IMPROVEMENT IN THE SIMULATION OF INJECTION MOLDED SHORT GLASS FIBER THERMOPLASTIC COMPOSITES

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Abstract

The mechanical properties of injection molded short-fiber reinforced thermoplastic composite parts are highly dependent on the orientation distribution of the fibers. A simulation tool capable of predicting fiber orientation accurately as a function of mold design and processing conditions is required as the predicted fiber orientation capabilities in commercial software show large discrepancies when compared with experimentally measured orientation. The presence of a fourth order tensor in the constitutive equation for fiber orientation makes both experimental determination and computation difficult.

In this work, a two dimensional axisymmetric simulation using Folgar Tucker model for predicting the flow-induced orientation of glass fibers in injection molded composite parts with a circular front is presented. The mass and momentum balance equations are discretized using Galerkin finite element method and the constitutive equation for fiber orientation is discretized using discontinuous Galerkin finite element method. To simplify the computation of the fourth order term, two closure approximations, Quadratic and Invariant-based Optimal Fitting (IBOF) closures are compared. Material parameters used in the model are determined using rheology and experimental fiber orientation is used for initial conditions. Simulation results are in close agreement with the trend seen in experimental data with still need for improving the simulation to capture the orientation in regions close to frontal flow and the walls.

Introduction

This Fiber reinforced thermoplastics made by injection molding is an attractive technology to develop lightweight, high-performance materials. The lightweight molded composites consist of a polymeric matrix reinforced with fibers because of the excellent mechanical properties obtained in the final product, the high throughput, and the cost reduction. The desired properties are only obtained when the orientation of the fibers is in the direction of mechanical interest. However, the fiber orientation varies through the part as a consequence of flow within the mold the forming, a phenomenon known as flow induced orientation. The fibers considered here are short glass fibers defined as fibers with high aspect ratio (a_r > 30) and absolute length below 1 mm.

Optimization of the technology requires a prediction tool using a computer model capable of designing the correct molding machinery, molding and processing conditions, and consistently controlling fiber orientation. The available simulations are able to predict the orientation only qualitatively due to several limitations in the modeling and numerical techniques used to solve the system of equations. Some of these limitations are the simulation of the flow with a flat front ignoring the effects of free-moving frontal flow region and assumption of random orientation as initial condition, especially for a center-gated disk. Other limitations are the use of models which ignore the fiber interactions (Jeffery model), or account for them in a concentration less than that of commercial interest (Folgar-Tucker model[1]), or ignore the viscoelastic effects of the polymer, and use a decoupled approach to solve the system of equations.

Previous work from our group has been in the development of a 2D solution for a coupled flow and fiber orientation using the Hele-Shaw (HS) approximation, which is the typical method of flow description in commercial simulators.[2] The material behavior was modeled using a modified version of Folgar-Tucker model[3] and a Newtonian model for the polymer matrix, with parameters determined from simple flow rheology. The modification in the Folgar-Tucker model accounts for the slow-down in the fiber motion due to inter-particle interaction occurring in highly concentrated fiber suspension.

This paper presents simulation results for prediction of fiber orientation in a center-gated disk using Folgar Tucker model ($\alpha = 1$) with Newtonian flow and experimentally measured orientation at the gate as initial condition. The flow was simulated using a decoupled approach and $\alpha = 1$ as a first step to simplify the physics of the problem in order to evaluate the frontal flow effects. A steady moving front with circular shape was included to capture the effects of the frontal flow on fiber orientation. Quadratic and IBOF closures have been considered for approximation of the fourth order tensor term in constitutive equation for fiber orientation and results are compared with experimental data.

Statement of Theory and Definitions

The isothermal flow of a polymer suspension in a center gated disk is described by

Momentum Balance: $$0 = \nabla \bullet \left(-p\mathbf{I} + 2\eta\mathbf{D} + \mathbf{T} \right) \quad (1)$$

