Composites Part A 115 (2018) 112–122

Contents lists available at ScienceDirect

Composites Part A

journal homepage: www.elsevier.com/locate/compositesa

# A new anisotropic viscous constitutive model for composites molding simulation

Anthony J. Favaloro[a,*], Huan-Chang Tseng[b], R. Byron Pipes[a]

[a] Composites Manufacturing and Simulation Center, Purdue University, West Lafayette, IN, United States
[b] CoreTech System (Moldex3D) Co., Ltd., ChuPei City, Hsinchu, Taiwan

ARTICLE INFO

*Keywords:*
A. Fibres
B. Directional orientation
B. Viscosity
C. Process simulation

ABSTRACT

Simulation methods, particularly those implemented in commercially available software, for the prediction of flow and fiber orientation in polymer composites molding processes typically neglect the coupling between flow and orientation which presents as anisotropic viscosity due to reinforcing fibers. While several particular solutions have been performed for simple geometries, the application of tensor based anisotropic constitutive behavior presents solution difficulties; thus, any potential consequences of neglecting coupling have been accepted in favor of developing and implementing additional complexity to the orientation evolution models. Here, a simple model is presented by which flow and orientation analysis can be coupled through a scalar viscosity function such that minimal adjustment to existing solvers is required for implementation.

## 1. Introduction

Understanding the final microstructure of parts produced through molding of fiber reinforced polymers is critical to understanding the resulting part performance [1]. In particular, injection moldings tend to display the so-called shell-core orientation structure in which the material near boundaries has experienced large shear, orientating fibers nearly in the flow direction, while material near the midplane experiences cross flow, producing an orientation state perpendicular to the flow direction [2,3]. The relative width of the core region then plays a critical role in the resulting part performance. It has been observed in long fiber thermoplastics that the core width is significantly increased as compared to short fiber thermoplastics [4,5]. Typically, modeling efforts to account for this observed increase in core width assume the flow field determined using orientation state independent, isotropic viscosity is correct and, thus, modify the expressions for orientation state evolution [6–8]. However, the problem of large core width has recently been addressed through the use of an isotropic yield stress in the viscosity definition [9] with the origin of the yield stress having been shown to be a result of inter-fiber or inter-bundle friction [10,11]. This investigation challenges the assumption that flow fields have been calculated correctly using unmodified, as compared to neat fluid, viscosity models, though parameters may have been adjusted.

In a similar fashion to orientation state affecting the performance of final parts, the evolving microstructure in flow processes is known to affect rheological properties [12–14] through anisotropic viscosity. In compression molding of glass mat thermoplastic (GMT), the investigations of Ericsson et al. [15] and Dweib and O'Brádaigh [16] both observe the development of elliptical flow fronts from initially circular disks due to initially anisotropic orientation states. Ericsson et al. [15] develop a simple model by which the ratio of in-plane extension rates can be determined, while Dweib and O'Brádaigh [16] show that the anisotropic nature of the GMT must be modeled to compare with experimental closure forces.

In this work, the authors propose that both effects, namely increased core width in long fiber thermoplastics and flow primarily transverse to the direction of largest alignment, are inherently coupled to the anisotropic nature of the suspension. However, contrasting prior investigations into the effect of coupling anisotropic viscosity and flow [17,18] which have suffered numerical difficulty when considering highly anisotropic fluids, a semi-phenomenological approach is taken to determine an appropriate method of coupling an isotropic viscosity model with the orientation state and deformation mode rooted in the established rheological models. Costa et al. [19] have previously demonstrated such a model through a proof-of-concept viscosity definition that is dependent on orientation state only, though the model was not based in established rheology. Maintaining an isotropic form of the constitutive behavior provides a necessarily simplification for numerical investigations. To this end, the development of a scalar viscosity model for suspensions that is a function of both the orientation state and deformation is presented. Additionally, a method by which the

* Corresponding author.
*E-mail address:* afavalor@purdue.edu (A.J. Favaloro).

https://doi.org/10.1016/j.compositesa.2018.09.022
Received 10 July 2018; Received in revised form 18 September 2018; Accepted 23 September 2018
Available online 25 September 2018

non-linearity of the matrix fluid may be coupled to the orientation state and deformation mode is investigated. These models have been implemented in a research version of the commercial software Moldex3D and have been applied to the problems of a compression molding center-gated disk and an injection molding center-gate disk.

