

EFFECTIVE MODULI OF 3-1 LONGITUDINALLY POROUS SOLIDS WITH REGULAR HEXAGONAL ARRAY

Adair R. Aguiar, Programa de Pós-Graduação Interunidades em Bioengenharia – EESC /FMRP/IQSC, Departamento de Engenharia de Estruturas-EESC-USP, São Carlos, SP, Brasil, aguiarar@sc.usp.br
Edmar B. T. Prado, Departamento de Engenharia de Estruturas-EESC-USP, São Carlos, SP, Brasil, edmarbt@sc.usp.br
Uziel Paulo da Silva, Departamento de Engenharia de Estruturas-EESC-USP, São Carlos, SP, Brasil, uziel@sc.usp.br

Abstract. Determining the effective properties of nonhomogeneous solids using analytical methods is generally based on the assumption that these solids have infinite dimensions. In laboratory experiments, however, samples have finite dimensions. Here, we are interested in verifying whether the analytical expressions provide accurate values for the constants measured in laboratory. We use the Asymptotic Homogenization Method (AHM) to determine the shear effective constant of an elastic solid of infinite dimensions containing a uniform and periodic distribution of circular cylindrical holes. We also use the Finite Element Method (FEM) to determine this constant in the case of a finite sample containing the same uniform distribution of cylindrical holes. Both solids have the same elastic properties and are subjected to similar anti-plane shear experiments. We show a table with effective constants calculated for different void volume fractions that allow verifying the good agreement between the values obtained through AHM, FEM, and a computational poroelastic model of Haversian bone found in the literature.

Keywords: Linear elasticity. Asymptotic homogenization method. Finite element method. Effective properties. Cortical Bone.

1. INTRODUCTION

Different multiscale models have been proposed for modeling cortical bone. For instance, Rho *et al.* (1998) surveys the available mechanical data, with an emphasis on the relationship between the complex hierarchical structure of bone and its mechanical properties. They observe that the application of composite rule of mixtures formulae in the prediction of the mechanical properties of bone have been only moderately successful. Hamed *et al.* (2010) introduce a hierarchical modeling approach to evaluate analytically the effective elastic constants of cortical bone. They use micromechanics methods and composite materials laminate theories to model the bone's elastic response at different scales, spanning from the nanostructural to the mesostructural levels. The results obtained at a lower scale serve as inputs for the modeling at a higher scale. The predictions are in good agreement with experimental data reported in the literature.

Determining the effective properties of a nonhomogeneous solid, such as bone, by means of analytical methods generally assumes that the solid has infinite dimensions. In laboratory experiments, however, samples have finite dimensions. It is, therefore, of interest to verify whether such expressions provide accurate values for the constants measured in the laboratory. In fact, a necessity has arisen for reliable mathematical models to explain the related data, obtained experimentally, in terms of effective elastic properties. The aim of this research is to develop a reliable and computationally efficient method of analysis suitable for predicting the response of elastic solids containing a distribution of heterogeneities, which, here, consists of a uniform and periodic distribution of circular cylindrical holes.

Some works related to this area of investigation are commented below. Swan *et al.* (2003) neglect the lamellar structure of cortical bone matrix and model the resulting Haversian bone matrix as a homogeneous and linearly elastic isotropic medium. They use a unit cell model with periodic boundary conditions and with 1% and 4% Haversian porosity together with Finite Element Method (FEM) to compute all the effective poroelastic moduli of Haversian bone with square-packed non-overlapping osteons. We also neglect the lamellar structure of the cortical bone matrix but, differently from these authors, we use a hexagonal array of holes to model non-overlapping osteons and we use finite element discretization of the whole domain, instead of the unit cell model, to compute all the effective moduli.

Grimal *et al.* (2008) introduce a method to obtain the elastic tensor of a cortical bone sample at the mesoscale from a mapping of its microscale elasticity. The mesoscale properties are estimated based on a finite element homogenization procedure and the results are compared with available experimental data. The authors observe, however, that, although experimental data indicate that the expressions $c_{66} < c_{55} = c_{44}$ always hold, their computed effective elastic coefficients do not obey these expressions, prompting them to question the validity of their computations for the case of effective c_{44} . In this work we do verify that $c_{66}^{ef} \leq c_{55}^{ef} = c_{44}^{ef}$ by using both analytical and computational methods.

