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A New Develop Model for Predict Micro Mechanical Properties of Composite Materials

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Abstract: Different analytical and numerical models are often used to predict the elastic properties of composite materials. However, accurate predictions and quick elasticity of composite materials in micro-scale is still more of challenging. In this study, the application of different analytical models such as: Rule of Mixture, Halphin-Tsai, Chamis are presented to predict the mechanical properties of composite materials. Then, finite element analysis (FEA) is used to verify the results obtained through Square RVE and hexagonal RVE models. This study focuses on evaluating the elastic properties of composite materials with the polymer background reinforced by the fiber distributed cyclically in a certain direction at a different volume fraction of fiber. We proceed to predict the mechanical properties of materials with a volume fraction of fiber from 10% to 70% using a microscale approach. In addition, this combination also provides a convenient platform for optimizing material design and composite geometry with different algorithms to solve a variety of problems in predicting the complex mechanical properties of composite materials. Finally, a computational software was developed to quick predict and efficient the mechanical properties of this complex materials. Compared with other studies, this study shows the possibility of high application in order to predict more accurate for composite complex materials.

Keywords: RVE, Composite Structure, Micro-scale RVE, Predict Mechanical Properties

1. Introduction

Composite materials have been widely developed and used in many fields in the past several decades. Composite materials with fibers reinforced are being utilized and widely developed in many technical fields from aerospace, marine until medical applications [1]. Lightweight, low abrasion, high hardness and durability, easy to be recycled or treated...are benefits compared with traditional materials. Therefore, the researchers and the industries have been showing great attention to the composites in recent years. By performing experimental analysis of scholars have been able to understand the effective mechanical properties of durability and other important properties of the composite materials [2, 3].

Nowadays, the researchers are trying to estimates the mechanical performance of composites material by various mathematical and numerical analysis. In order to reduce computational cost as well as time-consuming testing, then numerical and theoretical analysis are preferred to use [4]. This is a simple and useful method to behavior micro-scale mechanical properties of composite materials. The most famous, utilized and effective to predict the mechanical properties of composite are: Rule of Mixtures (ROM), Halphin-Tsai, Chamis' models [5, 6].

In this study, the mechanical properties of composite are characterized by using FEA, experimental and analytical analysis models mentioned above [4, 7]. From the analysis results, a comparison graph has been made to verify the predictive model which are in good agreement with experiment values.

Rafic Younes et. al. is compared the results obtained from mechanical theory analysis with experimental results for synthetic fiber reinforced composites [6]. Pal and Haseebuddin are predicted the effective elasticity of FRP by using analytical methods [7]. Balaco de Morais is applied micromechanical equation to predict the mechanical properties of continuously FRP composites [8]. Theocaris et al. has applied numerical homogenization for predicted effective transverse elastic modulus for FRP composites [9]. Sun and Vaidy applied FEA to estimate the mechanical properties of unidirectional composite material by established Representative Volume Element (RVE) [4]. Teng conducted FEA to predict the mechanical properties of composite materials through a unit cell [10].

In this study, different popular analysis models has been compared to provide an efficient analysis models for each micro-scale REV design of composite. At the same time, the numerical modeling approach using python programming language in computing environment Abaqus is also suggested. FEA results are compared with the results obtained from the analysis of popular models and the results obtained from experiments is conducted by other authors [4, 11, 12]. The results indicate that the FEA method is excellent agreement. Finally, a prediction software is developed based on the results obtained from the FEA.

2. Finite Element Approach

Two different types of RVE models, square RVE and hexagonal RVE models has been developed based on the periodic fibers distribution in the matrix. These numerical models are popular models can be used to predict the efficiency of composite materials. FE models using the Python programming language was implemented in Abaqus software are shown in Figure 1.

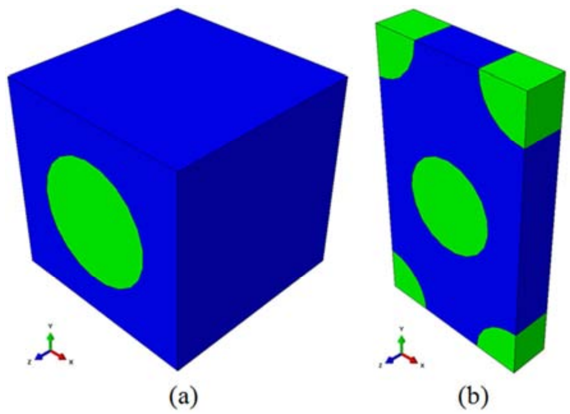


Figure 1. *Numerical models (a) Square RVE model; (b) Hexagonal RVE model.*

Composite is considered to be ideal without pores and other abnormalities, all fibers are evenly distributed in the matrix. Fiber is distributed straightly in certain direction.

