A Comparative Study of Analytical and Numerical Evaluation of Elastic Properties of Short Fiber Composites

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Abstract: Unlike the case of continuous fiber composites, the prediction of elastic properties of short fiber composites using the corresponding elastic properties of constituents is not a straight forward task. Many authors have attempted to predict the properties using either analytical or by experimental methods or a combination of both leading to empirical solutions. The current trend is to use the well known numerical solution Finite element method (FEM) to model the short fiber composite to predict their properties. In this paper, a RVE (Representative Volume Element) approach is used to model, with appropriate boundary and loading conditions and application of homogenization process to estimate elastic properties. The present values are compared with the available experimental and analytical solutions. The methods that best match with the current FE solutions are highlighted.

1. Introduction
The advantages of traditional long fiber composites such as high strength and high stiffness are well known\cite{1}. However, one common problem with these composites is their inability to manufacture intrinsic and complicated products using simple manufacturing techniques. In addition, achieving the isotropy at lamina level is virtually impossible. Though closer to isotropy is possible at laminate level, it’s again a contrived process. As against this, plastics are very good in their mold-ability and by nature are isotropic. But the plastics are not strong enough to be used in primary structures. A relative compromise between these two ends is a short fiber composite (SFC). The SFCs are also called as discontinuous fiber composites. The SFC is a composite made usually of plastic as the matrix phase and chopped short fibers as the reinforcing phase. The length of fiber is usually shorter than few millimeters \cite{1}. An SFC is better in strength than a typical plastic and yet it retains the isotropy and mold-ability of plastic.

The SFCs can be classified into two types based on their randomness i.e. Aligned Short Fiber composites [ASFCs] and Randomly Distributed Short Fiber Composites [RDSFCs]. In ASFCs the fibers have orientations along a particular direction in the matrix (Figure 1). Usually it is not possible to perfectly align these fibers in a particular direction, but a majority of them can at least be made to orient in a particular direction. Hence these are also known as preferentially oriented short fiber composites. These aligned fibers are usually transversely isotropic requiring at least 5 independent elastic constants are need to define them.

The RDSFCs on the other hand have fibers randomly distributed in all possible directions. Further, the randomness of short fiber composites is of two types i.e. 3D Randomness and 2D Randomness \cite{2}. The first type consists of short fibers distributed completely random in three dimensional spaces, usually in an isotropic polymer matrix. This means every orientation in the matrix has an equal chance
of having a fiber along it. This type of randomness (or at least randomness close to it) is observed in the products manufactured using injection molding machines. In the second type, the fibers are distributed randomly in a plane, meaning every direction in the plane has an equal probability of having a fiber along it. This type of randomness is observed in RDSFC specimens made by Hand-layup process. In such specimens, even though out of plane fibers do exist, the angle is usually very small [3].

In both the types, the matrix is normally isotropic in nature. But, the fibers can be isotropic as well as transversely isotropic, though the former is quite common. For example, Glass fibers are isotropic while carbon fibers are transversely isotropic.

2. Prediction of Mechanical properties of SFCs

Estimation of mechanical properties of SFC’s is not a straight forward task, because the properties of SFC’s are controlled by various parameters. For example, the stiffness and strength of SFC’s depend, inter alia, on [1] Properties of the constituent materials (fibers, matrix, binder, filler etc.), Relative proportions of each constituents (i.e. Volume Fractions), Orientations of the fibers, Aspect ratios of the fibers (l/d ratios), and Interaction between fiber and matrix.

Owing to these numerous factors involved in the determination of the stiffness and strength properties, physical testing of the SFC component is not always economical. Besides, the test data can easily become invalid if any of the governing parameters change. Hence, attempts have been made to predict the properties of SFCs analytically and numerically by using the properties of fibers, matrix and their relative proportions.

