

Thermal Conductivity of 3D Woven Composite Thermal Protection System Materials via Multiscale Recursive Micromechanics

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Multiscale micromechanics predictions have been made for the effective thermal conductivities and local thermal fields for a novel 3D woven composite thermal protection system material. The Multiscale Recursive Micromechanics approach, which enables micromechanics models to call other micromechanics models (or themselves recursively) to consider finer and finer length scales, has been employed. The multiscale model uses a recently developed version of the High-Fidelity Generalized Method of Cells micromechanics theory at each of three length scales. Results focus on the impact of the microstructural geometry representation at each length scale on the material's effective thermal conductivity, along with the local thermal flux and temperature fields induced in the microstructures.

I. Introduction

Novel thermal protection systems (TPS) for re-entry and hypersonic vehicles utilize 3D woven composite materials with blended carbon/phenolic filament tows (yarns) and a phenolic resin matrix. The presence of long carbon fibers provides superior stiffness and strength compared to legacy TPS, while the 3D weave pattern provides a great deal of design flexibility for both in-plane and through thickness thermomechanical behavior. However, modeling of 3D woven composites is notoriously complex and numerically intensive. The trend in model development for these materials has been to increase the geometric fidelity of the model [1]-[11]. However, the computational cost of these models can be exorbitant. Many of these models contain upwards of hundreds of thousands, or even millions, of

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degrees of freedom due to the complex nature of the woven microstructure. Of equal importance is the development of rapid engineering tools for material and structural design. With such tools, parametric and statistical studies can be conducted incorporating a variety of loading scenarios and levels of imperfections.

The primary purpose of TPS materials (as the name states) is to shield an underlying system from the effects of very high temperatures. The TPS must survive any mechanical loading it experiences, while also maintaining sufficient insulative characteristics, possibly in the presence of ablation. As such, TPS design and materials development are inherently multi-physics problems, with the TPS thermal performance playing a major role. The present investigation examines the thermal performance of 3D Medium Density Carbon Phenolic (3MDCP), which is a novel 3D woven composite TPS material. A unique modeling approach known as Multiscale Recursive Micromechanics (MsRM) has been employed, wherein recursive semi-analytical micromechanics methods are employed at various length scales within the composite [12]. The MsRM approach has recently been extended to solve for the effective thermal conductivity as well as the local temperature and thermal flux fields throughout the composite based on the High-Fidelity Generalized Method of Cells (HFGMC) micromechanics theory presented in ref. [13]. An introduction to HFGMC, as well as several simpler micromechanics theories, can be found in ref. [14]. This approach well-suited for inclusion in multi-physics TPS models, but this investigation focuses solely on the TPS material thermal properties. The MsRM approach has been applied to the 3MDCP TPS material to capture the microstructure at multiple length scales. Predictions, in the form of effective thermal conductivities and local thermal fields, are made and compared for different microstructural representations across the length scales. When available, model results are also compared to classical expressions from the literature and some available test data.

II. Multiscale Recursive Micromechanics Thermal Conductivity and Local Field Calculations

The MsRM approach for modeling materials with multiscale microstructures is shown in Fig. 1. The approach relies on recursive procedures, subroutines, and data structures that allow an arbitrary number of scales to be defined and to pass data between each other seamlessly. In the context of MsRM, the micromechanics theory provides a concentration tensor $\mathbf{A}_i^{(\alpha_i)}$, which, in terms of the heat conduction problem, relates the local average temperature gradient components within subvolumes in the material to the global temperature gradient components. The subvolumes (at a given scale, i) are denoted in general by α_i , where the number of subvolumes is N_{α_i} . The local average temperature gradients are denoted by,

$$\mathbf{X}_i^{(\alpha_i)} = -\frac{1}{V_{(\alpha_i)}} \int_{V_{(\alpha_i)}} [\nabla T]_i^{(\alpha_i)} dV_{(\alpha_i)} = -\frac{1}{V_{(\alpha_i)}} \int_{V_{(\alpha_i)}} \begin{bmatrix} \frac{\partial T}{\partial x_1} \\ \frac{\partial T}{\partial x_2} \\ \frac{\partial T}{\partial x_3} \end{bmatrix}_i^{(\alpha_i)} dV_{(\alpha_i)} \quad (1)$$

where T is the temperature field, whose gradients in the subvolume α_i are $\begin{bmatrix} \frac{\partial T}{\partial x_j} \end{bmatrix}_i^{(\alpha_i)}$ in coordinate direction j .

The temperature gradient concentration equation is given by,

$$\mathbf{X}_i^{(\alpha_i)} = \mathbf{A}_i^{(\alpha_i)} \bar{\mathbf{X}}_i \quad (2)$$

where $\bar{\mathbf{X}}_i$ are the global (homogenized or averaged) temperature gradients at scale i . At the highest scale ($i = 0$), the global temperature gradients are known from the applied conditions (an admissible combination of global temperature gradient and heat flux components) once the effective thermal conductivity tensor, $\mathbf{\kappa}_0^*$, has been computed as described below.

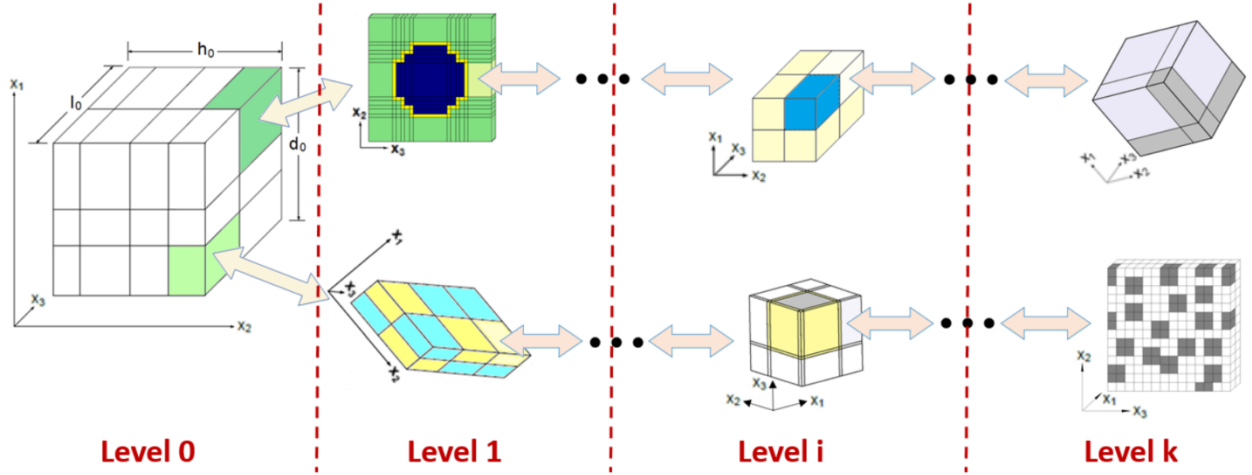


Figure 1. Schematic of the Multiscale Recursive Micromechanics (MsRM) approach wherein micromechanics models are embedded within each other to model microstructure at any number of length scales.

The local constitutive equation at scale i relates the average heat flux components in subvolume α_i ($\mathbf{q}_i^{(\alpha_i)}$ in tensor form) to the subvolume average temperature gradients and can be written as,

$$\mathbf{q}_i^{(\alpha_i)} = \boldsymbol{\kappa}_i^{(\alpha_i)} \mathbf{X}_i^{(\alpha_i)} \quad (3)$$

where $\boldsymbol{\kappa}_i^{(\alpha_i)}$ is the 2nd-order thermal conductivity tensor at scale i in subvolume α_i . Substituting Eq. (2) into Eq. (3) gives,

$$\mathbf{q}_i^{(\alpha_i)} = \boldsymbol{\kappa}_i^{(\alpha_i)} \mathbf{A}_i^{(\alpha_i)} \bar{\mathbf{X}}_i \quad (4)$$

The average (global) heat flux tensor at scale i is given by,

$$\bar{\mathbf{q}}_i = \sum_{\alpha_i=1}^{N_{\alpha_i}} v_{\alpha_i} \mathbf{q}_i^{(\alpha_i)} \quad (5)$$

where v_{α_i} is the volume fraction of subvolume α_i . Eqs. (4) and (5) lead to,

$$\bar{\mathbf{q}}_i = \sum_{\alpha_i=1}^{N_{\alpha_i}} v_{\alpha_i} \boldsymbol{\kappa}_i^{(\alpha_i)} \mathbf{A}_i^{(\alpha_i)} \bar{\mathbf{X}}_i \quad (6)$$

and recognizing that the effective constitutive equation at level i is given by,

$$\bar{\mathbf{q}}_i = \boldsymbol{\kappa}_i^* \bar{\mathbf{X}}_i \quad (7)$$

Eqs. (6) and (7) indicate that the effective thermal conductivity tensor at level i , $\boldsymbol{\kappa}_i^*$, is given by,

$$\mathbf{\kappa}_i^* = \sum_{\alpha_i=1}^{N_{\alpha_i}} v_{\alpha_i} \mathbf{\kappa}_i^{(\alpha_i)} \mathbf{A}_i^{(\alpha_i)} \quad (8)$$

Thus, as detailed in [13], once the concentration tensors for all subcells at a given scale are determined, all effective properties and field variables at that scale can be easily obtained. The effective thermal conductivity is given by Eq. (8), whereas the average temperature gradient and heat flux components for every subcell are given by Eqs. (2) and (3), respectively.

In MsRM, the scales are linked by equilibrating the homogenized global temperature gradient, heat flux, and thermal conductivity tensors at level i to the local average temperature gradient, average heat flux, and thermal conductivity tensors of a given subvolume at level $i-1$ (with appropriate transformation to account for the potential coordinate system change from scale to scale). That is,

$$\bar{\mathbf{X}}_i = \mathbf{T}_1^i \mathbf{X}_{i-1}^{(\alpha_{i-1})}, \quad \bar{\mathbf{q}}_i = \mathbf{T}_1^i \mathbf{q}_{i-1}^{(\alpha_{i-1})}, \quad \mathbf{\kappa}_i^* = \mathbf{T}_2^i \mathbf{\kappa}_{i-1}^{(\alpha_{i-1})}, \quad i = 1, \dots, k \quad (9)$$

where $\mathbf{T}_1^i$ and $\mathbf{T}_2^i$ are the appropriate first and second order coordinate transformation matrices, respectively. Hence, it is clear that starting with the lowest scale (k) microstructure (see Fig. 1), whose subvolumes contain only monolithic materials, the effective thermal conductivity tensor can be calculated using any standard micromechanics theory. This thermal conductivity tensor (after appropriate coordinate transformation) then represents the homogenized material occupying one of the subvolumes within a composite material at the next higher length scale. Given the transformed effective thermal conductivity tensors of all subvolumes at this next higher length scale, the effective thermal conductivity tensor of the composite at this level can be determined. This thermal conductivity tensor can then be transformed and passed along to the next higher length scale, and the process repeats until the highest length scale considered (0) is reached.