2.1. Finite Element RVE Model

The RVE is considered analysis with the same elastic constants and volume fraction of fiber as in the composites. Micro-scale RVE analysis models that are often used arranged in the square or hexagonal packing. The theoretical volume fraction of fiber distributed in the RVE depends on the type of RVE model. For square RVE array as shown in figure 1(a), the fiber distribution can be maximized 78.54% and hexagonal RVE array as shown in figure 1(b) can be maximized approximately as 90%. From that, the hexagonal packing geometry models of the composite structure can be arranged with thicker reinforced fiber than the square packing geometry.

2.2. Periodic Boundary Conditions

The multi-point constraints are applied on the nodes in the X, Y, Z directions to simulate 3D RVE composite materials. The load is applied to the face needed to obtain a uniaxial stress state. The simple Hooke's law is applied to predict the mechanical properties of composite materials.

The homogeneous method by numerical method, periodic boundary conditions are an necessary and important step.

When analyzing RVE, periodic boundary conditions must be applied to the RVE for accurate analysis of deformation and stress. Finite element method based on displacement theory is used in this analysis.

Composite materials can be represented in the form of multiple RVE arranged cyclically together called RVEs. Each RVE in the mixture has the same deformation and there is no isolation or overlap between the adjacent RVE after being deformed [13, 14]. After applying boundary conditions and displacement constants.

The corresponding technical constants are calculated as follows in the form of the respective stresses and deformations shown as:

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV \quad (1)$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \quad (2)$$

2.3. Meshing

Structural mesh of (C3D8R) type is used to divide the mesh for both types of RVE models surveyed. Mesh of RVE is obtained by using Abaqus software. The selection of meshing density is extremely important. It determines the accuracy of the predicted results as well as the calculation time.

In this study, the meshing as well as analysis is done through the Python programming language. Python scripts allow creating and modifying shapes, changing mesh sizes as well as the properties of RVE models before putting in Abaqus. The analysis process is performed automatically by Abaqus as well as read the output databases. This work is done very simply by running scripts. In addition, the python code are also allowed to automatically repeat the analysis process according to optimization requirements. This has important implications in performing optimization using optimal algorithms.

3. Analytical Analysis

The different analytical models as Rule of Mixtures (ROM), Halphin-Tsai and Chamis' models are used. The analysis results are compared with the results obtained from FEA and experimental results from other researchers. All models surveyed analysis are widely used to predict the elastic properties of composite materials.

In this study, analytical models have been developed into an application software. At the same time, this study used the optimal approrach to predict through data obtained from FEA. This predictive result can be allows to build the most accurate prediction formula compared to experiment. The interface software is shown in figure 2. Results obtained from different analytical models are compared with the value obtained from the FEA and other researchers. Therefor, which help designers choose reasonable RVE type of fiber distribution in matrix to obtain the optimal values of mechanical properties of composite materials.

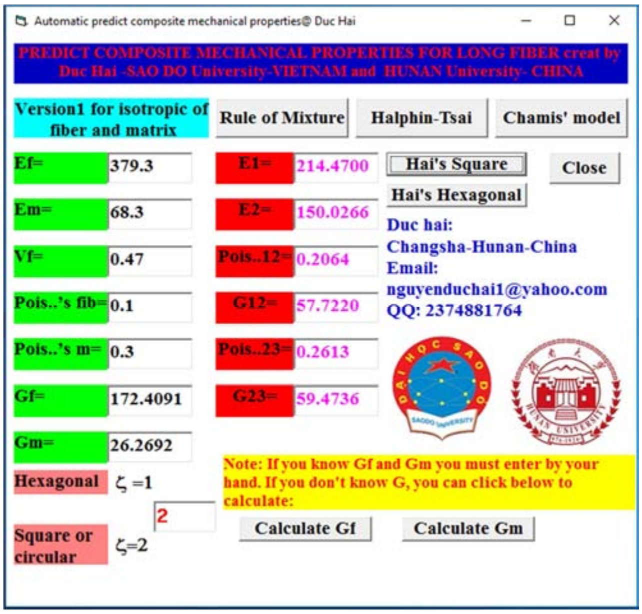


Figure 2. *The interface software software used for analytical micro-scale composite materials.*

4. Numerical Examples

In this section, the considered composite materials reinforced by unidirectional fiber form embedded in the matrix. Fiber and matrix are considered homogeneous and isotropic. There are many instances in composite where fibers are arranged randomly. Therefore, there are many difficulties in modeling, as well as analysis of mechanical behavior of this materials. In this study, composite materials with circular cross-sections are arranged in square RVE or hexagonal RVE and the periodic distribution in a unidirectional is considered. Conducting a survey to change volume fraction of fiber from 10% to 80%. Elastic properties are predicted by python code embedded in environment computing Abaqus.

