductivity tensor

$$k_{ij}^* \equiv \frac{1}{|Y|}\int_Y k_{ij}\left(\hat{e}^i + \nabla\omega^i\right)\left(\hat{e}^j + \nabla\omega^j\right) dy$$

where $\hat{e}^i$ is unit vector in $i$ -direction.

In summary, $\omega_i$ is a Y-periodic solution of

$-\nabla\left(k\left(\hat{e}^i + \nabla\omega^i\right)\right) = 0$ with boundary condition

$\left(\hat{e}_i + \nabla\omega^i\right)\cdot\hat{n} = 0$ .

This can be rewritten as

$$-\nabla\left(k\nabla\omega^i\right) = -\nabla\left(k\hat{e}^i\right) .$$

We have to find the weighting functions for each direction, x, y, and z.

The equation for Y-periodic $\psi$ satisfies;

$-\nabla\left(k\nabla\psi\right) = f_1$ with periodic boundary condition.

Above equation has unique solution if and only if $\int_Y f_1 dy = 0$.

We can obtain the detailed solution as;

$$\phi_\varepsilon \simeq \phi_0 - \sum_j \omega^j \frac{\partial \phi_0}{\partial x_j} + \psi .$$

This result is similar to Bensoussan's original derivation except a correction term for local periodic source term contribution $\psi$. Above four equations can be solved as a same linear matrix equation with different source terms.

### 3. Comparison with Maxwell's method

Folsom has made a detailed study on the effective conductivity problem of realistic TRISO particles using the finite element method.[4] We compared the two scale asymptotic model using typical PBMR TRISO parameters used by Stainsby and Folsom as shown at Table 1.

Table 1. TRISO parameters

| material | radius (cm) | conductivity (W/cm/K) |
|---|---|---|
| kernel | 0.0250 | 0.037 |
| buffer | 0.0345 | 0.005 |
| iPyC | 0.0385 | 0.040 |
| SiC | 0.0420 | 0.160 |
| oPyC | 0.0460 | 0.040 |
| matrix | PF=0.09344 | 0.15 |

Maxwell's model is written as [2];

$$k_e = \frac{3k_m k_p \alpha + \left(2k_m + k_p\right)k_m\left(1-\alpha\right)}{3k_m\alpha + \left(2k_m + k_p\right)\left(1-\alpha\right)} .$$

where $\alpha$ is the packing fraction and $k_e$ , $k_m$ , and $k_p$ is the effective, matrix, and particle conductivity, respectively.

It is not easy to find the effective TRISO conductivity $k_p$ . Stainsby has determined $k_p$ using analytic solution on a spherical symmetric TRISO problem as 0.041328 W/m/K[2, App. C]. For given packing fraction, Maxwell's formula gives 0.1370 W/cm/K. More precise finite element calculation by Folsom gives 0.1375 W/cm//K.[4]

A pebble fuel used in a PBMR is composed of randomly distributed TRISO particles. However it can be modeled as a periodic body centered cubic (BCC) lattice considering that the temperature variation outside of TRISO particle is relatively small.

We have made a BCC model to find the homogenized conductivity and local temperature variation due to heat generation at kernel region. We used a finite element method with cubic elements and quadratic Lagrange polynomial (L2) basis to solve the spherical TRISO.

In this case, the conductivity is a scalar and the geometry has symmetry in x-, y-, and z-directions, the weighting functions are symmetric and the effective conductivity is a scalar.

Cubic lattice calculation has a difficulty in cutting spherical boundary. To improve the error due to nodalization, we take the average of conductivities for different materials in the computational element when spherical boundaries intersect. We have compared two methods of averaging, one by volume average and the other by harmonic average.

Figure 1 displays the results with varying meshes. Figure 1 shows poor convergence of the harmonic average method. We have adopted the volume average method in succeeding analysis which converges rather fast.

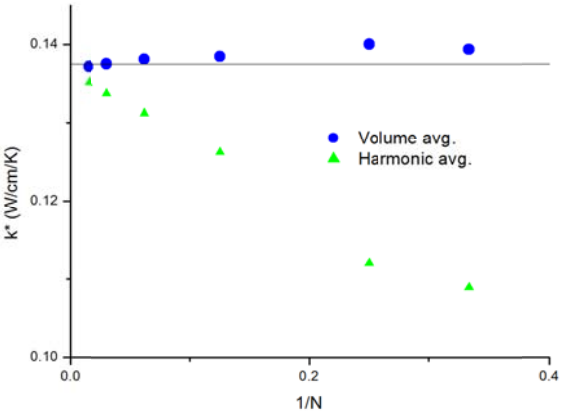


Figure 1. Homogenized conductivity by inverse number of nodes in a direction

Effective conductivity computed by two scale asymptotic expansion method is compared with Folsom as shown at Table 2.