As an example, for an MsRM analysis considering three length scales (0, 1, and 2), the overall effective thermal conductivity tensor can be written using Eqs. (8) and (9) as,

$$\mathbf{\kappa}_0^* = \sum_{\alpha_0} v_{\alpha_0} \left\{ \left(\mathbf{T}_1^1 \right)^{-1} \sum_{\alpha_1} v_{\alpha_1} \left[\left(\mathbf{T}_2^2 \right)^{-1} \sum_{\alpha_2} v_{\alpha_2} \mathbf{\kappa}_2^{(\alpha_2)} \mathbf{A}_2^{(\alpha_2)} \right]^{(\alpha_1)} \mathbf{A}_1^{(\alpha_1)} \right\}^{(\alpha_0)} \mathbf{A}_0^{(\alpha_0)} \quad (10)$$

Note that in Eq. (10), the superscript on the bracketed terms indicates that all variables within the brackets are a function of the subvolume indices from the next higher length scale (including lower scale volume fractions and subvolume indices). The intent of this notation is to fully define the subvolume at a given scale as one progresses down the length scales. For example, using this notation, the effective thermal conductivity tensor at level 2, from Eq. (9), can be written as,

$$\left\{ \left[\mathbf{\kappa}_2^* \right]^{(\alpha_1)} \right\}^{(\alpha_0)} = \left\{ \left[\mathbf{T}_2^2 \right]^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \mathbf{\kappa}_1^{(\alpha_1)} \right\}^{(\alpha_0)} \quad (11)$$

as there are distinct $\mathbf{\kappa}_2^*$ values for every level 1 subvolume, while there are distinct level 1 composites present within each level 0 subvolume.

Converse to this multiscale homogenization procedure, MsRM can perform multiscale localization of the heat flux and temperature gradient tensors. The multiscale localization is needed to calculate the heat flux, temperature gradient, and temperature fields at all length scales. For the three length scale example, for a known (applied) highest scale average temperature gradient, $\bar{\mathbf{X}}_0$, the local average temperature gradient tensor, in an arbitrary lowest scale (level 2) subvolume, can be written using Eqs. (2) and (9) as,

$$\left\{ \left[\mathbf{X}_2^{(\alpha_2)} \right]^{(\alpha_1)} \right\}^{(\alpha_0)} = \left\{ \left[\mathbf{A}_2^{(\alpha_2)} \right]^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \left[\mathbf{T}_1^2 \right]^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \mathbf{A}_1^{(\alpha_1)} \right\}^{(\alpha_0)} \left\{ \mathbf{T}_1^1 \right\}^{(\alpha_0)} \mathbf{A}_0^{(\alpha_0)} \bar{\mathbf{X}}_0 \quad (12)$$

Again, the superscript on the bracketed terms indicates that all variables within the brackets are a function of the subvolume indices from the next higher length scale. The average heat flux tensor for any subvolume at any length scale can be similarly determined through localization, or by simply using the average thermal gradient tensor, along with the constitutive equation (3) and thermal conductivity, at the appropriate length scale. Because of its ability to handle multiple length scales in a single analysis, MsRM is ideal for multiscale modeling of materials such as 3D woven composites that exhibit identifiable microstructures across multiple length scales.

Herein, the High-Fidelity Generalized Method of Cells micromechanics theory [14], [15], formulated for physics governed by vector constitutive laws (like thermal conduction) [13], has been used to calculate the concentration tensor, $\mathbf{A}_i^{(\alpha_i)}$, at each scale in the composite.

III. Multiscale Thermal Conductivity Analysis of a 3D Woven Composite TPS Material

The 3D woven composite TPS material whose thermal conductivity behavior has been investigated is shown in Figure 2, as presented by Fahy et al. [16]. The material labeled “Infused Lower Density Blended Yarn”, which is similar to 3D Medium Density Carbon Phenolic (3MDCP), consists of blended carbon/phenolic filament tows (yarns) and a highly porous phenolic resin matrix. Furthermore, its weave patterns are different in the warp and fill (a.k.a. weft) directions. As shown in Figure 3, in the fill direction, the tows are in a standard over one, under one pattern. In the warp direction the tows are wavier, each traversing further through the through-thickness direction. As such, this 3D woven composite does not consist of layers of the weave (as is the case for 2D woven composites). This is why, in the top view (Figure 3a) and in the warp direction view (Figure 3b), warp tows are penetrating the top of the figure.

As shown in Figure 3 and Figure 4, the primary features of this woven composite microstructural geometry have been captured in a MsRM repeating unit cell at the highest scale; that of the weave (macroscale). Examining the weave patterns in the warp (Figure 3b) and fill (Figure 3c) directions, a fairly simple geometric representation can be identified in which columns of HFGMC subcells represent either tow cross-over locations or the tow undulation regions between the tow cross overs. As shown, the difference between the warp and fill direction has been captured by assigning a greater undulation angle to the warp direction tows. This clearly represents more of an approximation in the warp direction, where multiple tows are grouped together, but it appears to be simplest (and most efficient) representation of the warp tow undulations. The undulation angles are captured through the coordinate transformations that may be applied between the scales (see Eq. (9) and Figure 1). It should also be noted that the standard “double homogenization” [18], [19] approach has been used, in which the through-thickness stacks of subcells (see Figure 4) are homogenized as a separate step prior to homogenization in the plane of the weave. This procedure has been shown to improve the model predictions, including the case of 3D woven composites [20].



Figure 2. Dual layer 3D woven TPS shown in Fahy et al. [16]. The “Infused Lower Density Blended Yarn” is very similar to the 3D Medium Density Carbon Phenolic (3MDCP) material modeled herein.

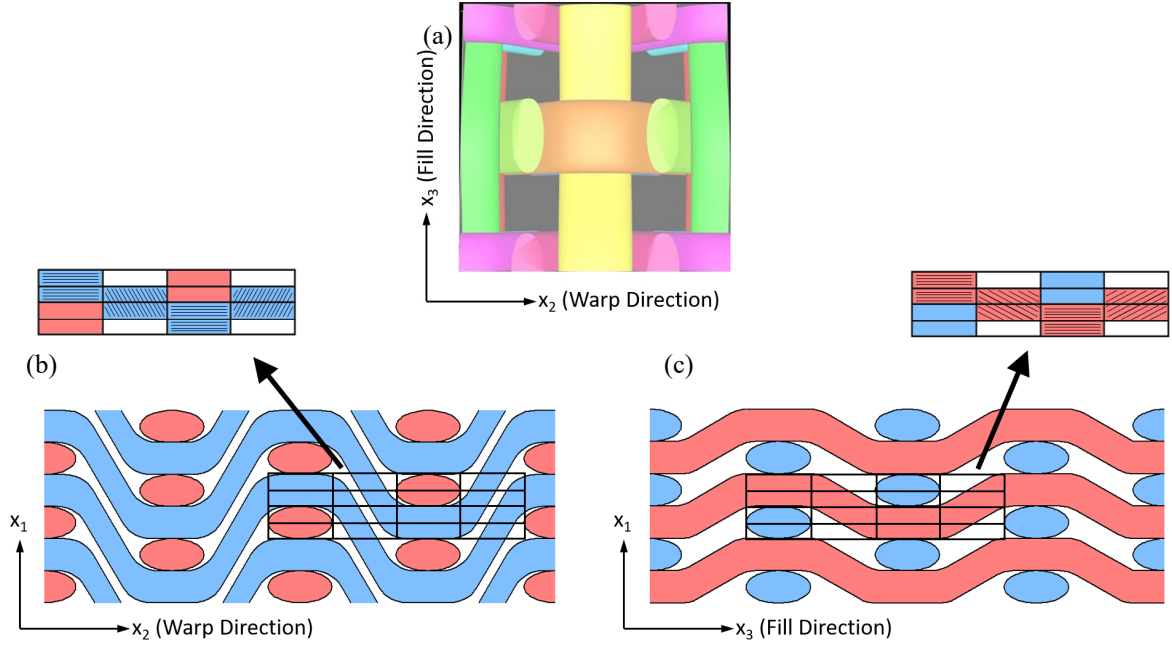


Figure 3 Schematic of the 3MDCP weave pattern. (a) Top view [17], (b) warp direction view, and (c) fill direction view.