4.1. The Homogenization Theory

The homogenization theory is the basic of composite material mechanics. In micro-scale, all materials are heterogeneous, in this section the homogenization of composite materials to culture aimed predict its mechanical properties is performed on RVE.

Drugan and willis [15] have shown that the minimum RVE size must is at least double the fiber diameter. With this RVE size, the maximum error is 5% in the elastic constants obtained.

In order to understand the mechanical behavior of composite, can reduce the computation time on the whole structure of material. Therefor, the micro-scale RVE analysis method is suggested. However, it requires appropriate boundary conditions so that RVE can be analyzed as a component of the material rather than an separate independent structure. That is why the periodic boundary conditions for RVE is very important. In order to solve the problem for this type of material, firstly must find the relationship between stress and strain. The relaxation stiffness matrix in the engineering is expressed through the stress and strain relationship according to Hooke's law given in Eq. (3):

$$\begin{Bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{Bmatrix}=\begin{bmatrix}C_{11}&C_{12}&C_{12}&0&0&0\\C_{12}&C_{22}&C_{23}&0&0&0\\C_{12}&C_{23}&C_{22}&0&0&0\\0&0&0&\frac{C_{22}-C_{23}}{2}&0&0\\0&0&0&0&C_{66}&0\\0&0&0&0&0&C_{66}\end{bmatrix}\begin{Bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\end{Bmatrix} \quad (3)$$

When the components of stiffness tensor are known in the directions, the mechanical properties homogeneous materials can be written as:

$$E_1 = C_{11} - \frac{2C_{12}^2}{C_{22}+C_{23}} \quad (4)$$

$$E_2 = \frac{[C_{11}(C_{22}+C_{23})-2C_{12}^2](C_{22}-C_{23})}{C_{12}C_{22}-C_{12}^2} \quad (5)$$

$$\nu_{12} = \frac{C_{12}}{C_{22}+C_{23}} \quad (6)$$

$$\nu_{23} = \frac{C_{11}C_{23}-C_{12}^2}{C_{11}C_{22}+C_{12}^2} \quad (7)$$

$$G_{23} = C_{44} = \frac{1}{2}(C_{22}-C_{23}) = \frac{E_2}{2(1+\nu_{23})} \quad (8)$$

$$G_{12} = C_{66} \quad (9)$$

4.2. Square RVE

In this section, the properties of the constituent materials are shown in table 1. The properties of the raw materials obtained from the previously published publications [4, 12, 16-18]. The distribution image of the unidirectional fiber is shown in figure 3. The volume fraction packaging is considered to be calculated at 47%, their major axes of the fiber are parallel to the Z axis direction of RVE.

Table 1. *Mechanical properties of the constituent materials boron/aluminum [4, 12].*

Properties	Fiber	Matrix
Young's modulus E (GPa)	379.3	68.3
Poisson's ratio ν	0.1	0.3

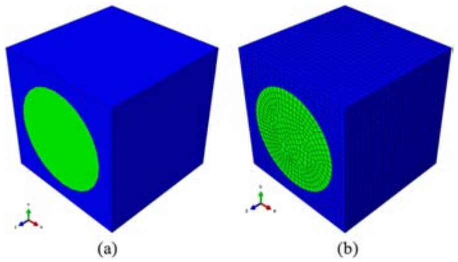


Figure 3. *Micro-scale Square RVE: (a) Square RVE arrangement; (b) Meshed RVE model.*

The relationship between the diameter of d_f and the volume fraction fiber V_f is defined as:

$$V_f = \frac{a_1(\pi/4)d_f^2}{a_1 a_2 a_3} \tag{10}$$

Simulation results are shown in table 2, the properties of micro-scale RVE mechanical behavior is consistent with the results analysed by the other author and figure 4 show the results obtained of stress and strain square packing RVE.

