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The use of shear-rate-dependent parameters to improve fiber orientation predictions for injection molded fiber composites

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Fiber orientation distribution in injection molded fiber composites has an important shell-core structure. Recently, significant theoretical orientation models, including RSC (Reduced Strain Closure), ARD (Anisotropic Rotary Diffusion), and iARD-RPR (improved ARD and Retarding Principal Rate), have been widely applied in commercial injection molding simulation software. However, there is a long-running problem requiring an urgent solution for the state-of-the-art predictive models: obvious deviation of fiber orientation was found in the core region, although the orientation in the shell layer was predicted well. According to the fiber motions of flow-induced orientation, we therefore aimed to introduce a relationship between the model parameters and the shear rate. As validation, the shear-rate-dependent parameters can effectively enhance the prior orientation results for short-glass-fiber composites and long-carbon-fiber-composites in injection molding simulations, with good agreement between the present predictions and the experimental data obtained thereby.

1. Introduction

Reducing vehicle weight by using lighter materials is a popular approach for improving fuel efficiency. Due to their ability to enhance mechanical performance as well as satisfy safety and durability requirements, fiber-reinforced-thermoplastic (FRTP) compounds are now commercially available as candidate materials. In general, the shell-core structure, as the orientation structure of the flow-induced orientation of fibers, is found in injection molded parts [1].

The classical hydrodynamic theory of a single axisymmetric fiber originated with the pioneer Jeffery [2] and was modified by Folgar and Tucker [3–5] in relation to the consideration of isotropic rotary diffusion (IRD) or the fiber-fiber interaction in concentrated suspensions. For state-of-the-art predictive engineering tools, the Folgar-Tucker equation has become a standard model for predicting flow-induced fiber orientation patterns in the injection molding simulation of fiber thermoplastic composites. Recently, there have been a significant number of objective theoretical models of fiber orientation; they include: RSC (Reduced Strain Closure) model [6], ARD-RSC (Anisotropic Rotary Diffusion and Reduced Strain Closure) model [6,7], iARD-RPR (Improved Anisotropic Rotary Diffusion and Retarding Principal Rate) model [8–10], which were developed in the field of suspension rheology. The modern orientation models have been incorporated into commercial injection molding simulation software, such as Autodesk Simulation MoldFlow Insight (ASMI) and Moldex3D (CoreTech System Co. of Taiwan).

However, some studies [11,12] have investigated the weaknesses and flaws in the RSC model due to the obvious deviations in fiber orientation between the simulation and actual experiment found in the core region, although the orientation in the shell layer was predicted fairly well. Over the last decades, the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge National Laboratory (ORNL) in the U.S. DOE (Department of Energy) Vehicle Technologies project of Lightweight Materials [13] have sought solutions to the long-running problem in using the RSC because inaccurate predictions of fiber orientation directly yielded non-reliable estimations of mechanical properties. In order to resolve this issue, the ASMI provided the inlet condition function set on the gate to improve the fiber orientation predictions in the injection molding simulation for the PNNL project of Nguyen et al. [14]; the inlet condition strongly influences the RSC predictions.

The iARD-RPR model and the RSC model are identical, given their specific values [8,9]. Unfortunately, the overestimation of fiber orientation (the degree of fiber alignment is higher than experimental data) at the core region was a result in the iARD-RPR model [15]. To solve this aspect of the prediction inaccuracy, therefore, we

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proposed a physical picture of the flow-induced orientation, and newly introduced a relationship between the shear-rate and the iARD-RPR orientation model parameters. To date, researchers have had no intention to consider such shear-rate-dependent orientation parameters. This point obviously differs from the previous method of setting a specific inlet condition at the gate, which is the solution implemented for the problem in MoldFlow.

