Three dimensional numerical simulations of fiber orientation in injection molding

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ABSTRACT: We present a fully three-dimensional computations of flow behavior and fiber orientation during filling of injection-molded parts. The fiber orientation is calculated by using a mathematical model based on orientation tensors and Folger-Tucker equation. The coupling between the flow kinematics and the fiber orientation is also taken into account. The influences of different parameters like fiber concentration, closure approximations are also considered. Moreover, on takes a special attention on the fiber orientation at the inlet of sprue regions. We points the influence of this initial orientation on the fiber orientation inside the mold.

Key words: Injection process, fiber orientation

1 INTRODUCTION

Composite materials made of glass fibers and thermoplastics matrix and obtained by injection molding are widely used in the industry. The fiber reinforcement improves the properties of the material such as the specific stiffness, the specific strength or the specific toughness, etc. The injection process, which is almost the same as the one used for non reinforced thermoplastics, allows the production of parts with an optimized total cost.

However, fiber suspensions can often exhibit an anisotropic behaviour due to a flow induced fiber-alignment in the flow direction. The fiber orientation has a major influence upon the properties of the composite as a whole. It is also important to measure this orientation in real composite parts in order to establish it’s link with the local properties.

The characterization of the flow or the calculation of fiber orientation in composite materials is of particular interest in current polymer processing research. Extensive numerical studies on the fiber suspension flows have been devoted to extrusion flow, squeezing flow and actually to the injection flow.

This paper focuses on the calculation of three-dimensional fiber orientation in injection molding process. A fully three-dimensional solution for the moving free surface flow and fiber orientation during injection molding is developed on the Rem3d software package. The approach adopted to determine the fiber orientation uses a second-order orientation tensor defined as a dyadic product of the orientation vector [1], whereas the material behaviour is based on the slender-body theory [2,3].

In the following sections, we successively describe the continuum model used including the fiber orientation, the rheological constitutive equation, the numerical method employed to solve our problem, and finally the numerical results obtained.

2 GOVERNING EQUATIONS

Numerical modeling of non-Newtonian fluid flows involves usually the coupling between motion equations, which lead to an elliptic problem, and the fluid constitutive equation introducing an advection problem. In the case of fiber suspensions, an extra-stress tensor is considered, which depends on the fiber orientation.

In this section, we briefly describe the governing equations of fiber orientation and introduce the continuum ones governing the flow of fiber suspensions.
2.1 Fiber Orientation

In order to predict the fiber orientation states, a second order orientation tensor is frequently used, defined as the dyadic product of the unit vector $\mathbf{p}$, averaged over all possible directions, with $\psi(p)$ as weighting function. $\mathbf{p}$ represents the unit vector aligned along the principal axis of the fiber and $\psi(p)$ is the probability distribution function of fiber orientation, defined as the probability of a fiber lying within a range $p$ and $p + dp$.

Orientation tensors was first suggested by Hand [4], and the idea was thoroughly investigated by Tucker and Advani [1]. The definitions of the second ($a_2$) and the fourth ($a_4$) order tensors are, respectively:

$$a_2 = \int p^2 \psi(p) \, dp$$

and

$$a_4 = \int p^4 \psi(p) \, dp$$

The starting point of fiber orientation modeling is the work of Jeffery [5] that has derived the equation of orientation evolution for an ellipsoidal particle immersed in a homogeneous flow motion. Folgar and Tucker [6] have added a diffusion term to Jeffery’s equation in order to consider the interaction among fibers. From Folgar and Tucker calculations, if $n$ is the spatial dimension and if $\Omega(v)$ and $\varepsilon(v)$ are respectively the volume averaged vorticity and strain rate tensors, the evolution equation for the second order orientation tensor becomes:

$$\frac{Da_2}{Dt} = (\Omega(v)a_2 - a_2\Omega(v)) + \lambda(\varepsilon(v)a_4 - a_4\varepsilon(v) - 2\varepsilon(v):a_2) + 2D(\mathbf{I} - na_2)$$

where the symbol “;” denotes the tensorial product twice contracted. For an ellipsoidal particle, $\lambda = \frac{\beta^2 - 1}{\beta^2 + 1}$ where $\beta$ is the aspect ratio of the ellipsoid defined as the ratio between the major and minor axes of the ellipsoid.

The last term in equation (3) has the form of an isotropic rotary diffusion with diffusivity $D$. Folgar and Tucker modeled the change in orientation caused by fiber-fiber interaction in the semi-concentrated regime by means of this isotropic rotary diffusion. Based upon their observations of fiber behavior in semi-concentrated suspensions, Folgar and Tucker suggested that the rotary diffusivity could be represented as $C_l \dot{\varepsilon}$, where $\dot{\varepsilon}$ is the magnitude of the strain-rate tensor and $C_l$ is the interaction coefficient, a dimensionless number taken to be a property of the suspension. Because the model is empirical there is no way, set apart direct simulation, to predict the value of $C_l$. Small values ($<10^{-2}$) typically provide a good fit to experimental fiber orientation data.