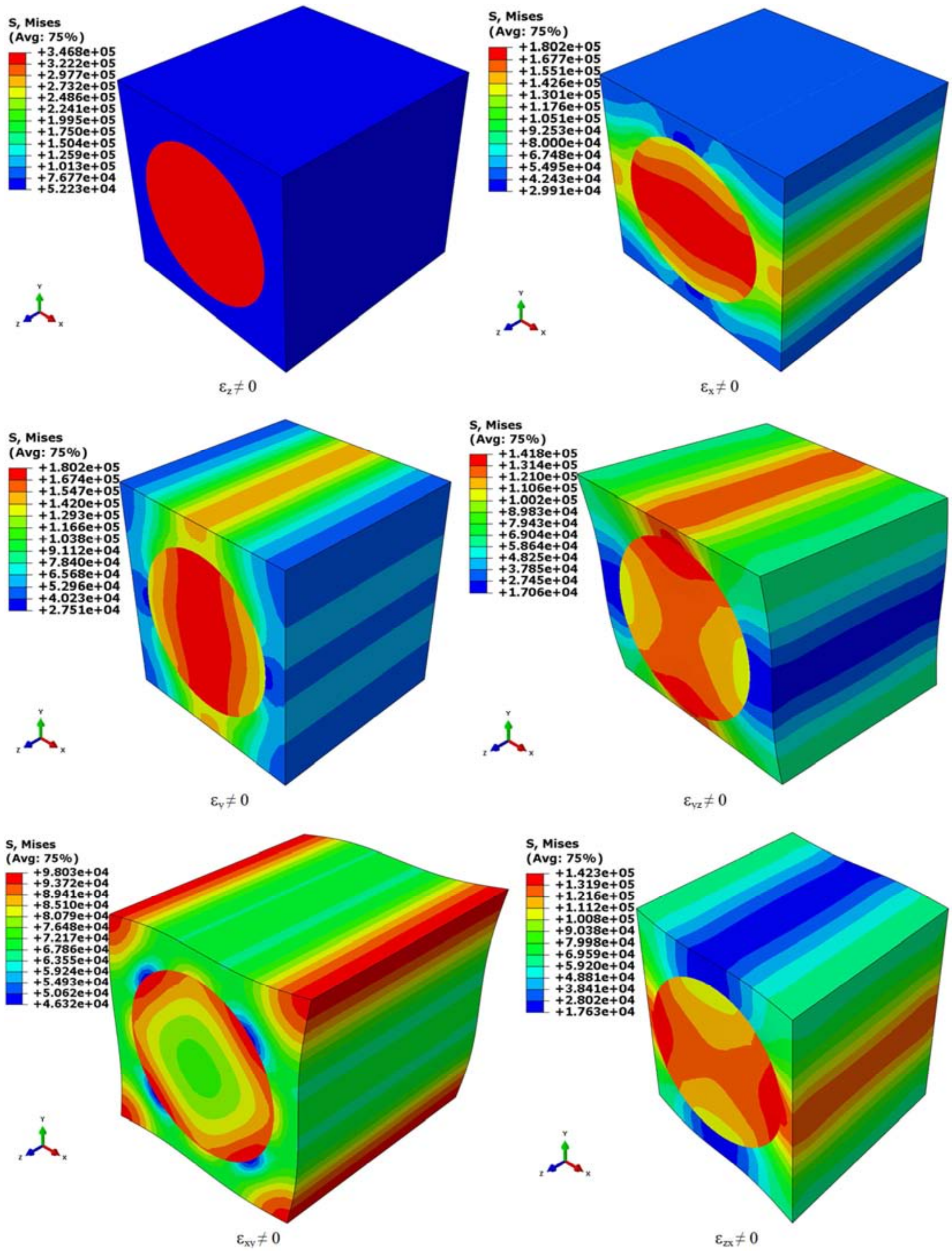


Figure 4. *The counter of stress in square micro-scale RVE.*

Table 2. *Results and comparison for unidirectional boron/aluminum (V_f=0.47).*

Material parameter	My predict	FEA	Fan Ye	C. T. Sun & J. L. Chen [17]	Hashin & Rosen [2]	M. B. Riley & J. M. Whitney [16]
E_1	214.4700	214.812	213	214	215	215
E_2=E_3	150.0266	144.081	143	156	135.2	123
G_{12}	57.7220	54.223	53.8	62.6	53.9	53.9
G_{23}	59.4736	57.469	45.4	43.6	52.3	-
ν_{12}	0.2064	0.1947	0.194	0.2	0.195	0.19
ν_{23}	0.2613	0.2535	0.256	0.31	0.295	-

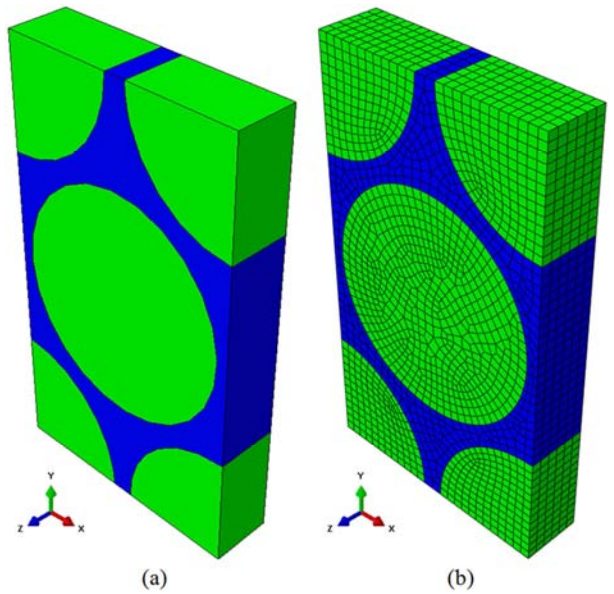


Figure 5. *Micro-scale hexagonally RVE: (a) Hexagonal RVE arrangement; (b) Meshed RVE model.*

