Injection moulding of fibre reinforced thermoplastics: integration of fibre orientation and mechanical properties computations

Hedi Miled [a]***, Luisa Silva*** [a]***, Thierry Coupez*** [a]***, Jean-François Agassant*** [a] [*]

[a] *Mines-Paristech, Centre de Mise en forme des Matériaux, UMR CNRS 7635, avenue Claude Daunesse, BP 207, 06904 Sophia Antipolis, France*

**Corresponding author : jean-françois.agassant@mines-paristech.fr*

Abstract. Injection moulding is widely used to process short fibre reinforced thermoplastics. The quality and especially the mechanical properties of the resulting part are linked to the mould conception (for example the gate(s) and the venting port(s) locations) and to the processing parameters which will govern fibre orientation distribution.
Fibre orientation modelling is based on the well known Folgar and Tucker equation which differ one from another by the interaction parameter, the closure approximation and by the coupling with the rheology of the reinforced melt. Quantitative comparison with experiments is very tedious and generally limited to simple part geometries (plaque or disk). As a consequence, in complex geometries, fibre orientation distribution is experimentally checked using several techniques and the resulting anisotropic thermomechanical properties are computed using various homogenization theories.
In this paper, we propose an integrated approach of the injection moulding of fibre reinforced thermoplastics starting from rheology of the material, orientation equation, interaction parameter and closure approximation. The resulting local fibre orientation distribution is then used in two ways in order to predict the mechanical properties of the part:
- First, using classical analytical homogenization theories but based on the computed orientation tensor and not on an experimental one,
- then, using numerical homogenization which consists in generating a Representative Elementary Volume (REV), by determining its unidirectional mechanical properties and finally, in computing directly the anisotropic properties of the part .

Introduction

Short fibre reinforced thermoplastics are widely used for plastic part production because they can be processed with the same machines as classical thermoplastics, but present enhanced mechanical properties. Nevertheless, fibres will orient during ,for example, the mould filling process due to the rate of strain and stress history they have encountered along their flow path untill solidification. As a consequence, fibre orientation will vary from one location of the injected part to another and, at a well defined position in the part, within the thickness (figure1) leading to anisotropic mechanical properties (figure 2). This is the main limitation for the development of these reinforced materials.
Short fibres orientation has been studied for decades, both experimentally and theoretically, by numerous authors (see, for example Vincent and Agassant,1986; Bay and Tucker,1992). Fibre orientation will be described generally by a second order orientation tensor which evolution as a function of time will account for several approximations: a closure approximation (Advani and Tucker,1990), an interaction coefficient when fibre concentration increases (Folgar and Tucker, 1984) . Rheology is modified by the presence (and the orientation) of fibres (see, for example Dinh and Armstong, 1984) but most of the authors decouple the flow field and the orientation field especially when complex injected parts are involved .There are many comparisons between experiments and computations in simple geometries (plaque, centre gated disk) but far less in industrial part geometries (Redjeb, 2007).

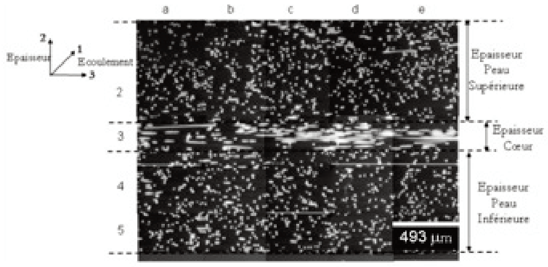

Fig. 1. Fibre orientation anisotropy though the thickness of an injected part

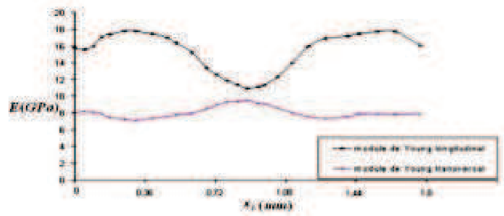

Fig. 2. Young Modulus through the thickness in the longitudinal and transverse directions

In fact, polymer part producers and end-users are not especially interested in the distribution of fibre orientation but on the resulting mechanical properties and, at a first glance, by the distribution of Young modulus (figure2). If they ignore fibre orientation mechanisms, they can measure this distribution (but this is a tedious task even for simple geometries), compute the resulting orientation tensor within the part and then develop an anisotropic thermo-elastic computation (see Advani and Tucker, 1987). The problem is to define the parameters of the stiffness matrix. Generally, classical composites homogenization theories have been used (see Halpin-Tsai, 1969; Eshelby,1957; Mori and Tanaka, 1973).

