APPLICATION OF THREE-PHASE AND FOUR-PHASE MODELS TO CALCULATE EFFECTIVE PROPERTIES OF A COMPOSITE

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Summary

In general, the effective properties of a n-phase composite material can be calculated by considering an (n+1)-phase composite model, where the (n+1)-phase consists of the equivalent homogeneous composite material. In the present study a three-phase composite which consists of spherical inclusions, an interphase and a matrix is considered. The effective properties of this three-phase composite can be calculated exactly using the four-phase composite model, and also by applying the less complicated three-phase composite model twice, in succession.

Here by applying these two methods to a typical composite, elastic properties of the interphase can be determined from the properties of the inclusion, matrix and composite. It is seen that the three-phase composite model yields results, which are very close to the results obtained from the four-phase composite model.

1. Introduction

The geometry and the properties of constituents of composites affect the effective properties of composites. In general, the effective properties of composites are obtained as bounds for inclusions of arbitrary shape [1-3] while for some particular shape of inclusion the effective moduli are exactly obtained [4-6]. It is advantageous that effective properties of composites can be determined from the properties of constituents of composites and the volume fraction. If effective properties of composites can be known in advance, composites which meet required properties can be made efficiently.

The three-phase composite sphere model for obtaining the effective elastic bulk modulus of a two-phase composite, composed of isotropic spherical inclusions and an isotropic elastic matrix was first presented by Hashin [2]. The quadratic equation to calculate the effective elastic shear modulus of the same model was obtained by Christensen and Lo [4]. The generalization of the three-phase composite sphere model to the multi-layer spherical inclusion was presented by Herve and Zaoui [5].

Many researchers have investigated the effective properties of concrete or cement mortar [7-11]. Concrete is considered as a three-phase composite material, composed of coarse aggregate, interfacial transition zone (ITZ) and mortar. A four-phase spherical model was used by Ramesh et al. [8] and a cylindrical model was used by Zhao and Chen [9,10] to study the effect of the ITZ on the effective properties of concrete and cement mortar. In general the thickness of the transition zone for concrete is about 10-30 μm. Many factors such as type of aggregate, water cement ratio, curing process and chemical compositions of concrete effect the properties of the transition zone.
Effective properties of concrete can be calculated from the elastic properties of mortar, aggregate and interface layer and the volume fractions. While it is difficult to determine elastic properties of the ITZ from experiments on the other hand effective properties of concrete can be measured by experiments. Hence in this paper a way to determine elastic constants of the ITZ is discussed. Hashin and Monteiro [11] considered the effective properties of cement mortar to determine the properties of the ITZ.

In Sections 2 and 3 the three-phase composite model and four-phase composite model are described. The two-step procedure to calculate the effective properties of a three-phase composite is given in Section 4. The four-phase composite model and the three-phase composite model with the two-step procedure is applied to concrete in Section 5. Using available experimental data for concrete, aggregate and cement mortar, the elastic properties of the interphase are estimated. Eshelby’s formula [12] used to obtain expressions for the effective properties are given in the Appendix.

2. Three-phase Composite Sphere Model

In calculating the effective properties of a two-phase composite material, which consists of spherical inclusions embedded in a homogeneous matrix material (Fig. 1), the three-phase composite sphere model is used. The model consists of a two-phase composite sphere surrounded by an equivalent homogeneous infinite medium as shown in Fig. 2. Each phase is homogeneous and isotropic elastic and perfect bonding is assumed at each interface. The derivation of the effective bulk modulus was presented by Hashin [2], while Christensen and Lo [4] obtained the quadratic equation to calculate the effective shear modulus.

2.1 Basic equations

The equilibrium equation when there are no body forces is

\[ \nabla \cdot \sigma = 0, \]  

where \( \sigma \) is the symmetric stress tensor and \( \nabla \cdot \sigma \) is the divergence of \( \sigma \).

The infinitesimal strain tensor \( \varepsilon \) is related to the displacement vector \( u \) by

\[ \varepsilon = \frac{1}{2} [\nabla \otimes u + (\nabla \otimes u)^T], \]  

where \( \nabla \otimes u \) is the gradient of \( u \) and superscript \( ^T \) denotes the transpose of a tensor.

