COMPARISON OF RECENT FIBER ORIENTATION MODELS IN AUTODESK MOLDFLOW INSIGHT SIMULATIONS WITH MEASURED FIBER ORIENTATION DATA

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Abstract - The *reduced strain closure* (RSC) and *anisotropic rotary diffusion* (ARD) models have been implemented in a research version of Autodesk Moldflow Insight software to improve the accuracy of fiber orientation predictions in simulations of injection-molded parts. The RSC model captures the slow fiber orientation kinetics, which are observed in experiments but over-predicted by the widely used Folgar-Tucker model. The ARD model accounts for fiber-fiber interactions using anisotropic diffusion to rectify the problem that for long-fiber materials, the Folgar-Tucker model does not match all aspects of measured fiber orientation data. Simulating the injection molding process in Autodesk Moldflow Insight software, the fiber orientation is predicted for a number of end-gated ISO plaques and center-gated disks of different thicknesses (from 1.5 to 6 mm) filled at different injection rates, with Midplane meshes as well as 3D meshes, using the RSC model for short-fiber materials and the ARD-RSC model for long-fiber materials. In Midplane models, with an appropriate inlet condition for fiber orientation applied at the gate, the RSC and ARD models show good agreement with measured fiber orientation data. In 3D models with random inlet orientation applied at the gate, the RSC model gives good agreement with one orientation component of the experimental data for short-fiber materials.

Introduction

Plastic materials are widely used as metal replacement in industrial applications owing to the advantages of higher strength-to-weight ratio and high corrosion resistance. Glass and carbon fibers are commonly added into plastic materials to reinforce the mechanical and thermal properties with negligible change of weight. The addition of fibers introduces anisotropy of the properties in injection-molded parts, mainly due to the preferential orientation of fibers induced by the flow during processing. For example, shearing flow, which is usually dominant during injection-molding processing of a thin part, tends to align fibers in the shearing direction. The part is much stronger and stiffer in the direction along which most fibers are aligned than in the direction crossing the major fiber alignment. In order to determine the properties in injection-molded parts and aid the design of mold and part and the selection of processing conditions, the fiber orientation must be accurately predicted.

Currently, most programs and commercial software, including Autodesk Moldflow Insight, use the Folgar-Tucker model (Folgar and Tucker, 1984) to predict the fiber orientation. The Folgar-Tucker model was developed based on Jeffery's equation (1922) for the motion of a single rigid fiber in an infinite Newtonian fluid by adding an isotropic rotary diffusion to represent interactions between fibers, and then the equation was recast in the term of the second-order orientation tensor for affordable computations.

However, recent experiments, including measurements of fiber orientation in injection-molded parts (O'Gara, J. F., personal communication, 2003) as well as measurements of rheology of fiber suspension (Sepehr et al., 2004), indicate that the Folgar-Tucker model predicts much quicker fiber orientation change with respect to strain than has been observed, and thus, usually over-predicts the overall fiber alignment. Wang et al. (2008) modified the Folgar-Tucker model by reducing the growth rates of the eigenvalues of the fiber orientation tensor by a constant scalar factor but keeping the rotation rates of the eigenvectors unchanged and developed the *reduced strain closure* (RSC) model. The RSC model exhibits slower orientation kinetics than the Folgar-Tucker model but exhibits a similar steady-state orientation and also provides excellent agreement with experimental data (Wang, 2007). United States patent No. 7,266,469 (Tucker et al., 2007) is held on the RSC model by Delphi Automotive LLP, and the model is used under license in this work.

Fibers longer than 1 mm are generally considered as long fibers. Usually, the fiber alignment in the flow direction is smaller in long-fiber materials than in short-fiber materials in injection-molded parts (Phelps and Tucker, 2009). The isotropic diffusion used in the Folgar-Tucker and RSC models is unable to capture the behavior of fiber-fiber interactions in long-fiber materials and cannot accurately predict all fiber orientation components simultaneously. The isotropic diffusion was replaced with the *anisotropic rotary diffusion* (ARD), which is defined on the surface of the unit sphere traced by all orientations of the unit vector, developed by Phelps et al. (2009). The RSC model can also be combined with the ARD model.

Both the RSC and ARD models were implemented in a research version of Autodesk Moldflow Insight software and were used to predict fiber orientation in injection-molded parts. The fiber orientation results were compared with the measured data.

