

# Prediction of Thermo-Mechanical Properties for Compression-Molded Composites

G. Lielens, P. Pirotte, A. Couniot, F. Dupret and R. Keunings

CESAME, Unité de Mécanique Appliquée, Université catholique de Louvain,  
Av. G. Lemaître, 4, B-1348 Louvain-la-Neuve, Belgium

## Abstract

We present a method to determine the thermo-mechanical properties of compression molded composite parts. The flow-induced fiber orientation is first calculated by numerical simulation, and the resulting orientation state is used as input in a micromechanical model that predicts the thermo-mechanical properties of the part. A two step homogenization scheme based on the grain model approach is followed. First, the properties of a reference composite with aligned fibers are estimated by means of a mixture rule between the upper and lower Hashin-Shtrikman bounds (derived by Willis). This method is in agreement with the Mori-Tanaka estimates for moderate concentrations, and gives better results for higher concentrations. Next, the properties of the composite are obtained by averaging several reference composites with different fiber directions. An example of a 3-D compression molded composite part is analyzed and the results are discussed.

## 1 INTRODUCTION

Fiber reinforced polymers are extensively used in mass production, in view of their short shaping time in processes like injection or compression molding, together with the good mechanical properties of the product. However, a non-homogenous fiber orientation field is often obtained, which is sometimes highly anisotropic and difficult to predict for complex geometries. Thermo-mechanical properties strongly depend on fiber orientation, but also on the presence of fillers or on the part porosity. The lack of numerical tools to predict these properties can cause over-dimensioning of the parts, which results in an unwanted weight and cost increase.

The purpose of this paper is to model the whole compression molding process, from the flow calculation to the properties prediction. We first briefly present our flow and fiber orientation model. The multi-level homogenization scheme used to predict thermo-mechanical properties is then explained. Various types of inclusions can be taken into account in this scheme, including long or short fibers, fillers or voids. Finally the example of a SMC compression molded container is analyzed, including mechanical loading simulation.

## 2 FLOW SIMULATION AND FIBER ORIENTATION PREDICTION

As our aim is to calculate the evolution of fiber orientation during the compression molding of thin parts, the flow field can be obtained using the lubrication approximation [1,10,12], which means that pressure variations across the thickness are neglected, while the pressure field  $P$  satisfies the following form of the mass equation :

$$\nabla \cdot (S \nabla P) + \dot{h} = 0 , \quad (1)$$

where  $S$  is the fluidity, which depends on the pressure gradient, the thickness of the cavity and the rheology of the suspension, and  $\dot{h}$  is the time derivative of the gap width (which differentiates the equation from the one governing injection molding). In complex parts,  $\dot{h}$  depends on the mold closing speed, but also on the local mid-surface orientation. Velocities can be deduced from the pressure field and are used as input for fiber orientation calculations. Although large concentrations of fibers are involved in most practical applications, the influence of fiber orientation on the flow kinematics is neglected in our model. Fibers are assumed to be long as compared to the gap width, and to remain parallel to the mid-surface, leading to a 2D orientation field. According to Advani and Tucker [2], orientation can be represented using a probability distribution function  $\psi(x, t, p)$ , which is a function of the location  $x$  and the time  $t$ , while  $p$  stands for the unit vector aligned with the fiber. Since calculating  $\psi$  means solving a four-dimensional problem in the 2D case, it is essential to simplify the model by introducing orientation tensors, which are defined as the successive moments ( $a_2, a_4, \dots$ ) of the distribution function  $\psi$ . In particular, according to such hypotheses, the second order evolution equation is written as

$$\overset{\Delta}{a}_2 = -2\lambda a_4 : D + 2C_i \dot{\gamma} (I_2 - 2a_2) , \quad (2)$$

where  $D$  is the rate of strain tensor, while  $\overset{\Delta}{a}_2$  stands for a mixed convected time derivative of  $a_2$ ,  $\lambda$  is a function of the fiber aspect ratio,  $C_i$  is a coefficient governing fiber-fiber interaction,  $\dot{\gamma}$  is the strain rate, and finally  $I_2$  stands for the second order unit tensor.

A drawback of this method is that the evolution equation for  $a_2$  involves the fourth-order tensor  $a_4$ , which means that a closure approximation (expressing  $a_4$  as a function of  $a_2$ ) is required in order to relate the evolution of  $a_2$  to the velocity field. We have used the natural closure approximation of Verleye and Dupret [3,13], which has been shown to be more accurate than the usual quadratic or hybrid closures, especially during the flow transients.

