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Applications of recently proposed closure approximations to injection molding filling simulation of short-fiber reinforced plastics

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Abstract

The present work is aimed at performing injection molding filling simulation of fiber suspension in polymer based matrix. The numerical simulation incorporates the coupling effect between the flow field and the fiber orientation state together with in-plane velocity gradient effect with recently proposed closure approximations. Predicted orientation components are compared with available experimental data of a film-gated strip and a center-gated disk. Predictions with IBOF closure approximation show excellent behaviors with regard to accuracy and numerical efficiency. However, predicted results seem to have consistent errors in comparison with experimental data. Diffusivity term which accounts for fiber-fiber interaction might have to be modified.

1. Introduction

Nowadays, injection/compression molded plastic parts with reinforced particles become more and more important due to its light weight, cost effectiveness, ease of manufacturing, etc., Fiber suspension in polymer based matrix is one of the kind and in this work, non-Brownian short fibers are considered. Fiber reinforced composite typically shows anisotropic mechanical, thermal and rheological properties. Prediction of thermo-mechanical properties with given fiber orientation has been well developed to some extent [Halpin and Kardo (1976)]. Therefore, prediction of fiber orientation during the transient mold filling is important for the prediction of such anisotropic properties of final plastic part.

Nowadays, many researchers have developed many numerical simulation programs with different methods. However, some of them using direct calculation of fiber motion [Yamamoto and Matsuoka (1993), Yamane *et al.* (1994), Mackaplow and Shaqfeh (1996), Sundararajakumar and Koch (1997), Fan *et al.* (1998)] require incredible computation time which is the reason why such a numerical simulation method cannot be accommodated. Calculation of fiber orientation state using the probability distribution function (DFC, in short) is one of them. Instead, a tensor representation of orientation state [Advani and Tucker (1987)], which is a pre-averaging concept of DFC, is widely used for its efficiency, compactness and above all, manageable computation time. However, it is necessary to introduce a closure approximation to express the higher order tensor in terms of lower order tensors for a closed set of equation since the evolution equation for orientation tensor involves the next higher even order tensor.

Various closure approximations have been proposed. Among them, a Hybrid closure approximation (HYB) [Advani and Tucker (1990)] has readily been used for its stable behaviors in spite of its over-prediction of orientation components compared with DFC. Recently, Cintra and Tucker (1995) developed Orthotropic fitted closure approximation (ORF, ORL) by assuming that the principal directions of 4^{th} order orientation tensor are functions of the eigenvalues of 2^{nd} order orientation tensor. Unknown parameters were determined by fitting selected flow data obtained from DFC. ORF (or ORL) shows better behaviors than previous closure approximations but unfortunately suffers from non-physical oscillations at low value of fiber-fiber interaction coefficient. Chung and Kwon have proposed ORW and ORW3 (1999, 2000a) which overcome such problems of non-physical oscillations. However, such Orthotropic type closure approximations (ORF, ORL, ORW and ORW3) requires additional computation time for the transformation between the global coordinate system and the principal coordinate system. In this respect, Chung and Kwon (2000b) have proposed IBOF (Invariant Based Optimal Fitting) closure approximation which significantly reduces the computation time.

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For proper numerical simulation, coupling effect between the flow field and fiber orientation state must be incorporated. Chung and Kwon (1995,1996) implemented the Dinh-Armstrong model [Dinh and Armstrong (1984)] incorporating the additional stress due to the existence of fibers into the governing equation based on the Hele-Shaw approximation in injection molding filling simulation of short-fiber reinforced plastic parts. Present work is aimed at injection molding filling simulations incorporating the coupling effect between the flow and fiber orientation along with the in-plane velocity gradient effect with recently developed closure approximations. Predicted values will be compared with available experimental data of a film-gated strip and a center-gated disk from Bay (1991).

2. Theory

2.1. Fiber Orientation

There are several different approaches describing the fiber orientation state in short-fiber-reinforced part during molding process, but among other things orientation tensors are mainly used for a compact representation of the orientation state of fibers because of the computational efficiency.

Fiber is considered to be rigid cylinder and its aspect ratio is assumed to be mono-disperse. Single fiber can be represented as a unit vector $\mathbf{p}$ (or θ, the polar angle, and ϕ, the azimuthal angle) as shown in Fig. 1. The orientation state of a group of fibers can be described by a probability distribution function $\Psi(\mathbf{p})$, defined so that the probability of a fiber being oriented within an angular range $d\mathbf{p}$ of the direction $\mathbf{p}$ is equal to $\Psi(\mathbf{p})d\mathbf{p}$. Combining the following conservation equation, Eq.1, for Ψ in $\mathbf{p}$ space and the fiber angular velocity equation, Eq.2, leads to the governing equation for $\Psi(\mathbf{p})$ [Folgar and Tucker (1984), Advani and Tucker (1987)].