Fiber Orientation Models

A concise description of fiber orientation is the second-order orientation tensor (Advani and Tucker, 1987), which is defined as

$$\mathbf{A} = \langle \mathbf{pp} \rangle \,, \tag{1}$$

where the unit vector **p** directs along the fiber length, and the bracket "⟨ ⟩" is the average over a volume domain. The trace of **A**, tr**A**, is unity due to the unit length of **p** and the normalization condition.

The Folgar-Tucker model in the term of the orientation tensor **A** is

$$\begin{aligned}\frac{D\mathbf{A}}{Dt} = (\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbb{A}{:}\mathbf{D}) \\ +2C_I\dot{\gamma}(\mathbf{I} - 3\mathbf{A}).\end{aligned} \tag{2}$$

Here, $D\mathbf{A}/Dt$ is the material derivative of **A**; **W** and **D** are the vorticity and the rate-of-deformation tensors, respectively; ξ is the particle shape parameter and is very close to unity due to the large length-to-radius ratio of fibers; C_I is the interaction coefficient, and a larger C_I implies more fiber-fiber interactions; and $\dot{\gamma}$ is the scalar magnitude of **D**. $\mathbb{A}$ is the fourth-order orientation tensor, defined as $\mathbb{A} = \langle \mathbf{pppp} \rangle$, and is approximated as a closure function of components of **A**.

In Autodesk Moldflow Insight software, for Midplane and Dual Domain meshes, the Folgar-Tucker model is further revised by a thickness moment of interaction coefficient D_z ($0 \le D_z \le 1$) (Autodesk Moldflow Insight help topic "Fiber orientation models"), and therefore Moldflow's orientation model is

$$\begin{aligned}\frac{D\mathbf{A}}{Dt} = (\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} - 2\mathbb{A}{:}\mathbf{D}) \\ + 2C_I\dot{\gamma}(\mathbf{I} - (2 + D_z)\mathbf{A}).\end{aligned} \tag{3}$$

Here, a smaller D_z implies less out-of-plane orientation. However, if $D_z < 1$, $D(\mathrm{tr}\mathbf{A})/Dt \neq 0$, given by Eq. (3). Thus, among the diagonal components of **A**, two in-plane components are calculated by Eq. (3), and the out-of-plane component is calculated by enforcing tr**A** = 1.

The RSC model introduces a scalar factor $\kappa < 1$ to slow the fiber orientation kinetics, and the equation is

$$\begin{aligned}\frac{D\mathbf{A}}{Dt} &= (\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} \\ &\quad - 2[\mathbb{A} + (1-\kappa)(\mathbb{L} - \mathbb{M}{:}\mathbb{A})]{:}\mathbf{D}) \\ &\quad + 2\kappa C_I\dot{\gamma}(\mathbf{I} - 3\mathbf{A}).\end{aligned} \tag{4}$$

Here, the fourth-order tensors $\mathbb{L}$ and $\mathbb{M}$ are functions of the eigenvalues λ_i (i = 1,2,3) and the eigenvectors $\mathbf{e}_i$ (i = 1,2,3) of the orientation tensor **A**, defined as $\mathbb{L} = \sum_{i=1}^{3} \lambda_i\, \mathbf{e}_i\, \mathbf{e}_i\, \mathbf{e}_i\, \mathbf{e}_i$ and $\mathbb{M} = \sum_{i=1}^{3} \mathbf{e}_i\, \mathbf{e}_i\, \mathbf{e}_i\, \mathbf{e}_i$. The scalar factor κ is a phenomenological parameter, and its value is determined by fitting the fiber orientation or rheology prediction to experimental data. Setting $\kappa = 1$ reduces the RSC model of Eq. (4) to the Folgar-Tucker model of Eq. (2).

The ARD model replaces the isotropic diffusion term with an anisotropic diffusion and the RSC version of the ARD model (ARD-RSC) is

$$\begin{aligned}\frac{D\mathbf{A}}{Dt} &= (\mathbf{W}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{W}) + \xi(\mathbf{D}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{D} \\ &\quad - 2[\mathbb{A} + (1-\kappa)(\mathbb{L} - \mathbb{M}{:}\mathbb{A})]{:}\mathbf{D}) \\ &\quad + \dot{\gamma}(2[\mathbf{C} - (1-\kappa)\mathbb{M}{:}\mathbf{C}] - 2\kappa(\mathrm{tr}\mathbf{C})\mathbf{A} \\ &\qquad - 5(\mathbf{C}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{C}) \\ &\qquad + 10[\mathbb{A} + (1-\kappa)(\mathbb{L} - \mathbb{M}{:}\mathbb{A})]{:}\mathbf{C}).\end{aligned} \tag{5}$$