## 3 THERMO-MECHANICAL PROPERTIES

Our goal is to predict the homogenized thermo-mechanical properties everywhere in a composite part using the fiber orientation state obtained after mold filling. The composite is assumed to consist of a continuous phase (the matrix) in concentration  $v_m$ , and of fibers in concentration  $v_i$ . Letting  $\sigma$ ,  $\epsilon$ ,  $\phi$  and  $\gamma$  denote the stress, strain, heat flux and thermal gradient, and assuming an isotropic matrix and transverse isotropic spheroidal inclusions of aspect ratio  $Ar$ , constitutive equations are written as follows:

$$\text{- in the matrix:} \quad \sigma = C_m : \epsilon - \beta_m \Delta T , \quad \phi = k_m \cdot \gamma ; \quad (3)$$

$$\text{- in the inclusions:} \quad \sigma = C_i : \epsilon - \beta_i \Delta T , \quad \phi = k_i \cdot \gamma ; \quad (4)$$

where  $C_{m \text{ or } i}$ ,  $\beta_{m \text{ or } i}$ ,  $k_{m \text{ or } i}$  are the stiffness tensor, the thermal stress tensor and the thermal conductivity tensor of the matrix or the inclusions, respectively. The orientation state of the inclusions is described by the second order orientation tensor  $a_2$ .

The homogenization volume is supposed to be large enough to contain a statistically representative amount of fibers, but small enough to let the orientation tensor be considered as uniform.

### 3.1 Homogenization of a two-phase composite with aligned inclusions

The homogenized thermo-mecanical properties of a two-phase composite depend on the properties of the inclusions and the matrix, and the distribution of strain and thermal gradient between them only. This distribution can be described by introducing a fourth order deformation concentration tensor  $B^\epsilon$  and a second order thermal gradient concentration tensor  $B^\gamma$ :

$$\langle \epsilon \rangle_i = B^\epsilon : \langle \epsilon \rangle_m , \quad \langle \gamma \rangle_i = B^\gamma \cdot \langle \gamma \rangle_m ; \quad (5)$$

where  $\langle \quad \rangle_{m \text{ or } i}$  denote the average in the matrix or the inclusions, respectively, in the homogenization volume. Using these tensors, the homogenized thermo-mecanical properties can be expressed as

$$\bar{C} = (v_i C_i : B^\epsilon + v_m C_m) : (v_i B^\epsilon + v_m I_4)^{-1} , \quad (6)$$

$$\bar{k} = (v_i k_i \cdot B^\gamma + v_m k_m) \cdot (v_i B^\gamma + v_m I_2)^{-1} , \quad (7)$$

$$\begin{aligned} \bar{\beta} &= v_i \beta_i + v_m \beta_m + \\ &v_i v_m (C_i - C_m) : (B^\epsilon - I_4) : (v_i B^\epsilon + v_m I_4)^{-1} : (C_i - C_m)^{-1} : (\beta_i - \beta_m) . \end{aligned} \quad (8)$$

Details are given in Appendix A.

Simple bounds for these tensors can be obtained without any assumption about the geometry of the phases by using the Voigt or Reuss hypotheses:

- for the Voigt bound, strain and thermal gradient are the same in the matrix and the inclusions:

$$B^\epsilon = I_4 , \quad B^\gamma = I_2 ; \quad (9)$$

- for the Reuss bound, stress and thermal flux are the same in the matrix and the inclusions:

$$B^\epsilon = C_i^{-1} : C_m , \quad B^\gamma = k_i^{-1} \cdot k_m . \quad (10)$$

These bounds are too wide to be useful, but tighter bounds can be obtained for the  $B$  tensors by using geometrical informations about the inclusions. The Hashin-Shtrickman-Willis bounds [4] are established for a randomly dispersed set of aligned ellipsoidal inclusions, which gives:

$$\begin{aligned} \text{- as lower bounds:} \quad & {}^{lo} B^\epsilon = (I_4 + E_{C_m, Ar} : (C_m^{-1} : C_i - I_4))^{-1} , \\ & {}^{lo} B^\gamma = (I_2 + E_{k_m, Ar} : (k_m^{-1} : k_i - I_2))^{-1} ; \end{aligned} \quad (11)$$

$$\begin{aligned} \text{- as upper bounds:} \quad & {}^{up} B^\epsilon = (I_4 + E_{C_i, Ar} : (C_i^{-1} : C_m - I_4)) , \\ & {}^{up} B^\gamma = (I_2 + E_{k_i, Ar} : (k_i^{-1} : k_m - I_2)) . \end{aligned} \quad (12)$$

