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Integration of a Multi-scale Homogenization Model into Finite Element Software for Predicting Mechanical Properties of Bulk Moulding Compound (BMC) Composite

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Abstract: Bulk Moulding Compound (BMC) is a short fiber composite with random orientation, used in many industrial sectors such as automotive, electrical,... Design and optimization of composite structures made of BMC meet difficulties due to the nature of this material and thus have not been integrated in the finite element software. This paper introduces a method to build and integrate a new computational model into finite element software (ABAQUS). The chosen model is a multi-scale homogenization model, which helps to calculate mechanical properties of composite materials by using the properties of the components and orientation tensor. This integration can be applied for prediction of composite properties on many kinds of materials, reducing time and cost for suppliers when it comes to optimization of mechanical properties.

Keywords: BMC, Short Fiber Composite, Multi-scale Homogenization, Abaqus Plugin

1. Introduction

With many interesting properties such as high specific strength, high corrosion and fatigue resistance, composite materials is widespread used in both civil and military applications. Mechanical properties of composite material depend strongly on its fiber orientation. Laminate composite structures with long fiber pre-oriented along some directions are widely used in aerospace. Thus, the precdiction of mechanical properties of laminate composie structure was intergrated in many finite element software such as Abaqus, ANSYS.

In automotive sector, short fiber composite with random orientation is used due to its low-cost price and simple manufacturing technology. However, the predicion of mechanical properties of short-fiber composite with random orientation is more complex and has not been integrated in the finite element softwares.

Nowadays, predicting mechanical behavior of composite is important for employing into real products. It includes many processes, which is supported by many softwares. Hence, integrating a new computational model to into a finite element software is more and more widely applied in the world. This helps people to use the tools most effectively and minimizing the timeconsumed.

In this paper, a multi-scale homogenization model is built to calculate the mechanical properties of BMC composite by using the two-step homogenization procedure [1], which stands on a classic approach in elasticity of T. Mori & K. Tanaka [2]. The BMC is considered an orthotropic materials. The calculated results are then compared with expermental results of two different materials carried out by N. Le et al. [3] to validate the model.

The model is then intergrated into ABAQUS FEA software to predict mechanical behaviours of short fiber composite. A program written in Python programming language is integrated in ABAQUS as a plug-in via ABAQUS GUI Toolkit [4].

2. Experimental Characterization of BMC Composite

2.1. Material

a) Injected plate

b) Xmold

Figure 1. *Two short fiber BMC composite samples: a) Injected plate; b) Xmold.*

Two types of short fiber BMC composite are consisdered: Injected plate and Xmold. Both types consist of 20% of E-glass fibers (6 mm long and 14 µm diameter) and 80% of polyester resin in weight. The fiber were randomly distributed before injection. The Young's modulus, Poisson's ratio of the matrix and the fiber are equal to 6.5 GPa, 0.27 and 74 GPa, 0.28, respectively. The samples of 100mm x 100 mm were cut from four corner of the Xmold and injected plate to do the microstructure test. Then five small samples were extracted from the square sample for the tensile test.

2.2. Orientation Tensor

In composite, the microstructure plays an important role in determining the physical and mechanical properties. According to several authors [1, 2, 5], among different parameters, fiber orientation is the most important. In general, there are two methods for measuring the orientation tensor: Ultrasonic method and Image Analysis method.

In the case of composites reinforced with short fibers, considering that they are of circular section, the intersection of a cutting plane (X, Y, Z) with a fiber forms an ellipse with major radius a and minor radius b. (Figure 2)

The software image analysis, Ellix [1], identifies each fiber as an ellipse and automatically determines the characteristics of the ellipse, it determinesthe coordinates (x_c, y_c) of its center, its radius a and b and its angle Φ in the cutting plane, compared to a reference direction. The angle θ is determined by the relationship:

$$\theta = \arccos\left(\frac{a}{b}\right) \tag{1}$$

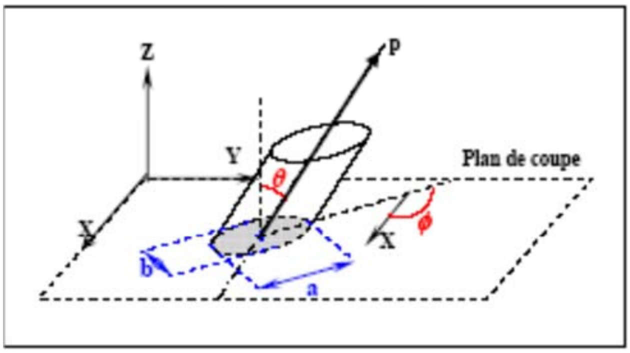


Figure 2. *Intersection of a fiber with a cutting plan.*

When a single fiber k is orientation (θ_k, Φ_k), we can infer the orientation tensor of the fiber k [6, 7]:

$$A_k = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{2}$$

$$\text{With} \begin{cases} a_{11} = \sin^2(\theta).\cos^2(\varphi) \\ a_{22} = \sin^2(\theta).\sin^2(\varphi) \\ a_{33} = \cos^2(\theta) \\ a_{12} = a_{21} = \sin(\varphi)\sin^2(\theta).\cos(\varphi) \\ a_{13} = a_{31} = \sin(\theta)\cos(\theta).\cos(\varphi) \\ a_{23} = a_{32} = \sin(\theta)\cos(\theta).\sin(\varphi) \end{cases}$$

In the case of BMC composites, Image Analysis method is used by N. Le et al. [3] to obtain the orientation distribution of fibers in the form of orientation tensor. These results confirm that the preferred orientation of fibers is in the direction of flow, BMC material is highlyanisotropic By averaging the tensor orientation in 16 layers of thickness, the 3D orientation tensor in the thickness of injected plate (I-Pl) and Xmold sample are:

$$A_{20F-I-Pl} = \begin{bmatrix} 0.551 & 0.076 & 0.025 \\ 0.076 & 0.416 & 0.004 \\ 0.025 & 0.001 & 0.032 \end{bmatrix} \tag{3}$$

$$A_{20F-Xmold} = \begin{bmatrix} 0.874 & 0.032 & -0.020 \\ 0.032 & 0.104 & 0.004 \\ -0.020 & 0.004 & 0.022 \end{bmatrix} \quad (4)$$

2.3. Tensile Test in Macroscopic Scale

Tensile tests were carried out to obtain mechanical properties of the BMC composites. The result shows a significant difference of behavior between the transverse direction and the longitudinal direction, which is consistent with the fiber's orientation distribution. The distribution of fibers in Xmold sample is less anarchic than those in the injected plate. Therefore, the value of the anisotropic ratio (E_{2c}/E_{1c}) of Xmold is larger than injected plate.

Table 1. *Mechanical properties of two types of BMC composite: Injected Plate and Xmold sample [8].*

Parameter	20F-Xmold	20F-I-Plate
E_1 (GPa)	10.76 ± 0.67	9.75 ± 0.82
E_2 (GPa)	9.24 ± 0.45	9.15 ± 0.52
E_2/E_1	0.86	0.95

3. Homogenization Model

3.1. Principle of Model

For the composite containing fibers with an orientation distribution, it is impossible to predict the effective elastic properties using a two-step homogenization procedure. In this case, the model is considered as a first step for a fictitious material where all fibers are aligned and the unidirectional composite properties are calculated by Mori-Tanaka model [2]. For example, stiffness tensors are calculated by the following formula:

$$C^{UD} = C_m + c_f\left(C_f - C_m\right) : A^{MT} \quad (5)$$

Where f and m refer to the fibers and the matrix, respectively, with stiffness tensors C_f and C_m; c_f is the volume fraction. The strain concentration tensor in the fibers A^{MT} that the model deduces is obtained from Eshelby tensor E which depends on the fiber aspect ratio and the matrix elastic constants.

$$A^{MT} = A\left[\left(1-c_f\right)I + c_f A\right]^{-1} \quad (6)$$

With

$$A = \left[I + E\left(C_m\right)^{-1}\left(C_f - C_m\right)\right]^{-1} \quad (7)$$

where I is the identity tensor.

