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Special *n*-sided Voronoi fiber/matrix elements for clustering thermal effect in natural-hemp-fiber-filled cement composites

Hui Wang [a,*], Qing-Hua Qin [b,*], Yi Xiao [b]

[a] *Department of Engineering Mechanics, Henna University of Technology, Zhengzhou 450001, China*
[b] *Research School of Engineering, Australian National University, Canberra, ACT 2601, Australia*

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ABSTRACT

The thermal effects of clustering in natural-hemp-fiber-filled cement composites are investigated and the effective thermal conductivity of the composites is numerically evaluated using the fundamental-solution-based finite element method in conjunction with special *n*-sided Voronoi fiber/matrix elements. In the numerical modeling, the special *n*-sided fiber/matrix elements are developed by a two-variable integral functional involving an independent non-conforming element interior temperature field and an auxiliary conforming element frame temperature field. The element interior temperature field is approximated by a combination of special fundamental solutions satisfying the fiber/matrix interfacial condition and the heat transfer governing equation in each material constituent, and the independent frame temperature field is interpolated by conventional shape functions. All integrals are performed only along the element boundary such that the mesh division associated with fiber/matrix domains can be significantly simplified by the *n*-sided Voronoi fiber/matrix polygonal elements which allow different numbers of sides for each element and permit calculation of fields everywhere in matrix and fibers. Numerical results demonstrate that these special elements are suitable for dealing with clustering distribution of fibers.

1. Introduction

Study of the distribution of fillers such as fibers [1,2], particles [3–6], carbon nanotubes [7,8], etc. in composites is important because the distribution significantly affects efficient load transfer from matrix to fillers, and thereby the functionality and reliability of composites. It has been noted that good distribution of fillers in matrix materials is difficult to achieve, for some well-known reasons such as chemical reactions, large difference of physical properties between fillers and surrounding matrix, and non-uniform mixture during the manufacturing process. Therefore, the effect of irregular or random clustering of fillers must be accounted for in the prediction of effective properties of periodic composites.

In this paper, our attention focuses on the effects of clustering of natural fibers on the thermal properties of cement composites, so that only work in this context is reviewed. As commonly used fillers, natural fibers have received much attention in the development of new composites due to excellent thermal characteristics that distinguish them from artificial fibers [9–17]. Most existing work has been performed under the assumption of uniformly distributed fibers, and the thermal effect of clustering of natural fibers on the performance of composites has rarely been studied. Moreover, the finite element simulations employed by most researchers are computationally intensive for the analysis of clustered fiber distribution in matrix, because very refined meshes within and around inclusions are usually necessary to obtain acceptable accuracy in the finite element method (FEM), resulting in large numbers of degrees of freedom. Moreover, the accuracy of the results depends somewhat on the mesh size in the FEM. Besides, the boundary element method (BEM) seems more complex for solving multi-material problems [18–20], because it requires separate boundary integral equation for each material domain and additional connective equations for satisfying continuous conditions on the boundary between any two adjacent material domains. The coefficient matrix in the final system of equations is full and nonsymmetrical.

To improve the computational efficiency and accuracy of clustered composite problems, in the present work, special *n*-sided Voronoi fiber/matrix elements are developed for numerical prediction of the effect of clustering on the effective thermal conductivity of cement-based composites filled with clustered natural hemp fibers. A representative unit cell containing random or regular

* Corresponding authors.
E-mail addresses: huiwang_china@163.com (H. Wang), qinghua.qin@anu.edu.au (Q.-H. Qin).

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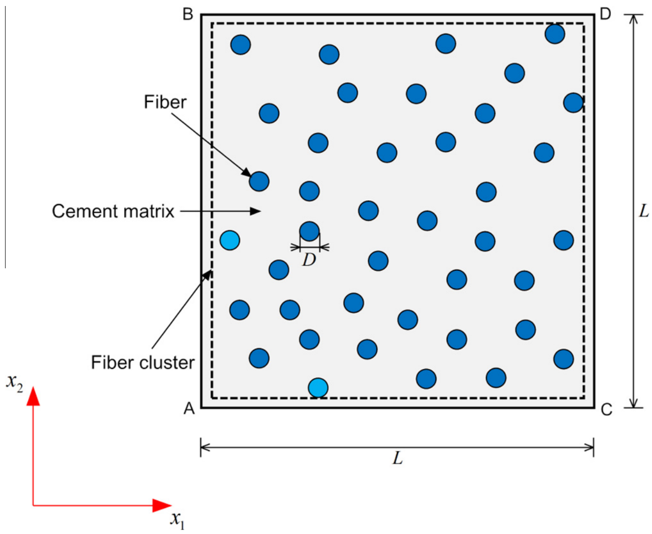

Fig. 1. Schematic representation of regularly and randomly clustered fibers within the cement matrix.