The Mori-Tanaka theory [5], which gives exact homogenized properties for dilute concentrations (i.e. when fibers do not interact), predicts  $B$  tensors that coincide with the lower bounds of eq. (11). The upper bounds of eq. (12) can also be obtained by using the Mori-Tanaka method, by considering that fibers become the continuous phase, and that the matrix becomes the dispersed phase with an ellipsoidal geometry. The upper bound is thus an accurate estimate of the  $B$  tensors for very high concentrations (which are reached above the maximum fiber packing, when the matrix becomes dilute and discontinuous). An accurate prediction of  $B$  can therefore be obtained in the intermediate concentration range by using a mixture rule between the lower and upper bounds:

$$\begin{aligned} B^\epsilon &= ((1 - F_{mel}(v_i)(^{lo}B^\epsilon)^{-1} + F_{mel}(v_i)(^{up}B^\epsilon)^{-1})^{-1} ; \\ B^\gamma &= ((1 - F_{mel}(v_i)(^{lo}B^\gamma)^{-1} + F_{mel}(v_i)(^{up}B^\gamma)^{-1})^{-1} . \end{aligned} \quad (13)$$

The mixture function  $F_{mel}(v_i)$  must be monotonously increasing and must satisfy  $F_{mel}(0) = 0$  and  $F_{mel}(1) = 1$ . Ideally, it has to be fitted on experimental data, although a simple function such as  $F_{mel}(v_i) = (v_i + (v_i)^2)/2$  gives very good results. This last mixture function has been used in the present work.

A comparison between this approach and other widely used predictive models, such as the Halpin-Tsai equations [6], is made in Ref. [14], where our method is shown to provide excellent results.

### 3.2 Extension to composites with non aligned inclusions

Predicting the  $B$  tensors is difficult for a two-phase composite containing non-aligned fibers, since no precise bounds can be established as in the previous case. To tackle this problem, we have used the grain decomposition approach [7]:

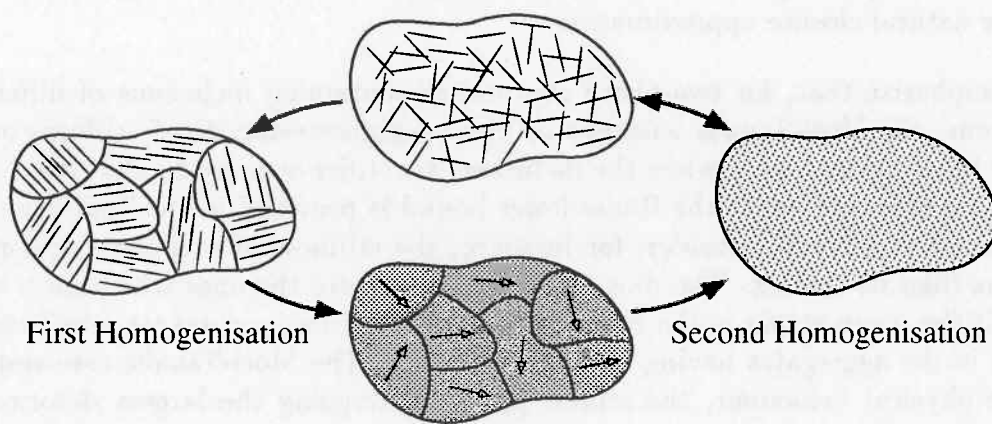


Figure 1 Grain model as a two step homogenization method.

The representative volume is decomposed into a set of aggregates containing the matrix in the same concentration  $v_m$  as in the representative volume, and aligned fibers with a concentration  $v_i = 1 - v_m$ . To keep unchanged the statistical description of the representative volume (i.e.

the concentration and orientation distribution of the fibers), the aggregates containing fibers of direction  $p$  must have a relative volume  $dV/V_r = \Psi(p)dp$ . Each aggregate is first homogenized using the above described technique, in order to provide an equivalent isotropic transverse homogeneous material. In a second step, the different aggregates are themselves homogenized into a single anisotropic material, using various assumptions for the distribution of strain and thermal gradient between the aggregates. Three possible hypotheses are :

- the Voigt upper bound, which assumes a parallel assembly with constant mean strain and thermal gradient over each aggregate:

$$\bar{\bar{C}} = \langle \bar{C} \rangle_{\Psi} , \quad \bar{\bar{k}} = \langle \bar{k} \rangle_{\Psi} , \quad \bar{\bar{\beta}} = \langle \bar{\beta} \rangle_{\Psi} ; \quad (14)$$

- the Reuss lower bound, which assumes a series assembly with constant mean stress and thermal flux over each aggregate:

$$\bar{\bar{C}} = (\langle \bar{C}^{-1} \rangle_{\Psi})^{-1} , \quad \bar{\bar{k}} = (\langle \bar{k}^{-1} \rangle_{\Psi})^{-1} , \quad \bar{\bar{\beta}} = \bar{\bar{C}} : (\langle \bar{C}^{-1} : \bar{\beta} \rangle_{\Psi}) ; \quad (15)$$