2.1. Analytical Methods

Researchers have approached the problem of prediction for properties of composite materials from various angles. A set of approaches known as Bounding value methods predict the bounds (maximum and minimum values) of elastic properties sought rather than the value itself[4-8]. Here the idea is, if the bounds are close enough, then bounds themselves are the solutions. The Self-Consistent methods [9-14] use the traditional elastic solution of an elliptical inclusion in an infinite media. Self-consistency here means the orientation average of the inclusion stress or strain is made equal to overall stress or strain. The popular Halpin-Tsai equations come under what are known as Semi-Empirical Methods [15-18]. In these methods, part of the solution is derived from theoretical work and other part from experimental works.

2.2. Numerical Methods to Predict the Elastic properties

With the advent of sophisticated Finite Element software, researchers are focusing their attention on FEM approaches in predicting the properties of SFCs. Owing to its numerical nature, FE methods can also be used to conduct parametric studies. Bohm [19] made FEM analysis of Spherical particles in a matrix and compared those with Hashin’s [6] Bounds and found a close agreement. Well-documented
results on FE based methods can be found in Gusev [20]. Recently in a well cited article Kari et. al. [21] have, made extensive study on the RDSFCs and transversely distributed composite materials. This was followed by Yi Pan [3] where various aspects of modeling an RVE were explored. But, when it comes to modeling of RDSFCs no final word is said yet, still a lot many numerical experiments are being carried out to simulate the behavior as close as possible to reality. Thus, owing to a large number of variables that control the behaviors of RDSFCs, a lot more needs to be done.

3. Methodology of Modelling

Two major approaches were attempted in this work. The first one was Analytical method where properties of the composite were predicted using some analytical equations. In the second method, Numerical modeling using commercial Finite Element codes was tried. Three elastic parameters studies were Young’s Modulus (E), Poisson’s Ratio (ν) and Shear Modulus (G). Though not attempted in the resent work, the other properties which are equality important for any structure design are σs, Ks, and αs. The details of the methods used in the current work are given below

3.1. Analytical methods

In the analytical method, three different equations available in literature were chosen to compare the results of the present work. The choice of these equations was based on the relevance of the model to our work. For analytical methods, wherever an explicit equation for shear modulus was not available it was obtained from usual isotropic relation E = 2G(1+ν).

3.1.1 Christensen Model [2]

In this model the properties of aligned SFRCs are used in predicting the properties of Random distributed short fibers. The aligned short fiber composites can be considered to be transversely isotropic and hence have five independent elastic constants. Christensen used these 5 independent constants already available in the literature and calculated

\[
E_{3D} = \left[ E_{11} + \left( 4\nu_1^2 + 8\nu_1 + 4 \right) K_{23} \right] \left[ E_{11} + \left( 4\nu_1^2 - 4\nu_1 + 1 \right) K_{23} + 6 \left( \mu_{12} + \mu_{23} \right) \right] \\
3 \left[ 2E_{11} + \left( 8\nu_1^2 + 12\nu_1 + 7 \right) K_{23} + 2 \left( \mu_{12} + \mu_{23} \right) \right]
\]

(1)

\[
\nu_{3D} = \frac{E_{11} + \left( 4\nu_1^2 + 16\nu_1 + 6 \right) K_{23} - 4 \left( \mu_{12} + \mu_{23} \right)}{4E_{11} + \left( 16\nu_1^2 + 24\nu_1 + 14 \right) K_{23} + 4 \left( \mu_{12} + \mu_{23} \right)}
\]

(2)

Here, \( K_{23} \) is Plain Strain Bulk modulus, \( \mu_{ij} \) is Shear modulus in ij plane, \( E_{11} \) is Young’s modulus in direction 1, and \( \nu_{12} = \nu_1 \) is major Poisson’s ratio.