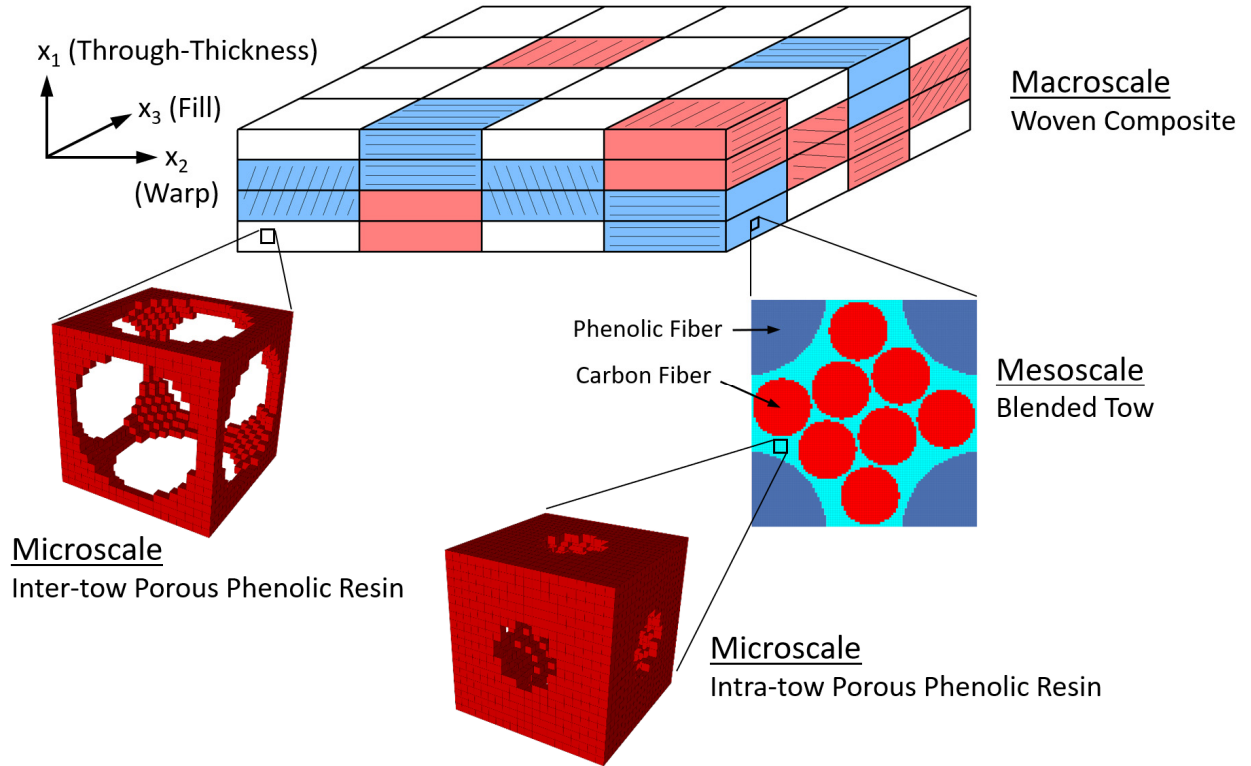


Figure 4. Schematic of the multiscale modeling approach indicating the lengths scales and sample repeating unit cell (RUC) geometries considered.

To represent the infiltrated fiber tows (mesoscale), a fiber/matrix repeating unit cell (RUC) has been used as shown in Figure 4. Note that the 3MDCP tows consist of blend of carbon and phenolic fibers. This is discussed in more detail in Section IV. Finally, at the microscale, due to the presence of significant porosity within the phenolic matrix, a pore/matrix repeating unit cell has been employed to represent this porous matrix material, both within the tows (intra-tow) and between the tows (inter-tow). Details of the microscale porous phenolic modeling are also given in the Section IV.

Based on the multiscale modeling approach shown in Figure 4, the required input properties/parameters for the model consist of the thermal conductivities of the AS4 carbon fiber, the phenolic fiber, the fully dense phenolic matrix (without voids), and the air assumed to be contained within the voids, along with the volume fractions of these constituents at each scale and the woven composite dimensions. The volume fractions considered and the woven composite dimensions are discussed in Section IV for each scale, while the employed constituent thermal conductivities are given in Table 1.

Table 1—Constituent material thermal conductivities. The AS4 fiber has been treated as transversely isotropic, while the phenolic fiber, phenolic matrix, and air have been treated as isotropic

	κ_{Axial} (W/mK)	$\kappa_{\text{Transverse}}$ (W/mK)
AS4 Carbon Fiber	6.83	0.5
Phenolic Fiber	0.25	0.25
Phenolic Matrix	0.25	0.25
Air inside voids	0.025	0.025

IV. Results and Discussion

Results for the multiscale HFGMC model of the 3MDCP woven composite (see Figure 4) have been presented in this section per scale, starting with the microscale (phenolic matrix plus voids). The modeling approach predicts not only the effective thermal conductivities, but also the local heat flux, temperature gradient, and temperature fields at each scale.

A. Microscale

The microscale of the multiscale 3MDCP woven composite consists of the phenolic matrix material located between the tows (inter-tow) and the matrix material within the tows (intra-tow), as shown in Figure 4. To decrease the thermal conductivity of this matrix material, and its contribution to that of the woven composite, a highly porous phenolic material is used. It has been assumed that the pores within the fully dense phenolic “skeleton” material are filled with air at 1 atm, whose thermal conductivity is an order of magnitude lower than the fully dense phenolic (see Table 1). Note that microscopy and CT-Scan studies on the 3MDCP porous matrix are underway, but results are not yet available. A recent microstructural study on a somewhat similar porous phenolic material was recently reported by Hamad et al. [21].

Two different microscale repeating unit cells (RUCs) have been considered for the porous phenolic, as shown in Figure 5. The first is a coarse representation (Figure 5a), consisting of $3 \times 3 \times 3$ subcells, which is the simplest (and most computationally efficient) RUC that can capture the skeleton material and the pore. This simple representation also has the advantage that it can easily be altered to represent any void volume fraction, as the skeleton material thicknesses can simply be made thinner or thicker. The second RUC (Figure 5b-d) is a much more refined $20 \times 20 \times 20$ representation, wherein the void shape approximates a sphere within a cubic region, and every subcell is a cube. A script was used to generate the refined RUC microstructure based on a target void volume fraction. As shown in progressing from a low void volume fraction (V_v) to a higher void volume fraction (Figure 5b-d), the internal void eventually penetrates the bounding cube surface (at a void volume fraction of approximately 0.45). This causes the RUC representation to transition from closed-cell to open-cell voids and represents a fundamental change in the RUC as there are no longer continuous planes of the skeleton material available to conduct heat. Furthermore, once the void penetrates the bounding cube, the representation no longer approximates spherical voids, but rather a regular network of interpenetrating spherical voids.

To evaluate the two microscale HFGMC porous phenolic models (coarse $3 \times 3 \times 3$ and refined $20 \times 20 \times 20$), the (isotropic) effective thermal conductivity was predicted as a function of the void volume fraction in Figure 6. A comparison has been made to some classical analytical expressions for the effective thermal conductivity of composites and cellular solids, along with some available test data for porous phenolic and phenolic foams from the literature (albeit for quite high void volume fractions).

The classical Hashin-Shtrikman bounds [22] for the effective thermal conductivity of an isotropic multiphase material are given by,

$$\kappa_{upper}^* = \kappa_m + V_v \left[\frac{1}{\kappa_v - \kappa_m} + \frac{1 - V_v}{3\kappa_m} \right]^{-1} \quad (13)$$

$$\kappa_{lower}^* = \kappa_v + (1 - V_v) \left[\frac{1}{\kappa_m - \kappa_v} + \frac{V_v}{3\kappa_v} \right]^{-1} \quad (14)$$

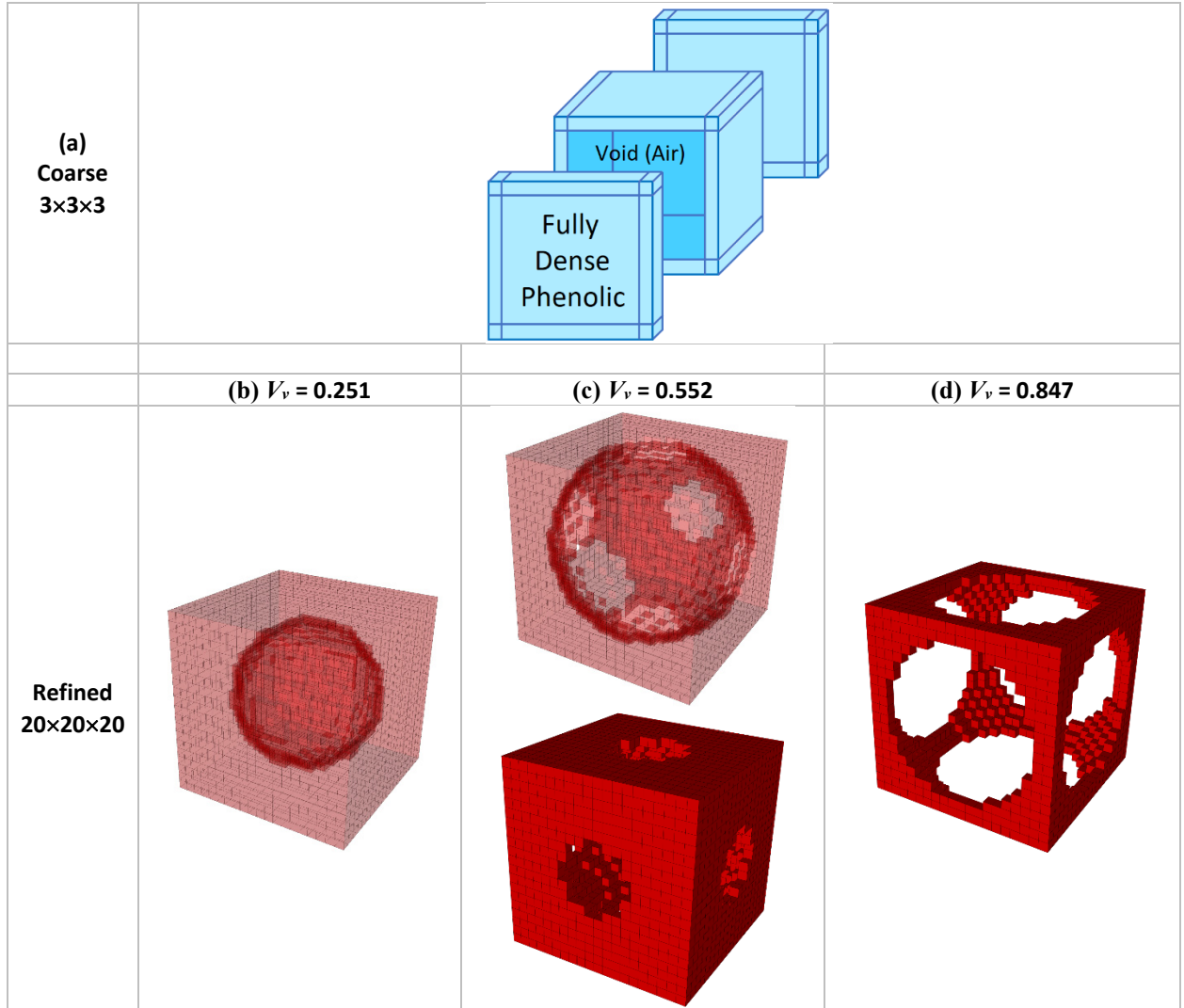


Figure 5. HFGMC RUCs representations of a material containing a spherical void. (a) Simple coarse $3 \times 3 \times 3$ subcell RUC (semi-exploded view), (b), (c), and (d) Refined $20 \times 20 \times 20$ subcell RUCs with volume fractions of 0.251, 0.552, and 0.847, respectively.