- and the Mori-Tanaka assumption, which assumes constant mean strain and thermal gradient over the matrix of each aggregate:

$$\begin{aligned} \bar{\bar{C}} &= (v_i \langle C_i : B^{\epsilon} \rangle_{\Psi} + v_m C_m) : (v_i \langle B^{\epsilon} \rangle_{\Psi} + v_m I_4)^{-1} , \\ \bar{\bar{k}} &= (v_i \langle k_i : B^{\gamma} \rangle_{\Psi} + v_m k_m) : (v_i \langle B^{\gamma} \rangle_{\Psi} + v_m I_2)^{-1} , \\ \bar{\bar{\beta}} &= \langle v_m \beta_m + v_i (\beta_i - C_i : (I_4 - B^{\epsilon}) : (C_i - C_m)^{-1} : (\beta_i - \beta_m)) \rangle_{\Psi} \\ &\quad + \bar{\bar{C}} : \langle v_i (I_4 - B^{\epsilon}) : (C_i - C_m)^{-1} : (\beta_i - \beta_m) \rangle_{\Psi} . \end{aligned} \quad (16)$$

Orientation averaging over the aggregates can be calculated directly using the  $a_2$  and  $a_4$  orientation tensors [2,7,11]. When the only known orientation tensor is  $a_2$ ,  $a_4$  can be determined using the natural closure approximation.

Let us emphasize that, for two-phase composites containing inclusions of different shapes or orientations, the Mori-Tanaka assumption gives a higher estimate of stiffness or conductivity than the Voigt upper bound when the inclusions are stiffer or more conductive than the matrix, and that an estimate below the Reuss lower bound is provided in the opposite case. This can be explained as follows: consider, for instance, the stiffness of a composite containing stiffer inclusions than its matrix. The most rigid aggregates are the ones which have the highest  $B^{\epsilon}$  tensor. If the mean strain is the same in the matrix of each aggregate, the total mean strain is higher in the aggregates having a larger  $B^{\epsilon}$  tensor. The Mori-Tanaka assumption thus leads to a non-physical behaviour, the stiffest grains undergoing the largest deformation. In this work, we have therefore chosen to use the Voigt upper bound for the second homogenization. Examples of aggregate averaging are given in Ref. [14].

### 3.3 Extension to multiphase composites

Although it is not possible to fully describe the thermo-mecanical behaviour of a multiphase composite by means of the two tensors  $B^{\epsilon}$  and  $B^{\gamma}$ , it is easy to extend the grain model to

composites containing more than one type of inclusions: in that case, the representative volume is decomposed into aggregates containing a matrix of concentration  $v_m$  and aligned inclusions of only one type of concentration  $1 - v_m$ . This set of aggregates is then homogenized using the same assumptions as previously. An example showing the prediction of conductivity for a two phase composite is given in Ref. [14].

## 4 EXAMPLE AND DISCUSSION

We consider the filling of a 5 mm thick container with Sheet Molding Compound (SMC). In view of symmetry, only a quarter of the part is analyzed. Data from a common polyester - glass fiber SMC have been used in isothermal flow calculations. The aspect ratio of the fibers is 1000. The fixed finite element mesh covering the whole part is represented in Fig. 2.a, while an example of temporary mesh generated during filling is shown in Fig. 2.c. The rectangular-shaped initial load and the successive fronts of material during compression are represented in Fig. 2.b. The orientation field is represented at different stages of the filling in Figs. 2.d, 2.e and 2.f by means of the two eigenvector-eigenvalue products of the second order orientation tensor. It is interesting to note that the final orientation state obtained by compression molding greatly differs from what can be observed for injection molded parts. The injection gate is indeed often followed by a divergent region, where fibers orient perpendicularly to the velocity. The final orientation is therefore rather anisotropic in injection molding. In compression molding instead, fibers tend to be less oriented (since a compressed isotropic disc remains isotropic, for instance). For multi-faceted parts like the container, important differences in gap width between the facets are observed during the flow, which induce a sharp contraction tending to align the fibers with the fluid velocity (Figs. 2.d and 2.e). The more compression progresses, the less this effect is important as the gap width becomes uniform at the end of the filling (Fig. 2.f). These effects, combined with in-plane deformation and transport, give rise to an unexpected final orientation pattern.