Mass Balance: $$0 = \nabla \bullet \mathbf{v} \quad (2)$$

where p represents the pressure, **I** the identity matrix, η the viscosity, **D** the rate of deformation tensor, **T** the fiber-contribution to the extra-stress tensor components and **v**, the velocity. These equations are supplemented by the typical boundary conditions for stress and velocity. The hydrodynamic extra-stress model is used to represent the fiber-contribution and is defined as

$$\mathbf{T} = \nu\zeta_{str}\left(\left(\nabla\mathbf{v} \right)^T + \nabla\mathbf{v} \right) : \mathbf{R_4} \quad (3)$$

where ν represents the fiber concentration, ζ_{str} the viscous drag, $\mathbf{R_4}$ the fourth order orientation tensor, respectively. The evolution of the second order orientation tensor is governed by:

$$\frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \bullet \nabla\mathbf{A} = \alpha\left[\left(\nabla\mathbf{v} \right)^T \bullet \mathbf{A} + \mathbf{A} \bullet \left(\nabla\mathbf{v} \right) - 2\left(\left(\nabla\mathbf{v} \right)^T + \nabla\mathbf{v} \right) : \mathbf{R}_4 - 6C_I II\left(\mathbf{A} - \frac{1}{3}\delta \right) \right] \quad (4)$$

where α represents the slip parameter, **A**, the second order orientation tensor and C_I the interaction coefficient and II the magnitude of the rate of deformation tensor. The inter-fiber interactions in a semi-dilute and concentrated regime are represented by the last term and the slip parameter in Eq. (4), respectively. With $\alpha = 1$ and $C_I = 0$, Eq. (4) reduces to the Jeffery model, which only accounts for the kinematic effects typical in dilute suspensions.

Orientation tensors represent an average orientation for a group of fibers evaluated from the information of individual fibers.[4] Therefore, they are commonly used to describe the local orientation in a molded part. The second (**A**) and fourth (**R**) order orientation tensors are the most widely used tensor representations in the literature on composites, defined as

$$\mathbf{A} = A_{ij} = \langle p_i p_j \rangle \tag{5}$$

$$\mathbf{R} = A_{ijkl} = \langle p_i p_j p_k p_l \rangle \tag{6}$$

where $\langle \_ \rangle$ represents the ensemble average of the dyadic product of the unit vector **p** over all possible orientations at a certain position and time.

R_4 can be expressed in terms of a quadratic closure according to the equation (7).

$$R_4 = AA \tag{7}$$

This is one of the simplest closures and estimates the fourth order tensor as a product of two second order tensors. It is exact for a perfectly aligned system and assures the symmetry of **A** tensor.[5] The IBOF closure approximates the fourth order tensor in terms of second order tensor and identity matrix with fifth order polynomial coefficients.[6]

$$\mathbf{R} = \beta_1 S(\mathbf{II}) + \beta_2 S(\mathbf{IA}) + \beta_3 S(\mathbf{AA}) + \beta_4 S(\mathbf{IA} \bullet \mathbf{A}) + \beta_5 S(\mathbf{AA} \bullet \mathbf{A}) + \beta_6 S(\mathbf{A} \bullet \mathbf{AA} \bullet \mathbf{A}) \tag{8}$$

where the coefficients β_1 through β_6 are polynomial expansions of second and third invariants of A and the operator S. Operator S is the symmetric part of its argument.[6] The fifth order polynomial expansions describing *β's* can be found elsewhere.[6] IBOF closure is efficient computation-wise and predictions from this closure closely match the fiber orientation in unsteady combined flows, homogenous flows, and radially divergent flows.[6]

Problem Description

A finite element simulation was developed for the flow of polymer/short glass fiber suspension through a center-gated disk, as show in Fig. 1. Effects of frontal flow were captured by including a circular front.

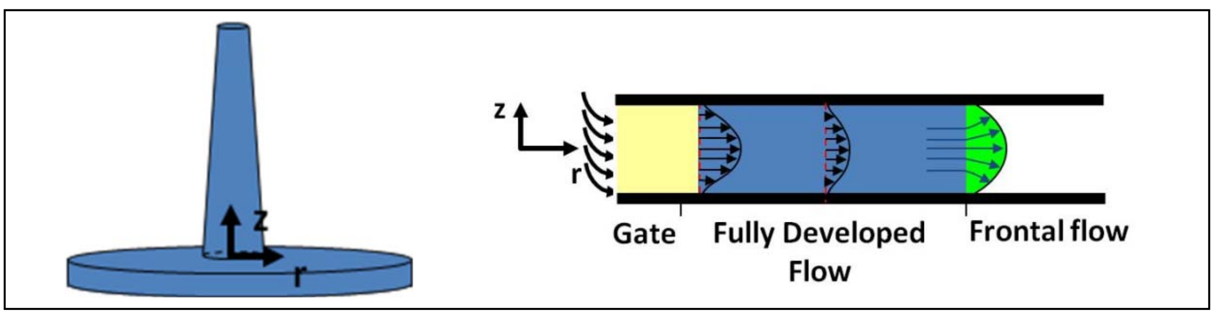


Figure 1: Geometry and Flow Regimes in a Center-Gated Disk.