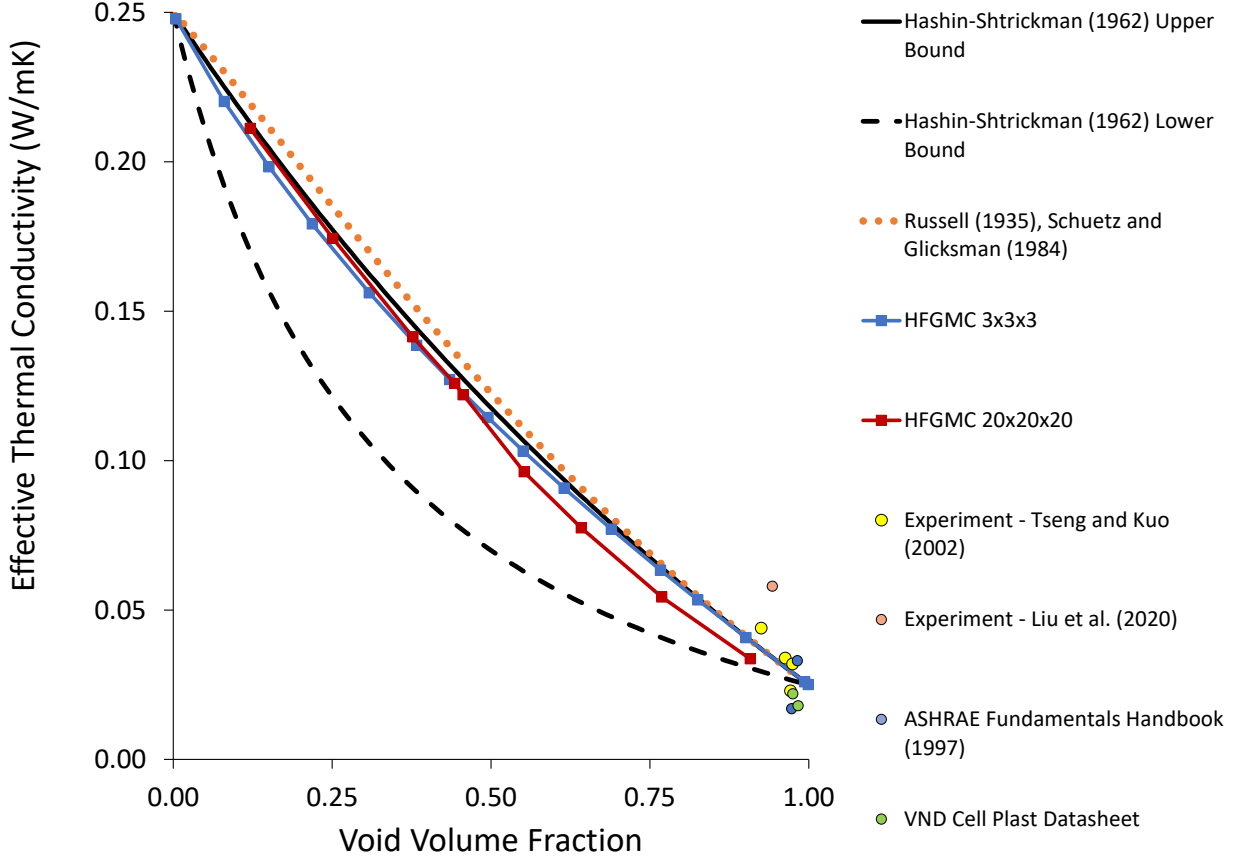


Figure 6. Predictions for the isotropic effective thermal conductivity of porous phenolic by HFGMC and classical analytical expressions as a function of void volume fraction, along with measurements from the literature.

where κ_v and κ_m are the thermal conductivities of the air within the void and the phenolic matrix skeleton material, respectively. The effective thermal conductivity expression derived by Christensen [23] using a micromechanics spherical inclusion model, along with the Mori-Tanaka [24] method-based solution presented by Benveniste [25] both correspond to the Hashin-Shtrickman upper bound. The results attributed to both Russell [26] and Schuetz and Glicksman [27] are based on a cellular solid expression, first presented by Russell [26] without derivation, based on analysis of conduction through a solid containing cubic pores, “By the laws of conductors, in series and in parallel ...” [26, p. 1]. This expression is given by,

$$\kappa^* = \kappa_m \left[\frac{V_v^{2/3} + \frac{\kappa_m}{\kappa_v} (1 - V_v^{2/3})}{V_v^{2/3} - V_v + \frac{\kappa_m}{\kappa_v} (1 - V_v^{2/3} + V_v)} \right] \quad (15)$$

which, according to Schuetz and Glicksman [27], corresponds to their cellular solid upper limit solution, which itself is based on an analogy to an electrical circuit with resistors representing the void and parts of the solid in series and parallel.

Comparing the HFGMC predictions to these classical analytical expressions for the porous phenolic in Figure 6, the HFGMC predictions are all within the Hashin-Shtrickman micromechanics-based bounds. The Russell-Schuetz-Glicksman cellular solid based results are above the Hashin-Shtrickman upper bound for lower void volume fractions (a significant shortcoming), but at higher void volume fractions, it matches the Hashin-Shtrickman upper bound quite

closely. This might be expected as materials considered to be cellular solids typically have very high void fractions. At low void volume fractions, the refined $20 \times 20 \times 20$ HFGMC prediction is quite close to the Hashin-Shtrikman upper bound, but at higher void volume fractions, the coarse $3 \times 3 \times 3$ HFGMC prediction is closer. There is clearly a discontinuity in the slope of the $20 \times 20 \times 20$ HFGMC prediction curve as the RUC transitions from closed cell to open cell (and the void microstructure transitions from spheres to interpenetrating spheres) at a void volume fraction of approximately 0.45. At void volume fractions above 0.45, the $20 \times 20 \times 20$ HFGMC predictions diverge from the classical expression results and the $3 \times 3 \times 3$ HFGMC predictions, all of which are based on closed cell geometries. The forthcoming microscopy results for the 3MDCP matrix material will shed light on how best to represent its porous geometry using HFGMC, but the cases examined herein serve to explore the options.

The experimental results shown in Figure 6, which represent void volume fractions ranging from 0.925 to 0.983, are from four sources: test results from Tseng and Kuo [28] and Liu et al. [29] on phenolic foam insulation, a handbook value for phenolic foam insulation [30], and a phenolic foam manufacturer datasheet [31]. Note that, in some cases, for these experimental data, the void volume fraction was deduced from the quoted phenolic foam density. Clearly, there is a great deal of scatter in the experimental data. However, the assumption in the model results is that the porous phenolic is isotropic, which implies that there is no bias in the void microstructure towards any of the coordinate directions. This may not be the case in the foam insulation tested. Other likely mismatches between the model and test data shown in Figure 6 include the skeleton material thermal conductivity and nonuniform density/microstructure.

As mentioned, the HFGMC thermal conductivity model not only predicts the effective thermal conductivity, but also the local fields within the heterogeneous materials. Figure 7 compares the local normalized heat flux and temperature fields in response to an applied global heat flux component, $\bar{q}_1$, for the coarse and refined porous phenolic RUCs with $V_v = 0.847$. Note that, at this V_v value, the refined RUC is open cell (while the coarse RUC is, as always, closed cell). The effective thermal conductivities for the two RUCs are also indicated in the figure (0.0498 W/mK vs. 0.0419 W/mK), which differ by $\sim 16\%$. For each RUC, the fields on two cross-sections are shown: a face cut cross-section and a center cut cross-section (as indicated near the top of Figure 7). The primary (highest magnitude) local heat flux component in response to the applied $\bar{q}_1$ is q_1 . For the coarse RUC, the q_1 heat flux is high through the closed face, while, on the center cut cross-section, the heat flux is high along the continuous edges, but low through the void. This is expected as the thermal conductivity used for the air in the void is one-tenth that of the skeleton phenolic material (0.025 W/mK vs. 0.25 W/mK, see Table 1. In contrast, the normalized q_1 fields for the refined RUC show the flux concentration that arises in the face cut cross-section as the heat flow path traverses around the opening in the face. The maximum heat flux occurs in the phenolic skeleton ligament at the “pinch-points” between the voids. On the center cut cross-section of the refined RUC, there is very little q_1 heat flux as the heat flow concentrates in the continuous phenolic ligaments present in the geometry. These differences in the q_1 heat flow between the coarse and refined RUCs are the primary source of the $\sim 16\%$ difference between these RUCs’ predicted effective thermal conductivities.

The normalized heat flux components normal to the applied global $\bar{q}_1$ component (normalized q_2 and q_3) are relatively minor compared to the primary heat flow direction flux component (q_1). These components do become locally appreciable in refined RUC face cut cross-section as the heat flow navigates the opening in the face. The temperature fields are related to spatial integrals of the local temperature gradient components, $\mathbf{X}_i^{(a)}$, and thus requires actual subcell dimensions to be calculated. In contrast, the local heat flux and temperature gradients are independent of the actual subcell dimensions and only depend on the relative dimensions of the subcells. The local temperature fields shown in Figure 7 are based on overall RUC dimensions of $1 \mu\text{m} \times 1 \mu\text{m} \times 1 \mu\text{m}$. These normalized temperature fields show very little difference between the two cross-sections for the coarse RUC, with some influence of the microstructure evident in the refined RUC results.

The void microstructures examined thus far all result in isotropic effective thermal conductivities for the porous phenolic material. To examine the impact of void shape on the effective thermal conductivities, the coarse $3 \times 3 \times 3$ microstructure was generalized to enable first-order representation of an oblate void shape. As shown in Figure 8, the void shape, which defined by the dimensions a , b , and c , becomes oblate by setting $a < b$, with $c = b$. That is, the void dimensions are taken to be the same in the x_2 - and x_3 -directions such that $c = b$, but the void is thinner in the x_1 -direction. The equations below enable the determination of all subcell dimensions for this oblate void RUC given the void volume fractions, V_v , and the void aspect ratio, A_R .