The calculated fiber orientation field in the part has been used as input to predict its thermo-mechanical properties. The bending and tension stiffness matrices have subsequently been computed on each element of the fixed mesh, using the classical Kirchoff theory, and have been introduced as a material property in the Finite Element structure computation code SAMCEF (which is able to deal with anisotropic materials). Fig. 3 shows the deformation and the von Mises stress in the container when it is clamped on its lower horizontal face and is loaded with an internal pressure of 1 bar. The behavior of the part (Fig. 3.a) is compared to a simplified case where fiber orientation is supposed to be isotropic (Fig. 3.b). One can observe that the shape of the deformed part and the stress distribution are mainly dependent on the geometry of the part. However, the camber is significantly lower in the case of flow-induced fiber orientation.

## 5 CONCLUSIONS

We have presented a global model that is able to predict the linear thermo-mechanical properties of complex composite parts from the flow-induced fiber orientation state. A decoupled approach has been used to calculate the flow kinematics and the fiber orientation during the compression molding process. This model leads to qualitatively good results in the case of

concentrated long fibers. The influence of fiber-fiber and fiber-polymer interactions on the flow is however neglected. Our micromechanical model is also appropriate when various types and concentrations of reinforcements are present in the composite. This model can provide a very efficient tool to optimize the design of composite parts, taking processing conditions into account. To validate this approach, comparisons with experimental results will be made to test both fiber orientation and thermo-mechanical properties.

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## List of Symbols

$P$  = Pressure ( $Pa$ ) ,  $\dot{\gamma}$  = strain rate ( $s^{-1}$ ) ,  $\dot{h}$  = Normal closure velocity ( $ms^{-1}$ )

$S$  = Fluidity of the fiber suspension in the mold ( $m^3s^{-1}Pa^{-1}$ )

$D$  = strain rate tensor ( $s^{-1}$ ) ,  $\omega$  = rotation rate tensor ( $s^{-1}$ ) ,

$I_2$  = second order unit tensor ,  $I_4$  = fourth order unit tensor

$p$  = fiber orientation unit vector ,  $\Psi(p)$  = fiber orientation distribution function

$a_2 = \oint pp\Psi(p)dp$  = second order orientation tensor

$a_4 = \oint pppp\Psi(p)dp$  = fourth order orientation tensor

$\lambda = (Ar^2 - 1)/(Ar^2 + 1)$  ,  $\dot{a}_2 = \frac{Da_2}{Dt} + a_2 \cdot \omega - \omega \cdot a_2 - \lambda(D \cdot a_2 + a_2 \cdot D)$

$\sigma$  = stress tensor ( $Pa$ ) ,  $\epsilon$  = deformation tensor ,  $\Delta T$  = Temperature difference ( $K$ ) ,

$\phi$  = heat flux ( $Wm^{-2}$ ) ,  $\gamma$  = thermal gradient ( $Km^{-1}$ ) ,

$C$  = Stiffness tensor ( $Pa$ ) ,  $\beta$  = thermal stress tensor ( $PaK^{-1}$ ) ,

$k$  = thermal conductivity tensor ( $WK^{-1}m^{-1}$ ) ,

$E_{C,Ar}$  = fourth order Eshelby tensor for eigenstrain concentration for a material of stiffness  $C$ , in an spheroidal inclusion of aspect ratio  $Ar$

$E_{k,Ar}$  = second order Eshelby tensor for eigen thermal gradient concentration for a material of conductivity  $k$ , in an spheroidal inclusion of aspect ratio  $Ar$

$\langle x \rangle$  = the average of the tensor  $x$  on the representative volume ,

$\langle x \rangle_y$  = the average of the tensor  $x$  on the matrix of the representative volume if  $y = m$ ,  
on the inclusions of the representative volume if  $y = i$

$\langle X \rangle_\Psi = \oint X(p)\Psi(p)dp$ , which mean average of the transverse isotropic tensor  $X$  over all the orientations.