Mesh

For the complex flow simulation through a center-gated, disk, a mesh was developed with a combination of quadrangle and triangle elements for the upper half of the center-gated disk geometry. The shape of the front was circular which is close to the experimentally observed front. The mesh had variable node-spacing with nodes closely spaced near the wall, inlet and circular front and sparsely placed in the center and the axis of symmetry. The circular front had 88 triangular elements and lubrication and entry region had 384 (48x8) quadrangle elements as shown in Fig. 2. All dimensions were normalized by half thickness of the disk.

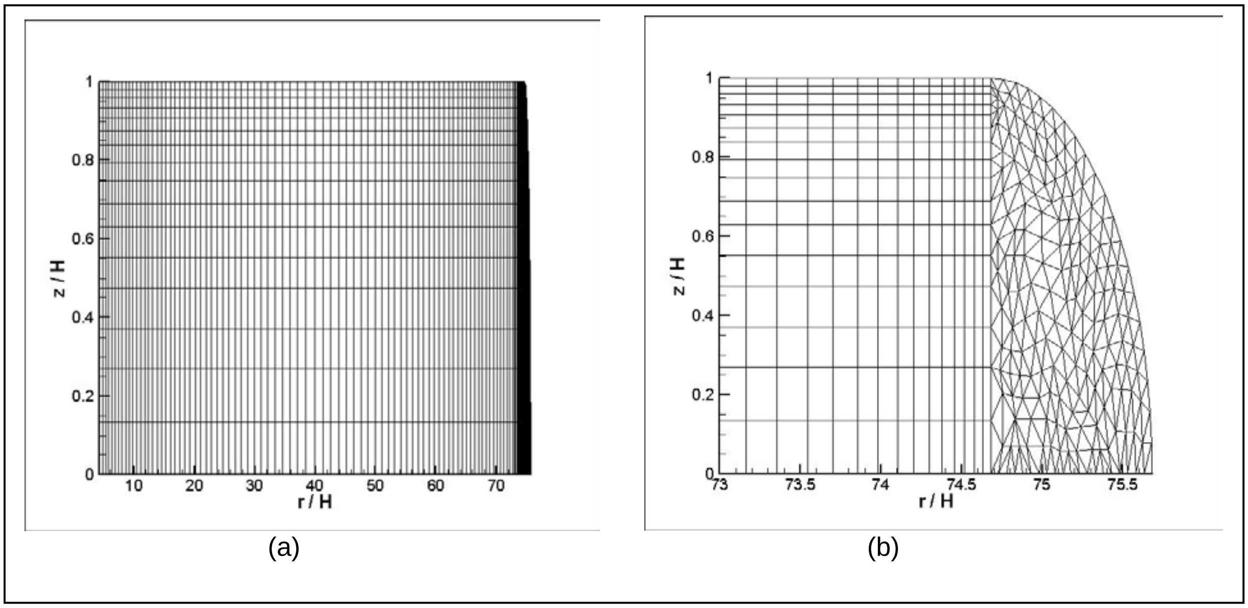
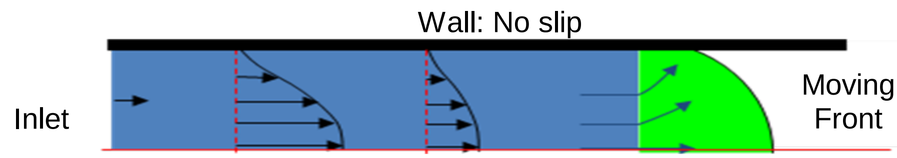


Figure 2: Mesh for center-gated disk geometry. Full mesh (a) and frontal flow region expanded to show the triangular elements (b).

