ESTIMATION OF THERMAL CONDUCTIVITY OF DIGITIZED HETEROGENEOUS MEDIA BASED ON LOCAL POROSITY THEORY

Jack Widjajakusuma

Jurusan Teknik Sipil, Universitas Pelita Harapan
e-mail: jack_w@uph.edu

ABSTRACT

Estimation of thermal conductivity of digitized heterogeneous media is the central problem in many engineering applications. Since effective thermal conductivity depend strongly on the microstructure of heterogeneous media, one has to incorporate more quantitative information about the underlying microstructure in estimating the thermal conductivity of such media. The present paper discusses estimation of effective thermal conductivity of heterogeneous media based on local porosity theory. To demonstrate the goodness of the mixing law based on the local porosity theory, we apply this mixing law to estimate thermal conductivity of digitized heterogeneous media, which have the same both porosities and two-point correlation functions. It is to find out that the local porosity theory provides good quantitative estimations with the exact results and the length of representative volume element.

Keywords: thermal conductivity, heterogeneous materials, mixing-law, local porosity theory, representative volume element

1. INTRODUCTION

Heterogeneous media are media, which are composed of different homogeneous constituents. Mostly media, which are used in civil engineering applications, are heterogeneous media such as soil, brick, concrete, rock, asphalt, wood and composite material. Therefore, understanding of thermomechanical phenomena of such media is a successful key in designing civil engineering structures. A key macroscopic parameter characterizing the thermomechanical characteristics of a heterogeneous media is the effective material constants. For example, in order to understanding the enhanced heat insulation for bricks, the enhanced safety in fire for high performance concrete, the pavement response, the energy transfer between two adjacent parts of rock, one has to know the effective thermal conductivity of brick, concrete, asphalt, and rock, respectively. In these instances, the effective heat conductivity is a key parameter.

The heterogeneous nature of such media causes variations of temperature gradient, heat flux and thermal conductivity from constituent to constituent. Within the constituent, the heat conductivity is uniform and equal to the heat conductivity of that constituent. The size scale of the constituent is called the micro-length-scale and it defines the domain of microscopic parameters. On larger scales (the macro-length-scale), the heterogeneous medium often behaves like a homogeneous medium with effective thermal conductivity which generally differ from those of the constituents. The effective heat conductivity of heterogenous medium depends strongly not only on the constituent’s thermal conductivity but also on the microgeometry (Beran, 1968, Torquato, 2002, Hilfer, 1996, Widjajakusuma et al., 2003).

The dependency of the effective thermal conductivity on the microgeometry can be illustrated as following. Consider biphasic media composed of 50% thermal conducting material and 50% thermal isolating material: (a) Dispersed isolating particles are embedded in the connected conducting matrix; (b) Dispersed conducting particles are spread out in the connected isolating matrix. It is evident that the first medium is impermeable material and the second medium is permeable material. Through this example, we can conclude that, for example, volume fractions and connectivity control the thermal conductivity of the heterogeneous medium. Volume fractions and connectivity are examples of microgeometrical quantities. Therefore, a mixing-law for estimating effective heat conductivity should contains information about the volume fractions and connectivity of heterogeneous medium.

Recently, local porosity theory, which was proposed by Hilfer (1991, 1993, 1996), can describe the fluctuations of volume fraction, of specific internal surfaces and connectivity of heterogeneous media in terms of local volume fraction distribution function, local specific internal surface distribution function and local percolation distribution
function, respectively. This paper concludes with quantitative estimation of effective thermal conductivity of digitized heterogeneous media, which have the same both porosities and two-point correlation functions.

This paper is organized as follows. In Section 2, we give microgeometrical characteristic functions. In section 3, we incorporate these characteristic functions into a mixing law. In section 4, we apply the mixing law based on local porosity theory to estimate the thermal conductivity of digitized heterogeneous medium. In section 5, we make some conclusions.