The stress and strain tensors, are split into isotropic and deviatoric parts as

\[ \sigma = \frac{1}{3} \text{tr}(\sigma)I + s, \quad \varepsilon = \frac{1}{3} \text{tr}(\varepsilon)I + e, \]  

where “\( \text{tr} \)” is the trace of a tensor, \( I \) is the second order identity tensor, \( s \) and \( e \) are the deviatoric stress and strain tensors, respectively. For phase \((i)\) Hooke’s law can be expressed as

\[ \text{tr}(\sigma^{(i)}) = 3K_i \text{tr}(\varepsilon^{(i)}), \quad s^{(i)} = 2\mu_i e^{(i)}, \]  

where \( K_i \) and \( \mu_i \) are the bulk and shear moduli of phase \((i)\).

Fig. 1. Two-phase composite material. Fig. 2. Three-phase composite sphere model.
where $K_i$ is bulk modulus and $\mu_i$ is shear modulus. The spherical coordinate system ($R, \psi, \theta$) is used in the following analysis.

### 2.2 Effective bulk modulus

The displacement field for phase ($i$) under uniform dilatation or uniform pressure at infinity can be written as

$$u^{(i)}_R (R) = F_i R + G_i R^{-2}, \quad u^{(i)}_\psi = u^{(i)}_\theta = 0,$$

where $F_i$ and $G_i$ are arbitrary constants. For the three-phase sphere model $i = 1, 2, 3$. From Eqs. (2)-(5) the expressions for stresses are

$$\sigma^{(i)}_{R R} = 3K_i F_i - 4\mu_i G_i R^{-3}, \quad \sigma^{(i)}_{R \psi} = \sigma^{(i)}_{R \theta} = 3K_i F_i + 2\mu_i G_i R^{-3}, \quad \sigma^{(i)}_{\psi \psi} = \sigma^{(i)}_{\psi \theta} = \sigma^{(i)}_{\theta \theta} = 0.$$

The non-singular stress condition at the origin and the continuity conditions at the interfaces are

$$\sigma^{(i)}(0) \text{ should be finite, } u^{(i)}(R_j) = u^{(j+1)}(R_j), \quad \sigma^{(i)}e_R(R_j) = \sigma^{(j+1)}e_R(R_j),$$

where $e_R$ is the base vector in the radius direction $R$. Substituting Eqs. (5)-(7) (for $i = 1, 2, 3; j = 1, 2$) into Eq. (A.3) the effective bulk modulus $K_{eff}$ is obtained as

$$K_{eff} = K_3 + \frac{f_1 (K_1 - K_2)}{1 + (1 - f_1)(K_1 - K_2)/(K_3 + 4\mu_2 / 3)},$$

where $f_1 = R_1^3/R_2^3$ is the volume fraction of the inclusion.

### 2.3 Effective shear modulus

The displacement field for phase ($i$) under simple shear deformation can be written as

$$u^{(i)}_R = (A_i R - \frac{3V_i}{1 - 2V_i} B_i R^3 + 3C_i R^{-4} + \frac{5 - 4V_i}{1 - 2V_i} D_i R^{-2}) \sin \psi \cos \theta,$$

$$u^{(i)}_\psi = (A_i R - \frac{7 - 4V_i}{1 - 2V_i} B_i R^3 - 2C_i R^{-4} + 2D_i R^{-2}) \sin \psi \cos \psi \cos \theta,$$

$$u^{(i)}_\theta = (-A_i R + \frac{7 - 4V_i}{1 - 2V_i} B_i R^3 + 2C_i R^{-4} - 2D_i R^{-2}) \sin \psi \sin \theta,$$

where $V_i$ is Poisson’s ratio and $A_i$, $B_i$, $C_i$, and $D_i$ are arbitrary constants ($i = 1, 2, 3$). From Eqs. (2)-(4) and (9) the relevant stresses are expressed as

$$\sigma^{(i)}_{R R} = 2(A_i + \frac{3V_i}{1 - 2V_i} B_i R^2 - 12C_i R^{-5} - 2 \frac{5 - V_i}{1 - 2V_i} D_i R^{-3}) \mu_i \sin^2 \psi \cos \theta,$$

$$\sigma^{(i)}_{R \psi} = (A_i - \frac{7 + 2V_i}{1 - 2V_i} B_i R^2 + 8C_i R^{-5} + \frac{2}{1 - 2V_i} D_i R^{-3}) \mu_i \sin 2\psi \cos \theta,$$

$$\sigma^{(i)}_{\psi \theta} = -2(A_i - \frac{7 + 2V_i}{1 - 2V_i} B_i R^2 + 8C_i R^{-5} + \frac{2}{1 - 2V_i} D_i R^{-3}) \mu_i \sin \psi \sin \theta.$$

