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Microstructure-guided numerical simulations to predict the thermal performance of a hierarchical cement-based composite material

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ABSTRACT

This paper presents a microstructure-guided numerical homogenization technique to predict the effective thermal conductivity of a hierarchical cement-based material containing phase change material (PCM)-impregnated lightweight aggregates (LWA). Porous inclusions such as LWAs embedded in a cementitious matrix are filled with multiple fluid phases including PCM to obtain desirable thermal properties for building and infrastructure applications. Simulations are carried out on realistic three-dimensional microstructures generated using pore structure information. An inverse analysis procedure is used to extract the intrinsic thermal properties of those microstructural components for which data is not available. The homogenized heat flux is predicted for an imposed temperature gradient from which the effective composite thermal conductivity is computed. The simulated effective composite thermal conductivities are found to correlate very well with experimental measurements for a family of LWA-PCM composites considered in the paper. Comparisons with commonly used analytical homogenization models show that the microstructure-guided simulation approach provides superior results for composites exhibiting large property contrast between phases. By linking the microstructure and thermal properties of hierarchical materials, an efficient framework is available for optimizing the material design to improve thermal efficiency of a wide variety of heterogeneous materials.

1. Introduction

Hierarchical materials contain structural elements which themselves have a structure [1]. The performance enhancements resulting from such structural hierarchy is of great interest since it offers an ability to tailor materials for desired properties. Several classes of composites including carbon fiber reinforced epoxy/clay, and glass fiber reinforced vinyl ester with carbon nanotubes [2–6], and biological materials such as wood and nacre [7,8] exhibit structural hierarchy. Thus, hierarchical materials with multiple design degrees of freedom associated with microstructural features and compositions at different length scales enable new avenues towards design of innovative materials. Microstructural design of such materials requires computational models capable of linking the material structure at different length scales to the performance, in addition to incorporating the influences of heterogeneity. The effective properties of hierarchical materials have been predicted using analytical schemes such as the Mori-Tanaka method [9–11], double inclusion method [11–14], and self-consistent schemes [15–17]. While popular because of their simplicity, these techniques are not adequately accurate when large contrast in constituent properties exist, or the volume fractions of the dispersed components are very high [18–20]. Computational techniques generally overcome these drawbacks [20–26].

This focus of this paper is on a suitable numerical modeling framework that integrates the material structure and component thermal properties to predict the thermal performance of a cementitious composite containing porous inclusions (lightweight aggregates (LWA)), which in turn are filled with different fluid phases. One of the constituents impregnated into the pores is a phase change material (PCM), which leads to several desirable properties of the composite as outlined later in this section. The PCM-impregnated LWA mortar system exhibits structural features

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at two different hierarchical length scales: (i) lightweight aggregate (LWA) inclusions embedded in the hardened cement paste matrix, and (ii) pore structure inside the LWAs manipulated through partial/complete impregnation of PCMs. In the latter length scale, the system typically consists of pores that contain air, water, and/or the PCM, depending on the amount of PCMs required for a given application, and the porosity and absorption capacity of the LWA. Such composites provide a wide array of benefits to buildings and infrastructure, including energy efficient building envelopes with adequate structural capacity [27–30], limiting the number and/or intensity of freeze-thaw cycles experienced by concrete in bridge-decks, thereby reducing damage [31,32], and reducing the temperature rise in fresh and hardened concrete thereby controlling thermal deformation and stress development [33]. A conceptual illustration of the hierarchical nature of this material (i.e., porous LWAs embedded in cement paste, and the pores of LWAs filled with different phases – water, air, or PCM – having vastly different thermal properties), is shown in Fig. 1.

The numerical technique presented in this paper provides a framework to predict the effective properties of such materials and enables their design for multifunctional applications. Here, a two-step, finite element-based microstructure-guided numerical homogenization scheme is used to develop design strategies that tailor the composition and microstructure of these systems for desired thermal performance.