In the second step, as in the method of Advani and Turker [7], the unidirectional properties are weighted by the orientation distribution function $\psi(\theta,\varphi)$.

$$C = \int_{\Omega} C^{UD}(\theta,\varphi)\psi(\theta,\varphi)d\Omega \quad (8)$$

Where Ω is the unit sphere, with:

$$d\Omega = \sin\theta d\theta d\varphi \quad (9)$$

$$\int_{\Omega} \Psi(\theta,\varphi)d\Omega = 1 \quad (10)$$

The prediction of mechanical behavior in the elastic phase is performed using the orientation tensor. Therefore, the stiffness tensor can be recalculated by the following equation:

$$\begin{aligned} C = C_{ijkl} &= C_1 a_{ijkl} + C_2\left(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}\right) \\ &+ C_3\left(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}\right) \\ &+ C_4\delta_{ij}\delta_{kl} + C_5\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \end{aligned} \quad (11)$$

Where δ_{ij} is the Kronecker symbol and five constants C_1,..., C_5 are calculated from the stiffness tensor C^{UD}; a_{ij} and a_{ijkl} are the second-order and the fourth-order orientation tensors.

Both of second-order and fourth-order orientation is needed for this method but the fourth-order one is unknown. In this case, this orientation tensor can be calculated from the second-order by using several closure approximations. They are given respectively by:

The linear equation, which is exact for a completely isotropic distribution of fiber orientations:

$$\begin{aligned} a_{ijkl}^{L} &= -\frac{1}{35}\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \\ &+ \frac{1}{7}\left(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}\right) \end{aligned} \quad (12)$$

The quadratic equation, which is exact for aligned fibers

$$a_{ijkl}^{Q} = a_{ij}.a_{kl} \quad (13)$$

The hybrid equation, which is intermediate between the linear and the quadratic:

$$a_{ijkl} = a_{ijkl}^{H} = \left(1-f\right)a_{ijkl}^{L} + f a_{ijkl}^{Q} \quad (14)$$

With

$$f = 1 - 27\det\left(a_{ij}\right) \quad (15)$$

The model was built in Matlab software to calculate the stiffness tensor of composite using the theory in this paper.

3.2. Results and Discussions

For validating the model, we compare three cases of composite with 20% of fibers in weight: 20F-0° (all of the fibers are aligned in direction 1), 20F-90° (all of the fibers are aligned in direction 2) and 20F-45°. Results of this validation can be found in Table 2.

In table 2, for the first case, all fibers are aligned in direction 1, and the Young's modulus of this direction is equal to 15.71 GPa. Because of orthotropic material, the value of E_{1c} is the same with E_{2c}. In the second case, all fibers are aligned in the second direction. We found a similar result compared with the first case. Finally, the direction in the third case is symmetric between first and second directions. So, the E_{1c} and E_{2c} values are identical. In conclusion, the model is validated for unidirectional composites. Basically, the maximum error of 7.5% between these results and the simulation results of N. Le et al. [3] is accepted.

Then, we apply this model for predicting the material's properties of two forms of BMC composite: 20F-Plate-I and 20F-Xmold. Results in Table 3 show that the Young modulus in the longitudinal direction of 20X – Xmold is maximum (11.8 GPa). An error of 12.6% of this simulation is little significant. One of the causes for this error may come from the avarage of orientation tensor. In case of 20F-I-Plate, the difference between simulation and experiment is less than 5.7%. Finally, this proves that our model is accepted for both types of BMC.

Table 2. *Validation of the model for simple cases.*

Unidirectional – direction 1	Unidirectional – direction 2	Unidirectional – direction 3
$A_{20F-0^\circ} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$A_{20F-90^\circ} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$A_{20F-45^\circ} = \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
E_{1c} = 15.71 GPa (Error: 7.5%)	E_{1c} = 8.45 GPa (Error: 4.1%)	E_{1c} = 8.49 GPa (Error: 1.7%)
E_{2c} = 8.45 GPa (Error: 4.1%)	E_{2c} = 15.71 GPa (Error: 7.5%)	E_{2c} = 8.49 GPa (Error: 1.7%)
E_{3c} = 8.45 GPa (Error: 4.1%)	E_{3c} = 8.45 GPa (Error: 4.1%)	E_{3c} = 8.45 GPa (Error: 4.1%)