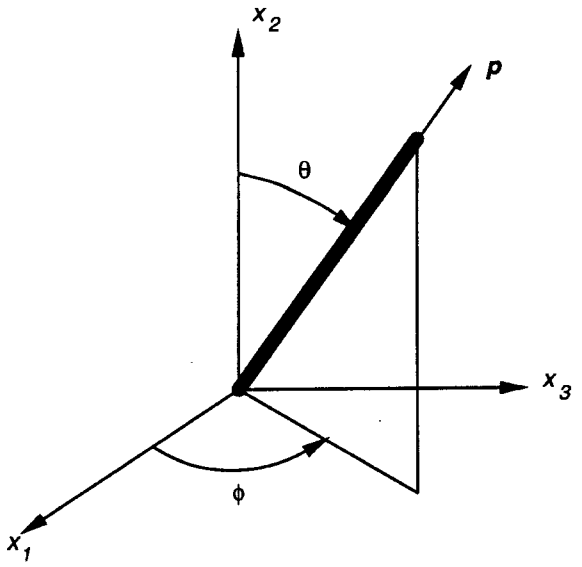

Fig. 1. Orientation of single fiber.

$$\frac{D\Psi}{Dt} = \frac{\partial}{\partial \mathbf{p}} \cdot (\Psi \dot{\mathbf{p}}) \tag{1}$$

$$\dot{p}_i = -\frac{1}{2}\omega_{ij}p_j + \frac{1}{2}\lambda(\dot{\gamma}_{ij}p_j - \dot{\gamma}_{kl}p_k p_l p_i) - \frac{D_r \partial \Psi}{\Psi \partial p_i} \tag{2}$$

Direct calculation of probability distribution function $\Psi(\mathbf{p})$ is referred to as 'DFC'.

The second and fourth order orientation tensors are defined as follows:

$$a_{ij} = \int p_i p_j \Psi(\mathbf{p})\, d\mathbf{p}$$
$$a_{ijkl} = \int p_i p_j p_k p_l Y(\mathbf{p})\, d\mathbf{p} \tag{3}$$

The evolution equation for the second-order orientation tensor a_{ij} can be expressed as follows [Advent and Tucker (1987)] :

$$\frac{Da_{ij}}{Dt} = -\frac{1}{2}(\omega_{ik}a_{kj} - a_{ik}\omega_{kj}) + \frac{1}{2}\lambda(\dot{\gamma}_{ik}a_{kj} + a_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl}a_{ijkl})$$
$$+ 2D_r(\delta_{ij} - 3a_{ij}) \tag{4}$$

where $\omega_{ij} = u_{j,i} - u_{i,j}$ is the rotation rate tensor, $\dot{\gamma}_{ij} = u_{j,i} + u_{i,j}$ the rate of deformation tensor, and δ_{ij} the identity tensor. $\lambda = \frac{(L/D)^2 - 1}{(L/D)^2 + 1}$ is a parameter related to the aspect ratio of the fiber L/D. The third term on the right hand side of Eq.4 accounts for fiber-fiber interaction. The rotary diffusivity term D_r is used to model fiber-fiber interaction in concentrated (semi-dilute) suspensions. Folgar and Tucker (1984) suggested $D_r = C_I\dot{\gamma}$, where an interaction coefficient C_I should be determined, to our present knowledge, in such a way that the predicted orientation can fit best the experimental data, $\dot{\gamma}$ being the generalized shear rate defined as follows

$$\dot{\gamma} = \sqrt{\frac{1}{2}\dot{\gamma}_{ij}\dot{\gamma}_{ji}} \tag{5}$$

The present study adopted $D_r = C_I\dot{\gamma}$ in the numerical calculations of fiber orientation.

2.2. Closure Approximations

A closure approximation is inherently required to obtain a closed set of evolution equations for orientation tensors: for instance, to solve Eq. 4 one needs to introduce a suitable closure approximation for the fourth-order tensor a_{ijkl} in terms of a_{ij} and δ_{ij}.

The present study employed several closure approximations which can be briefly described below.

Orthotropic fitted closure approximation (ORF,ORL)

Cintra and Tucker (1995) have developed Orthotropic fitted closure approximations (referred to as ORF, ORL)

by assuming the principal values of a_{ijkl} are functions of the eigenvalues of a_{ij}. Short summary might be presented as follows:

With full symmetry conditions and normalization conditions, there are only three independent components of principal values of 4th order tensor, which are taken to be functions of two largest eigenvalues of 2nd order tensor a_{ij} as follows :

$$\begin{aligned} \overline{A}_{11} &= f_{11}(a_1,a_2) \\ \overline{A}_{22} &= f_{22}(a_1,a_2) \\ \overline{A}_{33} &= f_{33}(a_1,a_2) \end{aligned} \tag{6}$$

where $\overline{A}_{11}$, $\overline{A}_{22}$, $\overline{A}_{33}$ are independent principal values of 4th order orientation tensor in contracted notation ($A_{11} = a_{1111}^{p}$, $A_{22} = a_{2222}^{p}$, $A_{33} = a_{3333}^{p}$, $A_{44} = a_{1122}^{p}$, $A_{55} = a_{2233}^{p}$, $A_{66} = a_{3311}^{p}$) and a_1,a_2 are two largest eigenvalues of 2nd order orientation tensor, that is, $a_1 \geq a_2 \geq a_3$. To determine unknown parameters in Eq.6 least square optimal fitting were used with selected flow cases generated by DFC.

Even if ORF and ORL satisfactorily predict most simple flows, one of the critical problems of ORF and ORL is that they suffer from non-physical oscillations in simple shear flow for low $\mathbf{C_I}$ values.

ORW and ORW3

ORW and ORW3 [Chung and Kwon (1999, 2000a)] were proposed as an improved version of ORF and ORL closure approximations to overcome non-physical oscillations ob-served in ORF and ORL. The main improvement was achieved by fitting additional flow data to cover the whole region of fiber orientation states. ORW3 outperforms ORW especially for non-homogeneous radial diverging flow for low $\mathbf{C_I}$ values.