2. MICROGEOMETRICAL CHARACTERISTIC FUNCTIONS

We consider that the heterogeneous medium is composed of a phase \( \phi^F \) and a phase \( \phi^S \), which have the volume \( V(\phi^F) \) and \( V(\phi^S) \), respectively. The total volume of the heterogeneous medium is given by \( V = V(\phi^F) + V(\phi^S) \).

The volume fraction of the phase \( \phi^F \) is defined as \( n^F = \frac{V(\phi^F)}{V} \). The volume fraction and is an example of the one-point correlation function (Beran, 1968, Torquato, 2002, Sahimi, 2008). The normalized two point correlation function is defined as

\[
S_2(L) = \frac{1^F(0)1^F(L) - (n^F)^2}{n^F(1-n^F)},
\]

where

\[
1^F(x) = \begin{cases} 1 & \text{for } x \in \phi^F \\ 0 & \text{for } x \notin \phi^F \end{cases}.
\]

Since the fluctuations of volume fraction, specific internal surface and connectivity of heterogeneous medium play significant roles in transport phenomena (Hilfer, 1993, 1996, Sahimi, 2003, Widjajakusuma et al., 1999, 2003), wave propagation (Debye et al., 1957, Sheng, 1995), and fracture (Botsis & Beldica, 1995) in heterogeneous media. In order to obtain the fluctuations of volume fraction, specific internal surfaces and connectivity of heterogeneous medium, we subdivide the heterogeneous medium into \( m \) non-overlapping cells \( K^1, K^2, \ldots, K^m \). We can measure microgeometrical quantities from these cells and then collect them into various histograms. From the histograms, we can find the probability density function of the corresponding geometrical quantities. Obviously, the probability density functions depend on the size and shape of the chosen cells. This kind of microgeometrical characterization is called local porosity theory (Hilfer, 1991, 1993, 1996, Biswal et al., 1998, Torquato, 2002, Widjajakusuma et al., 2003).

Local volume fraction distribution function

The local volume fraction, \( n^F(x_i, L) \), within the region \( K^i(x_i, L) \), and the local volume fraction distribution function, \( p(n^F, L) \), are defined by

\[
n^F(x_i, L) = \frac{V(\phi^F \cap K^i(x_i, L))}{V(K^i(x_i, L))}, \quad p(n^F, L) = \frac{1}{m} \sum_{i=1}^{m} \delta(n^F - n^F(x_i, L)).
\]

Here, \( K^i(x_i, L) \) denotes the cubical cell of length \( L \), \( x_i \) is the position vector of the center of \( K^i(x_i, L) \) and \( \delta(n^F - n^F(x_i, L)) \) is the Dirac delta function.

Local percolation distribution function

Consider a percolation parameter \( p_L \) which gives the average degree of connectivity between various subregions of a random medium. When \( p_L = 0 \), all subregions are totally isolated from every other subregion. When \( p_L = 1 \), all subregions are connected to neighbouring subregions. When the random medium is connected from one side to the other through paths which span completely across the system, a so-called spanning cluster exists. The term...
percolation threshold \( p_{Lc} \) can be defined in the following way. Starting from \( p_L = 0 \) if one creates connections among the subregions, at \( p_L = p_{Lc} \), a spanning cluster exists for the first time. When \( p_L \geq p_{Lc} \), there always exists a spanning cluster, although some isolated clusters can still be present.

Similar to the definitions of the local volume fraction and of the local specific internal surface, the indicator function for the connectivity of the phase \( \Phi^F \) within a subregion \( K^i(x_i, L) \) can be defined. This connectivity indicator function \( L(x_i, L) \) takes the value 1 if there is a connected path of the phase \( \Phi^F \) from one side to the opposite side and takes the value 0 otherwise:

\[
L(x_i, L) = \begin{cases} 
1 & \text{if } K^i(x_i, L) \text{ allows isotropic percolation} \\
0 & \text{otherwise}
\end{cases}
\]  

The local percolation probability \( p_L(n^F, L) \) is given by

\[
p_L(n^F, L) = \sum_{i=1}^{m} \frac{L(x_i, L)\delta(n^F - n^F(x_i, L))}{\delta(n^F - n^F(x_i, L))}.
\]  