Numerical Methods

Full mass and momentum balance equations were solved with Newtonian flow and Folgar Tucker model for the fiber orientation. In the numerical scheme, at each time step, the position of the front was calculated from mass balance and the mesh coordinates were shifted based on mass balance. Equations of motion were solved for pressure and velocity using Galerkin FEM. Orientation components were post-calculated from evolution equations using discontinuous Galerkin method.

The filling of a disk was simulated as described above. The simulation was performed upto a non-dimensional time of 648 units that reflected the filling of the disk upto 75% of the fill. The standard Galerkin method (GFEM) is used in the discretization of the balance equations. The discontinuous Galerkin method (DGFEM) with a standard implicit Euler scheme was used to discretize the evolution equations. In the simulation only the top half of the domain was considered with no slip velocity at the wall and symmetry boundary conditions at $z = 0$. Fiber orientation data in the gate region collected from experiments was used as the initial orientation. Boundary conditions used in simulation are shown in Fig. 3.



$$\underline{\underline{\sigma}} \bullet \underline{t} = \underline{0}, \quad \underline{v} \bullet \underline{n} = 0$$

Inlet: $\mathbf{A}(r_0, z) = \mathbf{A}_{Experimental}, \quad \mathbf{v}(r_0, z) = \dfrac{K}{r}\left(1 - \dfrac{z^2}{h^2}\right)$

Moving Front: Mass balance, circular shape

Figure 3: Boundary conditions used in the simulation.

To assess the effects of moving front in disk flow, the modified Folgar Tucker model was used with $\alpha = 1$ which eliminated the delay in evolution of fiber orientation and several values of C_I were considered. Results with coupled simulation and Hele Shaw flow with a flat front are presented elsewhere.[2]

Results and Discussion

Simple Flow Results

The rheometrical model predictions were made with the Folgar-Tucker model using Quadratic and IBOF closures and compared with the rheometrical predictions from solutions of full equations. Two cases were considered, shear and planar extension for various values of fiber interaction parameter, C_I. Fig. 4 shows a comparison of A_{rr} components in shear flow. The predictions using IBOF closure match the solution of full equations closely while the results from quadratic closures overpredict the orientation.

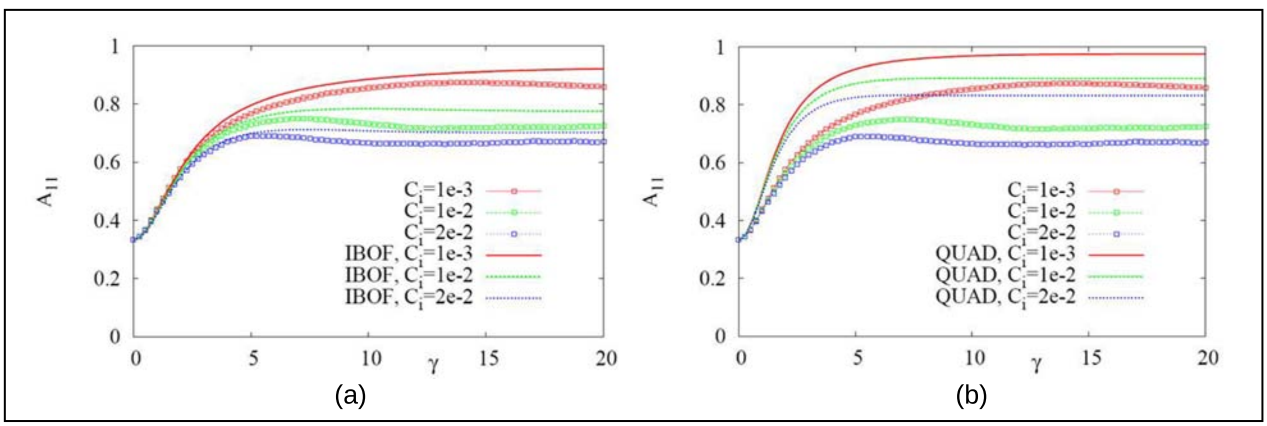


Figure 4: Rheometrical model predictions of A_{rr} component in shear flow, using IBOF closure (a) and Quadratic closure (b) compared with the solution of full equations without any closure.