Natural closure approximation (NAT)

NAT takes a general expression for a_{ijkl} in terms of a_{ij} and δ_{ij} and polynomial expansions in terms of principal invariants were adopted for unknown coefficients appearing in the general expression. The term "Natural" closure approximation is originated from the fact that it made use of the natural closure values, i.e., analytical solutions which exist only for $\mathbf{C_I} = 0.0$ with $\lambda = 1$ in a least square fitting procedure [Verleye and Dupret (1994)]. It showed good transient behaviors but results in a little over-prediction of steady state orientations. It may be noted, however, that singularities are reported to exist for axisymmetric orientation states, which is referred to as a significant drawback of using NAT in general flow cases without a special care of such singularities [Dupret and Verleye (1999)].

ORE

Recently, Wetzel (1999) and Verweyst (1999) introduced another version of Orthotropic fitted closure approximation, ORE, differing from ORF (or ORL) in that analytic solutions corresponding to $\mathbf{C_I} = 0$ and $\lambda = 1$ were adopted for the fitting flow data, as was done in NAT. It may be just mentioned that the performance of fiber orientation predictions in many flow cases is almost as good as ORW3.

Invariant Based Optimal Fitting closure approximation (IBOF)

IBOF [Chung and Kwon (2000b)] also starts with the most general expression of a full symmetric 4th order tensor a_{ijkl} in terms of a_{ij} and δ_{ij} as follows :

$$\begin{aligned} a_{ijkl} = {} & \beta_1\mathbf{S}(\delta_{ij}\delta_{kl}) + \beta_2\mathbf{S}(\delta_{ij}a_{kl}) + \beta_3\mathbf{S}(a_{ij}a_{kl}) + \beta_4\mathbf{S}(\delta_{ij}a_{km}a_{ml}) \\ & + \beta_5\mathbf{S}(a_{ij}a_{km}a_{ml}) + \beta_6\mathbf{S}(a_{im}a_{mj}a_{kn}a_{nl}) \end{aligned} \tag{7}$$

where the operator **S** indicate the symmetric part of its argument, for instance,

$$\begin{aligned} \mathbf{S}(T_{ijkl}) = \frac{1}{24}(& T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl} \\ & T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl} \\ & T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}+T_{ijkl}) \end{aligned} \tag{8}$$

IBOF assumes that the coefficients β_1~β_6 are polynomial expansions of the second and third invariants (II,III) of a_{ij}. It can be easily shown that, among the six β_i's in Eq.7, there are only three independent values with the rest being determined in terms of the three independent ones with the help of the normalization conditions and full symmetry between indices together with Cayley-Hamilton Theorem. Orthotropic type closure approximations (ORF, ORL, ORW, ORW3) requires additional computation time for the transformation between the global coordinate and principal coordinate and most of times are spent for this procedure. IBOF does not require such computation and total CPU time is about half the computation time Orthotropic type closure approximations required.

2.3. Mold Filling Flow

The anisotropic constitutive equation, including an additional stress due to the existence of fibers, should be introduced for the coupled analysis of the injection molding filling of fluid flow and the fiber orientation state. Using Batchelor's cell model [Batchelor (1971)], Dinh and Armstrong (1984) developed a rheological equation of state for semi-concentrated fiber suspensions where the average spacing h between neighboring fibers is greater than its diameter D, but less than its length L where hydrodynamic interactions between fibers dominates over mechanical contacts. The constitutive equation of this model can be described as follows:

$$\tau_{ij} = \eta(u_{i,j} + u_{j,i}) + \eta N u_{k,l} a_{ijkl} \tag{9}$$

where the dimensionless parameter N representing the

anisotropic contributions from the fibers is given by

$$N = \frac{\pi n L^3}{6 \ln(2h/D)} \tag{10}$$

with

$$h = \begin{cases} (nL^2)^{-1} & \text{for random orientation} \\ (nL)^{-1/2} & \text{for aligned orientation} \end{cases}$$

In the simulation, it is assumed that the average distance from a given fiber to its nearest neighbors h is linear in terms of the scalar measure of orientation f, which varies from zero to unity according to the orientation state of fibers. When the number of fibers per unit volume n is greater than $1/(DL^2)$, the average distance between fibers is assumed to be the same as for the aligned orientation state independent of the orientation state. Therefore, in this study, h is described as

$$h = (1 - f)h_{random} + fh_{aligned} \quad \text{for} \quad \frac{\pi}{4}\left(\frac{D}{L}\right)^2 < v_f < \frac{\pi}{4}\left(\frac{D}{L}\right)$$

$$h = h_{aligned} \quad \text{for} \quad \frac{\pi}{4}\left(\frac{D}{L}\right) \le v_f < \frac{\pi}{4} \tag{11}$$

$$f = 1 - 27 \det[a_{ij}] \tag{12}$$

where v_f stands for the fiber volume fraction.

