Composites Science and Technology 144 (2017) 51–56

Contents lists available at ScienceDirect

Composites Science and Technology

journal homepage: http://www.elsevier.com/locate/compscitech

Numerical prediction of fiber orientation and mechanical performance for short/long glass and carbon fiber-reinforced composites

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A R T I C L E I N F O

Article history:
Received 2 December 2016
Received in revised form
15 February 2017
Accepted 20 February 2017
Available online 22 February 2017

Keywords:
Fiber-reinforced thermoplastic composites
Shell-core orientation structure
iARD-RPR orientation model
Mechanical properties
Injection molding simulation

A B S T R A C T

Fiber reinforced polymer (FRP) composites offer exciting new possibilities for the green automotive industry, owing to their excellent mechanical properties, advantageous weight reduction and economical fuel consumption. In practice, accurately predicting fiber orientation is a critical issue in causing anisotropy in the mechanical properties of the FRP parts. Recently, an objective fiber orientation model, iARD-RPR (Improved Anisotropic Rotary Diffusion model combined with a Retarding Principal Rate model) proved significant in the field of fiber suspension rheology. Using state-of-the-art injection molding simulations, we therefore used the iARD-RPR model to explore the fiber orientation changes for various fiber components in regard to fiber length (short and long fibers) and fiber type (glass and carbon fibers). Under an extreme condition of higher fiber concentration and longer fiber lengths, a thicker core region and a narrow shell are always found in a typical orientation pattern of injection molded FRT parts. More importantly, these predicted orientation distributions provided to micromechanical material modeling computation of mechanical properties aid in the discussion on the reinforcing ability of short/long fibers and glass/carbon fibers based on the numerical simulation results. Comparisons with experimental data are also presented herein.

1. Introduction

Short/long fibers are routinely added to thermoplastics as fiber-reinforced composites in order to enhance mechanical performance and counter warpage deformation. Short fiber length is about 0.2–0.4 mm, while long fibers are generally longer than 1 mm. The use of fiber-reinforced thermoplastics (FRT) is enjoying continued growth, especially in automotive application. Fiber orientation markedly affects the mechanical properties, namely, strength, stiffness, and impact. However, an accurate orientation prediction is a primary requirement for ensuring a complete simulation from injection molding to structural analysis.

From a microscopic view, fiber orientation states in a general fluid are very complex. Over the last three decades, great efforts in fiber suspension rheology of theoretical research have succeeded in making it possible to describe the flow-induced variation in fiber orientation. Previously, the famous fiber orientation models, which contain the Folgar-Tucker model [1], the RSC (Reduced Strain Closure) model [2], and ARD (Anisotropic Rotary Diffusion) model [3], have been used available in commercial injection molding simulation software, ASMI (Autodesk Simulation Moldflow Insight). Significantly, the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge National Laboratory (ORNL) [4] have actively integrated the predictive orientation and engineering tools for injection-molded fiber composites. According to the disclosed PNNL-ORNL report, the use of the midplane-mesh (2.5D model) versions of ASMI with the ARD-RSC could obtain good agreement of fiber orientation between the experiments and the predictions regarding fiber composites in injection molding simulation. Regrettably, the ARD-RSC model used in the 3D numerical computation resulted in inaccurate predictions.

Based on the ARD-RSC [3], Tseng et al. [5–7] developed the iARD-RPR model (known as the Improved Anisotropic Rotary Diffusion model combined with Retarding Principal Rate model) which is suitable for predicting the core-shell structure orientation structure of both short and long fiber-filled materials. The iARD-RPR model has proven capable of describing anisotropic fiber orientation; as a result, it has been incorporated into the commercial software utilized for injection-molding simulation, Moldex3D. Using the Solid Mesh Model based on the 3D Finite Volume

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http://dx.doi.org/10.1016/j.compscitech.2017.02.020
0266-3538/

Method (3D-FVM) technology, Moldex3D can provide the transient flow field simulation involving complex 3D geometry, thanks to its robustness and efficiency. In the Manufacturing Systems Research Lab of General Motors (GM) Research and Development, Foss et al. [8] utilized Moldex3D to investigate the short-glass-fiber orientation predictions with injection-molding simulation. Their predicted orientation distribution exhibited the reliable, classic laminated structure: skin-shell-core-shell-skin.

Most researchers are interested in the dramatic changes of orientation states with respect to fiber length, including short and long fibers, as well as different types of fibers involving glass and carbon fibers. However, few studies on numerical simulations have attempted to demonstrate the reinforcing ability of short/long fibers and glass/carbon fibers. In the present study, we therefore aimed to perform accurate fiber orientation prediction via the iARD-RPR model implemented with the Moldex3D injection molding simulation. These predicted orientation distributions are compared to the related experimental data. Moreover, we explore the dramatic changes in fiber orientation with various fiber properties under the same fiber concentration and the same matrix resin. In addition, the predicted fiber orientation is provided to estimate tensile modulus and the stress-strain response.

2. Theoretical background

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. Orientation vector **p** is expressed in a surface spherical coordinate with the polar angle θ and the azimuthal angle ϕ. For a concise representation of the orientation of a large population of fibers, Advani and Tucker [9] defined the second order 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; **A** is the symmetric matrix and its trace is $A11+A22+A33 = 1$. Physically, $\mathbf{A} = \mathbf{I}/3$ represents the isotropic orientation state, wherein **I** is the identity matrix. Three diagonal components: *A11*, *A22* and *A33*, correspond to the flow, cross-flow and thickness directions, respectively.