natural fiber clusters is first taken from the cement composite under the assumption of microstructural periodicity, and then it is meshed by the present n-sided Voronoi fiber/matrix polygonal elements, which are rather unconventional elements due to the fact that (1) different elements can have a different number of sides, (2) each element is designed to enclose a centered natural fiber to avoid mesh division within the fiber and the surrounding matrix, (3) all integrals are evaluated along the element boundary, (4) it is possible to calculate fields everywhere in the matrix and the fibers. These special-purpose elements are constructed using the fundamental-solution-based hybrid FEM (HFS-FEM) recently developed for the study of functionally graded materials [21,22], isotropic/orthotropic homogeneous materials [23–25], and cellulous materials weakened by circular or elliptical holes [26–28] as well as cracks [29,30], by introducing two independent fields associated with each element. The HFS-FEM differs from the conventional FEM and the boundary element method (BEM) by virtue of features of element boundary integral, easy construction of special-purpose polygonal elements, and high accuracy and efficiency. For the particular clustering problem under consideration, the present n-sided Voronoi fiber/matrix polygonal element also involves two independent fields. One is the conforming temperature field along the element boundary, which is interpolated by conventional shape functions and is therefore appropriate for n-sided Voronoi polygonal elements having various numbers of nodes. The other field consists of the independent interior temperature and heat flux fields within the element, which are chosen to exactly satisfy equilibrium of matrix and fiber phases and the continuity between them by introducing the combination of fundamental solutions of the problem. These two independent interior and frame fields are finally linked by a two-variable integral functional to produce the stiffness equation and establish connections of all unknowns.

2. Micromechanical model of clustered composite

For a periodic cement-based composite containing clustered hemp fibers, the representative unit cell is the smallest repeated microstructure of the composite that can be isolated from the composite to estimate the composite's effective properties. It is assumed that the unit cell has same thermal properties and fiber volume contents as the composite under consideration.

Fig. 1 shows a representative unit cell containing clustered hemp fibers. In Fig. 1, L denotes the cell length, D is the diameter of the hemp fiber, and x_1 and x_2 are the global coordinate axial directions. Under the assumptions that (1) all material constituents are isotropic and homogeneous, and (2) the hemp fiber and the cement matrix are perfectly bonded, the steady-state local temperature fields in the matrix and the fiber, denoted by T_m and T_f, should satisfy the two-dimensional heat conduction governing equations respectively given by

$$\frac{\partial^2 T_m}{\partial x_1^2} + \frac{\partial^2 T_m}{\partial x_2^2} = 0, \quad \frac{\partial^2 T_f}{\partial x_1^2} + \frac{\partial^2 T_f}{\partial x_2^2} = 0 \tag{1}$$

and the continuous conditions at the interface between the hemp fiber and the matrix

$$\begin{aligned} &T_m = T_f \\ &k_m \frac{\partial T_m}{\partial n} = k_f \frac{\partial T_f}{\partial n} \end{aligned} \tag{2}$$

where n is the unit direction normal to the fiber/matrix interface.

According to Fourier's law of heat transfer in isotropic media, we have the following relationship of the temperature variable T and the heat flux component q_i:

$$q_i = -k\frac{\partial T}{\partial x_i} \qquad (i = 1, 2) \tag{3}$$

from which the effective thermal conductivity k_e of the homogenized composite can be determined by

$$k_e = \frac{\bar{q}_i}{\bar{\varepsilon}_i} \tag{4}$$

where $\bar{q}_i$ stands for the area-averaged heat flux component along the i-direction and $\bar{\varepsilon}_i$ the temperature gradient component along the i-direction. For example, for the applied temperature boundary conditions below

$$\begin{aligned} &T_m = T_0 && \text{on edge AB} \\ &T_m = T_1 && \text{on edge CD} \\ &k_m \frac{\partial T_m}{\partial n} = 0 && \text{on edges AC and BD} \end{aligned} \tag{5}$$

the effective thermal conductivity k_e of the composite can be calculated by the 1-directional average heat flux component $\bar{q}_1$ on the surface CD and the 1-directional temperature gradient component $\bar{\varepsilon}_1$ respectively given by

$$\bar{q}_1 = \frac{1}{L}\int_{AB} q_1(x_1, x_2)\mathrm{d}x_2 \tag{6}$$

$$\bar{\varepsilon}_1 = \frac{(T_1 - T_2)}{L} \tag{7}$$

3. Formulation of special *n*-sided Voronoi fiber/matrix element

The representative unit cell with the specified temperature conditions along the outer boundary of the cell is solved by a fundamental-solution-based hybrid finite element formulation with special n-sided Voronoi fiber/matrix elements. To efficiently treat regularly and randomly clustered distributions of hemp fibers in the unit cell and obtain a mesh with relatively high quality, the centroidal Voronoi tessellation technique is employed such that the generators for the Voronoi tessellation and the centroids of the Voronoi regions coincide [31]. The centroidal Voronoi tessellation technique can be viewed as an optimal partition corresponding to an optimal distribution of generators. Fig. 2 displays a typical n-sided Voronoi fiber/matrix element division for the composite cell including hemp fiber and cement material constituents. As an example, in Fig. 2, the centroidal Voronoi elements are