The injection mold filling flow for fiber suspensions including coupling effects between flow and fiber orientation with in-plane velocity gradient effects is governed by the following equations:

pressure equation [Chung and Kwon (1996)]

$$\frac{\partial}{\partial x}\left[(S-S^x)\frac{\partial P}{\partial x} - S^{xy}\frac{\partial P}{\partial y} - F^x\right] + \frac{\partial}{\partial y}\left[(S-S^y)\frac{\partial P}{\partial y} - S^{xy}\frac{\partial P}{\partial y} - F^y\right] = 0 \tag{13}$$

where

$$N^x = \frac{Na_{3113}(1+Na_{3223}) - N^2 a_{3123}a_{3213}}{(1+Na_{3113})(1+Na_{3223}) - N^2 a_{3123}a_{3213}}$$

$$N^y = \frac{Na_{3223}(1+Na_{3113}) - N^2 a_{3123}a_{3213}}{(1+Na_{3113})(1+Na_{3223}) - N^2 a_{3123}a_{3213}}$$

$$N^{xy} = \frac{Na_{3123}}{(1+Na_{3113})(1+Na_{3223}) - N^2 a_{3123}a_{3213}}$$

$$f^x = \eta Nu_{\alpha,\beta a} 31_{\alpha\beta}\big|_z + \int_0^{\tilde{z}} (\tau_{xx,x} + \tau_{yx,y}) d\tilde{z}$$

$$f^y = \eta Nu_{\alpha,\beta a} 32_{\alpha\beta}\big|_z + \int_0^{\tilde{z}} (\tau_{zy,z} + \tau_{yy,y}) d\tilde{z}$$

$$S = \int_0^{\tilde{z}} \frac{\tilde{z}^2}{\eta} d\tilde{z} \qquad S^x = \int_0^{\tilde{z}} N^x \frac{\tilde{z}^2}{\eta} d\tilde{z}$$

$$S^y = \int_0^{\tilde{z}} N^y \frac{\tilde{z}^2}{\eta} d\tilde{z} \qquad S^{xy} = \int_0^{\tilde{z}} N^{xy} \frac{\tilde{z}^2}{\eta} d\tilde{z}$$

$$F^x = \int_0^{\tilde{z}} \frac{\tilde{z}}{\eta}[(1-N^x)f^x - N^{xy}f^y] d\tilde{z}$$

$$F^y = \int_0^{\tilde{z}} \frac{\tilde{z}}{\eta}[(1-N^y)f^y - N^{xy}f^x] d\tilde{z}$$

Local Cartesian coordinates are chosen such that x and y coordinates are lying on the surface of thin cavity thickness molds, z being the gap-wise coordinate as shown in Fig. 2.

Boundary conditions on the pressure equation are

$P = 0$ on the moving flow front

$\bar{u} \cdot \bar{n}_x + \bar{v} \cdot \bar{n}_y = 0$ on the impermeable boundaries.

Pressure equation for fiber suspensions includes the extra terms (S_x, S_y, S_{xy}, F_x, F_y) due to the additional stress of fibers, and F_x and F_y represent the x and y directional in-plane velocity gradient effect. Refer to Chung and Kwon (1995,1996) for the details.

A modified Cross model has been employed for the viscosity of the thermoplastic medium:

$$\eta(\dot{\gamma}, T) = \frac{\eta_0}{1 + (\eta_0 \dot{\gamma}/\tau^*)}, \quad \eta_0 = B \exp\left(\frac{T_b}{T}\right) \tag{14}$$

where m, B, τ^* and T_b are constants for a given material.

energy equation

$$\rho C_p\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right) = k\frac{\partial^2 T}{\partial z^2} + \eta\dot{\gamma}^2 \tag{15}$$

Appropriate boundary conditions in the z-direction are the uniform temperature at the mold wall z = b and the symmetric condition at the mid-plane z = 0

A detailed implementation of numerical analysis is described in Chung and Kwon (1995,1996). In this work, fountain flow and the fiber-wall interaction have been neglected.

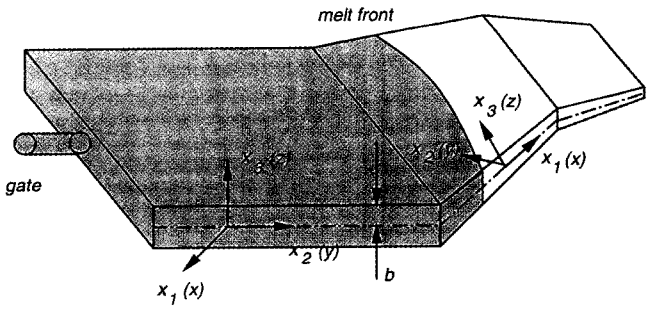

Fig. 2. Typical molded part for the analysis. A local coordinate system is chosen so that $x_3(z)$ is along the thickness direction, $x_1(x)$ and $x_2(y)$ lying on the plane.

3. Numerical analysis and discussion

We have performed coupled analysis of injection mold filling process including in-plane velocity gradient effects for a film-gated strip and a center-gated disk and compared with experimental measurements of fiber orientation of nylon 6/6 reinforced with 43 wt% ($v_f = 0.23$) of glass fibers (Du Pont: Zytel 101 L)[Bay (1991)]. Non-isothermal, non-Newtonian effects are incorporated. The average fiber length **L** =210 μm and the diameter D = 11 μm. The thermal properties and melt viscosity constants for the modified Cross model are shown in Table 1. Finite element meshes used for numerical analysis are shown in Fig. 3 and Fig. 4. Cavity geometry data are as follows.

Film-gated strip: length 1 = 203.2 mm, width W = 25.4 mm, and a thickness 2b = 3.18 mm.

Center-gated disk: outer radius R_0 = 76.2 mm and a thickness 2b = 3.18 mm.

N = 40.3 is used for simulation based on Dinh and Armstrongs theory with Eqs.9~10. Processing conditions are as follows:

Film-gated strip: inlet temperature T_{inlet} = 550 K, mold wall temperature T_{wall} = 297 K, and the filling time t_{fill} = 0.4 s.