## 2. Theoretical background

### 2.1. Orientation state representation & evolution

A single fiber is typically considered a cylindrical rod or a prolate spheroid. The orientation of a fiber is then completely described by a unit vector along the long axis of the fiber, $\mathbf{p} = p_i$. An orientation distribution function, $\psi(\mathbf{p})$, can be used to describe a large number of a fibers in a given volume [20]. However, for tractability in numerical solutions, Advani and Tucker [21] introduced the use of the second order orientation tensor:

$$\mathbf{A} = A_{ij} = \langle p_i p_j \rangle = \oint \psi(\mathbf{p}) p_i p_j \mathrm{d}\mathbf{p} \tag{1}$$

as the primary descriptor of orientation state. The second-order orientation tensor has all positive eigenvalues and trace of unity. Thus, $\mathbf{A}$ represents only five independent variables. A *collimated* orientation state is represented by the largest eigenvalue of $\mathbf{A}$ being equal to unity (i.e. all fibers are perfectly aligned along a particular direction), and a 3D isotropic orientation state is represented by . The fourth order orientation tensor is similarly defined as

$$\mathbb{A} = \mathbb{A}_{ijkl} = \langle p_i p_j p_k p_l \rangle = \oint \psi(\mathbf{p}) p_i p_j p_k p_l \mathrm{d}\mathbf{p} \tag{2}$$

While the $\mathbb{A}$ cannot be uniquely defined in terms of $\mathbf{A}$, the eigenvalue based orthotropic fitted closure (EBOF) of Cintra and Tucker [22] or the invariant based orthotropic fitted closure (IBOF) of Chung and Kwon [23] are typically used to approximate $\mathbb{A}$ in terms of $\mathbf{A}$ based on typical flow fields and a 3D isotropic initial conditions. Herein, the IBOF-5 closure presented in the Appendix of Ref. [23] by Chung and Kwon is used for all numerical calculations. Jack and Smith [24] have investigated the error associated with closure approximations and found the IBOF-5 to be near the lowest possible error for a fourth order closure approximation as compared to orientation distribution based calculations over a wide range of flow types.

Orientation evolution in response to deformation is based in Jeffery's hydrodynamic (HD) equation for prolate spheroids [12,13] followed by the addition of interaction behavior through rotary diffusion (DIFF) [6,7,20,25–27] and reduced orientation kinetics (ROK) [6,8,28]. Thus, the material derivative of $\mathbf{A}$ is expressed as a superposition of effects as

$$\dot{\mathbf{A}} = \dot{\mathbf{A}}^{\mathrm{HD}} + \dot{\mathbf{A}}^{\mathrm{DIFF}} + \dot{\mathbf{A}}^{\mathrm{ROK}} \tag{3}$$

The first term, being a result of Jeffery hydrodynamics, is

$$\dot{\mathbf{A}}^{\mathrm{HD}} = \mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W} + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbb{A}:\mathbf{D}) \tag{4}$$

where $\mathbf{L} = \mathbf{L}_{ij} = \partial\mathbf{u}_i/\partial\mathbf{u}_j = \nabla\mathbf{u}$ is the velocity gradient tensor, $\mathbf{W} = (\mathbf{L} - \mathbf{L}^{\mathrm{T}})/2$ is the vorticity tensor, $\mathbf{D} = (\mathbf{L} + \mathbf{L}^{\mathrm{T}})/2$ is the rate of deformation (or strain rate) tensor, and $\xi$ is a shape factor dependent on fiber aspect ratio typically set to unity. Extending the work of Folgar and Tucker [20], Phelps and Tucker [25] give a form for $\dot{\mathbf{A}}^{\mathrm{DIFF}}$ as

$$\dot{\mathbf{A}}^{\mathrm{DIFF}} = \dot{\gamma}[2\mathbf{D}_r - 2\mathrm{tr}(\mathbf{D}_r)\mathbf{A} - 5(\mathbf{D}_r\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D}_r - 2\mathbb{A}:\mathbf{D}_r)] \tag{5}$$

where $\dot{\gamma} = \sqrt{2\mathbf{D}:\mathbf{D}}$ is the strain rate magnitude of the suspension and $\mathbf{D}_r$ is a second order spatial tensor. The Folgar-Tucker model is recovered when $\mathbf{D}_r = C_I\mathbf{I}$ where $C_I$ is the interaction coefficient. Phelps and Tucker give $\mathbf{D}_r$ for anisotropic rotary diffusion (ARD) in their model as