In Parnell *et al.* (2009) the matrix phase is assumed to be homogeneous isotropic and the asymptotic homogenization method (AHM) is used to predict the influence of porosity on the induced anisotropy of cortical bone. For the case of circular pores, the authors show that the results obtained via homogenization are in good quantitative and qualitative agreement with finite element results from real two-dimensional microstructures obtained from images of cortical bone.

Later, Parnell *et al.* (2012) compare theoretical predictions of the effective elastic moduli of cortical bone at both the meso- and macroscales. They consider the efficacy of three alternative homogenization approaches: the AHM, the Mori–Tanaka scheme and the Hashin–Rosen bounds. The authors point out that, although the mesoscale behavior of bone is widely accepted as important, models incorporating its effect have started to appear only recently. Except for the work of Swan *et al.* (2003), the authors above have considered circular cylindrical holes arranged on a hexagonal lattice.

In addition to the above works on homogenization schemes to evaluate effective properties of bone, the impact of the elastic symmetry assumed for the bone matrix on the mesoscopic behavior was discussed by Sevostianov and Kachanov (2000), among others. These authors have proposed a micromechanics model to study the influence of porosity on the anisotropy of cortical bone. They have concluded that the differences between the cases of empty pores and pores filled with soft material were insignificant. Grimal *et al.* (2008) have quantified this influence and concluded that, on the contrary, it is significant.

In this work we consider that the solid has a uniform and periodic distribution of circular cylindrical holes in a linear elastic isotropic medium. The cylinders are centered in unit cells of hexagonal cross sections. We use closed form expressions obtained by Bravo-Castillero *et al.* (2009) to calculate analytically the effective shear elastic constant of the solid. A cross section of the solid is shown in Fig. 1. The procedure used to calculate this constant can be used to calculate the other elastic constants of the solid. In addition, the procedure may also be used in calculating the elastic constants of a solid with unit cells of different cross sections, such as the square cross section.

The rest of the paper is organized as follows. In Section 2 we present the statement of the anti-plane shear problem for the linear elastic isotropic medium with infinite dimensions and use this formulation together with the AHM in the calculation of the effective elastic constant c_{44}^{ef} . In Section 3 we consider finite dimensions for the elastic medium and we use the analogy between the associated elastic problem and the linear steady state heat conduction problem to formulate the problem that we solve numerically by using a finite element commercial package. In Section 4 we compare the results obtained via AHM and via FEM. In Section 5 we present the conclusions of this work.

2. PROBLEM STATEMENT

Consider a linear and isotropic elastic solid with infinite dimensions containing a uniform and periodic distribution of circular cylindrical holes centered in unit cells with hexagonal cross sections. In relation to a Cartesian coordinate system (x_1, x_2, x_3) with origin at O , the axes of the holes are parallel to the coordinate axis Ox_3 and the cross section of the region occupied by the solid in a stress-free undeformed configuration is parallel to the plane x_1x_2 . This cross section together with the cross section of the hexagonal unit cell are shown in Fig. 1, where M and Y correspond to the solid portions of the solid without holes and R and Γ correspond to the radius and the boundary of the hole in the cell, respectively.

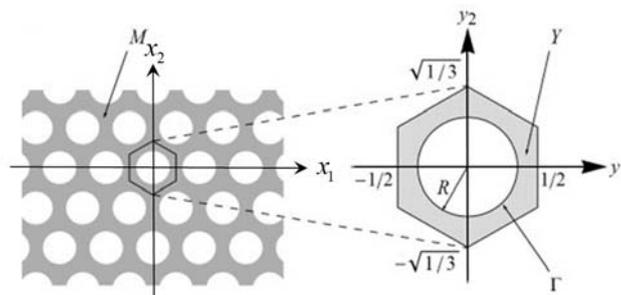


Figure 1. A cross section of a 3–1 longitudinally porous elastic periodic solid of infinite dimensions and the corresponding periodic cell for a hexagonal array. Adapted from Bravo-Castillero *et al.* (2009).

