Elastic Modulus Prediction of Particle Reinforced Composites Based on Sphere Model

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Abstract. The elastic modulus calculation of particle-reinforced composites is a classic but rather complex issue. By adopting analytic method, this paper is intended to seek solutions and calculations with the help of the symbolic integral operation function of the software Mathematica to derive the analytical expressions of the elastic modulus of particle-reinforced composites. Study shows that the representative volume unit of particle-reinforced composites may be expressed with spherical model. Two calculation methods which feature “first parallel and then serial” and “first serial and then parallel” respectively deliver two slightly different elastic modulus values, and the intermediate value may be deemed as the predicted elastic modulus.

1. Introduction
The elastic modulus calculation of particle-reinforced composites is a classic issue. Earlier studies adopted relatively simple models which can be calculated with analytic methods. These studies culminated in 50s and 60s in the last century, and representative studies include the corrected mixture ratio formula of Halpain-Tsai[1], Eshelby elastic inclusion model[2,3], Mori-Tanaka mean field model[4,5], Chamis model[6], Hill-Hashin-Christensen-Lo model[7-9] and bridging model[10], etc.

This paper is intended to attempt to resolve complex and vivid models by using analytic method in order to prevent the considerable error generated by simple models adopted by analytical method and meanwhile eliminate the consumption of excessive computer resource in the case of numerical method which provides non-universal calculation results among other deficiencies.

2. Spherical model
According to the idea of statistical averaging, it is feasible to assume that the particles used as reinforcement are evenly distributed in the space and surrounded by matrix material to form a series of small cubes; taking one of these small cubes as a representative volume unit while the particle in it is a sphere. Let the side length of this representative volume unit (calculating element) is 1, the radius of the particle is \( r \), and then the volume fraction of the particle is...
So the relationship between the radius and volume fraction of particle is

\[ r = \left( \frac{3}{4\pi V_p} \right)^{1/3} \]  

(2)

3. Derivation of elastic modulus formula

Taking the center of the sphere as the origin of coordinates, establish the horizontal rightward \( x \)-axis and the vertical upward \( y \)-axis. Assuming that a horizontal force is imposed on this representative volume unit.

3.1 The “series after parallel” calculation mode

Divide the portion falling within \(-r \leq x \leq r\) (the area between two dashed lines in the Figure 1) into \( n \) equal parts vertically to get \( n \) small cuboids (micro segments) which have an uniform width of \( \Delta x \) and an uniform height of 1; the middle part of all micro segments is particle material while the upper and lower parts are matrix material; the cross section at \( o-xy \) plane is shown in Figure 1.

Figure 1. Sphere model for calculation of series after parallel

Let the abscissa of one micro segment is \( x \) and the particle material is represented by shadow (the three-dimensional image is a disc which has a thickness of \( \Delta x \)), then the volume fraction of the particle material in the micro segment (including the matrix material) is

\[ V_{ps} = \pi \left( r^2 - x^2 \right) \]  

(3)

Under the action of the horizontal force, the shaded portion is arranged in parallel with the other portions in the cuboid, so the elastic modulus of this small cuboid is

\[ E_x = V_{ps}E_p + (1 - V_{ps})E_m = \pi \left( r^2 - x^2 \right)E_p + \left( 1 - \pi r^2 + \pi x^2 \right)E_m \]

\[ = \pi \left[ \left( \frac{3}{4\pi V_p} \right)^{2/3} - x^2 \right]E_p + \left[ 1 - \pi \left( \frac{3}{4\pi V_p} \right)^{2/3} + \pi x^2 \right]E_m \]  

(4)

Where: \( E_p \) and \( E_m \) represent the elastic modulus of the particle and matrix material respectively.
Under the action of the horizontal force, all these \( n \) micro segments are arranged in series within the range of \(-r \leq x \leq r\) (the portion between dashed lines in the figure), then according to series formula the reciprocal of the elastic modulus \( E_{n} \) of this portion is

\[
\frac{1}{E_{n}} = \frac{V_{1}}{E(x_{1})} + \frac{V_{2}}{E(x_{2})} + \cdots + \frac{V_{m}}{E(x_{m})} \\
= \frac{1}{E(x_{1})} \frac{\Delta x_{1}}{2r} + \frac{1}{E(x_{2})} \frac{\Delta x_{2}}{2r} + \cdots + \frac{1}{E(x_{n})} \frac{\Delta x_{n}}{2r}
\]