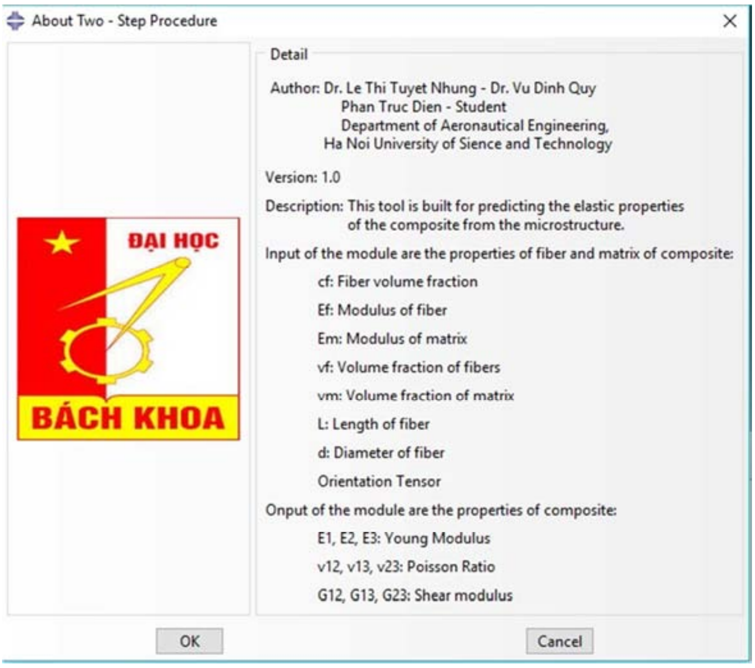
Table 3. *Comparison between Simulation and Experiment of the BMC elastics properties.*

	20F - Xmold			20F – I – Plate		
	Simulation	Experiment	Error (%)	Simulation	Experiment	Error (%)
E_{1c} (GPa)	11.18	10.76±0.67	3.9	9.41	9.75±0.82	3.5
E_{2c} (GPa)	8.07	9.24±0.45	12.6	8.63	9.15±0.52	5.7
E_{3c} (GPa)	8.01			8.30		

4. Integrating Multi-scale Homogenization Model into ABAQUS

Normally, two methods are used to integrate our model into ABAQUS: Writing User Subroutine and Writing Plugin[9]. In this section, we will present the method to integrate the multi-scale homogenization into ABAQUS by Writing Plugin.

The integrated process has been tested on Microsoft Window 7 with ABAQUS 6.10 version. Plugin is written Python programming language, must be placed in the Abaqus parent directory: Abaqus\6.xx\abaqus_plugins. For example, the default location for ABAQUS 6.10 on Windows is: C:\SIMULIA\Abaqus\6.10-1\abaqus_plugins.



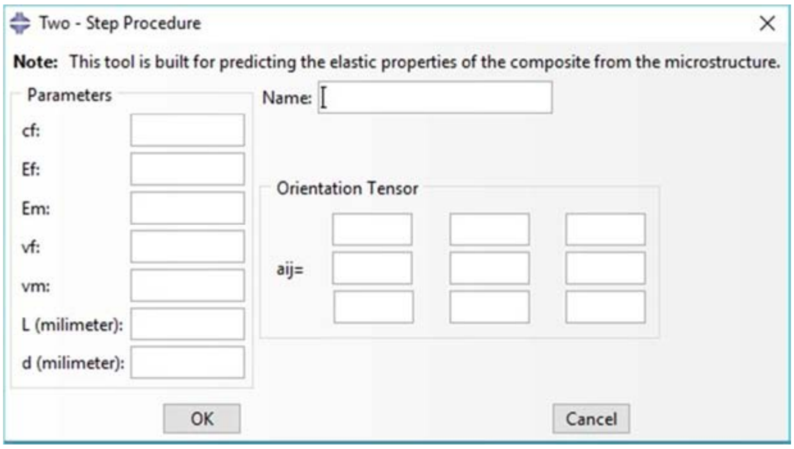


Figure 3. *Basic view of the interface GUI within ABAQUS /CAE.*

The main window of the interface contains many textboxes for the user to insert the parameters of our model.

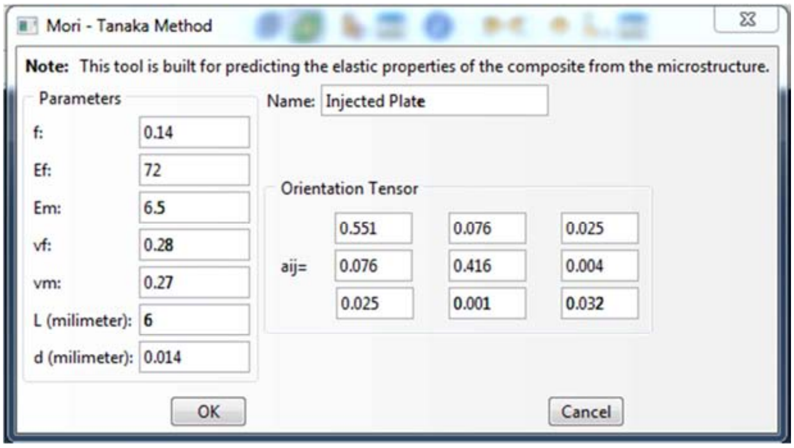


Figure 4. *Input parameters.*

Then, Abaqus will solve and create a new user-defined material automatically.