Table 1. Material properties and viscosity constants of nylon 6/6

Thermal properties (Du Pont: Zytel 70G43L)	
ρ	1.33×10^3 kg/m^3
C_p	1.97×10^3 J/(kg · K)
k	2.60×10^{-1} W/(m · K)
Viscosity constants for Cross Model (Du Pont: Zytel 70G43L)	
m	0.549
B	4.37×10^{-9} Pa · s
T_b	1.68×10^4 K
t*	3.04×10^4 Pa

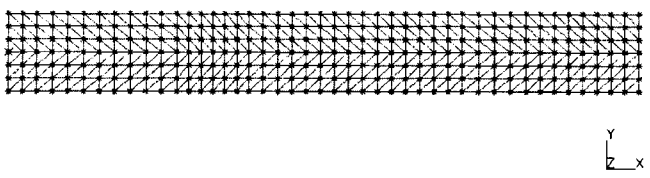

Fig. 3. Finite element mesh for rectangular film-gated strip with 528 elements and 315 nodes.

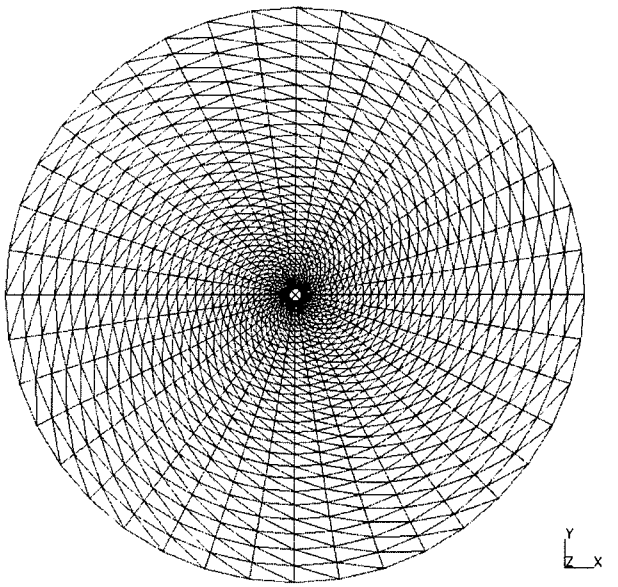

Fig. 4. Finite element mesh for a center-gated disk with 2400 elements and 1240 nodes.

Center-gated disk: T_{inlet} = 550 K, T_{wall} = 347 K, t_{fill} = 2.5 s.

Inlet (initial) orientation state is as follows:

Film-gated strip: $a_{11} = 0.5$, $a_{22} = 0.2$, $a_{33} = 0.3$, $a_{12} = a_{13} = a_{23} = 0$

Center-gated disk: $a_{11} = 1/3$, $a_{22} = 1/3$, $a_{33} = 1/3$, $a_{12} = a_{13} = a_{23} = 0$

Shown in Fig. 5 are flow and thickness directional orientation component (a_{11} & a_{33}) across the thickness at several flow directional locations (x/b) for a film-gated strip. To compare results obtained from various closure approximations with experimental data C_I = 0.001 is used for ORL and other models while C_I = 0.01 is used for HYB since results from HYB with C_I = 0.001 is too bad to compare. All of them seem to predict a_{11} and a_{33} qualitatively well compared with experimental data. However, a_{11} shows a little over-prediction of flow directional orientation component at far down-stream, resulting in a thinner core than the experimental data. This point is to be further discussed in conjunction with the center-gated disk case as below. a_{33} show qualitative agreements with experimental data except the symmetry region (z/b = 0) because of no shear deformation.

Shown in Fig. 6 are flow directional orientation component (a_{11}) across the thickness at several flow directional locations (r/b) for a center-gated disk. In this comparison, the same values of C_I are used as in the film-gated strip described above. As indicated in Fig. 6, closure models show excellent agreements with experimental data for the range of radial location between the inner radius and about half the radius of the disk. ORW,