In this paper, we propose an unified approach of injection moulding of reinforced thermoplastics. Starting with the rheology of the reinforced thermoplastic, the mould geometry and the processing conditions, we compute fibre orientation distribution in a complex part. At the same time, we build representative elementary volumes (REV) with a random orientation of the fibres in the volume and we submit these REV to several traction, compression and shear experiments in order to identify the parameters of the Advani and Tucker equation. We then apply these parameters to identify the stiffness matrix everywhere in the part and we deduce the anisotropic thermo-elastic properties.

Fibre orientation calculation

One assumes that the rheology of the reinforced polymer is not modified by fibre orientation. The second order orientation tensor will be influenced by the flow kinematics following Folgar and Tucker's equation (1984):

$$\frac{\partial \mathbf{a}_2}{\partial t} + \mathbf{v}.\nabla \mathbf{a}_2 = (\Omega \mathbf{a}_2 - \mathbf{a}_2 \Omega) + \lambda(\dot{\varepsilon}\mathbf{a}_2 + \mathbf{a}_2\dot{\varepsilon} - 2\dot{\varepsilon}\mathbf{a}_4) + 2dC_I\dot{\bar{\varepsilon}}(\mathbf{a} - \frac{\mathrm{I}}{d})$$

where $\lambda = \frac{\beta^2 - 1}{\beta^2 + 1}$ with $\beta = \frac{L}{D}$ Land D are respectively mean fibre lenght and fibre diameter, d is the spatial dimension (2 or 3) and $\dot{\bar{\varepsilon}}$ is the second invariant of the rate of strain tensor $\dot{\varepsilon}$

$\mathbf{a}_4$ is the fourth order orientation tensor which needs to be expressed as a function of the second orientation tensor using a closure approximation (see, for example, Advani and Tucker, 1990). In what follows we use the classical quadratic approximation: $\mathbf{a}_4 = \mathbf{a}_2 . \mathbf{a}_2$.

When solving this equation using a standard Galerkin finite element method, one may obtain serious oscillations of the orientation tensor.

Several stabilization techniques have been implemented , SUPG (Streamline Upwind Petrov-Galerkin Method, see Brooks et al, 1982) or RFB (Residual Free Bubbles, see Brezzi et al, 1998). Figure 3 shows that the development of orientation between two parallel plates is more regular when using stabilization techniques.

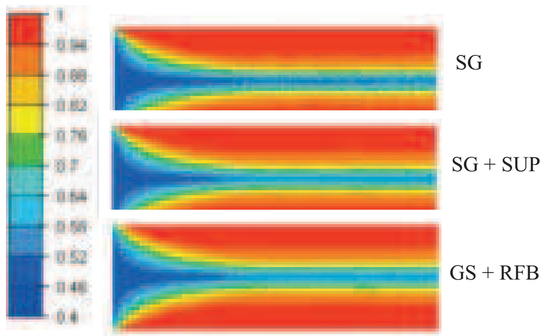

Fig.3. Comparison between the standard Galerkin method and two stabilization methods

REM3D software with a continuous finite element approximation for the different space variables, has been used (Miled, 2010). At each time step, it computes iteratively the flow and pressure fields, the temperature distribution and the orientation tensor. Continuous approximations allows significant reduction of the computation time when compared to the previous discontinuous approximation (Redjeb, 2007).
In the complex geometry presented figure 4a we illustrate at the end of the filling stage, the computed value of the firt component of the orientation tensor (a_{11}on figure 4b).

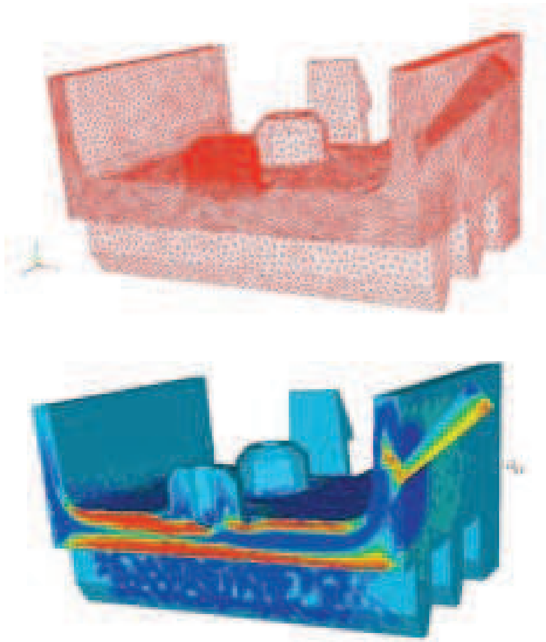

Fig. 4. Meshing of the injected part geometry (left) and distribution of the a_{11} component of the second order orientation tensor at the end of the filling stage (right)