The effective properties of the above periodic medium are calculated by means of AHM. The relevant essentials of these calculations can be found in Bravo-Castillero *et al.* (2009). Thus, for the problem at hand, which is to calculate analytically the effective shear elastic constant, c_{44}^{ef} , of the elastic solid, only the *Local Problem* $_{13}L$ over the unit cell Y must be specified at the outset. This problem consists of finding $U : Y \rightarrow \mathbb{R}$, harmonic and of zero average in Y , that satisfies the system of equations

$$\Delta U = 0 \quad \text{in } Y, \quad (1)$$

$$U_{,1}n_1 + U_{,2}n_2 = -n_1 \quad \text{on } \Gamma, \quad (2)$$

$$\langle U \rangle = 0, \quad (3)$$

where $\langle U \rangle \triangleq \int_Y F(\mathbf{y}) d\mathbf{y} / |Y|$, with $|Y|$ being the volume of Y , and Δ is the two-dimensional Laplacian in Y . The solution of Eq. (1)-Eq. (3) is sought in the class of doubly periodic harmonic functions, $U(z)$, which depends on the complex variable $z = y_1 + iy_2$, in the form of a series with undetermined real coefficients a_k , given by

$$U(z) = \text{Re}\{a_1[\zeta(z) - \pi z/\sin \mu] + \sum_{k=3,5,\dots}^{\infty} a_k \zeta^{(k-1)}(z)/(k-1)!\}, \quad (4)$$

where $\text{Re}\{\cdot\}$ stands for the real part of the argument, μ is the angle of the unit cell, which is $\pi/3$ for the hexagonal cell, and $\zeta(z)$ and $\zeta^{(k)}(z)$ are quasi-periodic Weierstrass zeta function and its k th derivatives of periods $\omega_1 = 1$ and $\omega_2 = e^{i\mu}$, respectively.

Once the local problem is solved, the homogenized effective modulus is given by the following expression

$$c_{44}^{ef} = \langle c_{44} \rangle + c_{44} \langle U_{,1} \rangle, \quad (5)$$

where c_{44} is the shear modulus of the solid part of the elastic medium and it can be shown that

$$\langle U_{,1} \rangle = (\pi R^2 - 2\pi a_1) / \sin \mu, \quad (6)$$

where a_1 is the solution of the infinite system

$$a_l = R^{2l} [(1 - \pi a_1 / \sin \mu) \delta_{ll} + \sum_{k=1,3,5,\dots}^{\infty} a_k \eta_{(kl)}] \quad \text{for } l = 1, 3, \dots, \quad (7)$$

where δ_{ll} is the Kronecker delta and

$$\eta_{(kl)} = C_{k+l-1}^l S_{k+l}, \quad S_{k+l} = \sum_{m,n}^* \beta_{mn}^{-k-l} \quad \text{for } k+l \geq 2, \quad \beta_{mn} = m\omega_1 + n\omega_2, \quad m, n = 0, \pm 1, \pm 2, \dots,$$

$$C_k^l = k! / [l!(k-l)!].$$

The star, *, in the summation sign indicates that the double sum excludes $m = n = 0$. For the hexagonal array of holes considered in this work, the series S_{k+l} and $\eta_{(kl)}$ are not null if $k+l = 6t$ for $t = 1, 2, 3, \dots$.

The solution a_1 of the infinite system in Eq. (7) is given by

$$a_1 = \frac{R^2}{1 + A_2 - \mathbf{V}_p^T \mathbf{M}_p^{-1} \tilde{\mathbf{V}}_p}, \quad (8)$$

in which $A_2 = \pi R^2 / \sin \mu$ and we recall from above that $\mu = \pi/3$ for a hexagonal cell. Also, for the case of the distribution of hexagonal cells considered in this work,

$$\mathbf{V}_p = \mathbf{V}_p(\omega_s), \quad \mathbf{M}_p = \mathbf{M}_p(m_{ts}), \quad \tilde{\mathbf{V}}_p = \tilde{\mathbf{V}}_p(\tilde{\omega}_t)$$

are vectors and matrices of infinite dimensions and

$$\omega_s = R^{12s} \eta_{(1-6s-1)}, \quad m_{ts} = \delta_{(6t-1-6s-1)} - R^{12s} \sum_{i=1}^{\infty} R^{12i} \eta_{(6t-1-6i+1)} \eta_{(6i+1-6s-1)}, \quad \tilde{\omega}_t = \eta_{(6t-1)}, \quad t, s = 1, 2, 3, \dots$$