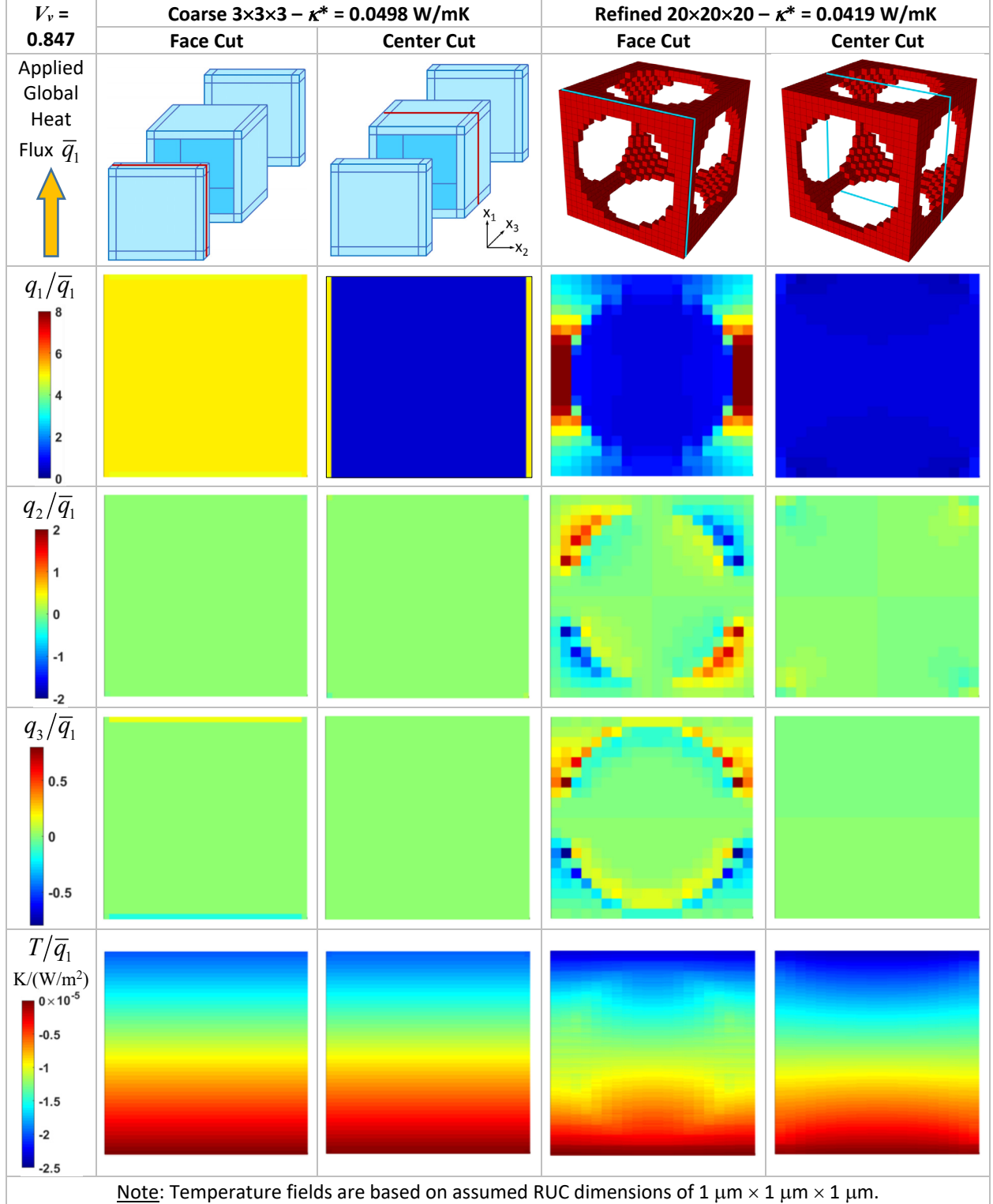


Figure 7. Local normalized heat flux and temperature fields induced by an applied global uniaxial heat flux, $\bar{q}_1$, considering face and center cut cross-sections, within the coarse ($3 \times 3 \times 3$) and refined ($20 \times 20 \times 20$) porous phenolic RUCs with a void volume fraction (V_v) of 0.847.

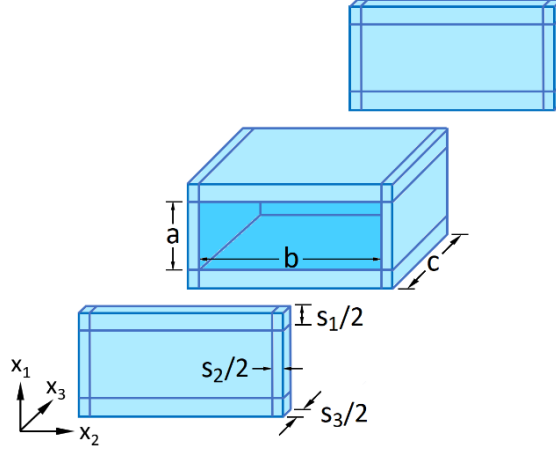


Figure 8. Coarse 3×3×3 subcell HFGMC RUC representation (semi-exploded view) of a material containing an oblate void.

The spacing between voids in each coordinate direction is s_1 , s_2 , and s_3 , respectively, where the spacing in the x_2 - and x_3 -directions is the same ($s_3 = s_2$), but greater in the x_1 -direction. The void aspect ratio (A_R) is defined as,

$$A_R = \frac{b}{a} \quad (16)$$

and the ratio of the spacing between voids in the different directions is also taken to be defined by the aspect ratio, such that,

$$\frac{s_1}{s_2} = A_R \quad (17)$$

The volume fraction of the void, V_v , is given by,

$$V_v = \frac{abc}{(a + s_1)(b + s_2)(c + s_3)} \quad (18)$$

and, because the size of the RUC is arbitrary, its length in the x_2 - and x_3 -directions can be taken to be 1. That is,

$$(b + s_2) = (c + s_3) = 1 \quad (19)$$

although the final subcell and RUC dimensions can be scaled as desired. Substitution of Eqs. (19) and (16) into Eq. (18) leads to,

$$V_v = \frac{a^3 A_R^2}{(a + s_1)} \quad (20)$$

With the aid of Eqs. (17), (19), and (16), it can be shown,

$$s_1 = A_R (1 - b) = A_R (1 - A_R a) \quad (21)$$

which, when substituted into Eq. (20) yields a cubic equation for a in terms of a specified void volume fraction and aspect ratio,

$$A_R^2 a^3 - V_v (1 - A_R^2) a - V_v A_R = 0 \quad (22)$$

which can be solved for a as this equation has one real root. Then b is obtained from Eq. (16), s_1 from Eq. (21), and s_2 from Eq. (19), thus providing all the needed dimensions of the oblate void RUC subcells. As mentioned, because the RUC size is arbitrary, the subcell dimensions can be scaled, provided that the ratios between all subcell dimensions are maintained.

Figure 9 shows the effect of the void aspect ratio on the effective thermal conductivity components of the porous phenolic with the coarse oblate void for void volume fractions (V_v) of 0.552 and 0.847. Note that, because the RUC dimensions are the same in the x_2 - and x_3 -directions, the effective thermal conductivities in these two directions are the same ($\kappa_{22}^* = \kappa_{33}^*$). At a void aspect ratio of 1, the void is not oblate, and the effective thermal conductivity is isotropic. As the void aspect ratio increases, the effective conductivity in the oblate x_1 -direction (κ_{11}^*) decreases as the continuous phenolic path in this direction decreases and the void cross-section increases. The opposite trend is evident in the predicted $\kappa_{22}^* = \kappa_{33}^*$ values, which increase with the void aspect ratio. The effect of the void aspect ratio is much greater for the lower void volume fraction as the phenolic skeleton is thicker in this case, and these dimensions change by greater percentages than in the higher void volume fraction case. In all cases, as the void aspect ratio increased, the effective thermal conductivity components tended to converge, with κ_{11}^* converging more slowly than $\kappa_{22}^* = \kappa_{33}^*$. As mentioned previously, microscopy and CT-Scan evaluation of the porous phenolic in the 3MDCP composite is underway. This will shed light on the actual void microstructure in the material and guide future modeling efforts at the microscale.

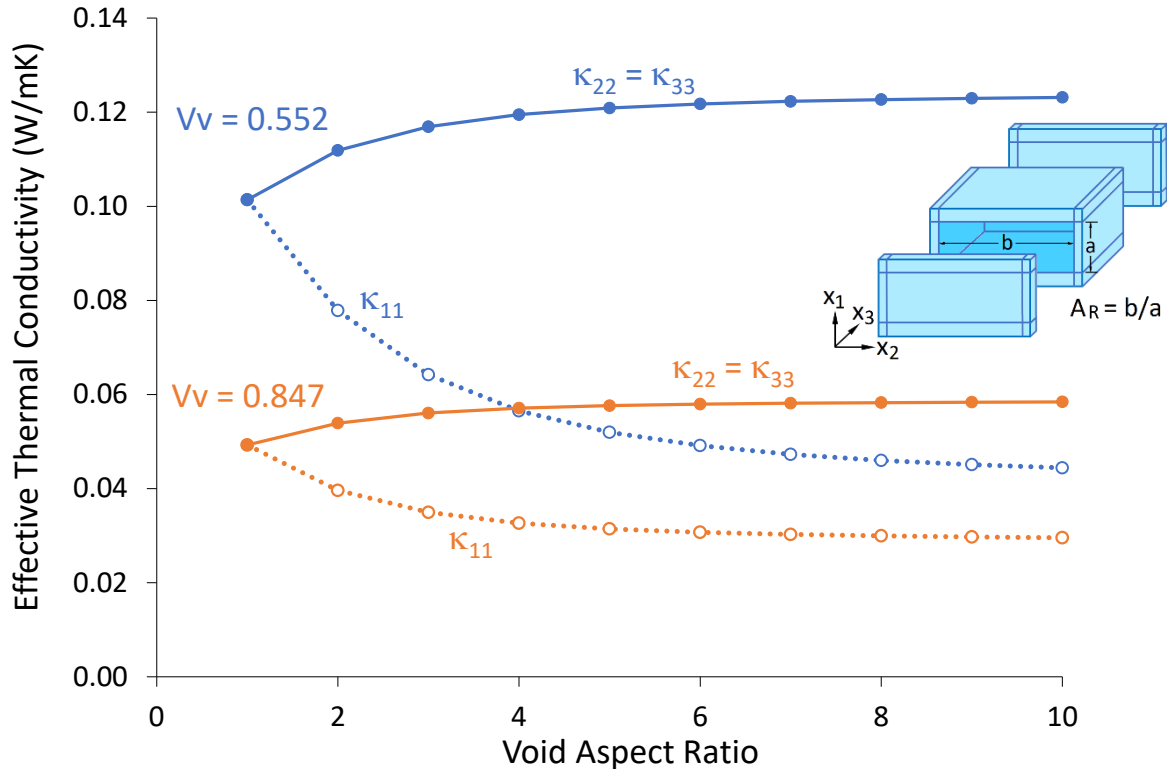


Figure 9. Effect of oblate void aspect ratio, b/a (see Figure 8), on the predicted effective thermal conductivity components for void volume fractions (V_v) of 0.552 and 0.847.