Thermoelastic anisotropic computation

The linear thermo-elastic constitutive equation writes:

$$\boldsymbol{\sigma}(T_0) = \mathbf{C}(\mathbf{a}, T_0)(\boldsymbol{\varepsilon}(T_0) - \boldsymbol{\alpha}(\mathbf{a}, T_0)\Delta T)$$

The rigidity tensor C and the dilatation tensor $\boldsymbol{\alpha}$ can be expressed , following Advani and Tucker (1987) , as a function of the second order and the fourth order components of the orientation tensors:

$$C_{ijkl} = b_1 a_{ijkl} + b_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + b_3(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jk}\delta_{il} + a_{jl}\delta_{ik}) + b_4(\delta_{ij}\delta_{kl}) + b_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

$$\alpha_{ij} = P_1 a_{ij} + P_2 \delta_{ij}$$

The different constants b_i are identified with a perfectly unidirectional composite, using for example Mori-Tanaka (1973) homogenization theory.
Knowing the modulus and the Poisson coefficient of the polymer matrix and of the fibres it is possible, starting from the values of the orientation tensor at each point of the part, to derive the distribution of the Young modulus in the different dircetions(figure5).

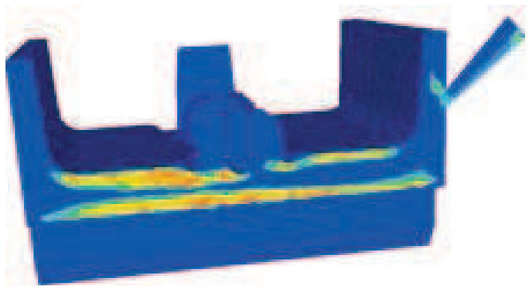

Fig.5. Illustration of the computed Young Modulus corresponding at one of the directionsE_{11}

Direct numerical simulation

An alternative way to compute the anisotropic thermo-elastic properties of the part is to proceed to direct numerical simulation at the fibres level and to identify b1... b5 parameters by generating several Representative Elementary Volumes (REV) (figure6). Knowing the stiffness and the thermal dilatation tensors for fibres and matrix we derive with a mixture law the stiffness and the thermal dilatation tensors everywhere in the REV. We then apply several elastic thermo-mechanical sollicitations on this REV and we deduce numerically homogenised stiffness and thermal dilatation tensors.

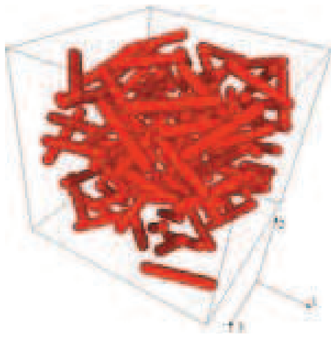

Fig. 6. Schematic representation of a typical representative elementary volume

The problem is to optimize the number of fibres in the REV in order to obtain a stabilized result. As an example, for unidirectional aligned fibres, we computed the E_1 modulus for the different REVs, varying the number of fibres and we compare it to the Mori-Tanaka semi analytical result (figure 7).In this case 22 fibres provide a stabilized result in a sufficiently refined mesh.

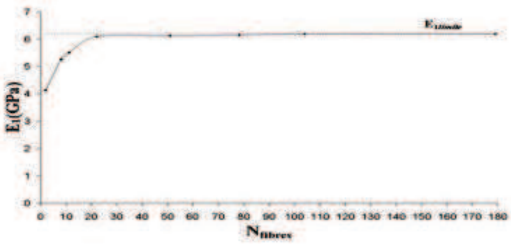

Fig. 7. Young modulus as a function of the number of fibres in the REV (the Mori-Tanaka modulus is 6.21 GPa)

On each REV we know the orientation p_i of each fibre which allows to calculate the second and the fourth orientation tensors and we have to deduce the five b_i parameters. For that purpose, we subject the REV to several deformations (tractions in the three directions, shear deformations in the different planes). We need to impose a minimum of five different deformations in order to determine the five parameters. Here we have used six different deformations modes and we have deduced the parameters with a least square method.As an example one considers a fibre reinforced composite with the following properties:

	$Matrice$	$Fibres$
$E(GPa)$	3	70
ν	0.35	0.2
$\alpha(10^{-6}K)$	108.3	4.9

Tab. 1. Elastic properties of fibres and matrix (the shape factor of the fibres is β =20 and the volume concentration is 15%)

We select several REV with different fibres orientation distributions and, for each sample we determine B = $(b_1, b_2, b_3, b_4, b_5)$ using the 6 deformation modes.