4.3. Hexagonal RVE

In this section, the model considered analysis is the hexagonal RVE packaging model shown in figure 5(a) and meshed as shown in Figure 5(b). The volume fraction of fiber packing V_f is 75.2%. The mechanical properties of the constituent materials are quoted from the literature [11, 18] are shown in table 3:

Table 3. *Mechanical properties of the constituent materials Carbon T300/epoxy [11].*

Properties	Fiber	Matrix
Young's modulus E (GPa)	230	3.12
Poisson's ratio ν	0.26	0.38

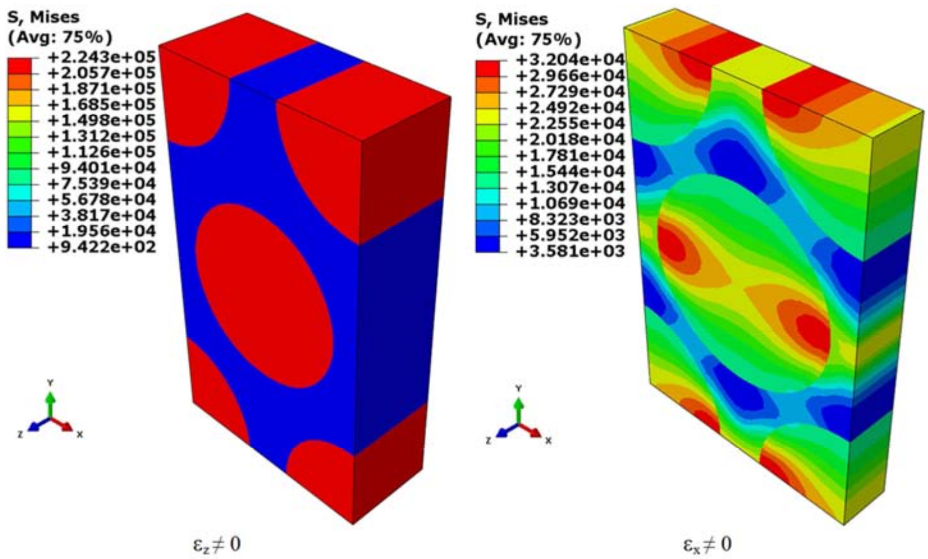
The relationship between the diameter of d_f and the volume fraction fiber V_f is defined as:

$$V_f = \frac{2a_1(\pi/4)d_f^2}{a_1a_2a_3} \tag{11}$$

Simulation results are shown in table 4, the properties of micro-scale RVE mechanical behavior is consistent with the results analysed by the other author and figure 6 show the results obtained of stress and strain square packing RVE.

Table 4. *Results and comparison for unidirectional Carbon T300/epoxy (V_f=0.752).*

Material parameter	My predict	FEA	Sheng and Hoa (2001) [11, 18]
E_1	173.7338	173.889	173.864
E_2=E_3	23.4204	24.432	22.135
G_{12}	7.3393	7.437	8.611
G_{23}	8.0878	8.758	7.796
ν_{12}	0.2833	0.2845	0.278
ν_{23}	0.4479	0.3947	0.42