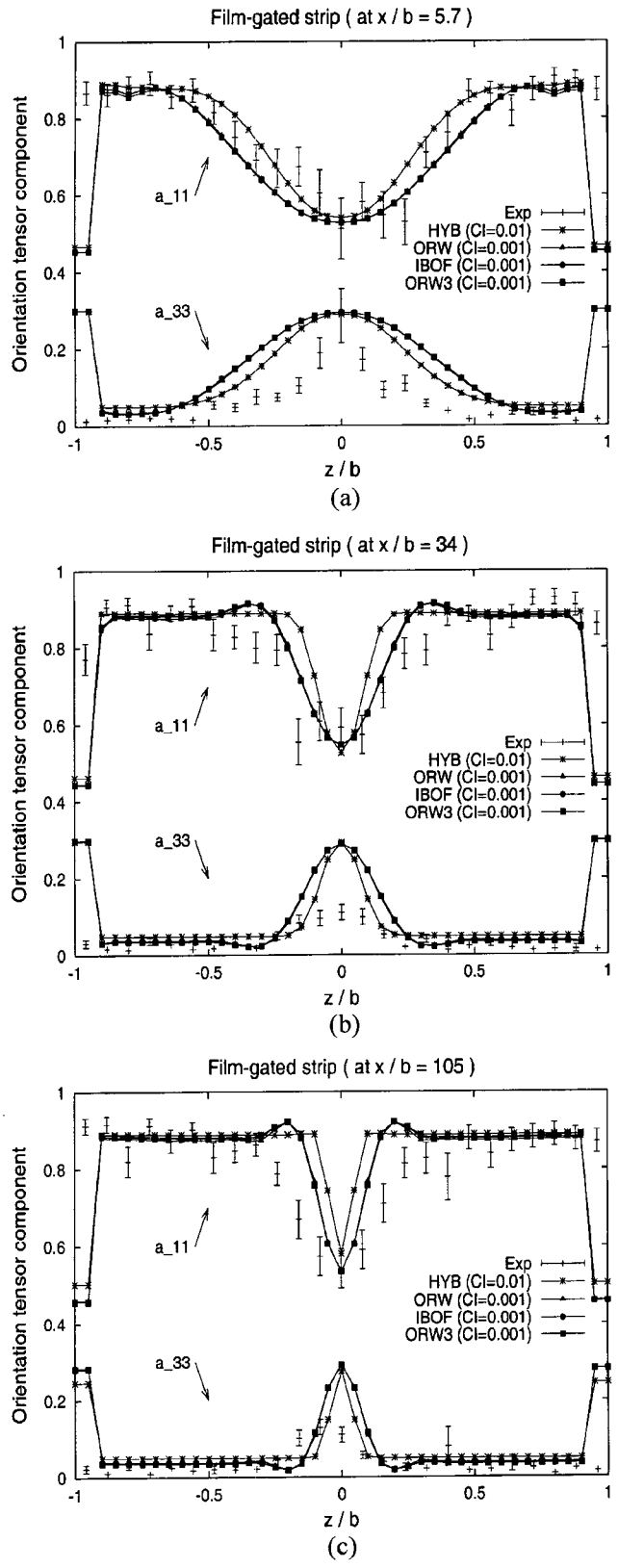

Fig. 5. Orientation component as a function of thickness positions (z/b) for various closure approximations of HYB, ORW,IBOF and ORW3 with experimental data for film-gated strip at (a) x/b = 5.7, (b) x/b = 34, (c) x/b = 105.

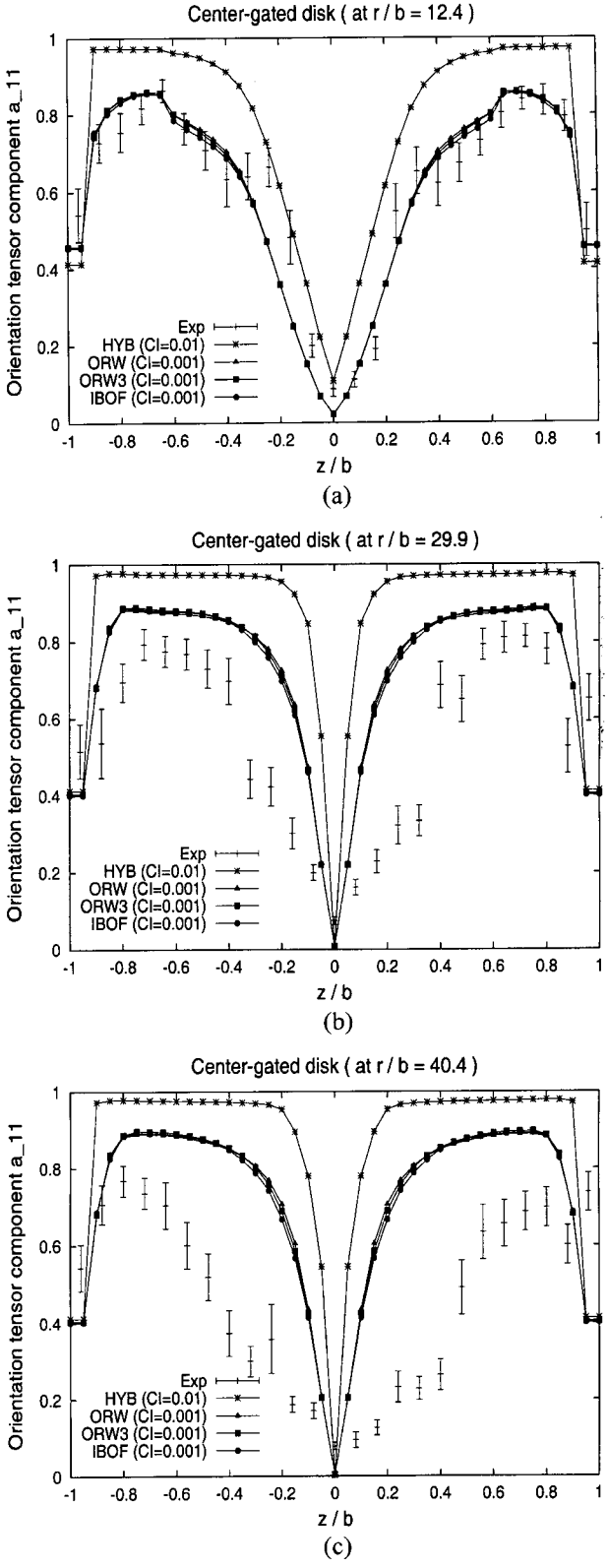

Fig. 6. a_{11} (flow-directional orientation) component as a function of thickness positions (z/b) for various closure approximations of HYB,ORW,ORW3 and IBOF with experimental data for center-gated disk at (a) r/b = 12.4, (b) r/b = 29.9, (c) r/b = 40.4.

ORW3 and IBOF almost show same behaviors.