2.2 Rheological constitutive equation

The rheological constitutive equation for suspensions of axisymmetric particles can be represented as follows for a quadratic closure approximation:

$$\tau_{ij} = 2\eta \varepsilon(v)_{ij} + 2\eta N_p (\varepsilon(v)_{ij} a_{ij}) a_{ij}$$

where $\tau_{ij}$ represent the deviatoric stress tensor, $\eta$ is the solvent viscosity. The coefficient $N_p$ which depends on particle volume fraction $\phi$ and shape factor $\beta$, is dimensionless parameters called “the particle number” and represents the anisotropic contribution of the fibers.

The full set of governing equation is obtained by adding the balance equations for mass and momentum to the constitutive equations for stress and orientation. Assuming an incompressible fluid and neglecting inertia and body forces, the balance equations are:

$$v_{ij} = 0$$

$$\sigma_{ij} = 0$$

$$\tau_{ij} = -P \delta_{ij} + \tau_{ij}$$

where $v_i$ is the $i$th component of the velocity, $\sigma_{ij}$ the Cauchy stress tensor and $P$ the hydrostatic pressure.

3 COMPUTATIONAL METHODS

The computations are made with Rem3d package, which uses a decoupled approach. That means that the problem is solved in two steps: the first step involves solution of the mechanical problem (5), (6) assuming an isotropic orientation at the first step or the orientation determined at the previous time. A classical mixed finite element method [7] is used in which the extra-stress term is implicitly considered; the second step involves the computation of fiber orientation due to velocity field obtained in the previous step. At each time step, the evolution equation (3) is solved by a space-time discontinuous
Galerkin method [8]. The moving free surface is also calculated at each time step by solving a convection equation associated to the characteristic function which defines the fluid domain.

4 NUMERICAL RESULTS

4.1 Planar Contraction flows

We consider an axisymmetric contraction. Lipscomb and al. [9] have shown experimentally that adding slender fibers to a Newtonian fluid greatly enhanced the size and strength of the corner vortex, even for low Reynolds numbers. As shown in Fig. 1 a long tube of half height $H = 10 \text{mm}$ is connected to a smaller tube of height $h = 1.25 \text{mm}$ giving a contraction ratio of 8. The mesh has an upstream tube length of $L_1 = 2H$ and a downstream length of $L_2 = L_1$. A flow rate is imposed at the inlet, placed at $x = -20$ and it corresponds to a parabolic velocity field (Fig. 3). A fully developed Poiseuille flow is also assumed up-and downstream of the contraction, with no-slip boundary conditions imposed along the wall, and symmetry conditions along the axis defined by $y = 0$. An isotropic orientation is imposed in the inlet, the interaction coefficient and the fiber aspect ratio are respectively $C_I = 0.001$ and $\beta = 10$. As shown in Fig. 1a, a small vortex is present in the corner. Fig. 1b shows a coupled solution with $N_p = 10$ and a greater vortex in the corner.

![Computed streamlines through a contraction](image)

(a)

(b)

Fig. 1. Computed streamlines through a contraction:
(a): decoupled case, (b) coupled case with $N_p = 10$

4.2 Injection molding flows

A rectangular cavity having holes are filled with a pseudo plastic fluid. The process conditions are the following: injection temperature $T_{\text{inj}} = 260^\circ \text{C}$, mold-wall temperature $T_m = 30^\circ \text{C}$, and the imposed flow-rate $d = 200 \text{mm}^3/\text{s}$. Moreover the fibers have initially a random orientation state; the shape factor and the interaction coefficient are respectively $\beta = 10$ and $C_I = 10^{-2}$. Finally the closure approximation is quadratic and $N_p = 0$.

![Evolution of the first orientation component at different filling steps](image)

Fig. 2: Evolution of the first orientation component at different filling steps

As shown in Fig. 2, the orientation is isotropic (spherical ellipses) in the empty domain (initial state). The evolution of the first tensor components $(a_{xx})$ in the fluid is plotted and the fountain flow effect is pointed out. It induces an orientation transverse to the flow direction and the last picture shows that the fibers are aligned with the interface of material fronts. In this way, the mechanical weakness of these regions can be explained.
4.3 3D divergent flows

This example looks at the orientation after a classical inlet die. It corresponds to a 3D divergent sprue with ratio 4:1. In Fig. 3, the isovales of the first components of orientation tensors are plotted in the half mid-plane. It is shown that after the divergent part, the fibers are less orientated in the core region. Moreover this difference of orientation between the core and the wall increases with the coupling.

Fig. 3: Evolution of the first orientation component in a divergent die: (a): decoupled case, (b) coupled case with \( N_p = 20 \)

5 CONCLUSIONS

Finite element methods for computing free surface flows of reinforced polymer are used. Theses methods are able to compute fiber suspensions flows involving a moving free surface. The first example point out the influence of the coupling between the fluid and fiber in a contraction die. The second example devoted to injection molded parts describes the influence of fountain flow on fiber orientation. The last example shows the influence of sprue inlet on the skin-core effect. Computations for industrial molds are in progress and will be displayed during the meeting.

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