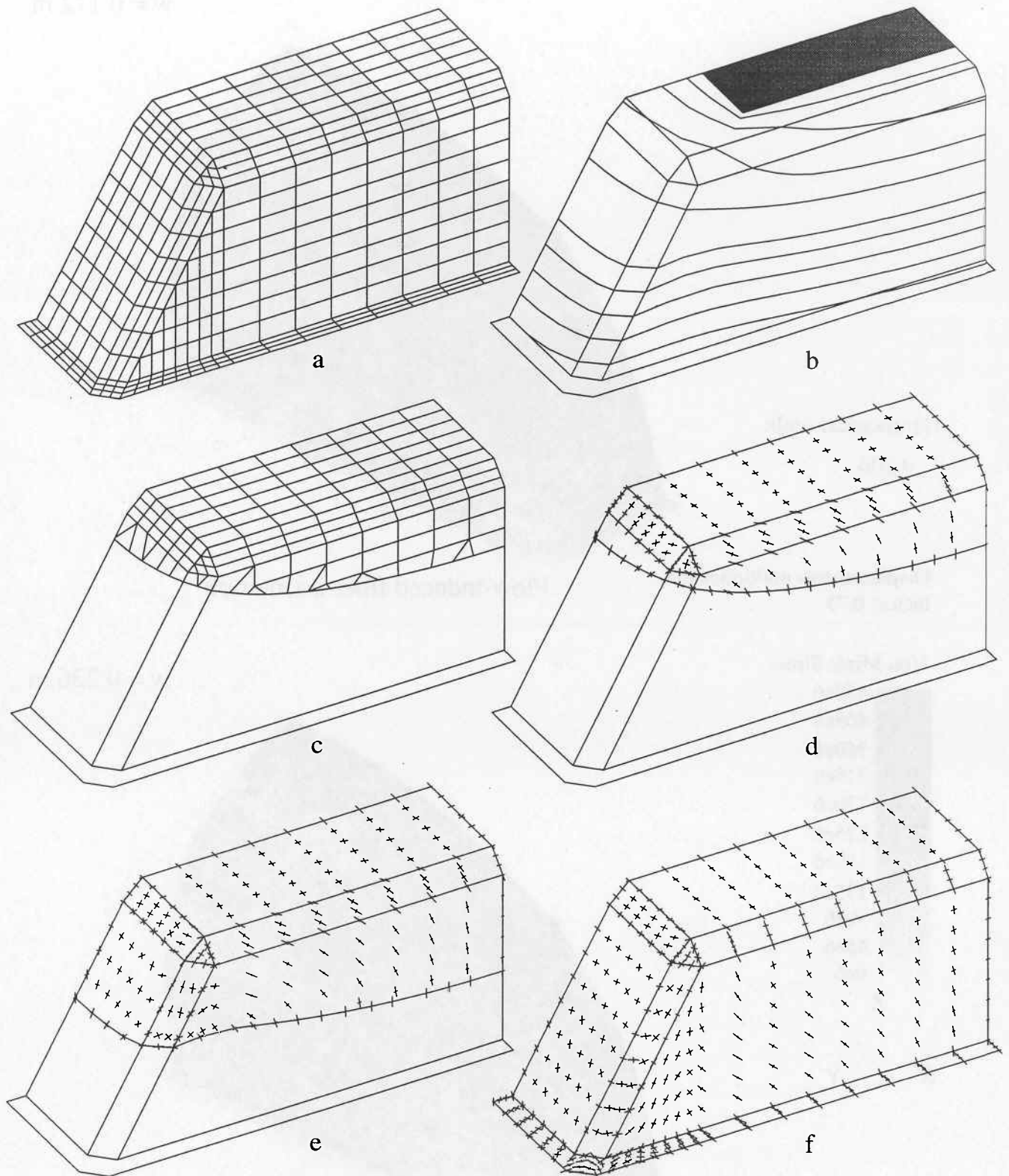


Figure 2 Compression Molding of a container;  
 a. fixed mesh; b. initial load and successive flow-fronts;  
 c. temporary mesh example; d. e. transient orientation fields during filling;  
 f. final orientation field.  
 Only a quarter of the part is represented.



