Efficient Volume Modules of Polydispersion Composites with Spherical Inclusion

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Abstract. The formula of R. M. Christensen [14], according to the definition of the volume modulus of polydisperse composites with spherical inclusion, is transformed to the dimensionless function \( k = k (\eta, \theta, w) \) of these modules, which depends only on three dimensionless parameters. For a given value of the parameters \( \eta \) and \( \theta \), the modulus formula becomes a function of \( k = k (w) \) of one argument (volume fraction of inclusion). In a flat space \( k - w \), the function \( k = k (w) \) is mapped by a curved segment between the points \((0, 1)\) and \((1, \theta)\) of the same space. For different values of \( \eta \), the function \( k = k (w) \) displays the spectrum of curved segments between the points mentioned above. This spectrum determines the position of a plane figure in the space \( k - w \). The shape of the figure and its position (in this space) changes with other values of the parameter \( \theta \). Examples are given of constructing two similar figures for characteristic subsets of the values of the function \( k = k (\eta, \theta, w) \).

1. Introduction
At present, the role of mathematical modeling as a means of studying phenomena and processes in plastic media, solids, including concrete and other composite materials, has sharply increased [1-13]. In the scientific and technical literature, to describe the physicomechanical properties of real solids, representative volumes with a minimum volume of material, which contains a sufficient number of carriers of the considered process mechanisms, are often considered [14-22]. In the mechanics of building composite materials, the representative volume model (PO model) for a granular composite quite often takes the form of a two-phase model, in which a spherical aggregate is included in the matrix (thick-walled sphere) (Fig. 1). The material of each phase is represented by an elastic solid (continuous homogeneous and isotropic).

![Figure 1. The diametrical section of the "model ON" granular composite.](image)

Under the action of a uniform external pressure \( q \), the PO model deforms, as a result of which contact pressure \( p \) arises at the points of the interface. The equilibrium state of such an inhomogeneous...
model can be described by a collection of homogeneous models composed of 3 calculation schemes (Fig. 2).

![Figure 2. Settlement schemes of the software model represented by: A) an effective homogeneous model (solid ball); B) a model of a homogeneous matrix (hollow ball); C) a model of a homogeneous filler (solid ball).](image)

Contact pressure $p$ can be found from the condition that the radial displacements are equal at adjacent points of the matrix and aggregate (see Fig. 2, b and c). Such a problem is solved in elementary algebraic expressions, if we use, as applied to the matrix (see Fig. 2, b), the solution of the Lame problem for a thick-walled sphere \[23-32, \ 37\]. As a result, without giving the mentioned calculations, we get the expression:

$$
\frac{1}{p} = q \left( \frac{1 + 2\eta}{(1 + 2\eta)w} + 2\eta\theta V \right),
$$

(1)

Where $w$ is the volume fraction of the aggregate material, $w = a^3 / R^3$ (see Fig. 1), $V$ is the volume fraction of the matrix material, $V = 1 - w$. In addition, the notation used by the authors of \[24-26,\ 32\] is accepted in formula (1):

$$
\eta = \frac{g_m}{e_m} = \frac{1 - 2\nu_m}{1 + \nu_m} = \frac{2G_m}{3K_m}, \quad \theta = \frac{e_m}{e_i} = \frac{K_m}{K_i},
$$

(2)

$$
e_m = \frac{E_m}{1 - 2\nu_m} = 3K_m, \quad g_m = \frac{E_m}{1 + \nu_m} = 2G_m,
$$

(3)

where $E_m$ and $\nu_m$ are Young's modulus and Poisson's ratio of the matrix material; $K_m$ and $G_m$ - volumetric modulus and shear modulus of the matrix; $e_m$ and $g_m$ are the spherical bulk modulus and the deviatorial matrix shear modulus; $\eta_m$ is the ratio of the modules of the matrix; $K_i$ and $e_i$ - volumetric and spherical modules of the filler material; $\theta$ is the ratio of volumetric modules of matrix materials and aggregate.

If we now equate, taking into account (1), the radial displacements at the external points of the effective model (see Fig. 2, a) and the matrix model (see Fig. 2, b), then as a result we obtain (again without calculations) the formula for calculating the dimensionless effective module of a two-phase composite:

$$
\frac{k}{K_m} = \frac{(1 + 2\eta w) + 2\eta\theta V}{V + \theta (2\eta + w)},
$$

(4)

where $k$ is the bulk modulus of the composite ($K$), expressed in fractions of the matrix module ($K_m$). In this case, the inverse formula for calculating the effective volumetric module $K$ will take the form:

$$
K = K_m k = K_m \left( \frac{(1 + 2\eta w) + 2\eta\theta V}{V + \theta (2\eta + w)} \right).
$$