(5)

Where: \( V_{i}(i=1,2,\ldots,n) \) is the volume fraction of the particle material of the \( i \)th micro segment, \( E(x_{i})(i=1,2,\ldots,n) \) is the elastic modulus of the particle of the \( i \)th micro segment, and \( \Delta x_{i}(i=1,2,\ldots,n) \) is the width (uniformly the height is 1) of the \( i \)th micro segment. When \( n \) approaches infinity, the above formula can be calculated with the integral method:

\[
\frac{1}{E_{n}} = \pi \sum_{i=1}^{n} \frac{1}{E(x_{i})} \frac{\Delta x_{i}}{2r} = \int_{-E_{n}/2r}^{E_{n}/2r} \frac{1}{E_{n}} \frac{1}{2r} \left[ \frac{3}{4\pi} V_{r}^{3/2} - x^{2} \right] dE_{n} + \pi \int_{-E_{n}/2r}^{E_{n}/2r} \left[ 1 - \frac{3}{4\pi} V_{r}^{3/2} + \pi x^{2} \right] dE_{n} = \frac{\sqrt{2\pi}}{2} \arctan \left( \frac{6\pi^{1/3} V_{r}^{1/2}}{E_{n}^{1/3} - E_{n}^{1/3}} \right)
\]

(6)

The above formula expresses the elastic modulus of all materials within the range of \(-r \leq x \leq r\) (the portion between the dashed lines in the figure), and the portion of pure matrix material on left and right side is also connected in series with it, so the reciprocal of the total elastic modulus \( E_{1} \) is

\[
\frac{1}{E_{1}} = 2r \frac{1}{E_{n}} + 1 - 2r \frac{1}{E_{n}} = \frac{4\arctan \left( \frac{6\pi^{1/3} V_{r}^{1/2}}{E_{n}^{1/3}} \right)}{\sqrt{\pi} \left( E_{n}^{1/3} - E_{n}^{1/3} \right)} \left[ 1 - \frac{6}{\pi} V_{r}^{1/3} \right]
\]

(7)

3.2 The “parallel after series” calculation mode

Similarly, we derived \( E_{2} \)

\[
E_{2} = 2rE_{n} + (1 - 2r)E_{n} = 2 \left[ \frac{3}{4\pi} V_{r}^{3/2} \right] E_{n} + \left[ 1 - 2 \left( \frac{3}{4\pi} V_{r}^{3/2} \right) \right] E_{n}
\]

\[
4E_{n}E_{r} \arctan \left( \frac{6\pi^{1/3} V_{r}^{1/2}}{E_{n}^{1/3}} \right) \left( E_{n}^{1/3} - E_{n}^{1/3} \right) = \frac{\sqrt{\pi} \left( E_{n}^{1/3} - E_{n}^{1/3} \right)}{\left[ 4 - \left( 36\pi V_{r}^{3/2} \right) E_{n} + \left( 36\pi V_{r}^{3/2} \right) E_{n}^{3} \right]^{1/2} E_{n}^{1/3}} + \left[ 1 - \frac{6}{\pi} V_{r}^{1/3} \right] E_{n}
\]

(8)

3.3 Prediction of elastic modulus
The calculations with two means - “series after parallel” and “parallel after series” deliver two different elastic modulus $E_1$ and $E_2$, and the former is larger than the latter. It is expected that the actual elastic modulus falls between $E_1$ and $E_2$, and the intermediate value may be deemed as the predicted elastic modulus value of particle-reinforced composites.

4. Conclusions

(1) The representative volume unit of particle-reinforced composites can be expressed with spherical model and sphere represents the shape of particle in a much better way than that in cube and other shapes; the problem of difficult integral computation can be solved by using symbolic computation software.

(2) Two calculation methods which feature “series after parallel” and “parallel after series” respectively deliver two slightly different elastic modulus values, and the intermediate value may be deemed as the predicted elastic modulus value of particle-reinforced composites.

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