2. Microstructure-guided numerical simulation for effective thermal properties of composite materials

This section elucidates the microstructure-guided numerical simulation approach for the prediction of effective thermal behavior of PCM-impregnated LWA mortars. At each length scale, the following methodology is incorporated: (1) generation of the representative volume element (RVE); (2) assignment of intrinsic thermal conductivities to the component phases in the RVE; (3) application of periodic boundary conditions [20,34,35] to account for the realistic periodicity of the RVE; (4) finite-element (FE) analysis on the meshed RVE with an imposed temperature gradient; and (5) determination of volume-averaged heat flux to obtain effective thermal conductivity through a post-processing module. The above-mentioned framework is generic and can be tailored to form an interactive module that integrates different length scales of hierarchical materials for effective property prediction. For instance, when the intrinsic elastic constants are assigned to the components, and appropriate boundary conditions are imposed on the RVE, effective elastic properties can be predicted.

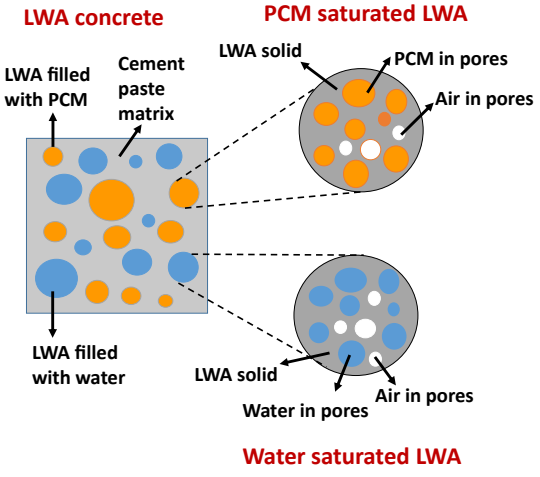

Fig. 1. A conceptual illustration of "structure within the structure" in LWA concrete/mortar. The inclusion phase is a multi-phasic porous solid which can host water, air and/or PCM.

2.1. Generation of representative volume element (RVE)

Lubachhevsky-Stillinger algorithm [36–39] is used to generate the RVE. This algorithm employs a hard particle contact model and hence particle overlaps are not allowed. The shape of the RVE is a cube. The desired number of particles in a periodic bounding box are randomly distributed in the cube. The initial velocities of the particles in the box are randomized, while the initial radius of each particle is set to zero. The radius of any particle in the next event is a function of the growth rate. This rate is designed to attain the desired particle size distribution. Through several iterations, the particles change position in the bounding box, collide and grow in order to obtain the desired volume fraction. The formulations of particle growth rate, velocity of particles in the bounding box, and updating of the particle positions that are integral to the microstructure generation procedure, are extensively described in Refs. [20,36–39]. The microstructural information thus obtained is implemented through a Python language script to enable it to be imported to a FE software such as ABAQUS™.

2.2. Boundary conditions

Periodic boundary conditions (PBC) [20,34,35,40] are used on the generated RVE. By taking advantage of periodicity, a smaller but computationally efficient domain is generated, and rapid convergence is obtained [20,34,35]. Periodic boundary conditions ensure temperature continuity and heat flux continuity at the boundary of the neighboring unit cells. Fig. 2(a) shows the schematic periodic arrays of repetitive unit cells and Fig. 2(b) shows the periodic boundary conditions applied to one of such unit cells. Here, s^+ and s^- are sth pair of two opposite parallel boundary surfaces of the unit cell as shown. The difference between the temperatures of the two opposite parallel boundary edges is given as:

$$T^{S+} - T^{S-} = \left(\frac{\partial T}{\partial x_j}\right)\Delta x_j^S \tag{1}$$

For a pair of opposite parallel boundary edges, Δx_j^s is constant for a specified temperature gradient. Equation (1) is applied as the nodal temperature constraint in the FE microstructural analysis. The temperature gradient is applied to the system of equations through a reference node that is not attached to any element and just acts as a carrier. These sets of linear constraint equations are appended to the previously generated Python language script containing microstructural information. Further details on periodic

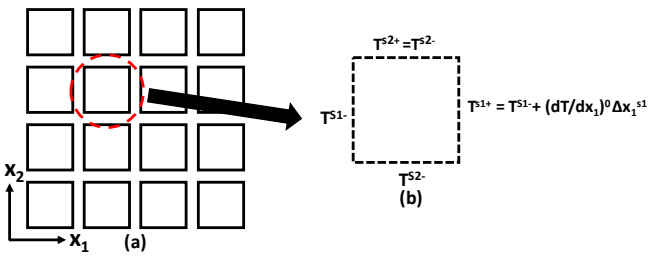

Fig. 2. Schematic representative element area (REA) under applied temperature gradient with periodic boundary conditions.