ON THE RELEVANCE OF THE JEFFERY AND THE FOLGAR & TUCKER MODEL IN THE SIMULATION OF SHORT FIBER SUSPENSIONS KINEMATICS

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Abstract
Numerous composite forming processes rely on the flow of short fibers suspensions such as the SMC. It has been proven that the final properties of the parts depend strongly on the final state of the microstructures, namely the fiber orientation and distribution. Then, reliable simulation tools have to be developed to predict the microstructure kinematics all along the process and in the whole part. Actually, most of the codes dealing with flowing particle suspensions use the kinematics derived by Jeffery in 1922 completed by a diffusion term introduced by Folgar & Tucker, that aims at mirroring fiber-fiber interactions in the semi-concentrated regime. However, the hypotheses on which relies these models are not adapted to the real cases encountered in the material forming processes. In this work, using the simulation of the SMC process as framework, the classical Jeffery and Folgar & Tucker model are analyzed using a kinetic theory based approach, testing the model hypotheses influence on the fiber kinematics. Finally, a first attempt to model SMC processes based on the previous framework is proposed.

1. Introduction

Numerous composite forming processes rely on the flow of short fiber suspensions such as the compression moulding of SMC, a composite manufacturing process largely considered in the automotive industry because of its high volume capabilities. In SMC processes, a charge of a composite material, which consists of a matrix reinforced with chopped glass fibres or carbon fibre bundles and fillers, is placed on the bottom half of the preheated mould. The upper half of the mould is closed rapidly at a speed of about 40 mm/s that causes the charge to flow inside the cavity.

It has been proven that the final properties of the parts depend strongly on the final state of the microstructures, namely the fiber orientation and distribution. The process simulation must then track the entire suspension flow history in order to be able to predict the final reinforcement structure as the defects generated by such a process are directly linked to the fiber orientation and distribution: (i) as the fibres tend to align themselves along the weld line (junction of two flow fronts), the part has poor mechanical properties normal to them; (ii) the fiber segregation results in regions in which the resin appears free of fibers, etc.

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When analyzing the process experimentally, different flow regimes are identified. At the beginning, the fiber suspension is dilute (or semi-dilute) and then the movement of fiber and the fluid remains indiscernible. All along the process, the fiber concentration increases and, at the end, when it is extremely high, percolated network of fiber contacts is established all along the suspension, fibers cannot move anymore and then the fluid flows throughout the rigid or moderately deformable entangled fibers skeleton, like a fluid flowing through a porous medium. In between these two limit cases, one could expect that fibers move but with a velocity lower than the one of the suspending fluid. Then, in order to predict the microstructure kinematics all along the process and in the whole part, the simulation tools developed have to be able to go from dilute fiber suspension regime to entangled net of fiber with fluid flowing through it.

1.1. On the fiber kinematics

Nowadays, most of the industrial codes dealing with flowing particle suspensions use the kinematics derived by Jeffery in 1922 [1] (at the microscopic scale) completed by a diffusion term introduced by Folgar and Tucker (at the macroscopic scale) [2], that aims at mirroring fiber fiber interactions in the semi-concentrated regime. However, taking a look at the hypotheses (**Hi**) on which relies the Jeffery kinematics, one can rapidly note that this model seems not adapted to the real cases encountered in tSMC for example:

H1 : Dilute to semi-dilute suspension. We just show that the fiber concentration increases all along the process to reach very concentrated regime;

H2 : Newtonian suspendant fluid. In most of the forming processes, the matrix used is visco-elastic;

H3 : Velocity gradient constant along the fiber (that implies an absence of size effect). Composite parts formed by SMC are plates and shells which implies a part thickness in the order of magnitude of the fiber length. Then, during the forming process, the fibers are immersed in flows having a characteristic length comparable to the fiber one;

H4 : Particles are rigid spheroids. Particles are generally fibers (spheroid with an infinite form ratio) which can deform (mainly bending) during the flow;

H5 : Flow in infinite media. As said for the third assumption, the flow occurs in a thin mold constituting a confined media for the suspension.

In this work, the different regimes observed during SMC process are studied separately and the associated models tested, using a generic micro to macro framework described in Section 2.1. Finally, a generalized flow model bridging the different flow regimes is proposed.