However, as fiber orientation reaches a steady state, one can observe an over-prediction of flow directional orientation component a_{11} at core layer (i.e., resulting in too thin core layer) as in the case of the film-gated strip. Assuming that the experimental data are correct, one may consider the following points to account for such a consistent deviation between the numerical prediction and experimental data.

① Compressibility effect by packing stage may affect orientation behaviors, but by intuition, additional velocity components induced by compressibility will further align flow directional orientation component and thus make the core layer thinner. Therefore, considering polymer compressibility effect may not be the right direction to remedy this kind of deviation.

② Diverging effect by thermal boundary layer at wall region (due to conduction from mold wall) induced by a long filling time at center-gated disk may reduce the flow directional orientation component around core layers as a kind of randomization effect. This phenomenon might be observed to some extent around core layer as indicated by the case of z/b = 0.2 in Fig. 7 which shows a_{11} as a function of radial location (r/b) at several thickness positions (z/b) in case of IBOF. a_{11} in the case of z/b = 0.2 starts decreasing around r/b = 30. This reveals the diverging effect, though not significant, in contrast to a_{11}at other layers (z/b = 0.5,0.7). However, a strip with a negligible thermal boundary layer due to a short filling time also shows a thin core. So the diverging effect does not make any difference between the film-gated strip and the center-gated disks despite their different filling time.

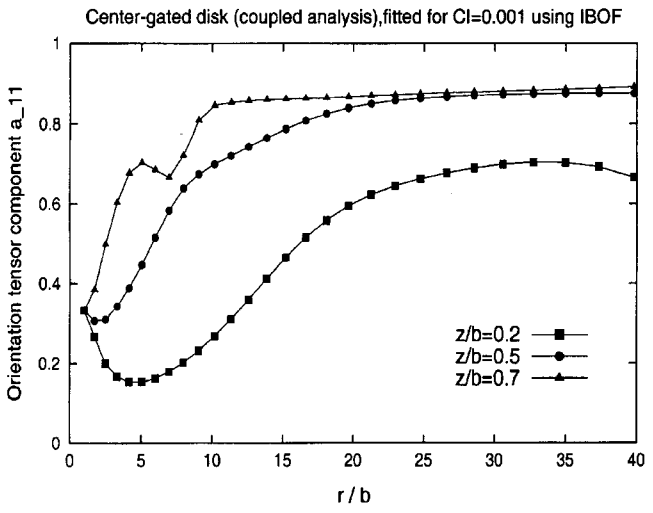

Fig. 7. Plot of a_{11} (flow-directional orientation) component vs. r/b for center-gated disk (coupled analysis with in-plane velocity gradient as well as usual shear effect) with $C_I = 0.001$ using IBOF closure approximation.

③ One may try to modify Folgar and Tuckers model for diffusivity term (more specifically, interaction coefficient C_I in $D_r = C_I\dot{\gamma}$), which accounts for the fiber-fiber interaction. According to this model, the orientation is known to reach the steady state rather quickly than the experimental data [Folgar and Tucker (1984)]. It seems natural to conceive that the magnitude of fiber-fiber interaction coefficient may depend on the orientation state especially during the transient and the steady periods. By intuition, C_I for the transient state must be larger than that of the steady state. This argument has been discussed by many researchers [Folgar and Tucker (1984), Shaqfeh and Fredrickson (1989), Rahnama *et al.* (1994), Stover *et al.* (1992), Fan *et al.* (1998)]. Also, we can verify this argument by performing the coupled simulation of the center-gated disk for $C_I = 0.0001$ with ORW3 and IBOF, which are shown in Fig. 8. At far downstream of r/b = 40.4, predicted orientation component is in much better agreement with experimental data than that for $C_I = 0.001$ (Fig. 6). On the other hand, near the gate (at r/b = 12.4) the predicted a_{11} with $C_I = 0.001$ is closer to experimental data than that with $C_I = 0.0001$. In summary, it looks plausible that near the gate where orientation state is still transient, $C_I = 0.001$ is appropriate and at far downstream where aligned orientation state is reached, $C_I \leq 0.0001$ is more appropriate. More study is in order along this line.

4. Concluding Remarks

We have extensively performed numerical analysis of injection molding filling process of fiber suspension in polymer based matrix with recently proposed closure approximations, namely ORW, ORW3 and IBOF. Coupling effect between the fluid flow and the fiber orientation is introduced via Dinh-Armstrong model, along with the in-plane velocity gradient effect in such analyses. Predicted fiber orientations are favorably compared with experimental data for cases of a film-gated strip and a center-gated disk. Simulation results show almost no differences among the fitted closure approximations (ORW, ORW3, IBOF). However, IBOF requires only half the computation time as compared with ORW or ORW3. HYB shows over-prediction of orientation components as expected. Systematic discrepancy between simulation results and experimental data may support, for a better prediction of fiber orientation, to modify the constant isotropic diffusivity term which was used to account for fiber-fiber interaction in the present analyses.