2. Theoretical background

A single fiber is regarded as a rigid cylindrical rod. The short-fiber and long-fiber lengths are typical 0.2–0.4 mm and 10–13 mm in fiber composite pellets with 2–3 mm diameter, respectively. The post-extruded average fiber length longer than 1 mm is generally considered as long fiber [7]. The fiber's unit vector $\mathbf{p}$ along its axis direction can describe the fiber orientation. For a concise representation of the orientation of a large population of fibers, Advani and Tucker [4] defined the second-rank orientation tensor as:

$$\mathbf{A} = \oint \psi(\mathbf{p})\mathbf{pp}d\mathbf{p} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{12} & A_{22} & A_{23} \\ A_{13} & A_{23} & A_{33} \end{bmatrix} \tag{1}$$

where $\psi(\mathbf{p})$ is the probability density distribution function over the orientation space; $\mathbf{A}$ is the symmetric matrix and its trace is $A_{11} + A_{22} + A_{33} + 1$. Physically, $\mathbf{A} = \mathbf{I}/3$ represents the isotropic orientation state, wherein $\mathbf{I}$ is the identity matrix. The diagonal components of the second order orientation tensor, A_{11}, A_{22}, and A_{33}, describe the degree of orientation in flow direction, cross-flow direction, and thickness direction, respectively.

$\mathbf{A}_4$ is the fourth-rank orientation tensor and is symmetric, defined as:

$$\mathbf{A}_4 = \oint \psi(\mathbf{p})\mathbf{pppp}d\mathbf{p}. \tag{2}$$

The $\mathbf{A}_4$ calculation decoupled in terms of $\mathbf{A}$ is obtained by higher order polynomial closure approximations, such as the Eigenvalue-Based Optimal Fitting (EBOF) Closure [16] and the Invariant-Based Optimal Fitting (IBOF) Closure [17,18]. Note that the accuracy of IBOF is as good as EBOF, and IBOF requires less computational time to obtain a solution [17].

Over the last three decades, theoretical researchers in the fiber suspension rheological field have made considerable efforts to determine the dynamic fiber orientation states. In general, the time-evolution equation of the second-rank orientation tensor $\mathbf{A}$ is fixed on the material derivative, denoted as $\dot{\mathbf{A}}$ [4]. The classic Folgar-Tucker IRD model is famous for predicting short fiber orientation. In seeking to achieve completeness, we summarize these modern models below, including the Phelps-Tucker ARD model [7], the Wang-Tucker RSC model [6] and the ARD-RSC model [7], as well as the iARD-RPR model of Tseng et al. [8–10].

2.1. RSC model and ARD-RSC model

In practice, the Folgar–Tucker model predicts a faster response rate of fiber orientation compared to experimental observation [19]. Thereby, Wang et al. [6] developed the RSC model with two parameters (C_I and κ) to slow down the response rate of fiber orientation kinetics:

$$\dot{\mathbf{A}}^{RSC} = \mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W} + \xi\{\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2[\mathbf{A}_4 + (1-\kappa)(\mathbf{L}_4 - \mathbf{M}_4 : \mathbf{A}_4)] : \mathbf{D}\} + 2\kappa\dot{\gamma}C_I(\mathbf{I} - 3\mathbf{A}), \tag{3}$$

$$\mathbf{L}_4 = \sum_{i=1}^{3}\lambda_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i, \tag{4}$$

$$\mathbf{M}_4 = \sum_{i=1}^{3}\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i, \tag{5}$$

where $\mathbf{L} = \nabla\mathbf{v} = \mathbf{W} + \mathbf{D}$ is the velocity gradient tensor with its component of $L_{ij} = \nabla_j v_i$; v_i is the component of the velocity in the x_i direction; $\mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T)$ is the vorticity tensor; $\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T)$ is the rate-of-deformation tensor; $\dot{\gamma}$ is the strain rate, namely $\dot{\gamma} = (2\mathbf{D} : \mathbf{D})^{1/2}$; L_f and d_f are fiber length and fiber diameter, respectively; $a_r = L_f/d_f$ is the fiber aspect ratio; $\xi = (a_r^2 - 1)/(a_r^2 + 1)$ is the particle shape factor, since $a_r >> 1$; and ξ is assumed to signify unity. The Folgar-Tucker fiber-fiber interaction coefficient C_I is experimentally measured between 10^{-2} and 10^{-4} [20,21]. The factor κ constrained between 0 and 1 is a slow-down factor fit by the experimental data, and generally suggested to be in the range of 0.05–0.2 [22]; note that when $\kappa = 1$ the RSC equation can recover to the standard Folgar-Tucker equation. In addition, λ_i and $\mathbf{e}_i$ are eigenvalues and eigenvectors of second-rank orientation tensor $\mathbf{A}$, respectively; and $\mathbf{L_4}$ and $\mathbf{M_4}$ are fourth-rank orientation tensors depending on λ_i and $\mathbf{e}_i$. Wang et al. [6] considered the rheological objectivity of material frame indifference to slow down the orientation rate and widen the core thickness. They employed a scalar factor κ to reduce the rate of eigenvalues for the orientation tensor, while the rate of eigenvectors remains unchanged.