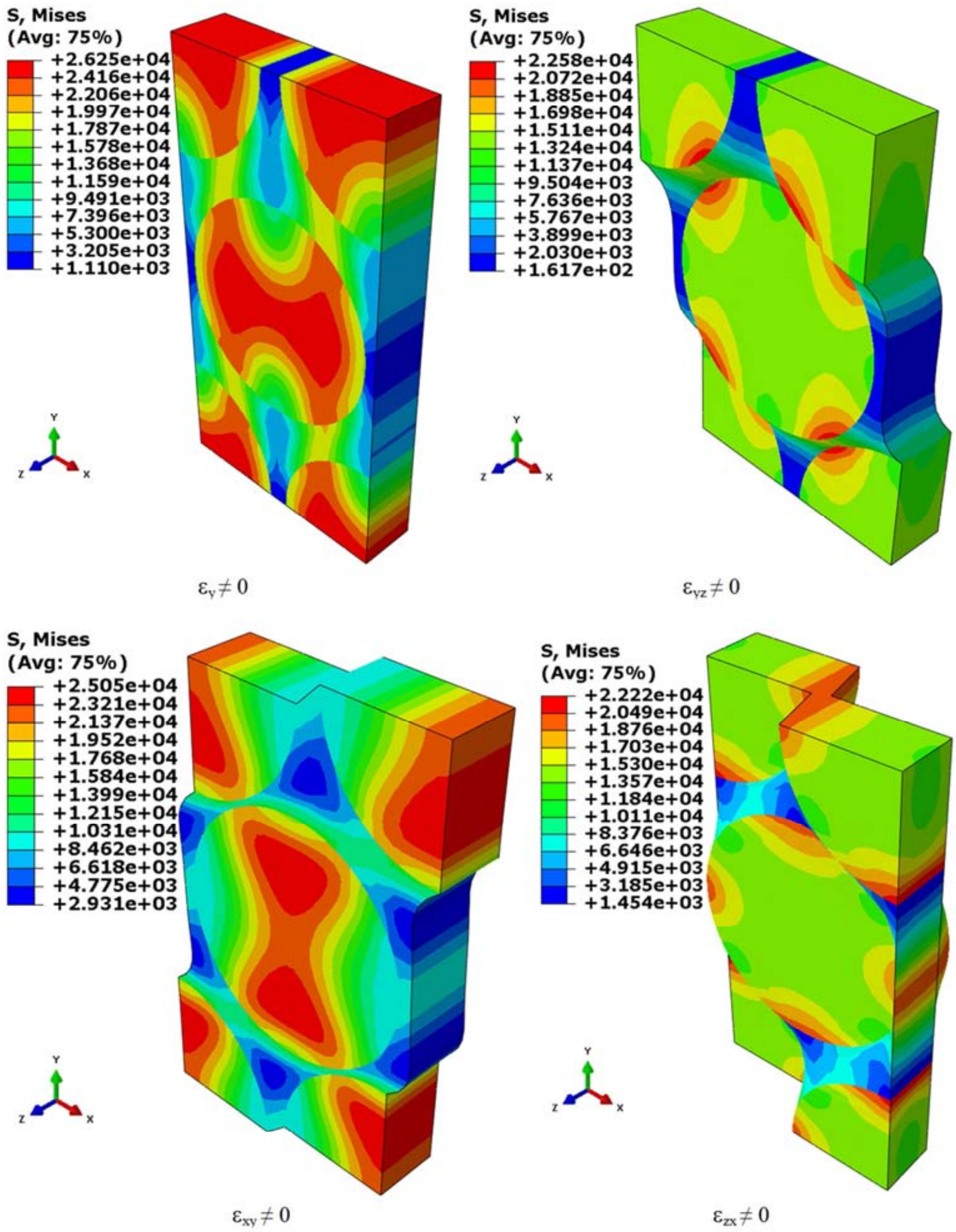


Figure 6. *The counter of stress in hexagonal micro-scale RVE.*

5. Results and Discussion

The longitudinal elastic modulus is the reaction of the composite materials in the case of applying the load parallel to the fiber direction. Figure 7(a) shows the effect of volume fraction of reinforecement fiber on the vertical module of composite materials using Rule of Mixture, Halphin-Tsai, Chamis' models and FEA combined python programming code with square RVE and hexagonal RVE.

From the comparison results, it can be observed that the vertical module gradually increases with the increase of V_f and from the graph that there is a good agreement between the results achieved by the methods. This is because the stiffness of the composite increases in parallel with an increase of V_f. Transverse elastic modulus is the yield stress of the composite materials during placement of the load perpendicular to the direction of the reinforcement fiber. The effect of V_f on the transverse module of RVE using these methods surveyed are illustrated in the graph in figure 7(b).

A great challenge for researchers to predict transverse Young's modulus E_2. Therefore, many analytical models using different micro-scale approaches has been developed. Additionally, the FEM is also studied to provide an accurate and effective prediction method for this complex materials.