Here, the rotary diffusion tensor **C** is constructed from **A** and **D** as (Phelps and Tucker, 2009)

$$\mathbf{C} = b_1\mathbf{I} + b_2\mathbf{A} + b_3\mathbf{A}^2 + b_4\frac{\mathbf{D}}{\dot{\gamma}} + b_5\frac{\mathbf{D}^2}{\dot{\gamma}^2}, \tag{6}$$

where b_i (i = 1, …, 5) are scalar constants and selected by matching experimental steady-state orientation and requiring stable orientation. Setting $b_1 = C_I$ and $b_i = 0$ (i = 2, …, 5) reduces the ARD-RSC model of Eq. (5) to the RSC model of Eq. (4).

Experiments

A series of end-gated ISO plaques and center-gated disks were molded by Delphi Automotive LLP and the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge National Laboratory (ORNL), to obtain the measured fiber orientation data which were compared with simulation results. The ISO plaques are 90 mm long and 80 mm wide, and the disks have a diameter of 177.8 mm. Delphi used a polybutylene terephthalate reinforced by 30% wt short glass fibers (General Electric Plastics Valox 420) and molded parts in thicknesses of 1.5, 2, 3, and 6 mm, filled at three different injection rates (slow, medium, and fast) for each thickness. PNNL-ORNL used a polypropylene with 40% wt glass fibers to mold plaques and disks of 3 mm thick, filled at two different injection rates (slow and fast) for each geometry, and the fibers have a nominal length of 13 mm and are considered as long fibers.

Fiber orientation through the thickness was measured by Delphi and PNNL-ORNL for their respective moldings using the optical system developed by Hine et al. (1996). Measurements were made at selected locations on the polished cross-section cut along the centerline of plaques and the radial direction of disks. Further details of the sample preparation and the orientation measurements can be found in O'Gara et al. (2003) and Nguyen et al. (2008).

Simulations

The research version of Autodesk Moldflow Insight software with the implementation of the RSC and ARD models was then used to simulate the injection molding process and predict the fiber orientation in these plaques and disks, with Midplane meshes as well as 3D meshes. The models and meshes for selected parts are illustrated in Figs. 1–4.

For Delphi parts molded with a short-fiber material, we applied the RSC model and used the scalar factor $\kappa = 0.05$, the same value which produces good agreement with experimental data in Wang (2007). For PNNL-ORNL parts molded with a long-fiber material, we applied the ARD-RSC model and used the same scalar factor $\kappa = 1/30$ and the same b_i parameters as suggested by Phelps and Tucker (2009).

As an essential nature of the RSC model, the development of fiber orientation is slowed down compared to the Folgar-Tucker model, and hence the predicted fiber orientation undergoes less change along the flow length of the part and is more strongly influenced by the inlet condition for fiber orientation at the gate. An accurate inlet orientation is therefore crucial to the accurate prediction of fiber orientation in the part. In the research version of the Autodesk Moldflow Insight Midplane solver, we added an option to specify the inlet orientation across the thickness at the gate. For the Midplane simulations presented in this paper, the fiber orientation measured near the gate is used as the inlet orientation for Delphi parts, and the fiber orientation similar to the measured orientation is used as the inlet orientation for PNNL-ORNL parts. However, in a 3D mesh, there is no generic definition of the thickness direction and no option for the inlet orientation, hence a random orientation is used at the gate in the 3D simulations.

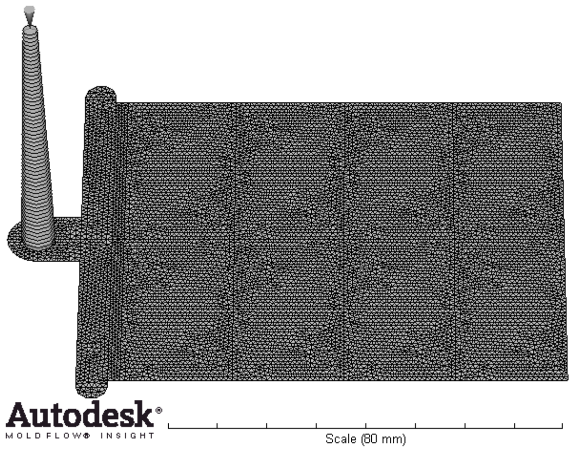

Figure 1. Model and Midplane mesh for an end-gated ISO plaque. The mesh size is about 1 mm.