(5)
Earlier, in the work of R. M. Christensen [33], a formula was obtained similar to formula (5), which, in our notation, has the form:

$$\frac{K - K_m}{K_i - K_m} = \frac{w}{1 + (1-w)(K_i - K_m)} \cdot \frac{K_m + \frac{1}{2}G_m}{K_m} \cdot$$

(6)

In this form, Christensen, taking into account the Hashin paradigm [34], obtained a formula for calculating the volume modulus of elasticity ($K$) in poly-dispersed composites with a spherical inclusion (filler). Simple transformations of formula (6), taking into account the notation (1) - (3), lead us again to formulas (4) and (5). Therefore, formulas (4), (5) and (6) are identical to each other. The method of obtaining formula (4) by using the solution of the Lame problem is less laborious, since it requires only elementary algebraic transformations. Christensen obtained formula (6) in a more complicated way, directly using the equations of the linear theory of elasticity.

2. The calculation formulas of the effective module ($k$) of the composites

In formulas (4) - (6), the fact is fixed that the material of the models, in the calculation schemes having the shape of a ball (fig. 2, a and c), is represented by only one elastic constant (module $k$ or $k_i$), and the matrix material having the shape of a thick-walled sphere (fig. 2, b) - two constants (modules $k_m$ and $g_m$). This fact, from the point of view of elastic properties, serves as a sign of the features of determining the effective modulus $k$ inherent only in two-phase composites, in contrast to the effective modulus of other (multiphase) composites.

Studying formula (4), we note that the parameters $\eta m$ and $w$ have the same and convenient range $(0, 1)$ of their values. However, the values of the modulus $k$ and the parameter $\theta$ change in another interval $(0, \infty)$ of numbers. Therefore, the interval $(0, 1)$ small and the interval $[1, \infty)$ - large numbers. In this case, we obtain two working versions of formula (4): option 1 - for module numbers ($k_1 \geq 1$) with values $\theta = \theta_1 \leq 1$

$$k_1 = \frac{K_i}{K_m} = \frac{(1+2\eta w)+2\eta_1 V}{V + \theta_1 (2\eta + w)};$$

(7)

option 2 - for module numbers ($k_2 \leq 1$) with values $\theta = \theta_2 \geq 1$

$$k_2 = \frac{K_2}{K_m} = \frac{(1+2\eta w)+2\eta_2 V}{V + \theta_2 (2\eta + w)}.$$  

(8)

We emphasize that in formulas (7) and (8), the parameters $\theta_1$ and $\theta_2$ have an inverse relationship (with an inversion coefficient equal to unity), since their product $\theta_1 \cdot \theta_2 = 1$. This property facilitates the analysis of calculation formulas. But first we recall the hypotheses of Voigt [35] and Reis [36].

3. The flat space of values of the modules $k$

Applying the “mixture rule”, we first determine, according to [16], the effective bulk modulus ($K$) of the composite (see Fig. 1, 2). As a result, we get the “according to Voig-tu” dependence

$$K_F = K_m V + K_i w.$$  

(9)

Then, applying the same rule, we will determine, according to [17], the effective volumetric compliance ($1/K$) of the material and obtain the “Reuss” dependence

$$\frac{1}{K_R} = \frac{V}{K_m} + \frac{w}{K_i}.$$  

(10)

In contrast to formulas (4) and (6), dependences (9) and (10) do not take into account the influence of the matrix shear modulus ($G_m$). This is precisely what lies mainly in the approximation of the Voigt and Reuss estimates.
The values of the moduli $K_F$ and $K_R$, respectively, serve as a rule, as the upper and lower boundaries of the values of real moduli $K$ of the composite. However, an analysis of the Christensen solution (6) represented by formulas (4), (7) and (8) allows us to refine this rule (in the sense of the upper and lower bounds for the Voigt-Reuss plug) as applied to the two-phase structure of granular SCMs. But first, we express the $K_F$ and $K_R$ modules in fractions of the $K_m$ module (matrix) and obtain formulas for dimensionless quantities of the same modules:

$$k_F = \frac{K_F}{K_m} = V + \frac{w}{\theta}, \quad k_R = \frac{K_R}{K_m} = \frac{1}{V + \theta w}. \tag{11}$$

In relation to the calculation formulas (7) and (8), expressions (11) will take the corresponding form:

option 1 (for $\theta \leq 1$)

$$k_{F1} = (1 - w) + \frac{w}{\theta_1}, \quad k_{R1} = \frac{1}{(1 - w) + \theta_1 w}; \tag{12}$$

option 2 (for $\theta \geq 1$)

$$k_{F2} = (1 - w) + \frac{w}{\theta_2}, \quad k_{R2} = \frac{1}{(1 - w) + \theta_2 w}. \tag{13}$$

In cases where the ratio $\theta$ is unchanged ($\theta = \text{const}$), expressions (12) and (13) become functions of one argument: $k_F = k_F(w)$ and $k_R = k_R(w)$. Therefore, these functions can be represented graphically in the flat space of the $k$ and $w$ axes (Fig. 3). The visibility of such a space used in the analysis of formulas (4) - (6) is evidenced by the contents of [12].