Table 2. Effective conductivity

| N | Effective conductivity (W/cm/K) | Relative error (%) to 0.1375 |
|---|---|---|
| 4 | 0.1400 | 1.85 |
| 8 | 0.1385 | 0.73 |
| 16 | 0.1381 | 0.47 |
| 32 | 0.1375 | 0.04 |
| 64 | 0.1372 | 0.21 |

Result of the two scale asymptotic method converges to that of Maxwell method. Larger error at fewer elements is mostly due to discretization error corresponding cubic section of spherical shape.

## 4. Application to Pebble fuel problem

Dimension and conductivities are adopted from Cho's paper[5] for the convenience of comparison of the results. Table 3 displays parameters used in this analysis.

Table 3. Fuel pebble parameters

| | |
|---|---|
| Power/pebble (W) | 1893.94 |
| No. of TRISO in a pebble | 9315 (PF=0.057162) |
| Materials | kernel/buffer/iPYC/SiC/ oPyC/matrix/shell |
| Radius (cm) | 0.025/0.03425/0.03824/ 0.04177/0.04577/2.5/3.0 |
| Conductivity (W/cm K) | 0.0346/0.01/0.04/0.183/ 0.04/0.25/0.25 |
| Helium Temperature (K) | 1173 |
| Heat transfer coefficient ($W/cm^2K$) | 0.01006 |

Figure 2 displays the shape of the conductivity weighting function $\omega^x$ in the BCC lattice. It apparently shows periodic shape as well as anti-symmetry along the central plane vertical to the x-axis. The magnitude is high at coating layers of TRISO and is decreasing as away from the center of TRISO.

Figure 3 displays local Y-periodic temperature distribution. The temperature distribution should be spherical near the center of TRISO particle. However, due to cubic element nodalization, the temperature distribution appears as cubic which will be disappear as number of mesh increases.

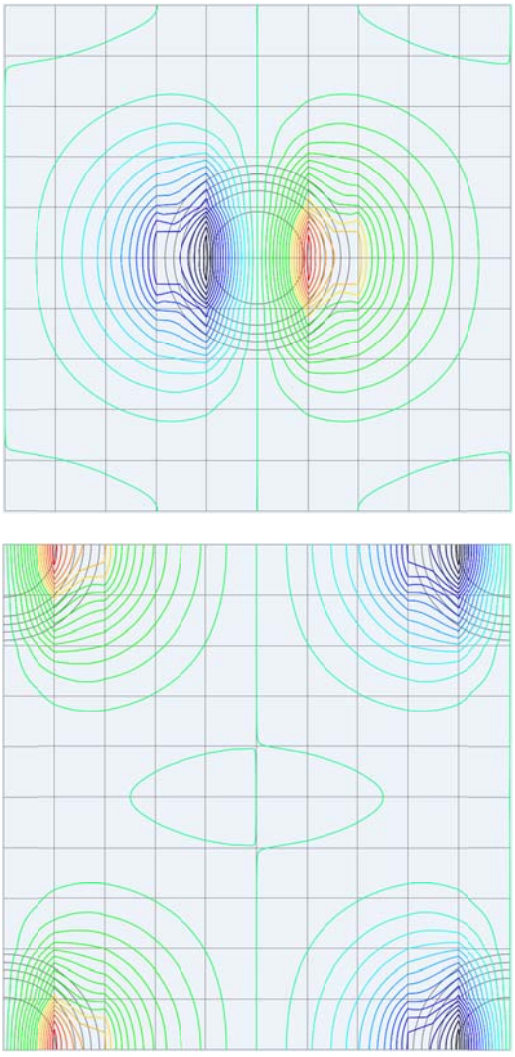

Figure 2. Conductivity weighting function $\omega^x$ in BCC lattice. (Up: central plane, Down: edge plane)

Table 4 displays the result with varying number of elements. The conductivity is a scalar due to symmetry in x-, y-, and z-direction.

Table 4 shows convergent behavior as finite element discretization becomes fine. Homogenized conductivity converges rather rapidly comparing the peak value. Slow convergence in $\psi$ is due to cubic nodalization in which heat generation and conductivity is smoothed.

We may adopt the homogenized conductivity as 0.2347 W/cm/K.