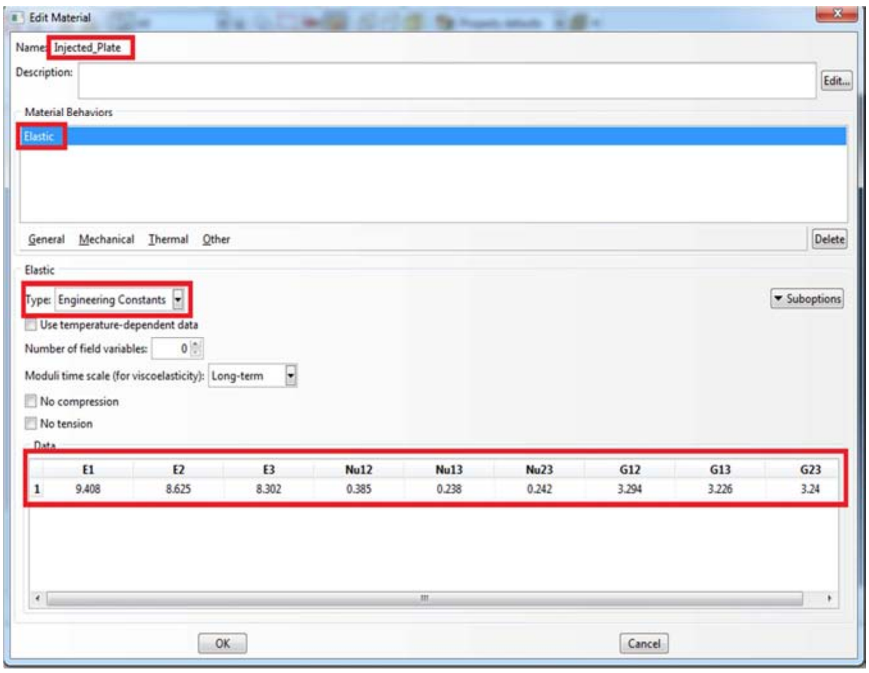


Figure 5. *New material is created.*

5. Testing of Integrated Model

Two simulations of composite plate BMC-Injected (0.5m x 0.5m x 0.005m) solicited by the same load and boundary conditions will be presented. A concentrated force of 500N was applied in the center of plate. Four edges of the plate were clamped.

In the first case, we use the material from the experiment, shear modules were calculated from Young modules and Poison's ratio [10], in the second case we use the material from the integrated model (Table 4). The results obtained by two simulations' will be compared to validate this model.

Table 4. *Material's properties of two simulations.*

	a) Experiment	b) Integrated model
Young's Module (GPa)	$E_1 = 9.75$ $E_2 = 9.15$ $E_3 = 9.15$	$E_f = 72$ $E_m = 6.5$
Poison's ratio	$v = 0.28$	$v_f = 0.28$, $v_m=0.27$
Orientation		$a_{ij=}$ $A_{20F\text{-}I\text{-}Pl}$

The Figure 6 shows the distribution of displacements in two simulations. The maximum displacement was founded in the same position, it is equal to 5.09 mm in the case a and 4.96 mm in the case b.