**Figure 3.** The region of flat space $k$ - $w$ bounded by the axes $k$, $\theta$ and $w$.

The dashed line marks 2 segments of the function $k_F = k_F(\theta, w)$ for the values $\theta = \theta_1$ and $\theta = \theta_2$

$$k_{F1} = (1 - w) + \frac{w}{\theta_1}, \quad k_{F2} = (1 - w) + \frac{w}{\theta_2}. \tag{14}$$

These functions are displayed by two families of straight-line segments starting from their common point with coordinates $(0, 1)$. In Fig. 3 dashed lines show 2 such segments, one of these two families. The right ends of the selected segments have coordinates $(1, \theta_2)$ and $(1, \theta_1)$; these ends in the figure are marked with bold dots.

The functions of the modules according to Reis and Christensen (in the same region of the space $k$ - $w$) have a curved outline; their graphs are located below the Voigt segments and are directly adjacent to these segments with their ends at the points $(0, 1)$, $(1, \theta_2)$ or $(1, \theta_1)$ (see Fig. 3). For a clearer description of these functions, we consider 2 numerical examples.

**4. Comparative analysis of estimates by Voigt, Reuss and Christensen**

Let us carry out a comparative analysis of the calculation formulas (7), (8) with formulas (12) and (13) in the sense of the upper and lower bounds for the effective elastic modulus in two-phase composites. For this purpose, we distinguish two groups of composites. In the first of them, we take the ratio of the
volume moduli of the components $\theta$ equal to 0.25, i.e., less than unity; in the 2nd group — more than one ($\theta = 4$).

Given a step $\Delta w = 0.125$, we calculate the modules $k_F$ and $k_P$ using formulas (12), (13) for both the 1st and 2nd groups of composites. The calculation results are presented in table 1.

Table 1. The values of the modules according to Voigt ($k_F$) and Reuss ($k_R$) for 2 groups of composites.

| Group | Module          | Volume fraction of aggregate ($w$) |
|-------|-----------------|-----------------------------------|
|       | according to Voigt |                                    |
| 1st   | $k_F$           | 1, 1.375, 1.75, 2.125, 2.5, 2.875, 3.25, 3.625, 4 |
|       | according to Reuss |                                  |
| 2nd   | $k_F$           | 0.906, 0.813, 0.719, 0.625, 0.531, 0.438, 0.344, 0.25 |
|       | according to Voigt |                                |
|       | $k_R$           | 0.727, 0.571, 0.471, 0.4, 0.348, 0.308, 0.276, 0.25 |
|       | according to Reuss |                              |

Then, for the same 2 groups, we calculate the modules $k$ by formulas (7) and (8) for $\eta_m$ ratios equal to 1, $\frac{1}{2}$ and 0, which correspond to the Poisson's ratio $\nu_m$, equal to: 0; 0.2 and 0.5. Results - see table 2.

Table 2. The values of the modules $k$ (according to Christensen) in 2 groups composites ($\theta = 1/4$ and $\theta = 4$) for three values of the parameter $\eta_m$.

| Options | Volume fraction of aggregate ($w$) |
|---------|-----------------------------------|
| $\theta$ | $\eta_m$ | 0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, $w \to 1$ |
| 0.25    | 1 | 1, 1.2, 1.429, 1.692, 2, 2.364, 2.8, 3.333, 4 |
| 0.25    | 0.5 | 1, 1.162, 1.353, 1.581, 1.857, 2.2, 2.636, 3.211, 4 |
| 0.25    | 0 | 1, 1.103, 1.231, 1.391, 1.6, 1.882, 2.286, 2.909, 4 |
| 4       | 1 | 1, 0.88, 0.769, 0.667, 0.571, 0.483, 0.4, 0.323, 0.25 |
| 4       | 0.5 | 1, 0.86, 0.739, 0.633, 0.538, 0.455, 0.379, 0.311, 0.25 |
| 4       | 0 | 1, 0.727, 0.571, 0.471, 0.4, 0.348, 0.308, 0.276, 0.25 |

Comparing the tables, we note that the values of row 3 of the table 2 coincided with the values of line 2 in the table 1. The values of row 6 of the table 2, in turn, repeat the values of row 4 of the table 1. Therefore, the lower bound of the values of the effective modules $k$ calculated “according to Christensen” (see Table 2) exactly coincided with the estimate of the modules $k_P$ “according to Flight” (see table 1). However, the Voigt and Christensen ratings are different. This follows from comparing other rows of the same tables.

For greater clarity, consider 2 graphical examples.