For planar extension, as shown in Fig. 5, both closures predict the orientation close to the solution of full equations. Quadratic closure overpredicts the orientation for small shear rates and then matches up very well the full equation results at high shear rates while IBOF is close to solution of full equation for the entire range. The effects of C_I are more significant in shear flow as compared to extensional flow for the values of C_I considered in this work. As we can see, the predicted orientation covers a greater range with a change in C_I in case of shear flow while the effect of changing C_I is not very significant in planar extensional flow.

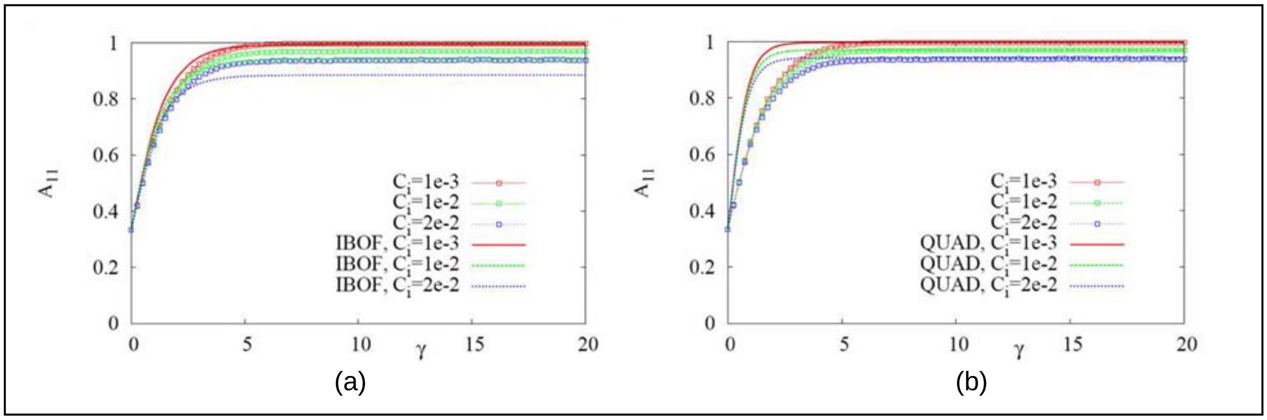


Figure 5: Rheometrical model predictions of A_{rr} component in planar extensional flow, using IBOF closure (a) and Quadratic closure (b) compared with the solution of full equations without any closure.

Prediction of Orientation

Flow kinematics predicted by the simulation were able to reproduce the axisymmetric diverging flow in a disk. As can be seen in the Fig. 6, streamlines are in radial direction through the lubrication region except at the front where they turn outward towards the wall, as expected in fountain flow.

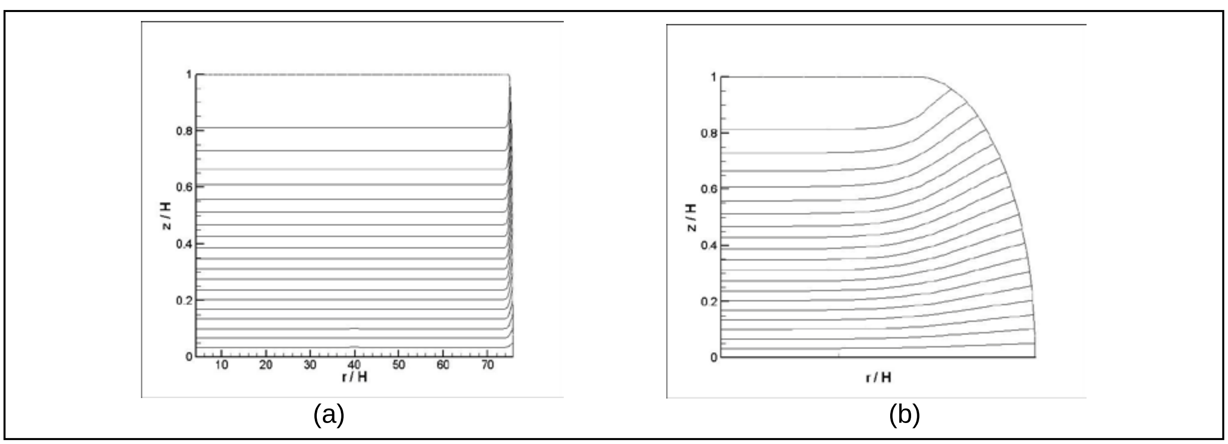


Figure 6: Streamlines for a center-gated disk for the full mesh (a) with the front expanded to show details in frontal flow region (b).