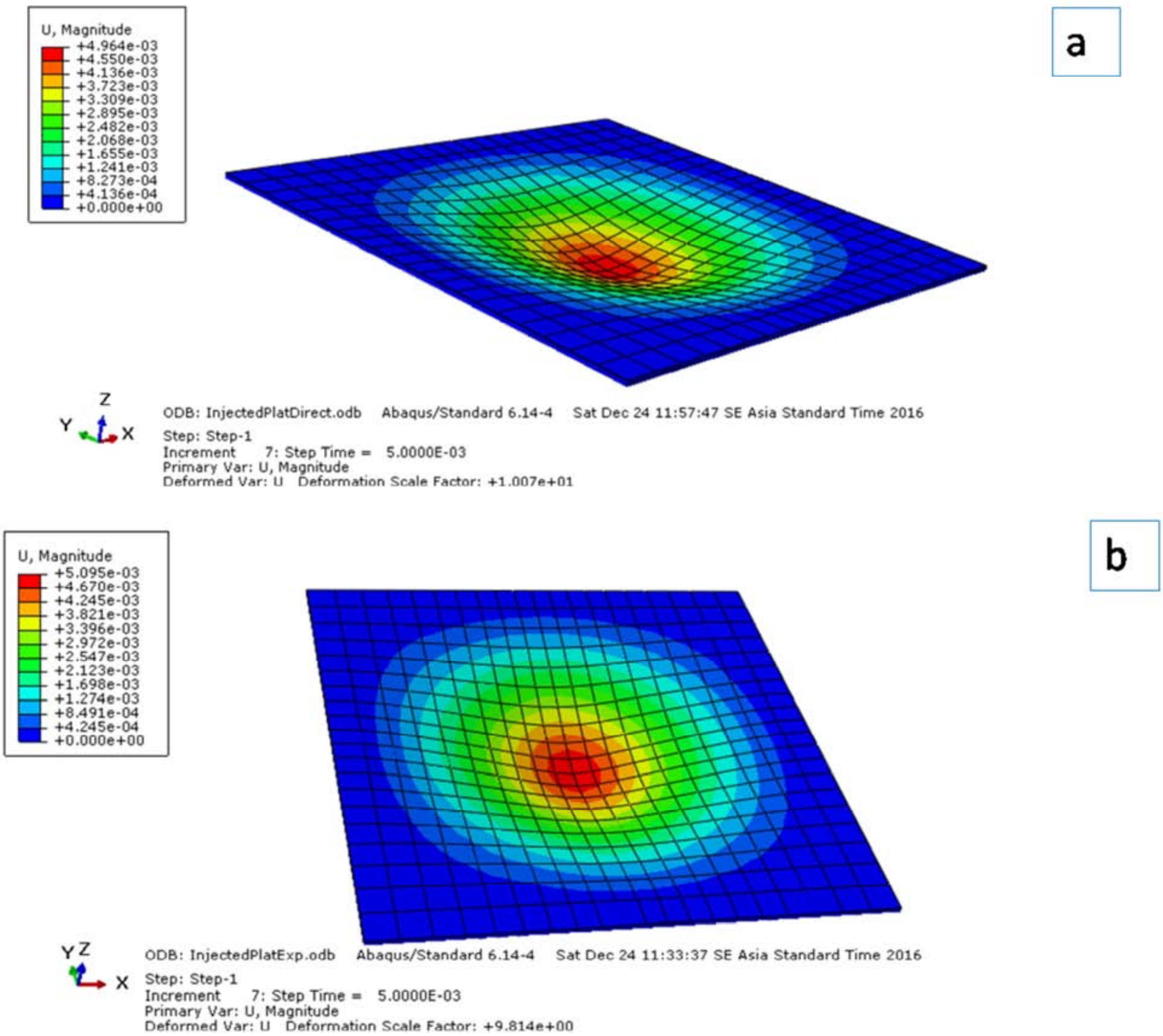


Figure 6. *Distribution of displacement (mm) of two simulation cases: a. Input parameters from experiment; b. Input parameters calculated from the integrated model.*

Table 5. *Comparison of two simulations.*

Results	Experiment	Integrated model	Error (%)
Von-Mise Stress (MPa)	22.19	22.71	2.3
Displacement (mm)	5.095	4.964	2.6

The Table 5 shows the correlation between the two simulations using integrated model results and the experimental results. The errors less than 5% were founded by comparing the stress and the displacement in the same position. The integrated model is valid for the structure simulation; the advantages of using this model are the quick results and low cost.

6. Conclusion

In this paper a homogenization model based on a two-step homogenization procedure was integrated into ABAQUS FEA software for predicting mechanical behaviors of short fiber composite. The comparison of calculated and experimental results shown a good agreement. This integration is helpful for users to calculate mechanical properties of many kinds of materials and to create them in ABAQUS FEA software quickly. Moreover, this plugin is simple and easy to use. This tool allows us to optimize the microstructure of the BMC.

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Biography

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