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 [10] and the famous Folgar-Tucker IRD (Isotropic Rotary Diffusion) model [1], include the Phelps-Tucker ARD (Anisotropic Rotary Diffusion) model [3], the Wang-Tucker RSC (Reduced Strain Closure) model [2] and the ARD-RSC model [3]. 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 injection molding FRT products [11].

From the aforementioned fiber orientation models, Tseng et al. [5–7] 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. [5] have improved such a non-objective issue and then proposed the objective iARD model. Here, we introduce the objective iARD-RPR model divided into three parts.

Firstly, the iARD-RPR equation contains three terms: the Jeffery Hydrodynamics (HD) $\dot{\mathbf{A}}^{HD}$, the iARD $\dot{\mathbf{A}}^{iARD}$, and the RPR $\dot{\mathbf{A}}^{RPR}$, presented as:

$$\dot{\mathbf{A}} = \dot{\mathbf{A}}^{HD} + \dot{\mathbf{A}}^{iARD}(C_I, C_M) + \dot{\mathbf{A}}^{RPR}(\alpha) \tag{2}$$

$$\dot{\mathbf{A}}^{HD} = (\mathbf{W}.\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbf{A}_4 : \mathbf{D}) \tag{3}$$

where $\dot{\mathbf{A}}^{\mathrm{iARD}}$ has two available parameters: the fiber-fiber interaction parameter C_I and the fiber-matrix interaction parameter C_M; $\dot{\mathbf{A}}^{\mathrm{PPR}}$ has one parameter α, which is meant to slow down the response rate of the fiber orientation; **W** is the vorticity tensor; **D** is the rate-of-deformation tensor; $\dot{\gamma}$ is the shear rate of **D**, $\dot{\gamma} = \sqrt{2\mathbf{D}:\mathbf{D}}$; $\xi = (a_r^2 - 1)/(a_r^2 + 1)$ is the particle shape factor; and a_r is the fiber aspect ratio. Since $a_r \gg 1$, ξ is assumed to signify unity. The fourth-order orientation tensor $\mathbf{A_4}$ is determined by using a higher order polynomial closure approximation in terms of the second-order orientation tensor **A**, such as the Eigenvalue-Based Optimal Fitting (EBOF) Closure [12] and the Invariant-Based Optimal Fitting (IBOF) Closure [13]. Note that the accuracy of IBOF is as good as EBOF, and IBOF requires less computational time to obtain a solution [13].

Secondly, it is significant that the rotary diffusion tensor $\mathbf{D}_r$ depends on the square of the objective rate-of-deformation tensor for defining a new iARD model [5], as below:

$$\dot{\mathbf{A}}^{\mathrm{iARD}} = \dot{\gamma}[2\mathbf{D}_r - 2tr(\mathbf{D}_r)\mathbf{A} - 5\mathbf{D}_r\cdot\mathbf{A} - 5\mathbf{A}\cdot\mathbf{D}_r + 10\mathbf{A}_4 : \mathbf{D}_r] \tag{4}$$

$$\mathbf{D}_r = C_I\left(\mathbf{I} - C_M\frac{\mathbf{D}^2}{\|\mathbf{D}^2\|}\right) \tag{5}$$

where **D** is the symmetric part of the velocity-gradient tensor **L**, $\mathbf{D} = \frac{1}{2}(\mathbf{L}^T + \mathbf{L})$. The scalar $\|\mathbf{D}^2\| = \sqrt{\frac{1}{2}\mathbf{D}^2 : \mathbf{D}^2}$ is the norm of tensor $\mathbf{D}^2$.

Eventually, the RPR model is introduced as:

$$\dot{\mathbf{A}}^{\mathrm{RPR}} = -R\cdot\dot{\Lambda}^{IOK}\cdot\mathbf{R}^T \tag{6}$$

$$\dot{\Lambda}_{ii}^{\mathrm{IOK}} = \alpha\dot{\lambda}_i, \quad i,j,k = 1,2,3 \tag{7}$$

where $\dot{\Lambda}^{\mathrm{IOK}}$ is the material derivative of a particular diagonal tensor and its superscript indicates the intrinsic orientation kinetics (IOK) assumption [6,7]; **R** is the rotation matrix and $\mathbf{R}^{\mathrm{T}}$ is the transpose of **R**; the superscript T is the transpose operator of a matrix throughout this paper; λ_i is the eigenvalues of **A**, $\lambda_1 \geq \lambda_2 \geq \lambda_3$; and $\mathbf{R} = [\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3]$ is defined by eigenvector columns of **A**.

In summary, the iARD-RPR model has only the three physical parameters: a fiber-fiber interaction parameter C_I, a fiber-matrix interaction parameter C_M and a slow-down parameter α. The available region of these three parameters is suggested in: $0 < C_I < 0.1$, $0 < C_M < 1$, $0 < \alpha < 1$. The iARD-RPR model has been implemented in the commercial injection molding simulation software, Moldex3D (CoreTech System Co. of Taiwan), to allow for the fiber orientation predictions. Accordingly, predictions of the fiber orientation model are contingent on the method and assumptions of the underlying numerical modeling during the mold filling.

Regarding a particular coupled problem, the flow and orientation equations must be solved simultaneously. To date, the coupled