Example 1. Compatible in one figure, the graphical dependencies constructed according to the table 1 and 2 for the 1st group of selected materials (Fig. 4). Moreover, all values of the effective modules lie in the range of numbers $1 < k < 4$. 
Figure 4. Dependences of the modules $k_{F1}$, $k_{R1}$ and $k_{1}$ on the volume fraction $w$.

The values of $k_{1}$ correspond to the values of $\eta$ equal to 1, $\frac{1}{2}$, and 0.

The endpoints of all curved graphs (see Fig. 4) are aligned with the endpoints of the Voigt straight-line segment. The lower graph of the module values “by Flight” gives a lower estimate of the values of effective modules of real composites. The area of flat space bounded by the upper and lower graphs gives us a visual image of the so-called Voigt – Reuss plug.

The same figure shows the dependences of the values of the modules $k_{1}$ "according to Christensen" - three curved graphs corresponding to the values of the Poisson's ratio $\nu_{m} = 0; 0.2$ and 0.5. In this case, the lower graph (with the value $\nu_{m} = 0.5$) exactly coincided with the graph of the $k_{R1}$ modules (according to Reuss). Consequently, the lower "Reuss" estimate, defined by the second of formulas (12), is also revealed as a special case of formula (7) with $\eta_{m} = 0$ (or $\nu_{m} = 0.5$, which is the same).

The Voigt estimate (upper graph) does not coincide with the upper Christensen estimate (2nd graph from above) (see Fig. 4), which, according to expression (7) for $\eta = 1$, is determined by the formula

$$\max_{\eta} k_{1} = \frac{(1 + 2w) + 20V}{V + 0_{1}(2 + w)}.$$  \hspace{1cm} (14)

The values correspond to the materials of the matrix, Poisson's ratio of which $\nu_{m} = 0$. Such materials are better than other materials (with $\nu_{m} > 0$) resist shear deformations. In other words, the smaller the coefficient $\nu_{m}$, the higher the stiffness (and strength) of the composites (if other premises are equal).

Example 2. We will do the same with the 2nd group of selected composites. The dependencies constructed in accordance with the data in Table 1 are compatible in one figure. 1 and 2, we get graphs similar to the graphs of the 1st group of materials (Fig. 5), but with modulus values $k \leq 1$.

Figure 5. Dependences of the modules $k_{F2}$, $k_{R2}$ and $k_{2}$ on the volume fraction $w$. 
The values of $k_2$ correspond to the values of the parameter $\eta = 1; \frac{1}{2}$ and 0.

The sequence in the arrangement of the graphs in Fig. 5 remains the same as in fig. 4. The main differences in the figures are that: 1) a straight line segment in Fig. 4 is shown ascending, and in Fig. 5 a similar segment - downward; 2) fig. 4 characterizes composites of the 1st group (for $\theta < 1$), Fig. 5 - composites of the 2nd group (for $\theta > 1$).

The dependences “according to Christensen” (2nd and 4th graphs in Fig. 5), defined by formula (8), for $\eta = 1$ and $\eta = 0$, take the form of functions:

$$\max k_2 = \frac{(1+2w)+20V}{V+\theta_2(2+w)},$$

$$\min k_2 = \frac{1}{V+\theta_3w}.$$  

(15)  

(16)

And thus, dependence (16), as a special case of the Cristensen formula (8), coincides with the Reiss formula (13).

5. Conclusion

Formula (6) by R.M. Christensen [14] for calculating the effective bulk modulus in polydisperse composites has been around for almost 40 years and has gained wide popularity. However, unfortunately, it is not actually used in building materials science. The above numerical studies of this formula made it possible to identify and graphically illustrate a number of its undoubted advantages.

Firstly, in the sense of upper and lower bounds for the volume moduli of real composites, this formula reveals a narrowed fork of estimates “according to Christensen” compared with the “Voigt-Reiss fork”.

Secondly, the lower bounds for Reuss (13) and for Christensen (16) coincide. This clarifies Christensen's position of the “plug” as part of the Voigt-Reuss plug.

Thirdly, the interpretations of the Christensen formula have the form of elementary algebraic functions of three dimensionless parameters ($\eta = 2G_m/3K_m$, $\theta = K_m/K_i$ and $w = a^3/R^3$). This greatly facilitates their numerical analysis and their practical use.

And finally, fourthly, the dimensionless form of representing the value of the effective modulus of the granular composite ($k = K/K_m$) allows you to build in a flat space $k$ - $w$ a system of an infinite number of graphical dependencies of the module $k$ on the quantitative content of the volume fraction of the filler. This allows in each concrete composite to determine the place of its effective module in the flat space of the modules defined by the Christensen formula. As a result, the possibility, if necessary, of strengthening (or weakening) of certain mechanical properties of the composite is clearly shown.

6. References

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