Sample 1: 1D orientation $\mathbf{a} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

→ B = (5.0065, -0.7719, 0.1161, 3,9611, 1.7339)

Sample 2: random orientation

$$\mathbf{a} = \begin{pmatrix} 0.658133 & -0.0251881 & -0.0271289 \\ -0.025881 & 0.185348 & 0.0236711 \\ -0.0271289 & 0.0236711 & 0.156519 \end{pmatrix}$$

→ B = (3.8625, -0.3669, 0.0106, 2.6732, 1.9394)

Sample 3: random orientation

$$\mathbf{a} = \begin{pmatrix} 0.470936 & -0.0799225 & 0.0593181 \\ -0.0799225 & 0.1809372 & 0.0135267 \\ 0.0593181 & 0.0135267 & 0.339692 \end{pmatrix}$$

→ B = (3.4553, -0.5213, 0.0661, 2.7698, 1.8389)

Sample 4: random orientation

$$\mathbf{a} = \begin{pmatrix} 0.256946 & -0.0967644 & -0.0149404 \\ -0.0967644 & 0.338103 & -0.0142976 \\ -0.0149404 & -0.0142976 & 0.404952 \end{pmatrix}$$

→ B= (4.3801, -0.5116, 0.1568, 2.8836, 1.7132)

We observe discrepancies between the different b_i values, but the order of magnitude remains identical. For the following thermo-elastic computations, an average of the values obtained is performed:

$\bar{B}$ = (4.2770, -0.5213, 0.0661, 2.7698, 1.8389)

When increasing the number of samples, the precision of this average value will increase too.

Application to a plaque with a complex gate geometry

We apply these numerically identified values of B to a Polyarylamide plaque (Solvay IXEF 1022) which has been experimentally studied by Vincent et al., 2005) (figure 8).

Fibre shape factor β is 10, volume concentration is 31.6%, the interaction coefficient in Folgar and

Tucker equation is $C_1=10^{-2}$. The viscosity of the reinforced thermoplastic follows a Carreau law (see Vincent et al, 2005).
The processing parameters are the followings: injection rate of 15 cm^3 /s injection temperature of 270°C, mould temperature of 130°C.

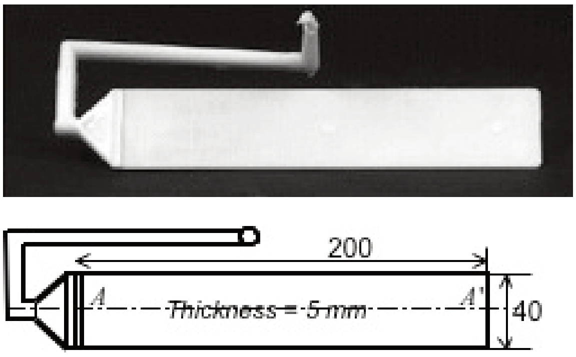

Fig. 8. Geometry of the plaque in the complex geometry case test

The geometry of the inlet gate is quite complex. (figure 9)

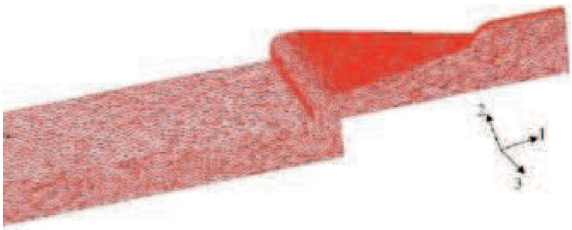

Fig. 9. Gate geometry

Figure 10 presents the different components of the second order orientation tensor obtained at the end of the injection moulding computation

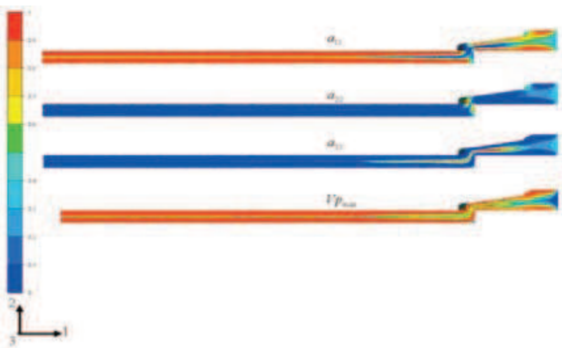

Fig. 10. Distribution near the gate of the different components of the second order orientation tensor, as well as the main eigenvalue of this tensor

These numerical results are compared to experimental measurements of fibre orientation (figure 11).