B. Mesoscale

Recall that the 3MDCP tows consist of both carbon and phenolic fibers. The tows are formed by twisting carbon fiber tows together with phenolic fiber tows. The microscopy and CT-scan studies of the 3MDCP material will provide details on the tow microstructure, but these results are not yet available. Therefore, to begin to examine the sensitivity of composite effective thermal conductivity to the geometry considered for the tows, three representations of the 3MDCP tows have been considered at the mesoscale; a coarse RUC, a refined RUC, and a multiscale RUC. These three RUCs are shown in Figure 10. Note that the phenolic and AS4 carbon fibers have nominal diameters of 15 μm and 7 μm , respectively. The coarse (4 $\times$ 8) and refined (100 $\times$ 100) tow RUCs attempt to maintain the relative fiber sizes, while also attempting to match the estimated volume fractions of the phenolic fiber (0.3344) and the carbon fiber (0.4225) within the tow. The multiscale tow represents the phenolic and carbon fiber tows individually at a lower length scale with 32 $\times$ 58 subcells and a hexagonally (hex) packed fiber arrangement. These are arranged to form the blended tow in a 4 $\times$ 4 subcell pattern wherein the subcells representing phenolic tows are smaller, resulting in rectangular subcells that produce the correct overall fiber volume fractions within the blended tow. In addition, as shown, half of the lower scale hex packed RUCs are rotated by 90° to ensure the effective thermal conductivities of the multiscale tow are identical in the x_2 - and x_3 -directions.

Predictions were made for the anisotropic effective thermal conductivities of the three tow representations for each of three porous phenolic matrix cases used to model the light blue porous phenolic shown in Figure 10 (see also Figure 4). The three chosen porous phenolic matrix cases are: (1) the refined (20 $\times$ 20 $\times$ 20) void RUC (Figure 5c), (2) the coarse (3 $\times$ 3 $\times$ 3) void RUC (Figure 5a), and (3) the coarse oblate void RUC (Figure 8) with an aspect ratio of 6. For all three porous phenolic matrix cases, the void volume fraction was kept at 0.552, which is close to the estimated matrix void volume fraction within the 3MDCP blended tows. Further, for the oblate void RUC, the orientation of the RUC within the matrix were specified such that the void's local x_1 -direction (see Figure 8) was in the blended tow x_3 -direction (see Figure 10) (thus the voids are flatter in the blended tow x_3 -direction). This required using different oblate void RUC local orientations within the two rotated orientations of the hex fiber packing tows used in the multiscale tow (see Figure 10).

The predicted anisotropic effective thermal conductivities of the blended tow are shown in Figure 11 for the nine cases considered (three tow RUCs, each with three different porous matrix RUCs). Because the axial thermal conductivity of the carbon fibers is much higher than all other constituent thermal conductivities (see Table 1), the predicted axial thermal conductivity (Figure 11a) is approximately an order of magnitude higher than the transverse thermal conductivity (Figure 11b). Note that the abscissa scale of the Figure 11a is over a very small range, and all model axial thermal conductivity predictions are all within 1% of each other. In Figure 11b, it is evident that the two predicted transverse thermal conductivity components are quite close when the refined and coarse void representations are used for the porous matrix (they are identical for the multiscale tow RUC). However, introducing the oblate void in the matrix, which, again, is oriented such that the thin void local x_1 void dimension (see Figure 8) is in the blended tow x_3 -direction, results in a significantly lower κ_{33}^* (20% - 29%) and a higher κ_{22}^* (4.1% - 6.6%). This trend is expected and is in accordance with the porous phenolic results in Figure 9. Differences between the 4 $\times$ 8, 100 $\times$ 100, and multiscale RUC blended tow predictions for the transverse effective thermal conductivity components are less than 5% (2.3% on average), excluding the 4 $\times$ 8 RUC with oblate void κ_{33}^* prediction, which is more than 10% lower than the other two tow RUC predictions. This lower κ_{33}^* prediction for the 4 $\times$ 8 RUC with oblate void is because of the heat flow path in the x_3 -direction in this RUC, which is discussed next.

Figure 12 shows the normalized local transverse heat flux fields and the temperature field in response to an applied $\bar{q}_3$ for all three blended tow representations for the case of the refined porous matrix RUC (see Figure 5b). Note that the transverse thermal conductivity of the carbon fiber is twice that of the phenolic fiber (see Table 1) and approximately five times that of the porous phenolic with $V_v = 0.552$ (see Figure 6). As such, for the 4 $\times$ 8 and 100 $\times$ 100 tow RUCs, in the primary x_3 heat flow direction, the local q_3 heat flux path is predominant through the carbon fibers, with lower flux in the phenolic fibers. Much of the porous matrix has very low local q_3 , but, because the carbon (and phenolic) fibers are not touching, in local regions between fibers, the heat flux in the porous matrix is high. For the coarse 4 $\times$ 8 RUC, wherein the carbon fibers are aligned in columns, the heat flux is high in these columns and low in the continuous matrix column between the fibers in the x_2 -direction. In the refined 100 $\times$ 100 RUC, the heat flux path is not as straight due to the arrangement of the carbon fibers and significant heat flux concentrations are present where the carbon fibers are closest to each other. The fact that the heat flux path is not straight can be seen in the normalized q_2 heat flux field, which indicates much more heat flux transverse to the applied heat flux direction compared to the

coarse 4×8 RUC q_2 heat flux field. There is not much heat flux variation across the blended tow RUC, but slightly higher q_3 is evident in the middle of the RUC compared to the side edges because more carbon tows are present in the middle two columns of subcells (see Figure 10).

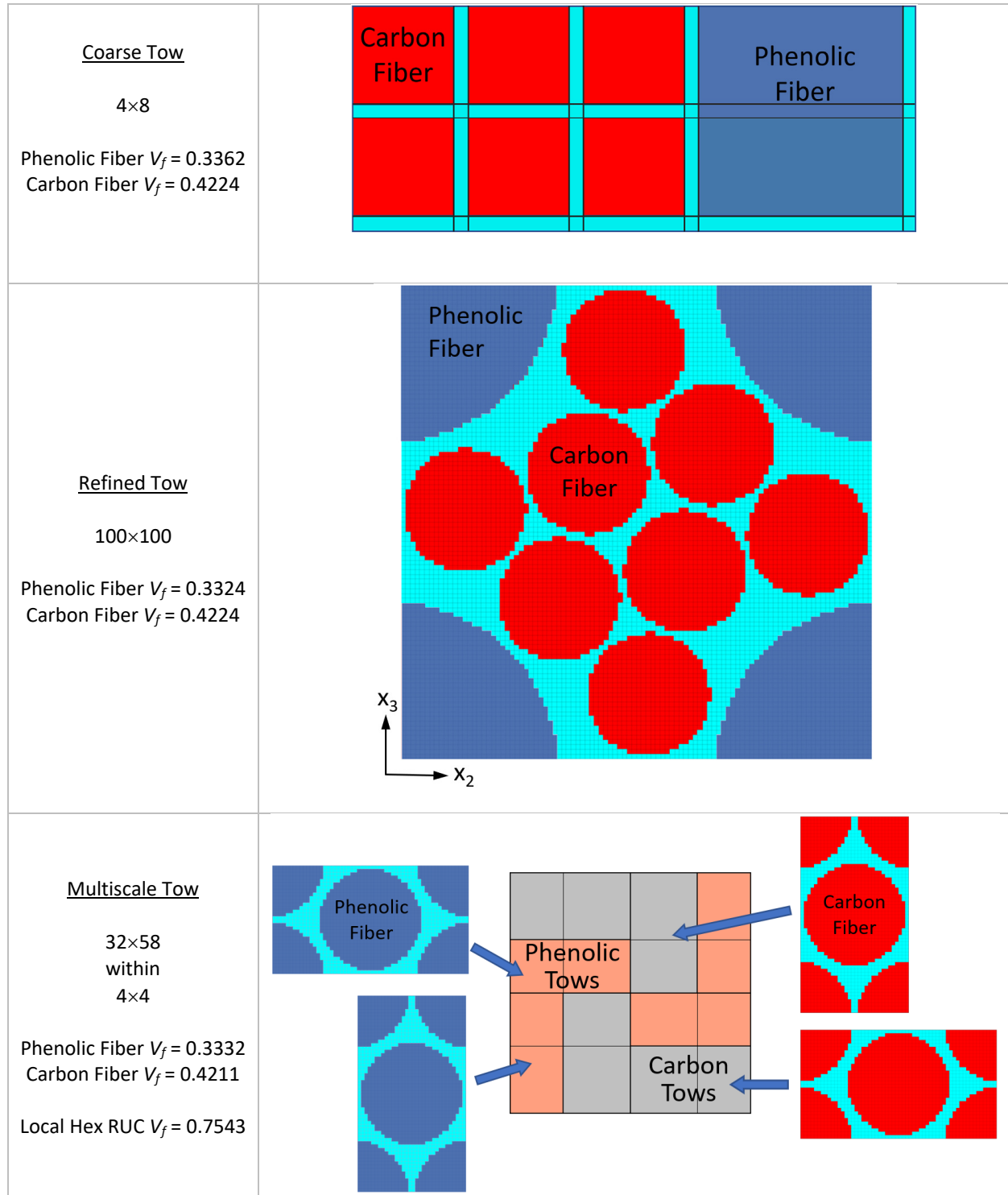


Figure 10. Coarse, refined, and multiscale RUCs used to simulate the tow in the 3MDCP material. Note that the x_1 -direction corresponds to the fiber direction.