Substituting Eqs. (7), (9)-(10) (for $i = 1, 2, 3; j = 1, 2$) into Eq. (A.3) and after some manipulation the effective shear modulus $\mu_{eff}$ can be obtained from
\[
a\left(\frac{\mu_{\text{eff}}}{\mu_2}\right)^2 + 2b\frac{\mu_{\text{eff}}}{\mu_2} + c = 0, \tag{11}
\]

where

\[
a = 8(\overline{\mu}_i - 1)(4 - 5\nu_i)\eta_i f_i^{10/3} - 2\left[63(\overline{\mu}_i - 1)\eta_i + 2\eta_i\eta_j\right]f_i^{7/3} + 252(\overline{\mu}_i - 1)\eta_i f_i^{13/3} - 50(\overline{\mu}_i - 1)(7 - 12\nu_i + 8\nu_i^2)\eta_i f_i + 4(7 - 10\nu_i)\eta_i\eta_j,
\]

\[
b = -2(\overline{\mu}_i - 1)(1 - 5\nu_i)\eta_i f_i^{10/3} + 2\left[63(\overline{\mu}_i - 1)\eta_i + 2\eta_i\eta_j\right]f_i^{7/3} - 252(\overline{\mu}_i - 1)\eta_i f_i^{5/3} + 75(\overline{\mu}_i - 1)(3 - \nu_i)\eta_i\nu_j f_i + \frac{3}{2}(15\nu_i - 7)\eta_i\eta_j,
\]

\[
c = 4(\overline{\mu}_i - 1)(5\nu_i - 7)\eta_i f_i^{10/3} - 2\left[63(\overline{\mu}_i - 1)\eta_i + 2\eta_i\eta_j\right]f_i^{7/3} + 252(\overline{\mu}_i - 1)\eta_i f_i^{13/3} + 25(\overline{\mu}_i - 1)(\nu_i^2 - 7)\eta_i f_i - (7 + 5\nu_i)\eta_i\eta_j.
\]

\[
\eta_i = (49 - 50\nu_i\nu_j)(\overline{\mu}_i - 1) + 35\overline{\mu}_i(\nu_i - 2\nu_j) + 35(2\nu_i - \nu_j),
\]

\[
\eta_j = 5\nu_j(\overline{\mu}_j - 8) + 7(\overline{\mu}_j + 4) , \quad \eta_j = \overline{\mu}_j(8 - 10\nu_j) + (7 - 5\nu_j), \quad \overline{\mu}_i = \mu_i/\mu_2.
\]

3. Four-phase Composite Sphere Model

The multi-phase composite sphere model presented by Herve and Zaoui [5] is a generalization of the three-phase composite sphere model. The four-phase composite sphere model [8] is a special case of the multi-phase composite sphere model. The composite consists of three-phases namely, spherical inclusions, interphase and the matrix material as shown in Fig. 3. Each phase is homogeneous and isotropic elastic and perfect bonding is assumed at each interface. The model consists of a three-phase composite sphere surrounded by an equivalent homogeneous infinite medium as shown in Fig. 4. The basic equations to analyze this model are the same as given in Section 2.

3.1 Effective bulk modulus

Substituting Eqs. (5)-(7) (for \(i = 1,4 ; j = 1,2,3\)) into Eq. (A.3) the effective bulk modulus \(K_{\text{eff}}\) is obtained in recursive form as

\[
K_{\text{eff}} = K_4 = K_3 + \frac{(f_i + f_j)}{1/(K_e - K_3) + (1 - f_i - f_j)/(K_3 + 4\mu_4/3)}, \tag{13}
\]

where

\[
K_e = K_2 + \frac{f_i}{(f_i + f_j)(K_1 - K_2) + f_j(K_2 + 4\mu_4/3)} \tag{14}
\]
and $f_1 = \frac{R_1^3}{R_3^3}$, $f_2 = \frac{R_2^3 - R_1^3}{R_3^3}$ are the volume fractions of inclusion and interphase phases, respectively.