Second invariant of rate of deformation tensor, which is indicative of shear flow, is shown in Fig. 7. As can be seen from the figure, it is close to zero at the axis of symmetry and near outer radius where the flow is dominated by extension, and increases near the gate and in the region where the front touches the wall which are shear dominated regions of flow.

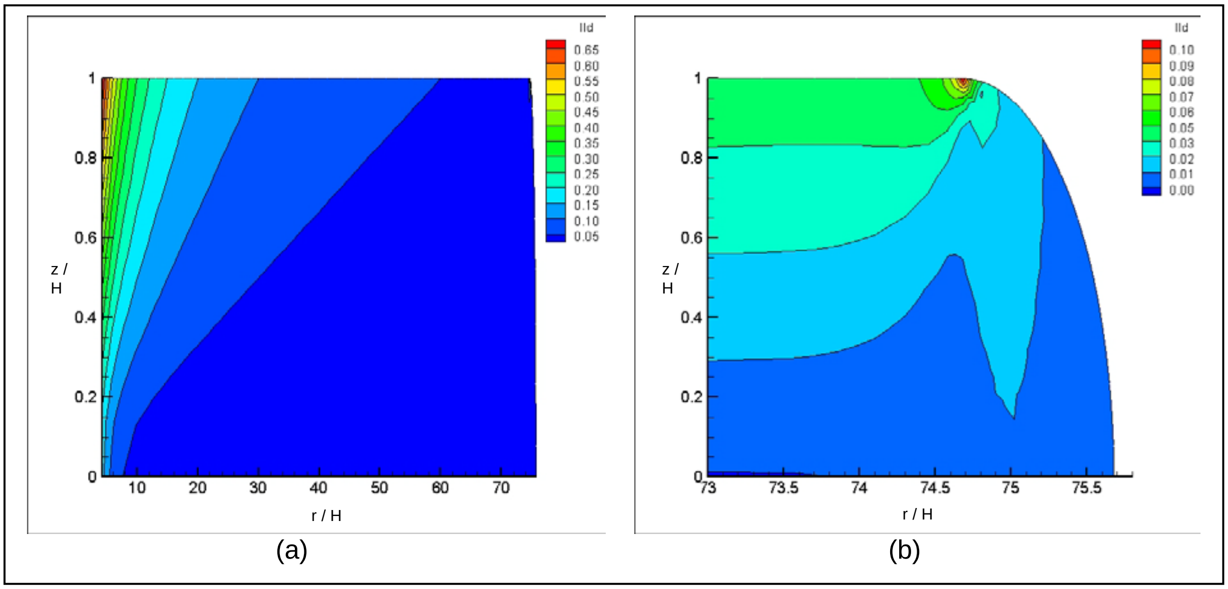


Figure 7: Second Invariant of rate of deformation tensor for a center-gated disk for the full mesh (a) with the front expanded to show details in frontal flow region (b).

The initial orientation matrix considered in the simulation had experimentally measured A_{rr}, $A_{r\theta}$, $A_{\theta\theta}$, and A_{zz} components only. Experimental data is presented elsewhere.[2] The predicted orientation after 648 time units are presented in Fig. 8. As can be seen in the figure, A_{zz} component is close to zero everywhere which is consistent with experimental data. Moreover, A_{rr} is close to zero in the center due to extensional flow with high values of $A_{\theta\theta}$, while close to the wall, A_{rr} dominates over $A_{\theta\theta}$ due to presence of shear flow close to the wall.

Quadratic and IBOF closures were compared with experimental evolution of fiber orientation through the disk. The experimental evolution of fiber orientation at 3 different heights of the center gated disk, i.e. close to axis of symmetry, midway between axis of symmetry and wall, and close to the wall were compared with results from two closure approximations. IBOF matches experimental data more closely as compared to quadratic closure in all the regions. Close to the axis of symmetry which is dominated by extensional flow, both closures are able to capture the trend in evolution of orientation. However, as we move close to the wall, which is shear dominated, the closures are not able to predict the local changes in orientation. The effects of frontal flow are also not captured by either closure. Experimental orientation at the front drops due to the complex nature of frontal flow and this phenomenon is not captured in the predictions using either closure. As can be seen in Fig. 9, both closures overpredict A_{rr} orientation at the front. However, IBOF is closer to experimental values as compared to quadratic closure.