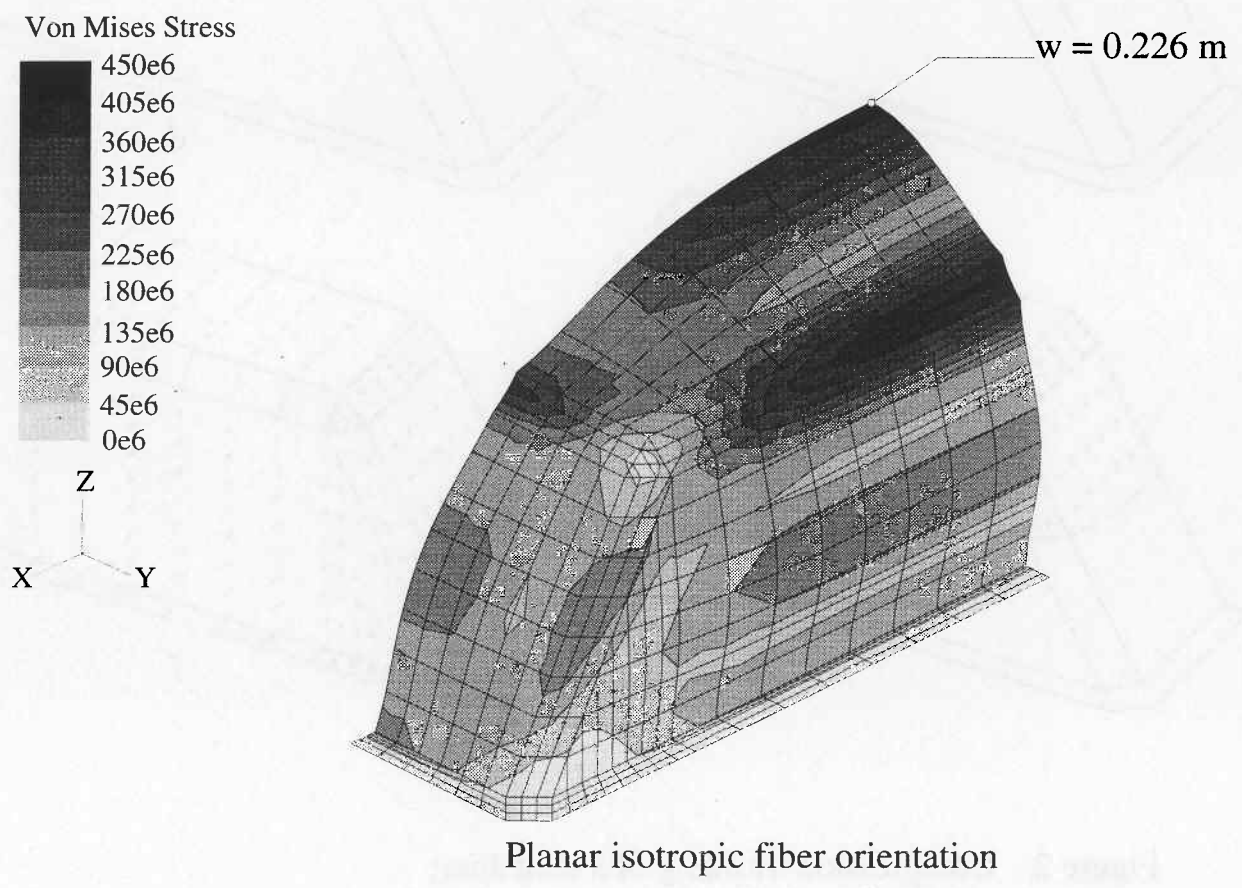
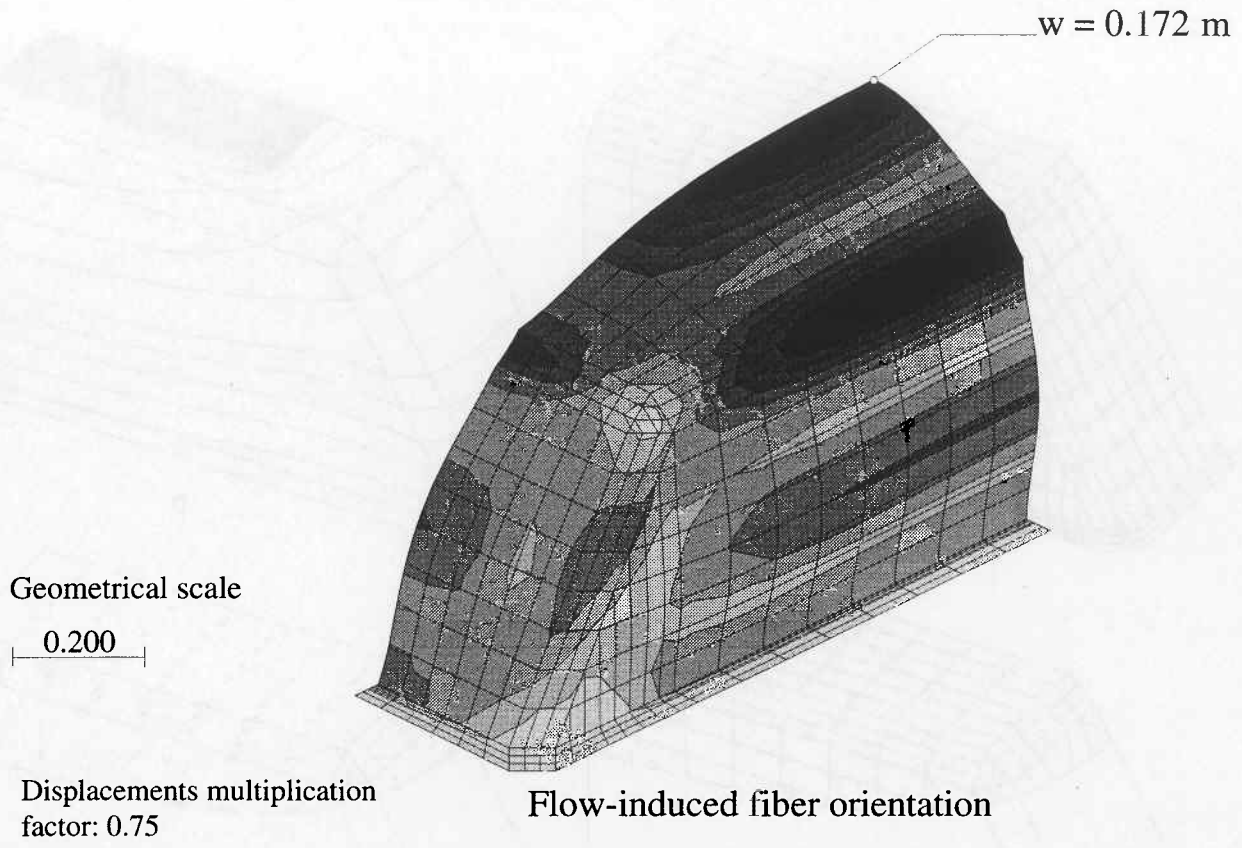