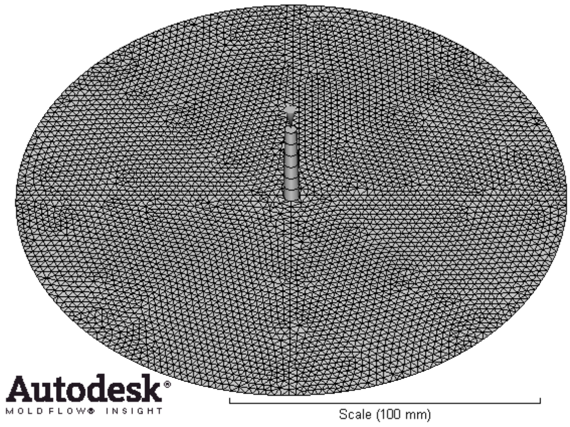

Figure 2. Model and Midplane mesh for a center-gated disk. The mesh size is about 2.47 mm.

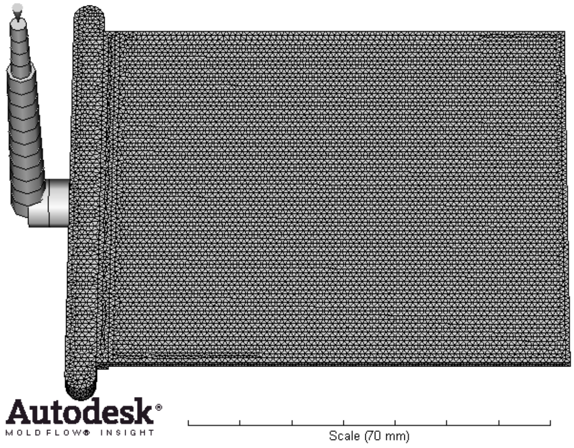

Figure 3. Model and 3D mesh for a 1.5 mm thick, end-gated ISO plaque. The surface mesh size is about 1.15 mm, and there are 12 mesh layers through thickness.

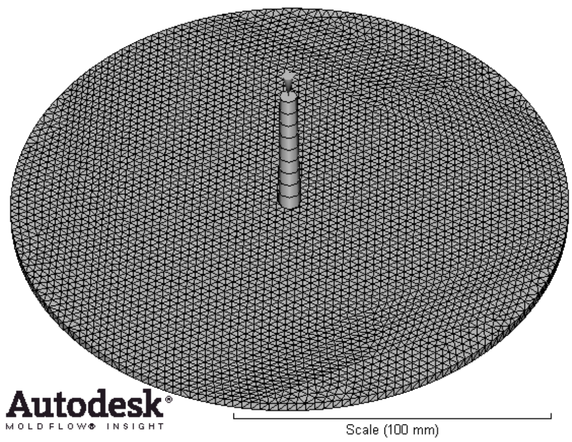

Figure 4. Model and 3D mesh for a 2 mm thick, center-gated disk. The surface mesh size is about 2.8 mm, and there are 12 mesh layers through thickness.

Results and Discussion

The orientation predictions by Autodesk Moldflow Insight are compared with measured fiber orientations in Figs. 5–10. Here, A_{11} denotes the component of the fiber orientation tensor in the flow direction, and A_{22} denotes the component in the cross-flow direction.

The fiber orientation data in plaques and disks exhibits the typical shell-core-shell structure through the thickness. The A_{11} component is small near the center, which is referred to as the core. At the core, A_{11} for plaques is similar to the inlet orientation due to low shearing in the core, while for disks it is transversely aligned due to strong stretching. The A_{11} component is large on both sides of the core, which are referred to as the shell layers. In the shell layers, fibers usually have strong alignment due to high shearing near the mold surface.

The Folgar-Tucker model over-predicts the fiber orientation change and hence gives a much narrower core than observed in experiments. Moldflow's D_z model attempts to broaden the core by decreasing the out-of-plane orientation, but the improvement is limited. Neither Moldflow's D_z model nor the Folgar-Tucker model is able to predict adequately the correct width of the core, as demonstrated in Figs. 5 and 6 and Figs. 7 and 8 for Midplane and 3D meshes, respectively, for Delphi plaques.