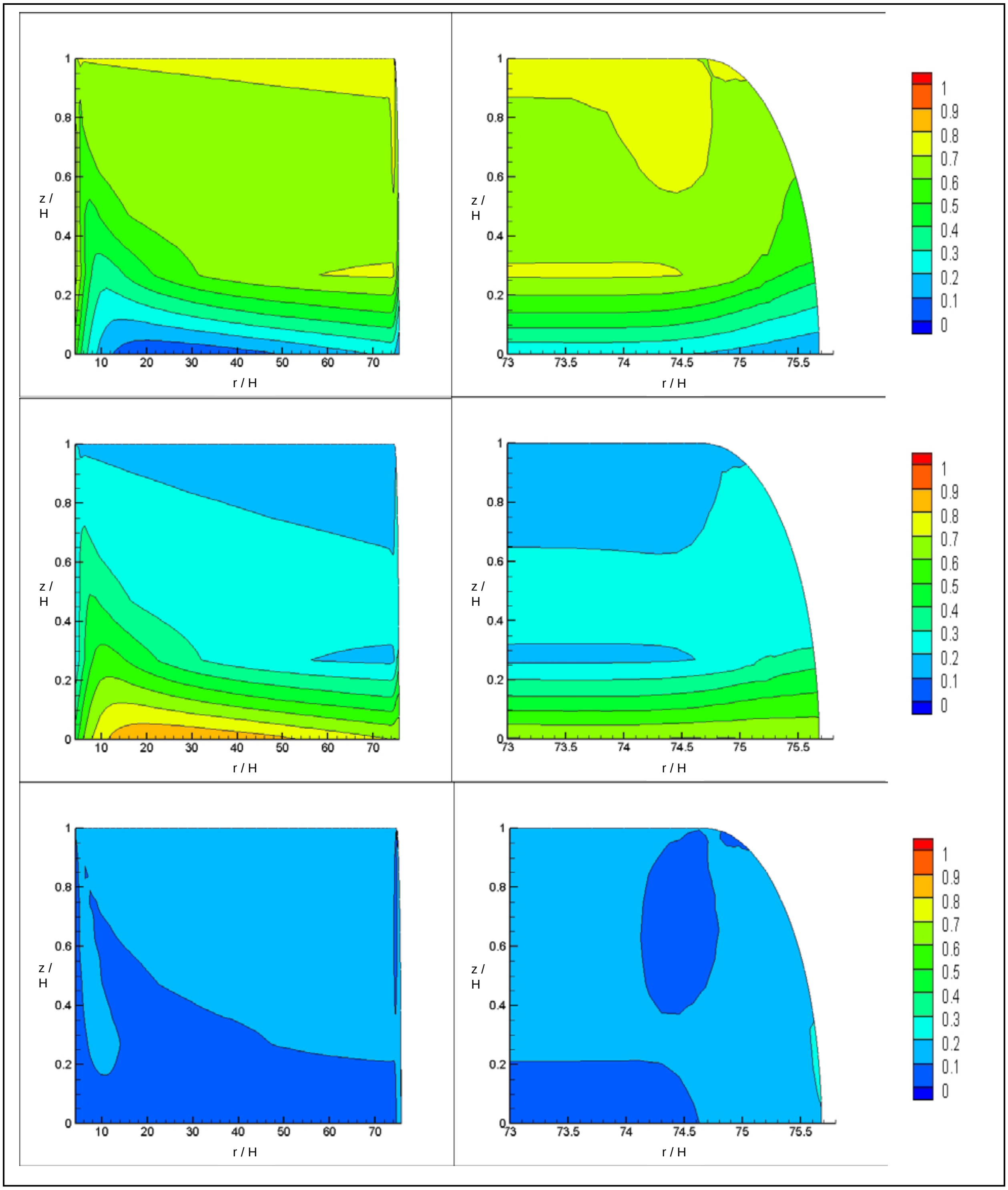


Figure 8. Predictions for diagonal components of orientation matrix with IBOF closure and C_I = 0.02. A_{rr} (top), $A_{\theta\theta}$, (center) and A_{zz} (bottom).

