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# Improved fiber orientation predictions for injection molded fiber composites



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#### ABSTRACT

Highly concentrated fiber suspensions exhibit complex rheological behaviors. There is a particular broader core region of the fiber orientation structure for fiber-filled parts in the injection molding process. However, there is a long-running problem requiring an urgent solution for the industry: to date, prior state-of-the-art predictive engineering tools have always provided unsatisfactory results pertaining to the narrow core. In accordance with insights derived from experimental results related to fiber suspension viscosity, yield stress viscosity does exist at low shear rates. By introducing the yield stress term to modify the standard Cross-WLF viscosity flow curve, namely the Yield-Cross-WLF, the core region can be realistically widened at present. Regarding validation, we employed the Yield-Cross-WLF viscosity model used in 3D injection molding simulation of an end-gated plaque for the concentrated long-carbon-fiber composite. Significantly, the predicted fiber orientation distributions show strong agreement with the measurements, as well as improvement compared to previous simulation attempts.

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#### 1. Introduction

Long fiber-reinforced thermoplastic (LFRT) composites have become familiar lightweight automotive materials since they satisfy safety and durability requirements. The configuration of the reinforcing fibers, including fiber orientation, fiber length, and fiber concentration, ultimately affects the mechanical performance of the finished part [1]. Primarily, the ability to accurately predict fiber orientation is critical for accurately determining the improvement of the mechanical properties of LFRT products. Over the last decades, the U.S. Department of Energy (DOE) has planned that the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge National Laboratory (ORNL) develop the predictive engineering tools to serve as LFRT accessories in the automotive industry [2,3].

In general, the shell-core orientation structure of fibers is found in injection molded parts. Two shell layers display the preferential orientation parallel to the flow direction, while the fiber orientation at a core region is perpendicular to the flow. Recently, the industrial trend has been moving towards applying a greater high-fiber-concentration (being over 40 wt%) of short/long fiber-reinforced thermoplastic composites in plastic product fabrication. The observations made on the great-width core region are signifi-

cant [4,5]. Such a material is a highly concentrated fiber suspension. However, predicting dramatic fiber orientation states that remains very challenging is a running problem in the industry, so far.

Theoretical models of suspension rheology to determine the anisotropic orientation of long fibers have been developed in which the ARD-RSC (Anisotropic Rotary Diffusion and Reduced Strain Closure) model derived by Tucker and coworkers is an integral part [6–8]. The Autodesk Simulation Moldflow Insight (ASMI) of commercial injection molding simulation software incorporated the ARD-RSC model to predict long fiber orientations. Following these famous orientation models of fiber suspension rheology, Tseng et al. [9–11] achieved a new, objective model, the iARD-RPR (Improved Anisotropic Rotary Diffusion and Retarding Principal Rate), which has been implemented into commercial software of injection molding simulation, such as Moldex3D (CoreTech System Co. of Taiwan).

According to the authoritative reports of PNNL project [2,3] using the ARD-RSC model incorporated in the ASMI mid-plane mesh computation with the inlet condition, the anisotropic orientation predictions for the injection molded long fiber composites evidently exhibited good agreement with the related experimental data. In practice, the 3D-mesh computation is preferable for truly analyzing complex geometric parts as it is superior to the mid-plane mesh model. Unfortunately, the ARD-RSC model in the use of 3D computation has produced unsatisfactory/inaccurate predictions [2,3,8], in which the orientation in the shell layer was

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predicted fairly well, while significant deviation was found in the core region [12].

In order to resolve this issue, the ASMI provided the "3D" inlet-condition function set around the gate to improve the fiber orientation predictions. Up to date, the ASMI proposed the Moldflow Rotational Diffusion (MRD) model [13], which is a modification of the ARD model to improves the prediction of the fiber orientation in 3D. On the other hand, Costa et al. [14] further proposed a preliminary orientation-dependent-viscosity model in order to enhance the predictions related to the fiber orientation core. They assumed that the viscosity is increasingly scaled by a constant factor if the degree of predicted fiber orientation in the flow direction is below a threshold value. It appears that such a simple aspect is intuitive without a serious rheological derivation.

Differing from the previous methods related to the inlet condition and the orientation-dependent-viscosity, here we aimed to understand what an real viscosity flow curve of the highly concentrated fiber suspensions were studied in rheological data. For the generalized Newtonian fluids, the polymer flow computation certainly adopted the Cross-WLF (Cross-William-Landel-Ferry) flow curve of the viscosity versus shear rate involving two regions: the Newtonian plateau at low shear rates and shear thinning at high shear rates. This is the prior understanding of general polymer rheology [15,16]. According to previous experimental investigations of fiber-filled suspensions [17–20], the yield-stress viscosity is obviously found at low shear rates. Hence, the Cross viscosity model should be not suitable for fitting the yield-stress viscosity.