$$\mathbf{D}_r = b_1\mathbf{I} + b_2\mathbf{A} + b_3\mathbf{A}^2 + b_4\mathbf{d} + b_5\mathbf{d}^2 \tag{6}$$

where $b_1$-$b_5$ are treated as constant coefficients and $\mathbf{d} = \mathbf{D}/\dot{\gamma}$ is a normalized rate-of-deformation tensor. As $\mathbf{d}$ is the rate-of-deformation tensor with the strain rate divided out, it encodes only the principal axes and relative magnitudes of the principal deformations. Thus, we defined $\mathbf{d}$ as the deformation mode. In this way, the ARD model depends upon deformation mode and orientation state. Tseng et al. [7] give $\mathbf{D}_r$ for the iARD model as

$$\mathbf{D}_r = C_I(\mathbf{I} - 4C_M\mathbf{d}^2) \tag{7}$$

depending on upon deformation mode where $C_I$ and $C_M$ are typically treated as constant parameters, though recent modeling efforts have utilized strain rate dependence [28]. Similarly, Tseng et al. have developed the pARD model depending only upon orientation state [26]. Finally, the diffusion model of Koch bears relevance to the topic of this work [27]. Koch gives a form for $\mathbf{D}_r$ as

$$\mathbf{D}_r = k_1(\mathbf{d}:\mathbb{A}:\mathbf{d})\mathbf{I} + k_2(\mathbf{d}:\mathscr{A}:\mathbf{d}) \tag{8}$$

where $\mathscr{A}$ is the sixth-order orientation tensor with similar definition to the second- and fourth-order orientation tensors. While appropriate closure models exist [29–33], the Koch model introduces the difficulty and computational expense of approximating $\mathscr{A}$ while providing limited benefits compared to the Folgar-Tucker model [25]. Specifically, when $k_2 = 0$, the Koch model reduces to an isotropic diffusion similar to the Folgar-Tucker model but with orientation state and deformation mode dependent magnitude through the kernel $(\mathbf{d}:\mathbb{A}:\mathbf{d})$. This kernel describes the degree to which stretching is along fiber axes. When stretching along fiber axes, the Koch model would predict stronger diffusion than when stretching is dominantly transverse to fiber axes. Next, to account for the discrepancy between orientation evolution rates in experimental observations and models, Wang et al. [8] have developed the reduced strain closure (RSC) model while Tseng et al. [6] have developed the retarding principal rate (RPR) model. The RPR model has the form

$$\dot{\mathbf{A}}^{\mathrm{ROK}} = -\mathbf{R}\cdot\alpha\dot{\Lambda}\cdot\mathbf{R}^{\mathrm{T}} \tag{9}$$

where $\mathbf{R}$ is the rotation matrix associated with the eigendecomposition of $\mathbf{A}$, $\dot{\Lambda}$ is the similarly ordered, diagonal, eigenvalue rate of change matrix as calculated by previous effects, and $\alpha$ is a modeling parameter. In this way, the RPR is always applied as the final orientation evolution term. The RSC and RPR models are equivalent provided the term $\kappa$ in the RSC model is set equal to $1-\alpha$. Again, $\alpha$ is generally treated as constant but has recently been utilized with strain rate dependence [28].

### 2.2. Fluid dynamics

In molding simulations under the assumption of creeping flow, the governing equations of the fluid mechanics which describe the transient flow motions are given as [34]:

$$\begin{gathered}\frac{\partial\rho}{\partial t} + \nabla\cdot\rho\mathbf{u} = 0\\ \frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u} - \sigma) = \rho\mathbf{g}\\ \boldsymbol{\sigma} = -P\mathbf{I} + \eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\end{gathered} \tag{10}$$

where $\rho$ is the density, $t$ is the time, $\boldsymbol{\sigma}$ is the total stress tensor, $\mathbf{g}$ is the gravitational acceleration vector, $P$ is the pressure, and $\eta$ is the isotropic viscosity. Typically, the isotropic viscosity is measured for a particular flow case; therefore, it is a measure of an effective viscosity of the suspension in that particular flow case. This is a deficiency of uncoupled approaches addressed in this work. The 3D finite volume method (3D-FVM) technique is adopted in Moldex3D to solve the governing equations efficiently and robustly for complex geometries. Specific details on the 3D-FVM are available in Ref. [35].

### 2.3. Anisotropic viscosity models

In the following, the notation of Beaussart et al. [36] that has direct