### Total fraction of percolating regions

The local percolation probability \( p_L(n^F, L) \) gives the local connectivity property of windows \( K^i(x_i, L) \). To obtain the global overall connectivity, one has to take the average of the local percolation probability over all windows. Thus,

\[
p(L) = \int_0^1 \int_0^1 p(n^F, L) p_L(n^F, L) \, dn^F.
\]  

The function \( p(L) \) gives the total fraction of percolating cells. If the value of \( p(L) \) of a given heterogeneous medium is above (under) some critical value \( p_c \), then there is a path of phase \( \Phi^F \) from one side to the opposite side. Obviously, \( \lim_{L \to L_{cr}} p(L) = 0 \) if the phase \( \Phi^F \) of a given heterogeneous medium is dispersed in the phase \( \phi^S \) and \( \lim_{L \to L_{cr}} p(L) = 1 \) if the phase \( \Phi^F \) is connected.

### 3. MIXING LAW

The effective thermal conductivity \( \overline{k} \) is defined by

\[
\overline{q} = -\overline{k} \, \text{grad} \, \Theta(x),
\]  

where \( \overline{q} \) is the average of the heat flux and \( \text{grad} \, \Theta(x) \) is the average of the gradient of the temperature field.

The mixing law based on LPT takes the form of

\[
\begin{align*}
\int_0^1 p(n^F, L) p_L(n^F, L) \frac{k_{cs}(k^F, k^S, 1 - n^F) - \overline{k}}{k_{cs}(k^F, k^S, 1 - n^F) + 2\overline{k}} \, dn^F & + \\
+ \int_0^1 p(n^F, L) [1 - p_L(n^F, L)] \frac{k_{cs}(k^S, k^F, n^F) - \overline{k}}{k_{cs}(k^S, k^F, n^F) + 2\overline{k}} \, dn^F & = 0,
\end{align*}
\]  

where
4. ESTIMATION OF EFFECTIVE THERMAL CONDUCTIVITY

In this section, the methods discussed in the previous section are applied to analyzing real digitized heterogeneous media. Sample A was obtained experimentally by computerized microtomography and the other two samples, R1 and R2, are obtained by the Gaussian field reconstruction method from the sample A (Adler, 1992, Biswal & Hilfer, 1999, Biswal et al. 1998). Both samples are numerically reconstructed from the same given real sample B, but with different length scales. R2 is two times coarser than R1. Thus, R2 has twice the actual size of R1. The basic idea of this method is to reconstruct a medium which should have the same two-point correlation function and volume fraction as the reference sample A. Thus, the volume fractions and the correlation functions of all samples should be the same, which can be seen from Table 1. column 4 and Figure 1c.

Through the digitization process, the samples are represented by a cubic lattice of voxels with a resolution \( a \). The dimension of the samples is denoted as \( M_1 \times M_2 \times M_3 \) (in unit of \( a^3 \)), the total porosity is \( \bar{\eta}^F \) (Table 1). The three-dimensional perspective of reference and reconstructed samples, A and R1, respectively, are shown in Figure 1a and 1b.

Table 1: Properties of digitized samples analysed

<table>
<thead>
<tr>
<th>Sample</th>
<th>( a )</th>
<th>( M_1 \times M_2 \times M_3 )</th>
<th>( \bar{\eta}^F )</th>
<th>( L_p )</th>
<th>( \frac{\varepsilon^f}{\varepsilon^s} = \infty ) (FVM)</th>
<th>( \frac{\varepsilon^f}{\varepsilon^s} = \infty ) (LPT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berea (A)</td>
<td>10 µm</td>
<td>128 x 128 x 128</td>
<td>0.1775</td>
<td>20</td>
<td>0.024021</td>
<td>0.048402</td>
</tr>
<tr>
<td>Reconstructed Berea (R1)</td>
<td>10 µm</td>
<td>128 x 128 x 128</td>
<td>0.1783</td>
<td>28</td>
<td>0.006836</td>
<td>0.019263</td>
</tr>
<tr>
<td>Reconstructed Berea (R2)</td>
<td>20 µm</td>
<td>128 x 128 x 128</td>
<td>0.1776</td>
<td>34</td>
<td>0.003084</td>
<td>0.034099</td>
</tr>
</tbody>
</table>

Figure 1. (a) Three-dimensional perspective of the pore space of Berea sandstone via microtomography. (b) Reconstructed Berea Sandstone R1. The pore space is grey and opaque and the solid phase is transparent. (c) The normalized two-point correlation function \( \overline{S}_2(L) \) of three samples.