Using the RSC model with Midplane meshes for the plaques and disks models accurately captures the core orientation and width, and also predicts the orientation in the shell layers reasonably well. The comparisons of the predicted fiber orientation with data are plotted in Figs. 5 and 6.

For 3D meshes of Delphi plaque and disk moldings, the RSC model gives an excellent fit to the A_{11} component through the thickness, but gives a poor fit to the A_{22} component, particularly in the core, as shown in Figs. 7 and 8. This poor prediction for the A_{22} component is probably due to the random orientation given at the gate. The A_{22} component at the center is always close to 1/3, which is almost the same as the inlet orientation. A more appropriate inlet orientation is therefore required in order to produce a good prediction.

The predictions by the RSC and the ARD-RSC models are compared with experimental data in Figs. 9 and 10 for a PNNL-ORNL plaque and a disk, respectively, molded with a long-fiber material. The RSC model is able to match the A_{11} component in the shell layers, but under-predicts the A_{22} component. Furthermore, adjusting the C_I value can produce a good match to either one component or the other but not to both simultaneously. The ARD-RSC model shows good agreement with the measured A_{11} and A_{22} components for both plaque and disk.

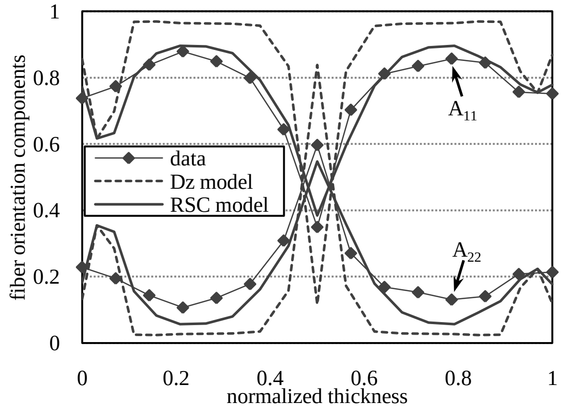

Figure 5. Comparison of fiber orientation data with Autodesk Moldflow Insight Midplane predictions in the Delphi 2 mm thick plaque filled at a slow injection rate. Moldflow's D_z model and the RSC model are used. The C_I and D_z values are automatically calculated by Autodesk Moldflow Insight, and $\kappa = 0.05$.

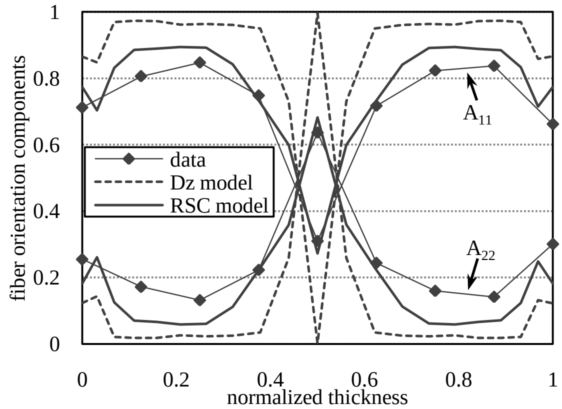

Figure 6. Comparison of fiber orientation data with Autodesk Moldflow Insight Midplane predictions in the Delphi 1.5 mm thick disk filled at a slow injection rate. Moldflow's D_z model and the RSC model are used. The C_I and D_z values are automatically calculated by Autodesk Moldflow Insight, and $\kappa = 0.05$.

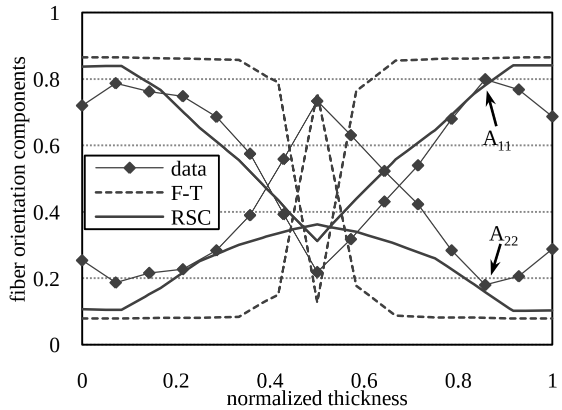

Figure 7. Comparison of fiber orientation data with Autodesk Moldflow Insight 3D predictions in the Delphi 3 mm plaque filled at a fast injection rate. The Folgar-Tucker and RSC models are used. The C_I value is automatically calculated by Autodesk Moldflow Insight, and $\kappa = 0.05$.