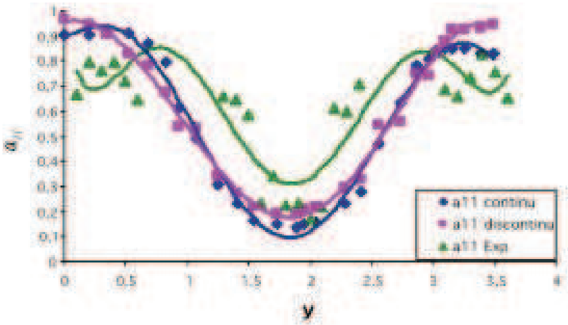

Fig. 11. Comparison of numerical computation of the a_{11} component of the orientation tensor (continuous approaches and discontinuous approaches) and experiments

Using the b_i parameters identified enough direct numerical simulation in the preceding section (mean values) we determine the different components of the Young modulus. One observes, figure 10 that fibres are oriented in the flow direction near the mould wall (i.e. along the plaque surface) which induces a value of the Young modulus E_{11} which is very near the value of the longitudinal Young modulus for a transverse isotropic composite. The minimum value of E_{11} is in the centre of the plaque where fibres are mostly oriented in the transverse direction. The Young modulus E_{22} and E_{33} are much lower, which means that the plaque is more rigid in direction 1 than in directions 2 and 3.

Fig. 12. Distribution of the anisotropic Young modulus (GPa)

The plaque is set in on the gate side and subjected to a simple traction in direction 1 (figure 13) at its extremity. Using the thermo-elastic computation we are able to compute the plaque deformation everywhere. On figure 13, we compare the displacement in direction 1 on the mid-plane of the plaque for an heterogeneous fibre orientation and for an isotropic fibre orientation (all the components of the Young modulus are then identical). We observe that the displacement is divided by a factor 2 when accounting for an anisotropic fibre distribution.

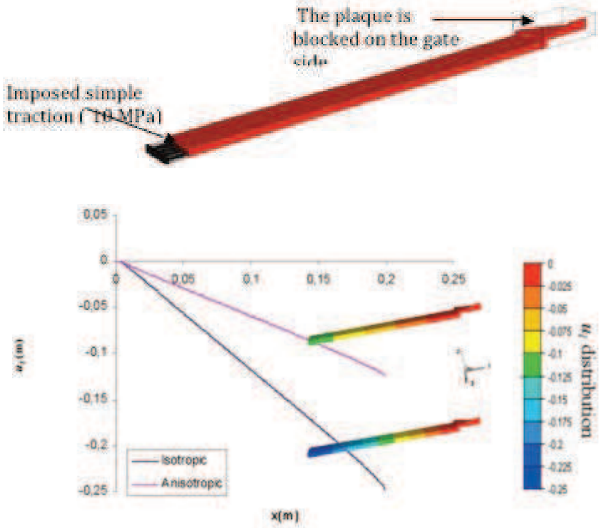

Fig. 13. u_1 component of the displacement; comparison between an isotropic and an anisotropic fibre orientation

Conclusion

This paper represents a first attempt to connect mould filling computation, resulting short fibre orientation, determination of the elasticity and dilatation tensors using direct numerical simulation, and resulting thermo-elastic properties. Measuring the distribution of fibre orientation, even in a simple plaque, is a tedious task as measuring plaque displacements when subjected to various solicitations is common and of easy practice. If confident, this kind of approach may significantly simplify gate positioning and injection moulding parameters optimization for target mechanical properties.
Nevertheless, the method needs to be improved at different levels: improvement of Folgar and Tucker equation in order to better account for fibre/fibre interaction and fibre/mould wall interaction, choose of appropriate closure approximations, optimization of REV (Representative Elementary Volumes) , improvement of the number of applied mechanical solicitations and of the optimization method for the b_l parameters identification.

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