2. Process beginning: Dilute / semi-dilute flow regime

In the dilute and semi-dilute cases, the flow model of the suspension can then be described using the four following equation defined in $\Omega_f(t)$:

$$\begin{cases} \nabla\cdot\boldsymbol{\sigma} = \mathbf{0} \\ \nabla\cdot\mathbf{v} = 0 \\ \boldsymbol{\sigma} = -P\mathbf{I} + 2\eta\mathbf{D} + 2\eta N_p\mathbf{a}^{(4)} : \mathbf{D} \\ \frac{D\mathbf{a}}{Dt} = \nabla\mathbf{v}\cdot\mathbf{a} + \mathbf{a}\cdot(\nabla\mathbf{v})^T - 2a^{(4)} : \mathbf{D} - 6D_r\left(\mathbf{a} - \frac{\mathbf{I}}{3}\right) \end{cases}, \qquad (1)$$

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where the first two equations are the equilibrium and the fluid incompressibility, the third is the constitutive equation related to the macroscopic micro-structural description of the suspension (whose derivation is described in detail in [3]). The fourth describes the evolution of the microstructure (orientation tensor evolution equation) based on the classical Folgar & Tucker model. In what follows, the derivation of this last equation is going to be described and analyzed in detail.

2.1. Generic micro to macro framework

At the microscale, each fiber is modeled as a rod and two beads located at both rod ends. The microstructure is described by the centre of gravity location and the unitary vectors defining the orientation of each fibers of the suspension, $\mathbf{x}_i^G$ and $\mathbf{p}_i, i = 1 \cdots N$ respectively. The evolution of the microstructure is then described by deriving the evolution of these $\mathbf{p}_i, i = 1 \cdots N$. In the classical case of a dilute non Brownian suspension of rigid fibers, the rod is only subjected to hydrodynamic forces that are assumed to apply on the beads. The forces and torques balance on the rod implies that i) the rod center of gravity moves at the same velocity as the fluid at this point and ii) the rod orients with the kinematics predicted by Jeffery [1] :

$$\dot{\mathbf{p}}_i = \nabla\mathbf{v} \cdot \mathbf{p}_i - \left(\mathbf{p}_i^T \cdot \nabla\mathbf{v} \cdot \mathbf{p}_i\right) \mathbf{p}_i \tag{2}$$

At the mesoscale, using kinetic theory principles, the microstructure is described at a certain location $\mathbf{x}$ and time t from the orientation distribution function $\psi(\mathbf{x}, t, \mathbf{p})$ giving the fraction of rods that, at position $\mathbf{x}$, and time t are oriented in the direction $\mathbf{p}$. The balance ensuring the rods conservation implies:

$$\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial\mathbf{x}}(\dot{\mathbf{x}}\psi) + \frac{\partial}{\partial\mathbf{p}}(\dot{\mathbf{p}}\psi) = 0 \tag{3}$$

with $\dot{\mathbf{x}}$ and $\dot{\mathbf{p}}$ defined by the expressions derived at the microscale: $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t)$ and Equation (2). Eq. (3), known as Fokker-Planck equation, is a well balanced compromise between the macroscopic scale that defines the overall process, and a finer microscopic information describing the rods kinematics. The price to pay is the increase of the model dimensionality.

At the macroscale, the orientation distribution function is substituted by its moments defined in standard physical domains, i. e. involving space and time but averaging the conformational coordinates. Because of the possible symmetric description of a fiber, the first moment vanishes. Then, the commonly used macroscopic descriptor for the suspension is the second order moment of the distribution function, know as the orientation tensor [4]:

$$\mathbf{a}^{(2)} = \int_{\mathcal{S}(0,1)} \mathbf{p} \otimes \mathbf{p}\, \psi \, d\mathbf{p} \tag{4}$$

whose evolution reads, in the case of a non-brownian dilute suspension of rigid fibers:

$$\dot{\mathbf{a}}^{(2)} = \nabla\mathbf{v} \cdot \mathbf{a}^{(2)} + \mathbf{a}^{(2)} \cdot (\nabla\mathbf{v})^T - 2\mathbf{a}^{(4)} : \nabla\mathbf{v} \tag{5}$$

where $\mathbf{a}^{(4)}$ is the fourth order moment of the distribution. In order to limit the calculation complexity and because the second order moment of the distribution is (a priori) sufficient to describe the microstructure, closure relations are used to express the fourth order moment as a function of the lower order moments. For the sake of notational simplicity in the sequel the exponent $^{(2)}$ will be omitted and the orientation tensor will be referred as $\mathbf{a}$.