Upon substituting Eq. (8) in Eq. (6) and the resulting expression in Eq. (5), we obtain the analytical expression

$$c_{44}^{ef} = c_{44} (1 - 2A_2 K^0), \quad (9)$$

where

$$K^0 = \frac{1}{1 + A_2 - \mathbf{V}_p^T \mathbf{M}_p^{-1} \tilde{\mathbf{V}}_p}.$$

3. COMPUTATIONAL PROCEDURE

In the preceding section we have obtained the effective constant c_{44}^{ef} by considering a solid with infinite dimensions containing uniformly distributed circular cylindrical holes. In this section we simulate numerically the antiplane shear of a cylindrical sample with rectangular cross section containing the same uniform distribution of circular holes and we determine the corresponding effective elastic constant. The cross section of the solid is illustrated in Fig. 2. The material of the sample is isotropic and linearly elastic with the same elastic constant adopted for the solid with infinite dimensions.

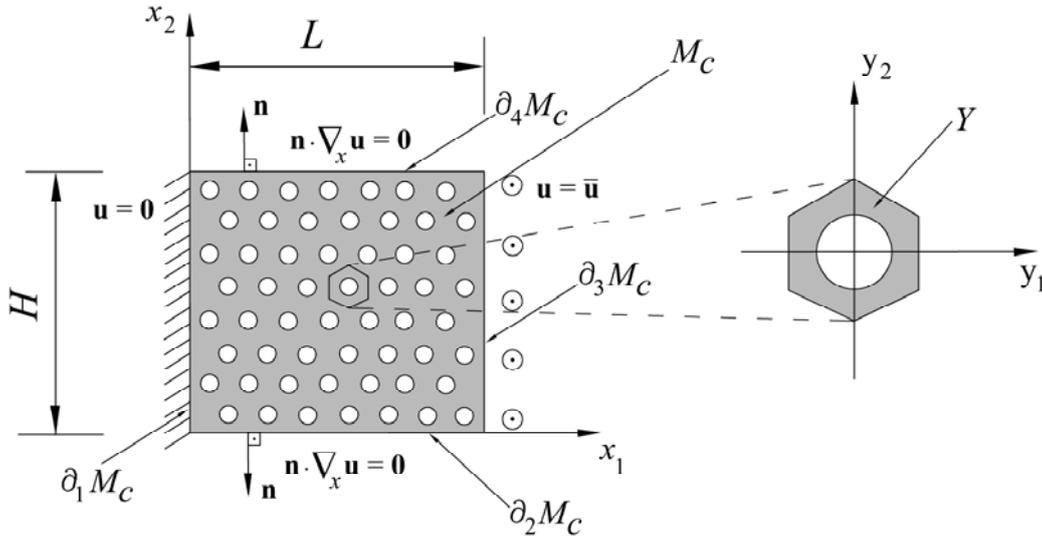


Figure 2. Cross section of a cylindrical sample containing a uniform distribution of circular cylindrical holes and the corresponding periodic cell for a hexagonal array.

The governing differential equation and the boundary conditions at the walls of holes have the same form of Eq. (1) and Eq. (2), respectively. Here, however, M and Ω are replaced by, respectively, M_C and Ω_C , where M_C is illustrated in Fig. 2 and Ω_C is the union of all the contours of the holes. On the external boundary of the sample, we impose the conditions illustrated in Fig. 2, where L and H are the sides of the sample, \mathbf{n} is the outward normal vector to the external boundary, and the symbol \odot represents the direction of $\bar{\mathbf{u}}$ applied normal to the plane $x_1 x_2$ on $\partial_3 M_C$.