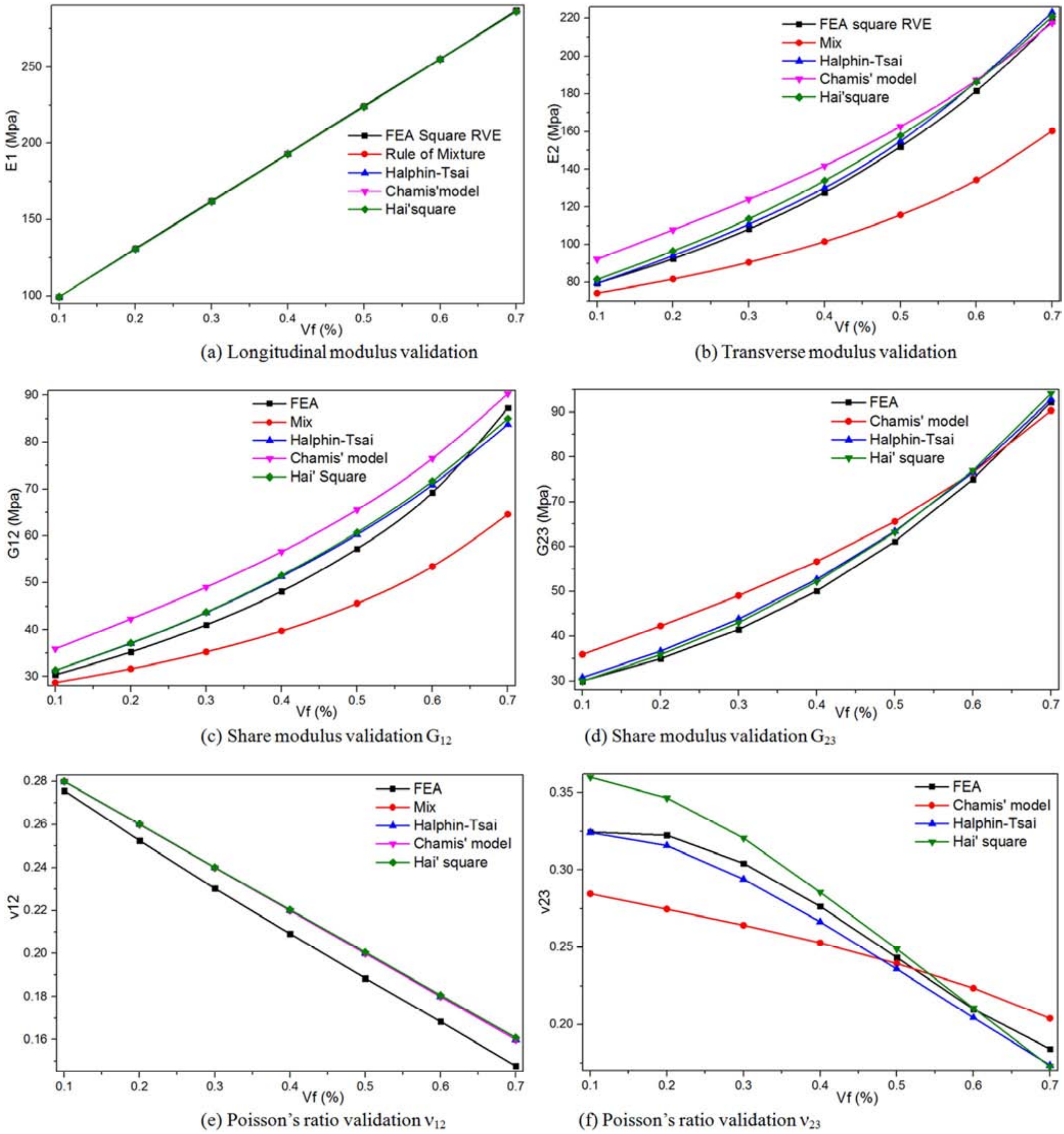


Figure 7. *Results of square RVE using FEA with other model.*

From the graph clear that, the transverse elastic modulus increased with the increase in V_f. Transverse elastic modulus is predicted by FEA with hexagonal RVE for results good agrrement than square RVE analysis. Figure 8 shows the effect of V_f on the poisson ratio of composite materials. From the graph, it is clear that poisson's ratio decreases with the increase of V_f.

Figure 8(c) shows the effect of V_f on the composite shear modulus G_{12}. It is clear from the models that the shear modulus increases with the increase of V_f. The numerical approarch yielded very good results when compared with the experiment results is performed by Luciano and Barbero [11, 12].

From the above graphs, we can also see that there is a good agreement between the results obtained from the analysis method using Abaqus scripts with the previous analysis models including Rule of Mixture Model, Halpin-Tsai Model, Chamis' model.

For transverse shear modulus G_{23}, comparisons are made between the results of the FEA approarch and the analytical models. Chamis' model yield the good results compared with numerical results. The results from the analytical models and FEA are compared and are shown in figure 8(d).