Using the equations (3), (5), \( p(n^F, L) \), \( p_L(n^F, L) \), the function of percolating regions \( p(L) \) can be computed for these three digitized samples. In Figure 2d, \( p(L) \) is plotted versus \( L \) (in units of \( a \) ) for all samples. For all samples, \( p(L) \) is sigmoidal in shape. Figure 2d shows that \( p(L) \) of sample A is much higher than of samples R1 and R2. The total fraction of percolating cells \( p(L) \) of both samples R1 and R2 are almost the same. It means that the connectivity of the original sample A is better than those of both reconstructed samples R1 and R2. This results can
be qualitatively confirmed from the pictures of the cross sections of these three samples as depicted in Figure 2a, 2b and 2c, because the reconstructed samples R1 and R2 have more isolated pore spaces.

Obviously, the mixing-law based on the local porosity theory (8) estimate effective thermal conductivity $\kappa$, which depend on the length of the measurement cell $C^l$. Therefore, it is important to determine the length, over which (8) provide reasonable estimations of $\kappa$. This length can be seen as the length of the representative volume element (RVE) (Nemat-Nasser & Hori, 2000, Widjajakusuma 2002b). For scales larger than the RVE, we can assume that the heterogeneous medium behaves as the homogeneous medium, while for the scales smaller than the RVE, we have to take into account the heterogeneity of such medium.

Various length scales relevant to the transport properties are proposed in earlier works on local porosity theory (Boger et al., 1992, Hilfer, 1996, Widjajakusuma 2002b, Widjajakusuma et al., 1999, 2003). In our earlier works (Widjajakusuma 2002b, Widjajakusuma et al., 2003), we found that for percolation length $L_p$, which is defined as $d^2 p/d L^2 |_{L=L_p} = 0$, the mixing-law (8) provides a good estimation of the effective material parameters in the infinite contrast $\kappa/\kappa = \infty$. Therefore, in this work, we will also use the percolation length $L_p$. The percolation length $L_p$ of the three samples is given in Table 1 column 5.

Table 1 presents the detailed comparison between the predictions of mixing-law (column 7) and the exact values (column 6) for infinite contrasts ($\kappa/\kappa \to \infty$). We found that estimation based on local porosity theory gives good agreement with the exact values. The exact values were obtained through finite volume method (FVM), which can be found in Widjajakusuma (2002a).

5. CONCLUDING REMARKS

In this paper, we estimated the effective thermal conductivity of real digitized heterogeneous media using the mixing-law based on local porosity theory. In the case of the infinite contrast, $\kappa/\kappa = \infty$, we found that at the percolating length $L_p$, the estimation based on the local porosity theory gives good agreement with the exact results. Furthermore, the percolating length $L_p$ can be seen as the length of RVE, which is the central question in the theory of the heterogeneous media.

The results establish that $n^f (x_i, L)$, $p_L (n^f, L)$ and $p(L)$ contain useful microscopic information which can lead to reasonable prediction of effective thermal conductivity. Therefore, in addition to the volume fraction, in predicting the effective material parameters, one has to include connectivity information of the microstructure. It should be emphasized that mixing-laws, which solely use volume fraction as the input parameter, cannot correctly estimate the effective thermal conductivities of these three samples, since all of them have the same porosities. We have shown through three digitized samples, which have the same porosities, that the total fraction of percolating cells $p(L)$ can distinguish the connectivity of these samples. It means that $p(L)$ can quantitatively capture the connectivity information of heterogeneous media.
REFERENCES