Figure 3: Same problem as in Fig.6. Behaviour of the container under a 1 bar pressure. Comparison between the effect of the flow induced orientation and the isotropic case. Isovalues indicate the von Mises stress, and  $w$  is the camber.

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## Appendix A

The homogenised properties of a representative volume of composite are defined for imposed mean strain  $\langle \epsilon \rangle$ , temperature difference  $\Delta T$  and mean thermal gradient  $\langle \gamma \rangle$  by the following relations:

$$\text{- stiffness } \bar{C} \text{ and thermal stress } \bar{\beta} : \langle \sigma \rangle = \bar{C} : \langle \epsilon \rangle - \bar{\beta} \Delta T ; \quad (17)$$

$$\text{- thermal conductivity } \bar{k} : \langle \phi \rangle = \bar{k}_i \cdot \langle \gamma \rangle . \quad (18)$$

To derive the expression of  $\bar{C}$ , a mean strain  $\bar{\epsilon}$  is supposed to be imposed on a representative volume of composite. This mean strain can be expressed as a function of the mean strain in

the matrix phase using the definition (5):

$$\langle \epsilon \rangle = v_i \langle \epsilon \rangle_i + v_m \langle \epsilon \rangle_m = (v_i B^\epsilon + v_m I_4) : \langle \epsilon \rangle_m . \quad (19)$$

The mean stress is obtained using the constitutive equations (3,4) with  $\Delta T = 0$ :

$$\bar{\sigma} = v_i \langle \sigma \rangle_i + v_m \langle \sigma \rangle_m = v_i C_i : \langle \epsilon \rangle_i + v_m C_m : \langle \epsilon \rangle_m = (v_i C_i : B^\epsilon + v_m C_m) : \langle \epsilon \rangle_m . \quad (20)$$

By inverting relation (19), the mean stress can be expressed as a function of mean strain in the representative volume of composite, giving the expression (6) for  $\bar{C}$

The expression (7) for  $\bar{k}$  is obtained in exactly the same way.

Computing  $\bar{\beta}$  is less immediate. The representative volume is supposed to undergo a temperature difference  $\Delta T$  and a constant strain  $\epsilon$  is imposed in all this volume. The stress must be equal in the inclusions and the matrix for equilibrium:

$$\sigma_i = C_i : \epsilon - \beta_i \Delta T = \sigma_m = C_m : \epsilon - \beta_m \Delta T \Rightarrow \epsilon = (C_i - C_m)^{-1} : (\beta_i - \beta_m) \Delta T \quad (21)$$

Next, an opposite mean strain  $-\epsilon$  is superposed, in such a way that the total mean strain vanishes. Using the relation (19) and (5), the mean strain in the matrix and the inclusions can easily be computed:

$$\langle \epsilon \rangle_i = \epsilon - B^\epsilon : (v_i B^\epsilon + v_m I_4)^{-1} : \epsilon ; \quad (22)$$

$$\langle \epsilon \rangle_m = \epsilon - (v_i B_i^\epsilon + v_m I_4)^{-1} : \epsilon . \quad (23)$$

It is easy to verify that  $v_i \langle \epsilon \rangle_i + v_m \langle \epsilon \rangle_m = 0$ . With the help of the constitutive equations (3,4), the mean stress in the matrix and the inclusions is:

$$\langle \sigma \rangle_i = C_i : (I_4 - B^\epsilon : (v_i B^\epsilon + v_m I_4)^{-1}) : \epsilon - \beta_i \Delta T ; \quad (24)$$

$$\langle \sigma \rangle_m = C_m : (I_4 - (v_i B_i^\epsilon + v_m I_4)^{-1}) : \epsilon - \beta_m \Delta T . \quad (25)$$

Finally, the expression (8) for the homogenised thermal stress tensor  $\bar{\beta}$  is finally obtained using the definition (19).