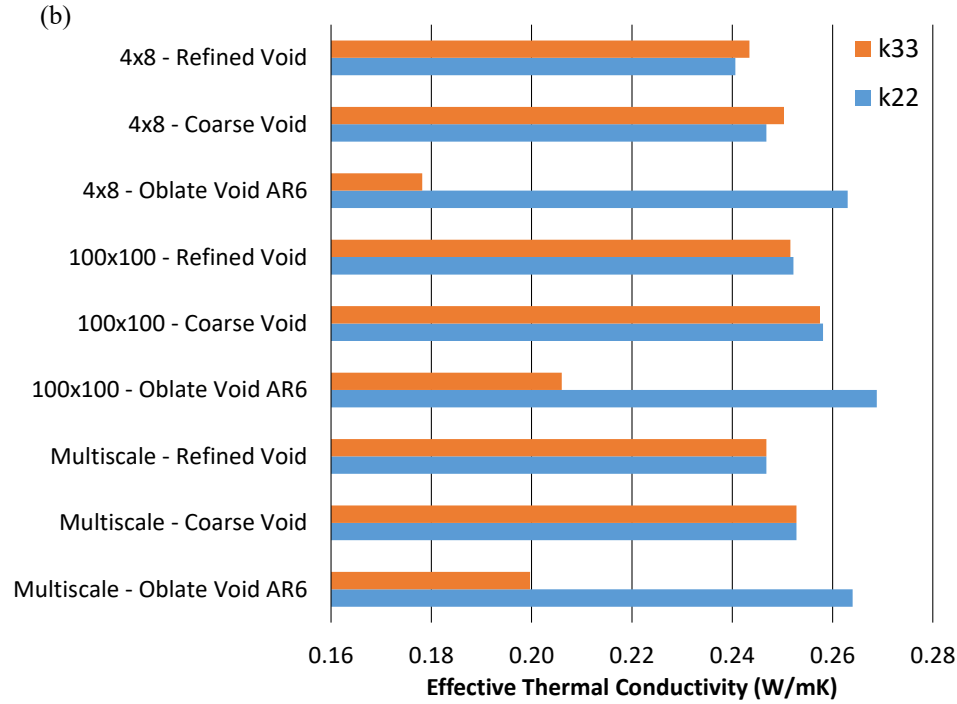
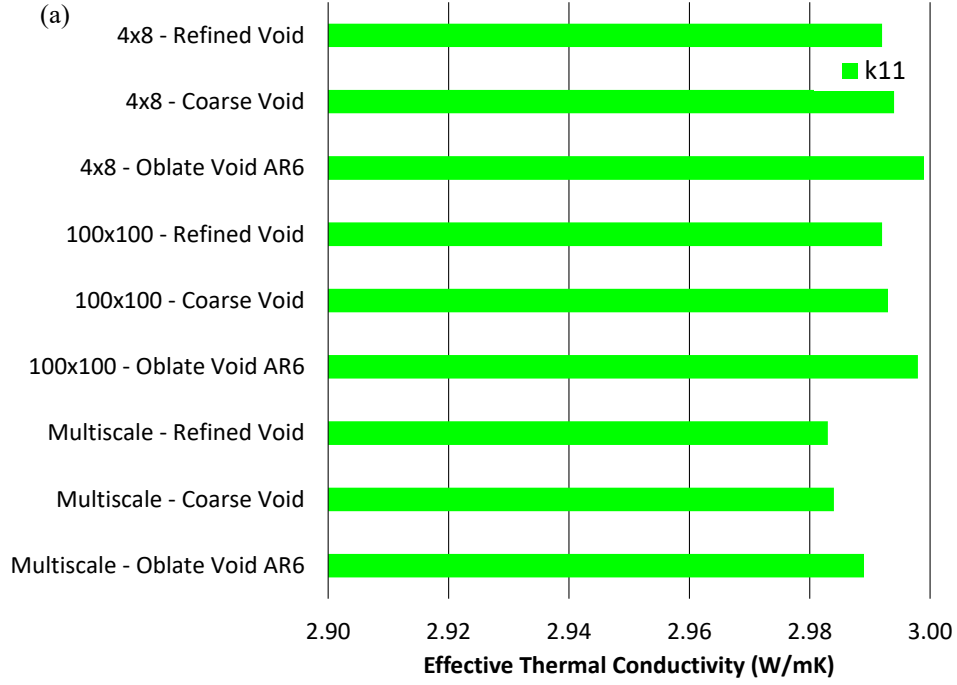


Figure 11. Predicted anisotropic effective thermal conductivities for the 4x8, 100x100, and multiscale blended tow RUCs shown in Figure 10, wherein, for each, three different porous matrix RUCs (refined, coarse, and oblate voids) were used. (a) Axial (fiber direction) effective thermal conductivity, κ_{11}^* . (b) Transverse effective thermal conductivities, κ_{22}^* and κ_{33}^* .

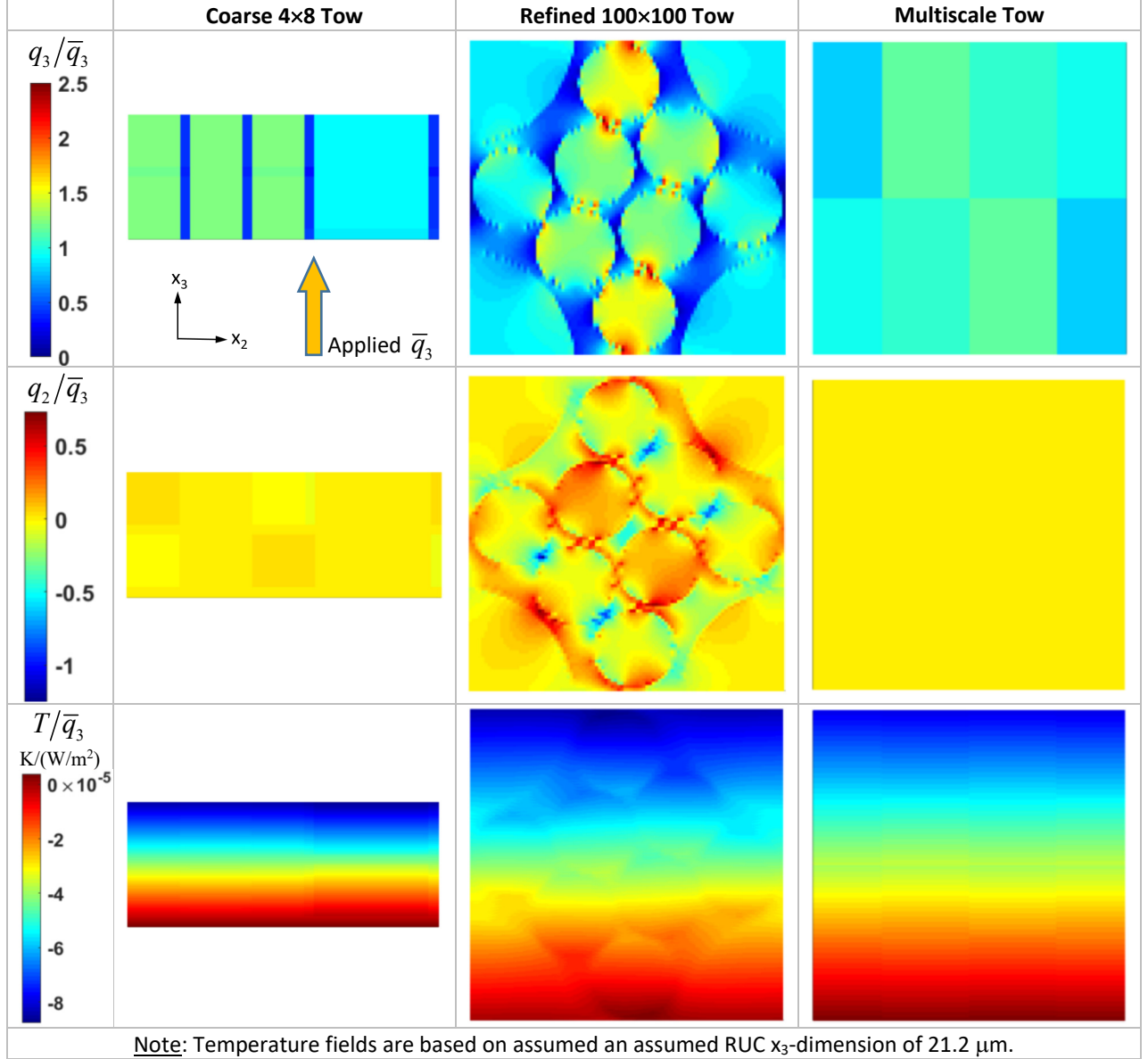


Figure 12. Normalized predicted local transverse heat flux component and temperature fields for the three blended tow RUCs considered (see Figure 10), wherein the porous matrix was modeled with the refined pore RUC with $V_v = 0.552$ (see Figure 5b), in response to an applied global $\bar{q}_3$ heat flux component.

The reason for the greater impact of introducing the oblate void within the coarse 4×8 RUC can also be gleaned from Figure 12. As mentioned, in this RUC, the columns of high local q_3 force high heat flux through relatively thick porous matrix subcells (see Figure 10). When the oblate void is used for the porous matrix, the thermal conductivity of these thick porous matrix subcells is lowered considerably, and, unlike the refined 100×100 tow RUC, heat flow is primarily unidirectional, with no closely spaced offset fibers to provide low resistance heat flow paths.

C. Macroscale

Results for the macroscale 3D woven 3MDCP composite are shown in Figure 13, wherein the effective anisotropic thermal conductivities have been predicted considering the same nine blended tow cases considered in Section IV.B.

The employed coarse 3MDCP RUC, which was discussed in Section III, is also shown, along with the coordinate convention for the fill (x_3), warp (x_2) and through-thickness (x_1) directions. As described in Section II, in the MsRM modeling approach, the orientation of the material occupying any subcell may be assigned an orientation with respect to the higher-scale coordinate system. This is how the fill and warp tows are assigned their proper orientations to represent the weave pattern in the macroscale RUC. This is also how an orientation is given to the oblate void RUC for the porous matrix at each scale. For the inter-tow matrix (white subcells in Figure 13), the thinner oblate void dimension was oriented in the x_1 -direction to simulated planar voids in the x_2 - x_3 plane. This same global oblate void orientation was maintained in tow cross-over subcells, in which the fibers are oriented in the x_2 - or x_3 -directions. For tows representing undulations in the weave pattern, these same x_2 - x_3 planar voids were rotated along with the fiber direction to simulate the voids following the tows in the weave. This may or may not be representative of the actual void microstructure in the 3MDCP composite, but more information will be forthcoming based on the in-progress microstructural studies mentioned previously.