Previously, Phan-Thien et al. [21] proposed that the Folgar–Tucker IRD constant C_I be extended to an ARD tensor $\mathbf{D}_r$. Furthermore, Phelps and Tucker [7] constructed the ARD model:

$$\dot{\mathbf{A}}^{ARD} = (\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbf{A}_4 : \mathbf{D}) + \dot{\gamma}[2\mathbf{D}_r - 2\mathrm{tr}(\mathbf{D}_r)\mathbf{A} - 5\mathbf{D}_r\cdot\mathbf{A} - 5\mathbf{A}\cdot\mathbf{D}_r + 10\mathbf{A}_4 : \mathbf{D}_r] \tag{6}$$

In addition, the ARD model is coupled with the RSC model as ARD-RSC:

$$\dot{\mathbf{A}}^{ARD-RSC} = \mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W} + \xi\{\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2[\mathbf{A}_4 + (1-\kappa)(\mathbf{L}_4 - \mathbf{M}_4 : \mathbf{A}_4)] : \mathbf{D}\} + \dot{\gamma}\{2[\mathbf{D}_r - (1-\kappa)\mathbf{M}_4 : \mathbf{D}_r] - 2\kappa\mathrm{tr}(\mathbf{D}_r)\mathbf{A} - 5(\mathbf{D}_r\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D}_r) + 10[\mathbf{A}_4 + (1-\kappa)(\mathbf{L}_4 - \mathbf{M}_4 : \mathbf{A}_4)] : \mathbf{D}_r\} \tag{7}$$

For the anisotropic rotary tensor $\mathbf{D}_r$, Hand [23] focused a theory of anisotropic fluids and given a general second-order polynomial tensor-valued function form, which depends on the orientation tensor and the rate-of-deformation tensor with nine parameters b_{1-9}:

$$\mathbf{D}_r = b_1\mathbf{I} + \frac{b_2}{\dot{\gamma}}\mathbf{A} + \frac{b_3}{\dot{\gamma}^2}\mathbf{A}^2 + \frac{b_4}{\dot{\gamma}}\mathbf{D} + \frac{b_5}{\dot{\gamma}^2}\mathbf{D}^2 + \frac{b_6}{\dot{\gamma}}(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D}) + \frac{b_7}{\dot{\gamma}}(\mathbf{D}\cdot\mathbf{A}^2 + \mathbf{A}^2\cdot\mathbf{D}) + \frac{b_8}{\dot{\gamma}^2}(\mathbf{D}^2\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D}^2) + \frac{b_9}{\dot{\gamma}^2}(\mathbf{D}^2\cdot\mathbf{A}^2 + \mathbf{A}^2\cdot\mathbf{D}^2) \tag{8}$$

In simplifying it, Phelps and Tucker [7] constrain the b_i coefficients to be scalar constants, and set $b_{6-9} = 0$,

$$\mathbf{D}_r = b_1\mathbf{I} + b_2\mathbf{A} + b_3\mathbf{A}^2 + \frac{b_4}{\dot{\gamma}}\mathbf{D} + \frac{b_5}{\dot{\gamma}^2}\mathbf{D}^2 \tag{9}$$

The RSC and ARD-RSC models have been incorporated into the commercial injection molding simulation software, ASMI. In general, a so-called inlet condition set for the gate is suggested in the ASMI computation of fiber orientation for injection molding simulation, with the aligned orientation at the shell layer and transverse/random orientation at the core region. Wang et al. [24] examined the midplane-mesh computation with ARD-RSC; with an inlet condition set around the gate area, they were able to obtain good orientation predictions of long-carbon-fiber composites. However, the 3D-mesh computation results were not satisfactory.

The ARD-RSC model contains a set of six parameters (κ and b_1-b_5), which can be measured/computed. In principle, the target orientation state chosen is one in which the injection filling flow