To solve numerically the equilibrium problem described above, we observe that this problem is analogous to a linear steady state heat conduction problem, which consists of finding the temperature field $T : M_C \rightarrow \mathbb{R}$ that satisfies

$$\Delta_x T = 0 \quad \text{in } M_C, \quad (10)$$

$$\mathbf{n} \cdot \nabla_x T = 0 \quad \text{on } \Omega_C \cup \partial_2 M_C \cup \partial_4 M_C, \quad (11)$$

$$T = 0 \quad \text{on } \partial_1 M_C, \quad T = \bar{T} \quad \text{on } \partial_3 M_C, \quad (12)$$

where Δ_x e ∇_x are, respectively, the Laplacian and the gradient operators defined in M_C and ∂M_C is the external boundary of M_C . We use the finite element commercial package COMSOL 4.4[®] to obtain approximate solutions of Eq. (10)-Eq. (12). The temperature field T is approximated by quadratic triangular finite elements.

Once an approximate solution of the thermal problem is obtained for a given discretization, we associate the temperature T with the displacement u and the conductivity k with the elastic constant c_{44}^{ef} . Thus, the effective elastic constant c_{44}^{ef} is determined from the expression

$$c_{44}^{ef} = \frac{\int_{\partial_3 M_C} \mathbf{n} \cdot \nabla_x T dx_2}{\bar{T}/L}, \quad (13)$$

where $\int_{\partial_3 M_C} \mathbf{n} \cdot \nabla_x T dx_2$ is the heat flux on $\partial_3 M_C$.

4. RESULTS AND DISCUSSION

In Fig. 3 we show graphs of the effective elastic constant c_{44}^{ef} versus the void volume fraction A_2 obtained via AHM, by means of Eq. (9), and via FEM, using Eq. (13), for the elastic samples with rectangular cross sections having the dimensions $L \times H \in (0.0756 \times 0.0714, 0.1623 \times 0.1520, 0.3173 \times 0.2947, 0.6397 \times 0.5925)$ [m²], where we recall from Fig. 2 that L and H are the dimensions of the sides of a cross section. These dimensions correspond to FEM Fi, $i=1, \dots, 4$ in the legend of Fig. 3. In both cases, finite and infinite media, the elastic constant of the solid part is $c_{44} = 1$ GPa. In the case of the elastic samples, the holes are contained in a rectangular frame having a thickness that is held fixed at 0.0031 m. Observe from the figure the good agreement between analytical and numerical solutions as $L \times H$ increases. In particular, observe the good agreement of these solutions for higher values of void volume fraction and as these values approach the limit for which the walls of the holes touch each other. In the case of cells with regular hexagonal cross section, this limit is 0.9069. We then see from these results that analytical results obtained via AHM for an infinite medium yield good approximations of results obtained from the numerical simulation of the behavior of a finite medium.

Next, we compare our results with results obtained by Swan *et al.* (2003) for the corresponding effective shear elastic constant using the same properties given by these authors. In their work, however, the holes are centered in a square unit cell (instead of the hexagonal cell). In Table 1 we present the void volume fraction A_2 , which can have the values 0.01 and 0.04, the effective shear elastic coefficient obtained from their Table 2 for the fully drained case, the coefficient c_{44}^{ef} obtained via both AHM and FEM, and relative errors in percentage between their coefficients and c_{44}^{ef} obtained via both AHM and FEM. Observe from their Table 2 together with their Table 1 that $A_2 = 0.01$ is associated with Young's modulus $E = 11$ GPa and Poisson's ratio $\nu = 0.39$ and that $A_2 = 0.04$ is associated with $E = 12$ GPa and $\nu = 0.38$. The fully drained case corresponds to the response of bone in which the fluid carries no excess pressures from applied loadings. Observe from Table 1 the very good agreement between our calculations and theirs for the case $A_2 = 0.04$ and a larger discrepancy in the case $A_1 = 0.01$, which is being investigated.