To obtain the orientation tensor evolution equation given in Equation (1), a diffusion has been added by Folgar & Tucker in order to mimic the effect of fiber fiber interactions, whose macroscopic counterpart results:

$$\dot{\mathbf{a}}^{(2)} = \nabla\mathbf{v} \cdot \mathbf{a}^{(2)} + \mathbf{a}^{(2)} \cdot (\nabla\mathbf{v})^T - 2\mathbf{a}^{(4)} : \nabla\mathbf{v} - 6D_r\left(\mathbf{a} - \frac{\mathbf{I}}{3}\right) \tag{6}$$

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with D_r the diffusion coefficient that scales linearly with the shear rate and the fiber concentration. However, as said in the introduction, this equation relies on numerous hypotheses that are not fulfilled in the SMC process case. To check the relevance to use this equation in our SMC simulations, each of the hypotheses have been studied separately in the generic framework just described and its influence on the microstructure kinetics prediction has been observed.

2.2. On the relevance of the Folgar & Tucker model

Each of the hypothesis used by Jeffery to derive his equation (**Hi**) has been studied, *i.e.* the appropriate physics have been introduced at the microscale and their impact on the evolution of **a** has been studied [5–8]. The main conclusions in term of fiber orientation predictions are:

1. The Folgar & Tucker model is appropriate to account for the interactions occurring in concentrated suspensions, using a diffusion coefficient scaling linearly with the shear rate and the fiber concentration.
2. When the suspendant fluid is non-newtonian, at low Weisenberg number, the Folgar & Tucker model is not appropriate as it does not predict the correct direction of alignment of the fibers (which in this case is no more in the flow direction but in the vorticity one). However, in the case of forming processes where the Weisenberg number tends to large values, this deviation is no more observed as in this case the fibers recover an alignement in the shear direction.
3. In order to take into account the fiber bending and in particular the fiber breakage during the flow, the calculation of the bending energy in the suspension appears as a reasonable route in terms of computing time and model complexity.
4. In the case of confined distributions, the orientation tensor **a** used to described the distribution at the macroscale seems no more relevant and renders inaccurate predictions based on the Folgar & Tucker model. However, as the orientation tensor is the usual descriptor of fibers suspension, instead of proposing new descriptors, in first approximation, new evolution laws have been proposed based on lubrication hypothesis or more phenomenological considerations.

Finally, in the first part of our SMC process simulations, the Folgar & Tucker model appears to be a good compromise to be used as it is appropriate to mirror the fiber-fiber interactions and as the non-Newtonian character of the fluid does not influence the microstructure kinematics. The increase of the fiber concentration along the process is also easily taken into account using an appropriate law for the diffusion coefficient D_r evolution.

3. Process final configuration: concentrated percolated regime

At the end of the process, however, the fibers do not move anymore and therefore the fluid flows through the porous medium associated to the entangled fibrous skeleton, flow that can be described by using the standard Darcy's model defined in $\Omega_f(t)$:

$$\begin{cases} \nabla \cdot \mathbf{v} = 0 \\ \mathbf{v} = -\mathbf{K}(\psi(\mathbf{p}))\nabla P \end{cases}, \tag{7}$$

where $\mathbf{K}(\psi(\mathbf{p}))$ represents the permeability that depends on the fiber orientation distribution $\psi(\mathbf{p})$.

The objective is now to bridge these two extreme case to obtain a continuous evolution of the fluid and the microstructure behaviors.