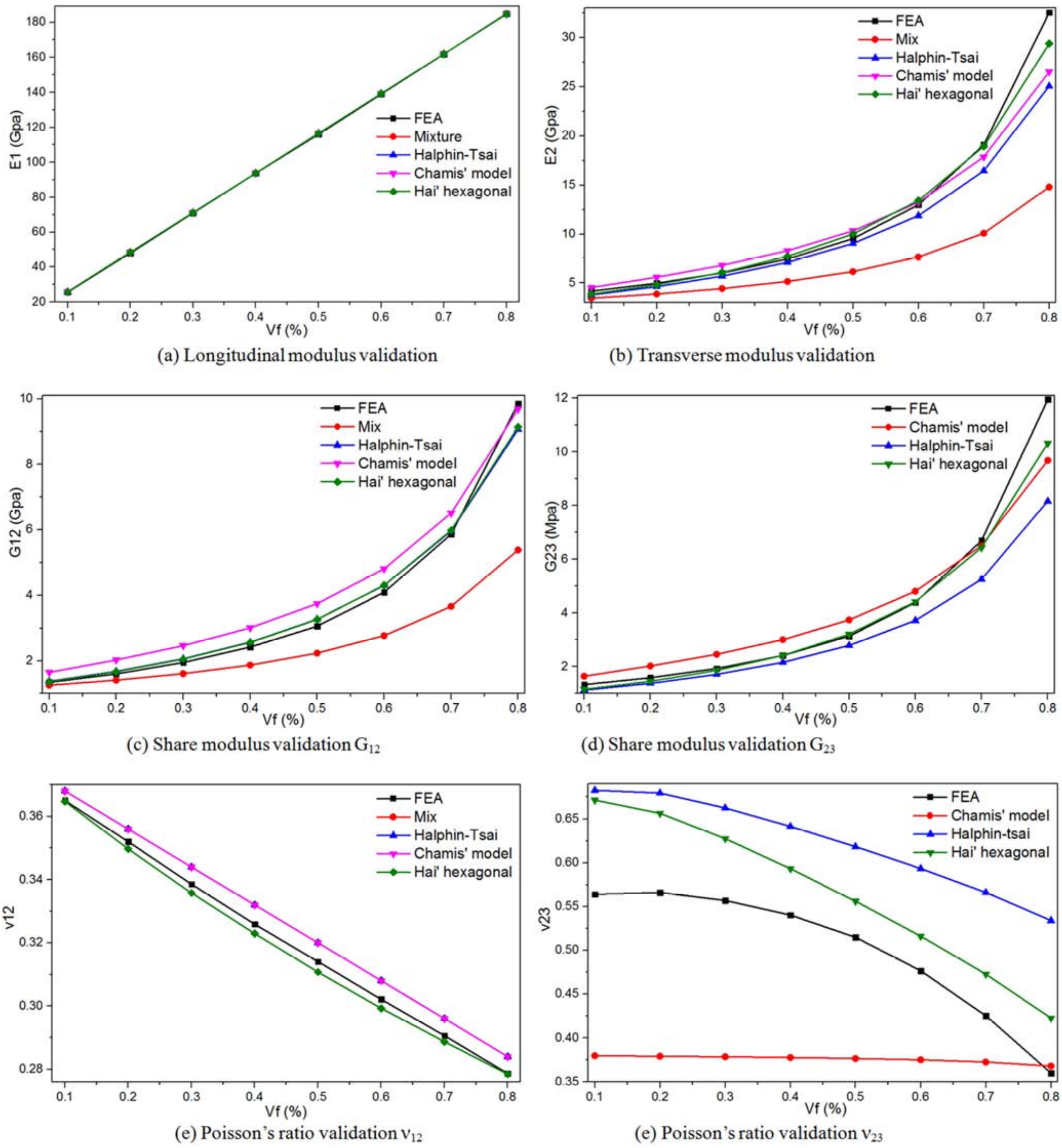


Figure 8. *Results of hexagonal RVE using FEA with other model.*

6. Conclusion

In this paper, comparative results obtained from analytical analysis, FEA and other researchers have been performed. From the results achieved in order to accurately evaluate the most suitable model that can accurately predict the effective mechanical properties of composite materials. The analysis of the results are compared, showing that all analytical models and the numbers models are obtained E1 and v12 were in good agreement with FEA results and experiments. However, the ability to predict the the shear modulus and the transverses Young's modulus has not reached high accuracy. From the above analysis, it can be concluded that:

(1) Depending on how to design structure of RVE models, it is necessary to use it to reasonably analysis models. At the same time, FEA approach indicates is an effective method to predict the mechanical properties of

composite materials.

(2) Abaqus software application approach with a Python code helps process of model building and analysis faster by changing the command. Investments that helps the design process predict the mechanical behavior of materials quickly and accurately.

(3) The results obtained by the tool are developed by us, it allows for predicting quickly, efficiently and close predictions of the FEA models. Moreover, the tool is designed with an intuitive interface, convenient, easy to use to reduce computational time.

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