Table 4. Homogenized conductivity and maximum value of $\psi$

| N | k* (W/cm/K) | $\psi_{peak}$ (K) |
|---|---|---|
| 3 | 0.239549 | 0.079 |
| 4 | 0.238245 | 0.450 |
| 6 | 0.236863 | 1.610 |
| 8 | 0.235964 | 5.586 |
| 10 | 0.235878 | 11.414 |
| 16 | 0.235288 | 16.291 |
| 32 | 0.234925 | 23.160 |
| 64 | 0.234689 | 25.802 |

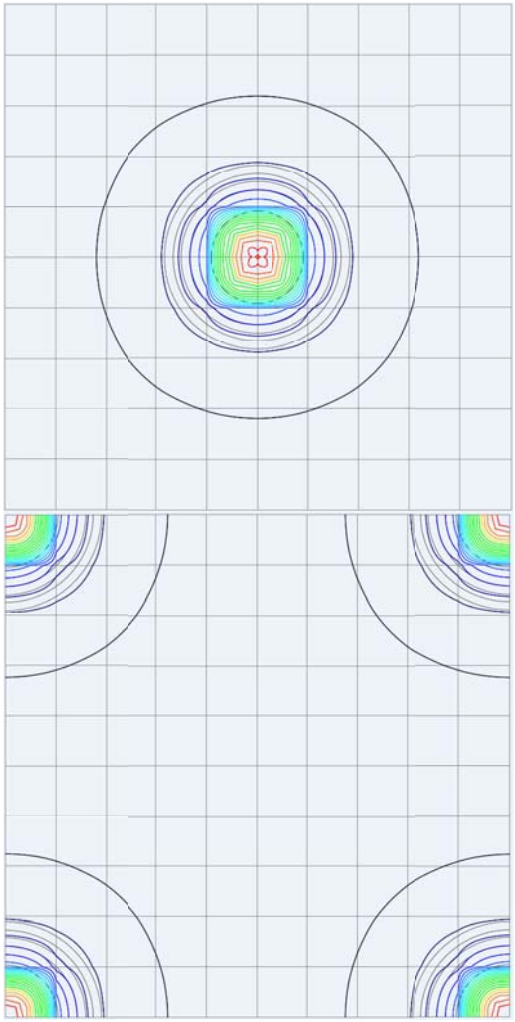

Figure 3. Y-periodic temperature $\psi$ (Up: central plane, Down: edge plane)

Using Stainsby's analytic method, effective TRISO conductivity is 0.047775 W/cm/K. Stainsby's Maxwell method gives the homogenized effective conductivity as 0.2345 W/cm/K which is practically same to present method. The peak value of $\psi$ is converging slowly due to sufficiently. To preserve total power generation in the problem region, the power density at kernel region is reduced which results low temperature rise at kernel. This situation can be improved by refined nodalization at kernel location. We can estimate the peak value of $\psi$ using the analytic solution assuming spherical symmetry around a TRISO. The analytic peak value is found as 28.95 K.

We can construct the heterogeneous temperature distribution after finding the homogenized temperature distribution. For our pebble fuel problem, there exists an analytic solution for the homogenized problem. Using the homogenized conductivity, 0.2347 W/cm/K, obtained in present study, we obtain 1380K as the temperature at the interface between shell and fuel region and 1508K as homogenized centerline temperature.

Figure 5 of Cho's paper[5] reads as 1515K for the center line temperature and 1380K as the interface temperature. The value is equivalent to homogenized conductivity of 0.223 W/cm/K. Present homogenized conductivity is about 5% higher comparing the one by Monte Carlo approach used by Cho.

## 5. Conclusion and Further Study

Two scale homogenization theory developed by Bensoussan and applied to various diffusion problem by Allaire was extended for conductive diffusion problem with periodic heat source. The result was compared with Stainsby's Maxwell method and Cho's two temperature model. For multi-materials in a finite element, the volume average strategy of conductivity approaches more rapidly.

Further simplification can be achieved by considering the fact that Y-periodic temperature is strongly varying only inside TRISO particle which has spherical symmetry. The weighting function can be computed with consideration of symmetries in y- and z-direction as well as anti-symmetry on x-direction. We can also consider a further simplification using the homogenized TRISO particle in the BCC lattice.

Present method converges to Maxwell's method for TRISO problem by sufficiently large number of computational elements. Stainsby's method can be used for TRISO problem where analytic solution exists. However, for more complex geometry such as prismatic fuel block, two scale asymptotic expansion approach can be used with finite element method to obtain the weighting functions.

We will extend present method for homogenization of the prismatic fuel block composed of many fuel compacts and coolant holes. In this case, the effective conductivity is a tensor which has non-zero off diagonal components.

Present method can be applied for the neutron diffusion problem since the thermal conduction problem is an elliptic problem like a neutron diffusion problem.

Current flux reconstruction practice which is solving an eigenvalue problem on an (or several color set)

assembly may be modified to rather simple group-wise source problem.

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