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4. Generalized model bridging the flow regimes

In between the two limits case previously presented, intense hydrodynamic interactions and contacts are at the origin of a relative velocity between the fibers and the suspending fluid. In order to control this relative velocity we consider an extended micro-mechanical model where an extra force applies on the rod centre of gravity that scales with the relative velocity between the fiber and the mould velocity. We consider the mould velocity because when the contacts percolation occurs it is expected that fibers remains at rest with respect to the moud in which the flow takes place. In this case, the torques and forces balances lead to a relative velocity between the fiber and the fluid: $\mathbf{v}_r = \mathbf{v}_0 - \mathbf{v}_G = (1-\alpha)\mathbf{v}_0$, where α is a parameter mirroring the relative importance of the hydrodynamic forces to the hydrodynamic interactions.

Moreover, in that situation the flow is constituted of one contribution coming from the suspension flow with a velocity that coincides with the one of the fibers, and another one, in which the fibers are assumed at rest and the fluid flows through the fibrous skeleton with the fluid/fibers relative velocity. The fluid velocity is denoted by $\mathbf{v}$, the one of the fibers that defines the suspension velocity by $\mathbf{v}^s$ and the relative velocity of the fluid with respect to the fibers by $\mathbf{v}^r$. As discussed in Section 2 we have the equalities:

$$\begin{cases} \mathbf{v} = \mathbf{v}^s + \mathbf{v}^d \\ \mathbf{v}^s = \frac{\xi}{\xi+\mu}\mathbf{v} = \alpha\mathbf{v} \\ \mathbf{v}^r = \frac{\mu}{\xi+\mu}\mathbf{v} = (1-\alpha)\mathbf{v} \end{cases} . \tag{8}$$

Now, by adding the pressure drop related to both flow contributions (both contributions are assumed acting in parallel like in the Kelvin-Voigt viscoelastic model)

$$\nabla P = \eta\Delta\mathbf{v}^s + 2\eta N_p \nabla\cdot((\mathbf{D}^s : \mathbf{a})\mathbf{a}) - \mathbf{K}^{-1}(\mathbf{a})\cdot\mathbf{v}^d, \tag{9}$$

and writing both velocities $\mathbf{v}^s$ and $\mathbf{v}^r$ as a function of the total fluid velocity $\mathbf{v}$ according to Eq. (8), it results

$$\nabla P = \alpha\left\{\eta\Delta\mathbf{v} + 2\eta N_p\nabla\cdot((\mathbf{D} : \mathbf{a})\mathbf{a})\right\} - (1-\alpha)\left\{\mathbf{K}^{-1}(\mathbf{a})\cdot\mathbf{v}\right\}, \tag{10}$$

that is no more than the Brinkmann model where the viscous and Darcy's contributions are weighted by α and $(1-\alpha)$ respectively.

The flow model must be complemented with the Folgar & Tucker equation governing the evolution of the orientation tensor $\mathbf{a}$ associated to the rods population,

$$\frac{D\mathbf{a}}{Dt} = \nabla\mathbf{v}\cdot\mathbf{a} + \mathbf{a}\cdot(\nabla\mathbf{v})^T - 2\mathbf{A} : \mathbf{D} - 6D_r\left(\mathbf{a} - \frac{\mathbf{I}}{3}\right), \tag{11}$$

and the one governing the evolution of the fluid phase field needed for defining the flow domain at each time $\Omega_f(t)$,

$$\frac{DI}{Dt} = 0. \tag{12}$$

Using this generalized flow model, all the scenarios previously discussed can be addressed as indicated in Table 1.

5. Conclusion

In this work, a 3D modeling framework for SMC process has been proposed. For the fiber orientation prediction, the usually used Folgar & Tucker model has been deeply studied and its hypotheses has

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Flow regime	N_p	D_r	α
Pure fluid	0	–	1
Dilute	> 0	0	1
Semi-dilute	> 0	> 0	1
Semi-concentrated to concentrated non-percolated	> 0	> 0	< 1
Concentrated percolated	–	–	0

Table 1. Bridging model parameters for the different flow regimes.

been tested in the case of real process conditions. It appears finally that the interactions and the non-Newtonian character of the matrix are well taken into account by this model (in the SMC modeling), but the flow confinement remains a tricky issue as the orientation tensor model seems no more relevant in this condition.

Finally, a generalized model allowing to go from the dilute suspension regime at the beginning of the process to the fluid flow through fiber network regime at the end has been proposed as a all-in-one model of the SMC process.

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