Researchers so far have not been concerned about the yield stress viscosity to improve the core width in fiber orientation predictions. In the present study, we therefore considered such a yield stress viscosity added to the standard Cross-WLF viscosity model, namely, Yield-Cross-WLF. We further discussed the viscosity data on highly concentrated fiber suspensions from high shear rates to low shear rates as measured by capillary rheometer and rotational rheometer. A numerical analysis of an injection molding simulation attached with the Yield-Cross-WLF viscosity proved significant; it revealed the relationship between yield-stress viscosity and fiber orientation. Moreover, we validated the prediction of fiber orientation for the 50 wt% long-carbon- fiber-reinforced polypropylene in injection molding simulation, as compared with the PNNL experimental data [21].

#### 2. Theoretical background

The flow-induced fiber orientation indicates that changes in the fiber orientation are strongly driven by the flow field. For injection-molded fiber composites, the actual flow of the fibers dispersed in the polymer melt is transient, non-Newtonian and non-isothermal, with frozen layers building up as the complex mixture flows through the mold cavity. The process is highly nonlinear, as the material properties are dependent upon the rheological and thermal conditions. For completeness, here we summarize the theoretical equations involving two parts: the fiber orientation kinetics and fluid mechanics.

#### 2.1. Time-evolution equation of orientation tensor

A single fiber is regarded as a rigid cylindrical rod. The fiber's unit vector 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 [22] defined the second-rank orientation tensor as:

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

where  $\psi(\mathbf{p})$  is the probability density distribution function over the orientation space.

The second-rank orientation tensor **A** is the symmetric matrix and its trace is  $A_{11} + A_{22} + A_{33} = 1$ . Physically, **A** = **I**/3 represents the isotropic orientation state, wherein **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 (x1-direction), cross-flow direction (x2-direction), and thickness direction (x3-direction), respectively.

The orientation tensor is given as:

and 
$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
 for the perfect alignment. (3)

The principal directions of the orientation tensor A are numbered in the order of the respective principal values, from the largest to the smallest. The first principal direction represents the direction along which the most fibers are aligned, and the third principal direction represents the one along which the fewest fibers are aligned. The larger principal value indicates a stronger alignment in the corresponding principal direction.

A physical interpretation of the orientation tensor is very similar to that of the stress tensor. The diagonal components of a fiber orientation tensor represent the strength of alignment in the respective directions. The values of the diagonal components range between 0 and 1, and the sum of all three diagonal components is 1. The off-diagonal components of a fiber orientation tensor represent the amount that alignments vary from the coordinate axes; they are zero when the coordinate axes coincide with the principal directions of the orientation tensor. Therefore, non-zero off-diagonal components indicate that x1, x2, and x3 axes are not the principal axes [23].

A time-evolution equation of the second-order orientation tensor is fixed on the material derivative, denoted as  $\dot{\mathbf{A}}$ . Over the last three decades, theoretical researchers in the fiber suspension rheological field have made considerable effort to determine the dynamic fiber orientation states involving short and long fibers. The modern models, based on the classic fiber orientation models, the pioneering Jeffery hydrodynamic model [24] and the famous Folgar-Tucker IRD (Isotropic Rotary Diffusion) model [25], include the Phelps-Tucker ARD (Anisotropic Rotary Diffusion) model [7], the Wang-Tucker RSC (Reduced Strain Closure) model [6] and the ARD-RSC model [7]. These famous and modern models are available in commercial injection molding simulation software, the Autodesk Simulation Moldflow Insight (ASMI), providing the fiber orientation predictions practiced in most of injection molded fiber-reinforced thermoplastic products [26]. On the other hand, Férec et al. [27] particularly considered these significant contacts of fiber interactions for long fiber orientation in non-dilute fiber suspensions.

From the aforementioned fiber orientation models, Tseng et al. [9–11] developed a new model, the iARD-RPR (improved ARD model and Retarding Principal Rate model). However, the iARD tensor does not pass the classic rheological rule of Euclidean objectivity, namely, material frame indifference. It is hard to ignore the non-objective effect due to the fact that different coordinate systems can yield different answers. More recently, Tseng et al. [11] have improved such a non-objective issue and then proposed the objective iARD model. Significantly, there is application value of the iARD-RPR model to provide good orientation predictions

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