3.1.2 Manera’s Approach [22]

Manera used the Puck’s equation and made some benign simplifications and assumptions which led to simple utility functions for the prediction of Elastic properties of glass fiber composites. In addition, Manera also conducted tests on the glass fiber specimens and found out the utility value of those equations. The equations are
\[
\overline{E} = V_f \left( \frac{16}{45} E_f + 2E_m \right) + \frac{8}{9} E_m
\]  
(3)

\[
\overline{G} = V_f \left( \frac{2}{15} E_f + \frac{3}{4} E_m \right) + \frac{1}{3} E_m
\]  
(4)

\[
\nu = \frac{1}{3}
\]  
(5)

\[
\overline{G} = \frac{\overline{E}}{2(1+\nu)}
\]  
(6)

Where, \( V_f \) = Fiber volume fraction, \( E_f \), \( E_m \) are the Young’s Moduli of fiber and matrix respectively.

### 3.1.3 Pan’s Modified Rule of Mixture [23]

Pan showed that the fact in aligned FRP’s: ‘the volume fraction is same as area fraction’, cannot be applied by default in RDSFCs. Pan suggested a relation between \( A_f \) and \( V_f \) and obtained the final relation as

\[
E^{3D}_c = E_f \frac{V_f}{2\pi} + E_m (1 - \frac{V_f}{2\pi})
\]  
(7)

\[
\nu^{3D}_c = \nu_f \frac{V_f}{2\pi} + \nu_m (1 - \frac{V_f}{2\pi})
\]  
(8)

Where, \( V_f \) = Fiber volume fraction,

\( E_f \), \( E_m \) are the Young’s Moduli of fiber and matrix respectively.

\( \nu_f \), \( \nu_m \) are Poisson’s Ratios of fiber and matrix respectively.

### 3.2. Numerical Modeling and Analysis

The numerical modeling involved series of MATLAB [24] programs and Python [25] scripts that interact with Abaqus [26]. The following major steps are involved.

#### 3.2.1 Generation of RVE

An RVE is a sample part of the composite whose properties are expected to be same as that of composites as a whole. For this expectation to be valid, the RVE must be big enough to accommodate sufficiently large number of constituents. In addition, it should also have orientation of fibers which also is representative of orientation seen in the composite.

In the present work the generation of RVE was done using the Modified Random Sequential Algorithm [27]. The orientations of fibers to be placed in the RVE are generated using the MATLAB software, owing its crisp and intuitive vector operational capabilities. Typical RVEs generated for three volume fractions are shown in figure 2.
Figure 2. RVEs at various volume fractions (2a) $V_f = 2\%$, (2b) $V_f = 6\%$ and (2c) $V_f = 10\%$

3.2.2 Importing the RVE into commercial FE software for analysis
The automation of modeling and meshing in Abaqus is achieved via its scripting language which is based on open source programming language Python. In the present case, the fiber orientations are generated in MATLAB and rest of the modeling was done using this scripting language. The script used could accommodate variation of fiber length, aspect ratio, the minimum gap between fibers etc. The script could call the Abaqus and have the problem solved.

3.2.3 Homogenization Scheme
The RVE so generated is subjected to homogeneous load and displacement boundary conditions [28]. In applying homogenization scheme, the following volume averaging techniques are used. When homogeneous boundary conditions are applied to the RVE, average stress and average strains are defined by

$$\overline{\sigma}_{ij} = \frac{1}{V} \int_{V} \sigma_{ij} dV \quad \overline{\epsilon}_{ij} = \frac{1}{V} \int_{V} \epsilon_{ij} dV$$

Homogeneous boundary conditions applied on the surface of a homogeneous body that will produce a homogeneous field [28]. The equation for the homogeneous boundary conditions are given by

$$u_i(S) = \epsilon^0_{ij} x_j$$

where $\epsilon^0_{ij}$ are constant strains.

As far as the load is concerned, a uniform pressure scheme is applied. The pressure is applied in three faces in each of the three perpendicular directions.

3.2.4 Post Processing
In addition, another script is written exclusively for the post processing. The script could open the binary results file of Abaqus (i.e. *.odb file) generated by the analysis of previous steps and calculate the average values stress and strain and elastic moduli in each direction. A typical displacement plot is shown in Figure 2(b). The computed values are written in a text file which is used for post processing and plotting using Matlab.