The RUC dimensions, a , b , and t in Figure 13, which represent the tow cross-over length, tow undulation length, and constant subcell layer thickness (equal to one-half tow thickness), were chosen to be representative of the 3MDCP composite. The employed values are $a = 1.41$ mm (0.0556 in.), $b = 1.13$ mm (0.0444 in.), and $t = 0.177$ mm (0.00695 in.). The tow undulation angles in the fill and warp directions were taken as 17.4° and 46.8° , respectively. The inter-tow void volume fraction was specified as 0.847 with the intra-tow void volume fraction set to 0.552, which are in accordance with current estimates for the composite. These volume fractions and dimensions across the scales result in the overall volume fractions for the constituents within the macroscale 3MDCP model given in Table 2. All overall material volume fractions are within 0.1% of each other.

As one would expect given the lower scale results, Figure 13 indicates good overall agreement among the predictions using the different tow and porous RUC void representations. In the fill direction, the effective thermal conductivity (κ_{33}^*) is highest due to the presence of relatively straighter continuous carbon fibers. In the warp direction, which has significantly higher undulation angles for the tows, the effective thermal conductivity (κ_{22}^*) is approximately half that in the fill direction. In the through-thickness direction, there are no continuous carbon fibers, and the thermal conductivity (κ_{11}^*) is very low, approximately one-third that in the warp direction.

As was the case in the tow results, the presence of the oblate void has its greatest impact on reduction of the through-thickness effective thermal conductivity, with the 4×8 tow case exhibiting the greatest effect. The oblate void shape reduced κ_{11}^* significantly, by 27% to 32% compared to the isotropic coarse void representation. Because the oblate void within the tows follows the tow undulations, the oblate void shape reduces the all three effective thermal conductivity components (11% to 18% for κ_{22}^* and 6% to 9% for κ_{33}^*).

For the cases that did not include the oblate void, the effect of the tow representation was quite minor, with all predicted effective thermal conductivity components having an average difference of 1.3% and a maximum difference of 2.1% for a given porous matrix representation. The porous matrix representation (refined $20 \times 20 \times 20$ vs. coarse $3 \times 3 \times 3$) had greater effect within each tow representation, causing differences (averaged across the three tow RUC cases) of 8.3%, 4.8%, and 2.3% in the through-thickness, warp, and fill direction effective thermal conductivities, respectively. As one might expect, the porous matrix representation has its greatest impact on the lowest, most matrix-dominated effective thermal conductivity component, κ_{11}^* , and its least impact on the most fiber-dominated effective thermal conductivity component, κ_{22}^* . These results indicate that the 3MDCP effective conductivity predictions are more sensitive to the chosen microstructural representation of the matrix voids compared to that of the blended tow. Of course, the results of the ongoing 3MDCP microscopy study will provide a great deal insight into the actual microstructure across all scales considered for this composite.

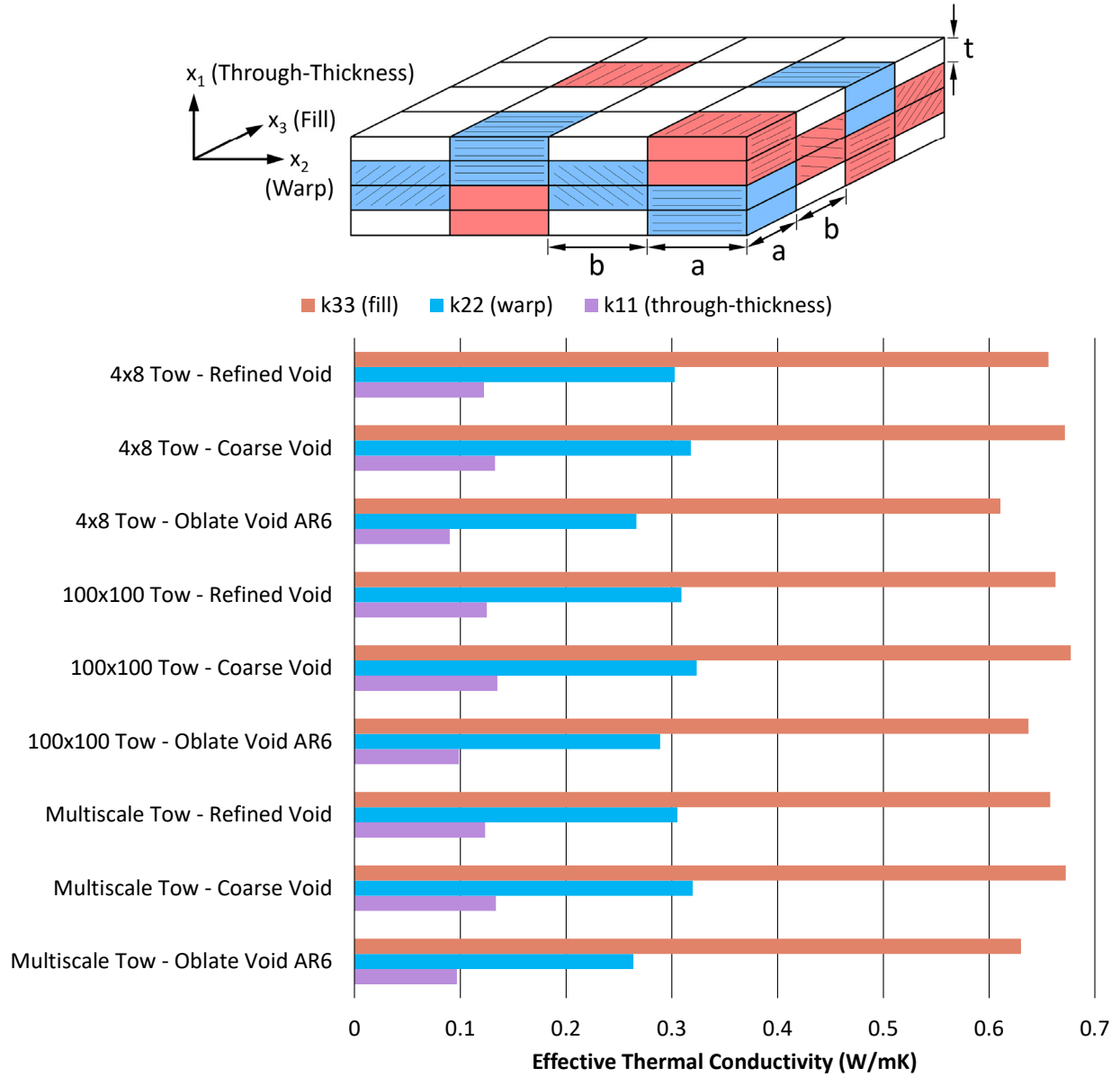


Figure 13. Predicted anisotropic effective thermal conductivities for the 3MDCP TPS composite for the nine different blended tow and porous matrix RUC representations considered in Section IV.A. Consistent porous matrix representations were maintained in the intra-tow matrix, which are represented by the white subcells in the RUC diagram.

Table 2—Material volume fractions for the macroscale 3MDCP model.

	Phenolic Fiber	Carbon Fiber	Intra-Tow Matrix	Inter-Tow Matrix	Fully Dense Phenolic Matrix	Void
4x8 Tows	0.1869	0.2349	0.1342	0.444	0.1281	0.4501
100x100 Tows	0.1858	0.2349	0.1363	0.444	0.1290	0.4513
Multiscale Tows	0.1852	0.2341	0.1366	0.444	0.1291	0.4515

V. Conclusion

This paper presented the Multiscale Recursive Micromechanics (MsRM) approach for calculating the effective thermal conductivity components and determining the local heat flux, temperature gradient, and temperature fields for composite materials with an arbitrary number of length scales. At each length scale, the High-Fidelity Generalized Method of Cells micromechanics theory, formulated for physics governed by vector constitutive laws (like thermal conduction), has been used. This approach was applied to a novel 3D woven TPS material, 3D Medium Density Carbon Phenolic (3MDCP), composed of blended phenolic fiber/carbon fiber tows and a highly porous phenolic matrix. Effective thermal conductivity and local field predictions were made starting with the porous phenolic microscale, wherein two microstructures were considered, consisting of the air-filled void and the fully dense phenolic skeleton material. The isotropic effective thermal conductivity predictions of these microstructures were compared to classical micromechanics and cellular solid effective thermal conductivity solutions, along with some limited experimental data, across a range of void volume fractions. The effect of an oblate void shape was also investigated and shown to have a major impact on the effective thermal conductivity for two realistic void volume fractions.

Next, at the mesoscale of the 3MDCP composite, three microstructures were considered for the tow, which includes a blend of carbon and phenolic fibers. Coarse, refined, and multiscale tow RUCs were developed, each of which considered the porous matrix RUCs at the lower length scales. Effective anisotropic thermal conductivities and local fields were presented. Inclusion of the oblate void to represent the porous matrix was again shown to have a significant impact.

Finally, at the macroscale, using a relatively simple RUC representation for the overall 3MDCP microstructure, effective thermal conductivities were predicted for the range of different mesoscale (tow) and microscale (porous phenolic matrix) microstructures. It was found that these global, composite-level effective thermal conductivities were more sensitive to the void microstructure used for the porous matrix at the microscale as compared to the microstructure used to represent the tow at the mesoscale. The results also indicated that the effective thermal conductivity in the fill direction (with lower tow undulation angle) is approximately double that in the warp direction (with significantly higher undulation angle). The through-thickness effective thermal conductivity, which is the most matrix dominated, had the lowest predicted effective thermal conductivity, at approximately one-third that of the warp direction and one-sixth that of the fill direction.

Detailed microscopy and CT-scan investigations are underway that are expected to provide a great deal of insight into the actual microstructure of the 3MDCP material across all the considered length scales. This will enable refinement of the microstructures employed herein to make them more realistic. Thermal conductivity testing is also planned in the near future, thus providing validation data for the effective thermal conductivity predictions. Planned future work will also involve coupling the MsRM thermal conductivity predictions with mechanical progressive damage simulations and TPS ablation simulations to capture the effects of local damage and erosion on the thermal insulation performance of the 3MDCP composite material.

Acknowledgment

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