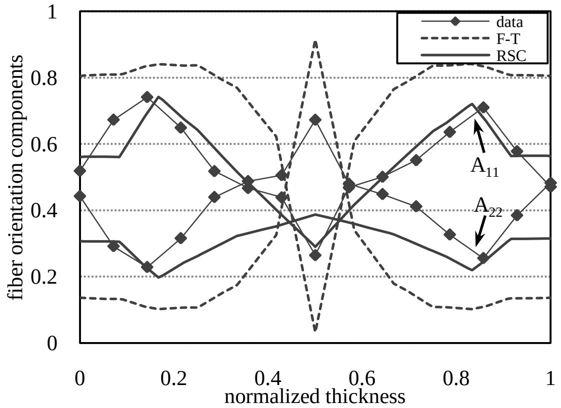

Figure 8. Comparison of fiber orientation data with Autodesk Moldflow Insight 3D predictions in the Delphi 6 mm disk filled at a slow injection rate. The Folgar-Tucker and RSC models are used. The C_I value is automatically calculated by Autodesk Moldflow Insight, and $\kappa = 0.05$.

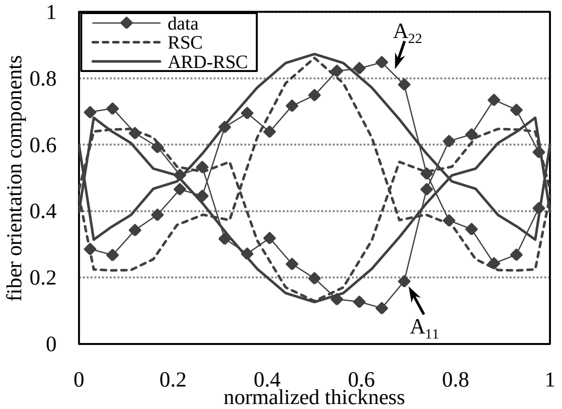

Figure 9. Comparison of fiber orientation data with Autodesk Moldflow Insight Midplane predictions in the PNNL-ORNL 3 mm thick plaque filled at a fast injection rate. The RSC and the ARD-RSC models are used. $C_I = 0.03$ for RSC, and $\kappa = 1/30$ for RSC and ARD-RSC.

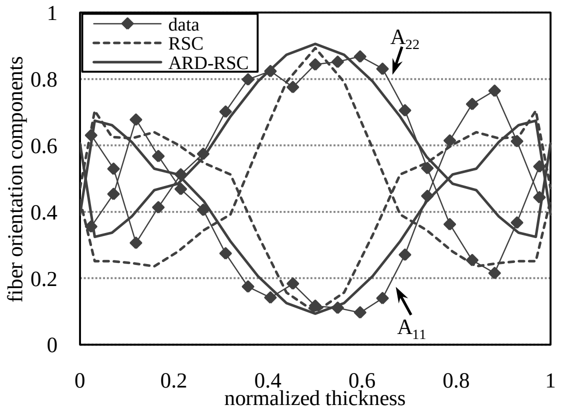

Figure 10. Comparison of fiber orientation data with Autodesk Moldflow Insight Midplane predictions in the PNNL-ORNL 3 mm thick disk filled at a slow injection rate. The RSC and the ARD-RSC models are used. $C_I = 0.03$ for RSC, and $\kappa = 1/30$ for RSC and ARD-RSC.

Conclusions

Two recent orientation models, the RSC and ARD models, were successfully implemented in a research version of Autodesk Moldflow Insight software used for fiber orientation analysis. The program reasonably predicts the fiber orientation, and the prediction agrees well with the measured orientation data for a short-fiber material using the RSC model and for a long-fiber material using the ARD-RSC model. Overall, the RSC and ARD models are superior to the commonly used Folgar-Tucker model and the default Moldflow's D_z model implemented in Autodesk Moldflow Insight software available commercially.

The RSC model slows down the orientation kinetics, and the fiber orientation in a part strongly depends on the inlet orientation at the gate. A careful selection of the inlet orientation condition is required for an accurate orientation prediction in a part. How to specify the inlet orientation across thickness in a 3D mesh and how to automatically give a reasonable inlet orientation need to be addressed to make the RSC model more useful for general cases.

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