4. Results and discussions
Most of the work in the field of short fiber composite is directed towards the 2D Randomly Distributed Short Fiber Composites (RDSFCs). However, the literature in the 3D RDSFCs is rapidly growing. In
this work an attempt is made to analyze the 3D RDSFCs using FEM. It is well known that the 3D 
RDSFCs are isotropic in nature and hence only two elastic constants are sufficient to describe its 
complete elastic behavior. This work is therefore restricted to analysis and to estimate three important 
elastic properties namely Young’s modulus, Shear modulus and Poisson’s ratio. Before estimating the 
esthetic properties of RDSFCs the isotropic nature of the model is to be verified, the same is discussed 
below.

4.1. Isotropic Material
As 3D RDSFCs are isotropic in nature, the properties are independent of the direction of measurement. 
To verify this from the generated RVE model, young’s moduli is measured in three perpendicular 
directions. In Abaqus, three cases were analyzed as separate steps and in each step appropriate 
boundary conditions are used. The resulting local stresses are then homogenized as per the equation 
(9). Table. I gives the results obtained for three volume fractions 1%, 7% and 14%, respectively. As 
can be seen from the table, the variation of E among all the three directions is less than 2% validating 
the isotropic nature of RVE model.

| Fiber Volume Fraction | E1 (in GPa) in direction 1 | E2 (in GPa) in direction 2 | E3 (in GPa) in direction 3 | %Variation from Mean |
|-----------------------|-----------------------------|-----------------------------|-----------------------------|----------------------|
| 1%                    | 2.3398                      | 2.3406                      | 2.3603                      | 0.5715               |
| 7%                    | 2.8639                      | 2.8947                      | 2.8422                      | -0.8629              |
| 14%                   | 3.6549                      | 3.6599                      | 3.5538                      | -1.9075              |

4.2. Elastic Modulus
The properties of the fiber and the matrix used are given the Table 2

| Constituents | E, GPa | ν  |
|--------------|--------|----|
| Reinforcement| 73     | 0.25|
| Matrix       | 2.25   | 0.4 |

Young’s modulus and Poisson’s ratios were directly computed using the homogenization technique, 
whereas the shear modulus was derived using isotropic relation $E = 2G(1+\nu)$.

In this work, fourteen RVEs with fiber volume fraction varying from 1 to 14% are generated. For 
each of these RVEs, three analytical methods mentioned earlier and the present FE method are used to 
compute the elastic properties. The results of the computed Young’s modulus are plotted in Figure 3. 
Similarly plots for G and $\nu$ are shown in the Figures 4 and 5 respectively.

The results indicate that at lower volume fractions all the four methods show closer values. As the 
volume fraction increases, the Manera and Christensen equations tend to give higher values of elastic 
modulus. The Pan’s equation and the FE method predict consistently similar values over the range of 
volume fraction. Similar trend can be observed even in the case of Shear modulus. However, for the 
case of Poisson’s ratio, The Pan’s and Manera’s predictions show mostly constant values while the FE 
method and Christensen’s predictions show a decreasing trend with the increase in the fiber volume 
fraction.
**Figure 3.** Variation of Young’s Modulus with Volume fraction

**Figure 4.** Variation of Shear Modulus with Volume fraction
5. Conclusions
In the present work a comparative study of analytical and numerical methods for the predictions of the elastic properties of 3D RDSFCs is conducted. The results show that E values estimated by RVE approach are accurate and simulate the isotropic behavior well. As expected E and G values increase with increasing volume fraction is well demonstrated by all the four methods. However, the variation in $\nu$ with volume fraction is almost constant. This can be attributed to the fact that addition of fiber in all three directions is nullifying the possible increase or decrease in the Poisson’s ratio.

The FE results are much closer to the Pan’s Model than other two models. For this reason, in 3D RDSFCs, the estimation of elastic properties by Pan’s model is computationally less expensive than FE estimations. It appears that, whenever a quick and yet fair estimation of elastic properties can be computed by Pan’s equations similar to “Rule of Mixtures” for 3D RDSFCs. However, efforts are on to extended FE analysis over large range of volume fraction to conclusively estimate the same.

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