3.2 Effective shear modulus

Substituting Eqs. (7), (9)-(10) (for $i = 1, 4$; $j = 1, 2, 3$) into Eq. (A.3) and after some manipulation the effective shear modulus $\mu_{\text{eff}} = \mu_3$ can be obtained from

$$4d_{12}^{(3)}\left(\frac{\mu_{\text{eff}}}{\mu_3}\right)^2 + (d_{23}^{(3)} - 2d_{13}^{(3)} - 2d_{14}^{(3)} + 3d_{24}^{(3)}) \left(\frac{\mu_{\text{eff}}}{\mu_3}\right) - d_{34}^{(3)} = 0,$$

where

$$d_{ij}^{(3)} = P_{ij}^{(3)} - P_{ij}^{(1)} - P_{ij}^{(2)} - P_{ij}^{(3)},$$

$$\mathbf{p}^{(n)} = \mathbf{p}^{(n-1)} \mathbf{s}^{(n)}, \quad \mathbf{p}^{(1)} = \begin{bmatrix} 1 - 2\nu_1 & 1 - 2\nu_1 & 1 - 2\nu_1 & 1 - 2\nu_1 \end{bmatrix} \begin{bmatrix} -6\nu_1 & -7 + 4\nu_1 & 3\nu_1 & -7 - 2\nu_1 \end{bmatrix},$$

$$\mathbf{s}^{(n)} = \begin{bmatrix} -2(5 - \nu_n) & 24\bar{f}_{n-1}^{2/3} & -2\nu_n & -14\bar{f}_{n-1}^{1/3} & 14 & 14 & 14 & 14 \\ 3(1 + \nu_n) & -24\bar{f}_{n-1}^{2/3} & 7 + 2\nu_n & -21\bar{f}_{n-1}^{1/3} & 6\nu_n & 7 - 4\nu_n & -3\nu_n & 7 + 2\nu_n \\ -5 - 4\nu_n & 6\bar{f}_{n-1}^{2/3} & -4\nu_n & 14\bar{f}_{n-1}^{1/3} & 9\bar{f}_{n-1}^{5/3} & -6\bar{f}_{n-1}^{5/3} & -36\bar{f}_{n-1}^{5/3} & 24\bar{f}_{n-1}^{5/3} \\ -(3 - 6\nu_n) & -6\bar{f}_{n-1}^{2/3} & -(7 - 4\nu_n) & 21\bar{f}_{n-1}^{1/3} & 5 - 4\nu_n & 2 - 4\nu_n & -2(5 - \nu_n) & 2(1 + \nu_n) \end{bmatrix},$$

and $\bar{f}_{n-1} = \sum_{i=1}^{n-1} f_i / \sum_{i=1}^{n} f_i$, $\bar{\mu}_{n-1} = \mu_{n-1} / \mu_n$.

4. Two-step Method

In determining the effective bulk modulus $K_{\text{eff}}$ and the effective shear modulus $\mu_{\text{eff}}$ of a three-phase composite, it is possible to use a two-step procedure.

Step 1: The three-phase composite model is used for medium “1” and “2” and the effective properties $K_e$ and $\mu_e$ are determined.

Step 2: The three-phase composite model is used for the equivalent homogeneous medium of step 1 and phase “3” and the effective properties $K_{\text{eff}}$ and $\mu_{\text{eff}}$ are calculated. When $K_{\text{eff}}$ and $\mu_{\text{eff}}$ are determined by this method $K_{\text{eff}}$ is exact while $\mu_{\text{eff}}$ is not so.

A similar method was applied for composites with coated fibers by Sutcu [14].

![Fig. 5. The two-step method to calculate effective properties.](image-url)
5. Numerical Results

In this section the effective properties of a three-phase composite is determined by using the four-phase composite sphere model and the three-phase composite sphere model with the two-step method. The three-phase composite considered is concrete which can be considered as consisting of coarse aggregate, interfacial transition zone (ITZ) and mortar. The elastic constants of gravel and mortar are given in Table 1, where the data for Young’s moduli are taken from Hirsch [7] and the data for Poisson’s ratios are those assumed by Ramesh et al. [8]. The measured Young’s moduli of concrete given in Table 2 are from Hirsch [7]. Since \( E_1, \nu_1, E_3, \nu_3 \) are known, for \( E_2 = E_2/E_3 = 0.25, 0.5, 0.75, 1.0 \) and \( 0.25 \leq \nu_2 \leq 0.4 \), the effective Young’s modulus of concrete \( E_{\text{eff}} \) is calculated and plotted in Fig. 6. The measured Young’s modulus of concrete \( E_{\text{con}} \) is also plotted in Fig. 6 and if the volume fraction of ITZ is known combinations of \( (\nu_2, E_2) \) for the ITZ can be postulated. In Fig. 7 contours of \( E_{\text{eff}} \) and \( \nu_{\text{eff}} \) are plotted for \( f_1 = 0.3, \ f_2 = 0.1 \) and if the Poisson’s ratio of concrete is known it is possible to obtain \( E_2 \) and \( \nu_2 \) of the ITZ.