5. FINAL REMARKS

We have presented analytical and numerical results related to the calculation of the effective elastic constant c_{44}^{ef} of an isotropic and linear elastic solid containing a uniform and periodic distribution of circular cylindrical holes. The holes are centered in unit cells with regular hexagonal cross sections. The analytical results are obtained via AMH for an elastic solid of infinite dimensions and the numerical results are obtained via FEM for a solid of finite dimensions with rectangular cross section. The graphs of c_{44}^{ef} versus volume concentration A_2 for different values of length of the sides of the rectangular cross sections indicate a good agreement between analytical and numerical results. We shall present results for the other effective elastic constants of the solid at the conference.

This work represents the initial efforts of the research group to determine the effective elastic constants of nonhomogeneous solids through analytical, computational and experimental methods.

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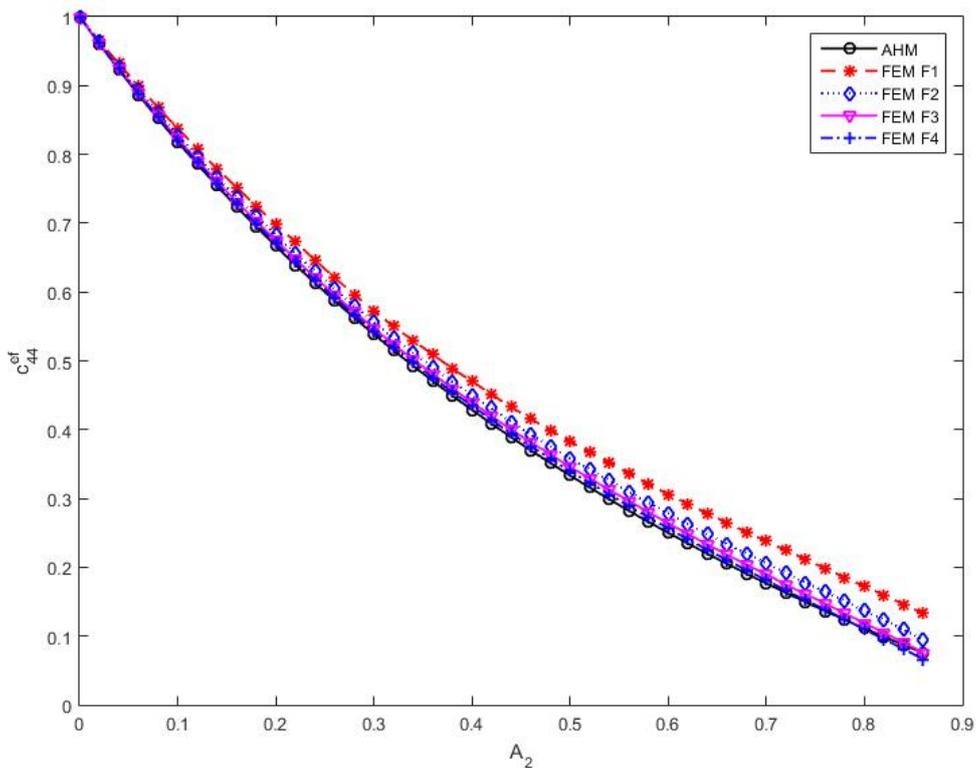


Figure 3. Curves of effective elastic coefficient c_{44}^{ef} versus void volume fraction A_2 for an infinite medium and for samples of finite dimensions containing an increasing number of uniformly distributed circular cylindrical holes in a hexagonal lattice.

Table 1. Calculated effective constant c_{44}^{ef} and relative errors between results obtained via AHM and FEM and results presented by Swan *et al.* (2003) for the fully drained case.

A_2	C_{44}^{ef} (GPa)	C_{44}^{ef}	C_{44}^{ef}	Relative Error (%)	Relative Error (%)
	Swan <i>et al.</i> (2003) Fully drained	(GPa) AHM	(GPa) FEM		
0.01	3.5587	3.8784	3.8776	8.9836	8.9613
0.04	4.0161	4.0134	4.0098	0.0672	0.1572

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8. ACCOUNTABILITY FOR INFORMATION

The authors are solely responsible for the information included in this work.