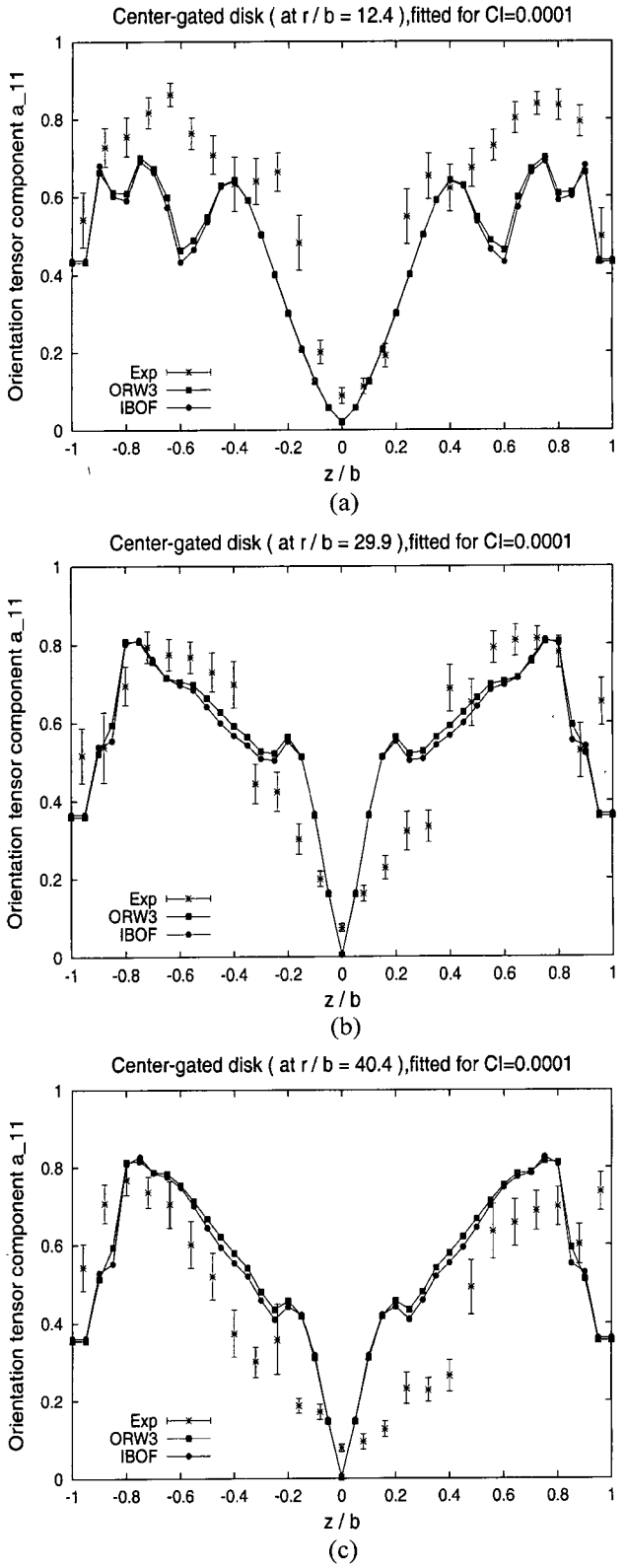

Fig. 8. a_{11} (flow-directional orientation) component as a function of thickness positions (z/b) with $C_I = 0.0001$ for closure approximations of ORW3 and IBOF with experimental data for center-gated disk at (a) r/b = 12.4, (b) r/b = 29.9, (c) r/b = 40.4.

5. List of symbols

a_{ij} = Second-order orientation tensor.
a_{ijkl} = Fourth-order orientation tensor.
a_{ijkl}^{p} = Fourth-order orientation tensor in reference to eigenspace of second-order orientation tensor (Defined to be principal values of fourth-order orientation tensor in this paper).
a_1, a_2, a_3 = Eigenvalues of second-order orientaton tensor in descending order in magnitude.
$\overline{A}_{mm}$ = Principal values of fourth-order orientation tensor in contracted notation.
b = Half gap thickness of molded part.
C_I = Interaction coefficient for fiber-fiber interaction
C_p = Thermal capacity of the thermoplastic medium.
D = Fiber diameter.
D_r = Diffusivity term which accounts for fiber-fiber interaction
f = Scalar measure of orientation
h = Average distance from a given fiber to its nearest neighbor.
k = Thermal conductivity of the thermoplastic medium.
l = Chracteristic length of injection molded part.
L = Fiber length.
n = Number of fibers per unit volume.
n_x, n_y = Components of unit outward normal vector on the boundary.
N = Dimensionless number accounting for anisotropic contribution from fiber.
p = Fiber unit direction.
p_i = Fiber angular velocity.
P = Pressure.
R_0 = Outer radius of center-gated-disk.
t_{fill} = Filling time.
T = Temperature.
T_{inlet} = Inlet melt temperature.
T_{wall} = Mold wall temperature.
u, v = In-plane velocity components with respect to local coordinate.
$\bar{u}$, $\bar{v}$ = Gapwise average velocity.
$u_{i,j}$ = $\partial u_i / \partial x_j$, velocity gradient tensor.
v_f = Volume fraction of fibers.
W = width of injection molded part.
w = Gapwise velocity components with respect to local coordinate.
x,y,z = Local coordinate system.
m, B, τ^*, T_b = Coefficients of viscosity function.
D/Dt = Material derivative.
I, II, III = First, second and third principal invariants of a_{ij}

Greek letters

Ψ = Probability distribution function.
$\dot{\gamma}$ = Generalized shear rate.
$\dot{\gamma}_{ij}$ = Rate of deformation tensor.
δ_{ij} = Unit tensor.
η = Viscosity of the thermoplastic medium.
η_0 = Zero shear rate viscosity.
λ = Geometric parameter related to the particle aspect ratio.
ρ = Density of the thermoplastic medium.
τ_{ij} = Stress tensor.
ω_{ij} = Vorticity tensor.

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