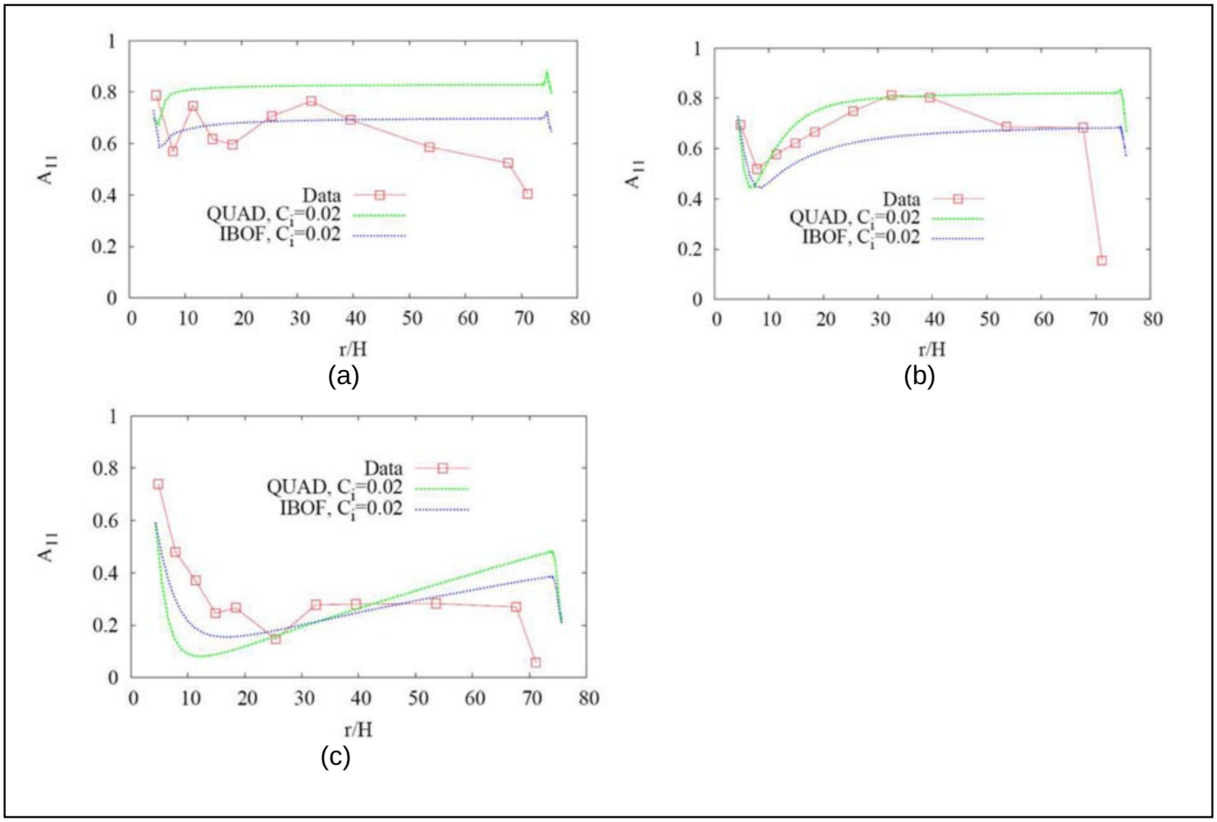


Figure 9: Experimentally determined radial evolution of A_{rr} orientation compared with predictions from IBOF and Quadratic closures with a value of C_I = 0.02 at different heights in the disk, z/H = 0.75 (a), z/H = 0.42 (b) and z/H = 0.08 (c).

Summary and Next Steps

Simulation results indicate that rheometrical model prediction is better in planar extensional flow than in shear flow. Both quadratic and IBOF closures can be used for extensional flow as the variations in results from both the closures are similar and they are able to match the solutions of full equations very well. In shear flow, IBOF closure predictions are more close to the solution of full equations. IBOF closure is a better candidate for approximating the fourth order orientation tensor because of better performance in shear flow without any loss of performance in extensional flow. Also, IBOF closure is close to experimental evolution of fiber orientation in the disk at all three heights considered in this work. However, at the front, both the closures overpredict fiber orientation in radial direction due to complex nature of frontal flow. Some additional modifications are needed in the proposed method to predict the local changes in A_{rr} close to the wall and a drop in orientation in the frontal flow region.

Acknowledgements

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