<table>
<thead>
<tr>
<th>Table 1 Elastic constants of constituent materials</th>
<th>Table 2 Measured Young’s moduli of concrete</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>Poisson’s ratio*</td>
</tr>
<tr>
<td>Gravel</td>
<td>( E_i = 59.6 ) (GPa)</td>
</tr>
<tr>
<td>Mortar</td>
<td>( E_i = 19.17 )</td>
</tr>
<tr>
<td>0.5</td>
<td>32.5</td>
</tr>
</tbody>
</table>

\( \nu_2 = 0.4, E_2 = 1.25 \)
\( \nu_2 = 0.1, E_2 = 1.25 \)
\( \nu_2 = 0.4, E_2 = 1.0 \)
\( \nu_2 = 0.1, E_2 = 1.0 \)
\( \nu_2 = 0.4, E_2 = 0.75 \)
\( \nu_2 = 0.1, E_2 = 0.75 \)
\( \nu_2 = 0.4, E_2 = 0.50 \)
\( \nu_2 = 0.1, E_2 = 0.50 \)
\( \nu_2 = 0.4, E_2 = 0.25 \)
\( \nu_2 = 0.1, E_2 = 0.25 \)

--- Four-phase composite sphere model, ······ Two-step method, ——— Experimental results

Fig. 6. Effective Young’s modulus of concrete \( E_{\text{eff}} \) for \( E_1 = 59.6 \) GPa, \( \nu_1 = 0.15 \), \( E_3 = 19.17 \) GPa, \( \nu_3 = 0.26 \), (a) \( f_1 = 0.3 \), (b) \( f_1 = 0.4 \) and (c) \( f_1 = 0.5 \).
In this calculation, since each phase is assumed to be homogeneous and an isotropic elastic material, Young’s modulus and Poisson’s ratio are related to the bulk modulus and shear modulus by

\[
E_i = \frac{9K_i\mu_i}{3K_i + \mu_i}, \quad \nu_i = \frac{3K_i - 2\mu_i}{2(3K_i + \mu_i)}.
\]  

(19)

It is seen from Figs. 6 and 7 that the two-step method gives results close to the four-phase sphere model results.

6. Conclusions

The effective elastic moduli of a three-phase composite are calculated by using the four-phase sphere model and by using a two-step method. The bulk modulus calculated using both methods is the same while the shear modulus is not the same. The four-phase sphere model is exact while the two-step method is an approximate scheme. However the two-step method gives sufficiently correct answers. These models are applied to concrete and by comparing with the experimental results the elastic properties of the interfacial transition zone are conjectured or if the parameters of the transition zone are known the effective properties of concrete can be predicted.

References


**Appendix: Elsheby’s Formula**

Elsheby [12] gave an expression for the strain energy $U$ stored in a composite medium subjected to a uniform field at infinity as

$$U = U_0 \pm \frac{1}{2} \int_S \left( t_i u^i_0 - t_i u_i \right) dS,$$

(A.1)

where $t_i$ and $u_i$ are the traction and displacement components of the composite medium on the surface $S$ of the inclusion, $t_i^0$ and $u_i^0$ and $U_0$ are traction and displacement components on the surface $S$ and the stored strain energy of the homogeneous medium (with no inclusion) subjected to the same uniform field. The $+$ or $-$ sign in Eq. (A.1) is used when the uniform strain field or stress field is prescribed, respectively.

The strain energy of the composite model shown in Fig. 2 is $U$ and when the inclusion and matrix are replaced by the equivalent medium the strain energy is $U_0$, therefore the energy condition to be satisfied is

$$U = U_0.$$  

(A.2)

By analyzing the boundary value problem under uniform conditions at infinity combined with the energy conditions in Eqs. (A.1) and (A.2) the effective properties may be obtained from the condition,

$$\int_{\theta=0}^{2\pi} \int_{\psi=0}^{\pi} \left[ \sigma_{RR}^0 u_R + \sigma_{R\psi}^0 u_\psi + \sigma_{\psi R}^0 u_\psi - u_\psi^0 \sigma_{RR} - u_R^0 \sigma_{R\psi} - u_\psi^0 \sigma_{\psi R} \right] R_\theta^2 \sin \psi d\psi d\theta = 0,$$  

(A.3)

where $n = 2$ or 3 for the three-phase or the four-phase sphere model, respectively.