NUMERICAL PREDICTION OF FLOW INDUCED FIBERS ORIENTATION IN INJECTION MOLDED POLYMER COMPOSITES

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ABSTRACT

Since the filling stage of injection molding process has important effect on the determination of the orientation state of the fibers, accurate analysis of the flow field for the mold filling stage becomes a necessity. The aim of the paper is to characterize the flow induced orientation state of short fibers in injection molding cavities. A dog-bone shaped model is considered for the simulation and experiment. The numerical model for determination of the fibers orientation during mold-filling stage of injection molding process was solved using Computational Fluid Dynamics (CFD) software called MoldFlow. Both the simulation and experimental results showed that two different regions (or three layers of orientation structures) across the thickness of the specimen could be found: a shell region which is near to the mold cavity wall, and a core region at the middle of the cross section. The simulation results support the experimental observations that for thin plates the probability of fiber alignment to the flow direction near the mold cavity walls is high but low at the core region. It is apparent that the results of this study could assist in decisions regarding short fiber reinforced polymer composites.

Keywords: Computational Fluid Dynamics (CFD); Fiber orientation; Non-Newtonian fluid.

INTRODUCTION

Nowadays, fiber reinforced plastic composites are replacing metals which are being used for many years. This is due to the fact that fiber reinforced plastics have high strength to weigh ratio, low cost compared to metals, and high resistance to corrosion. However, the production of the composites nowadays is very challenging to meet the market requirement. Moreover, the study of the flow of fiber-filled polymers in injection molding process is quite complex due to the fact that the flow of fiber filled thermoplastics in the molten state is modified by the presence of fibers and vice versa, i.e., the fiber motion and rotation are also affected by the flow [1]. These add considerable complexities to the flow study of the polymer matrix. Above all, the study of the flow properties of concentrated suspensions in polymer melts remains most challenging. Therefore, it is very important to fully understand the flow behavior of the polymer-fiber mixture inside the injection molding cavity in order to be able to accurately predict the orientation state of the fibers.

To date numerous researchers have reported on the patters of fibers orientation in injection molded fiber reinforced polymer composites [2-5]. The first author who studied the flow of fiber suspensions and found distribution function of the orientation angle of the particle is Jeffery [6]. In his model, Jeffery assumed that the particle is rigid, neutrally buoyant, axisymmetric, and large enough so that Brownian motion (motion arising from collision of molecules in the fluid medium with the suspended particles) can be negligible. However, most commercially available reinforced thermoplastics are concentrated suspensions as they contain around 30% by weight, or 15% by volume of fibers [7].

Hence, some modifications to Jeffery's model are necessary to account for the fiber-fiber interactions for concentrated fiber suspensions. Folgar and Tucker [8] have modified the Jeffery's model by introducing a fiber-fiber interaction coefficient. Moreover, the flow and fiber motion calculations are coupled through the stress terms. One of the well-known numerical methods for the stress contribution from the fiber suspension is solving of the stress tensor in the flow field. In this case, the fiber stress is modeled by the constitutive equation of the fiber orientation tensor. Instead of calculating the orientation distribution function directly, the orientation tensor method is used. However, tensor approximation inevitably encounters a closure problem of a higher-order orientation state. To tackle this problem, many researchers have developed different closure models [9, 10].

The aim of the paper is to numerically characterize the flow induced orientation state of short fibers in three dimensional injection molding cavities. The data obtained from the simulation are compared to qualitative experimental data. A bone shaped model was considered for the simulation and experiment. The model is intended to predict the fiber orientation across the through thickness of the specimen at various locations along its length.

MATHEMATICAL MODEL

The mould cavity considered for this study is a bon-shaped tensile testing specimen cavity as shown in Figure 1 with dimensions 164 mm x 18 mm x 3 mm. Highly viscous nylon/glass fiber mixture enters the cavity through the origin at the right side of the cavity.
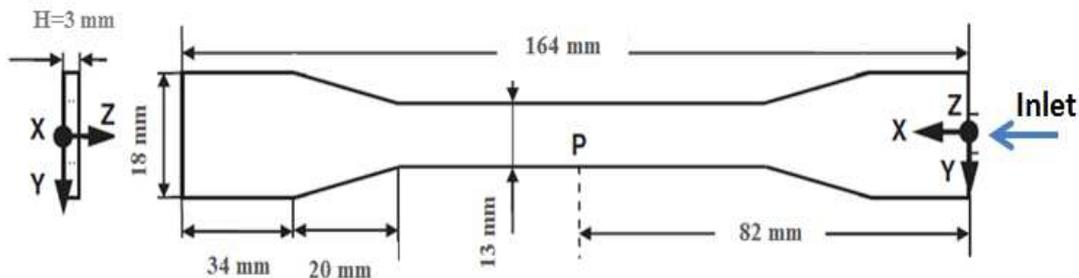

Figure 1. Schematic of the mold cavity

During the filling stage, the polymer/fiber mixture flow field is considered to be incompressible, non-isothermal and behaves as non-Newtonian fluid. Since the mixture under consideration is highly viscous, the inertia and body force terms in the

momentum equation are neglected. Therefore, the general form of the mass, momentum and energy equations can be written as [11]:

$$\nabla \cdot (\boldsymbol{u}) = \boldsymbol{0} \tag{1}$$

$$0 = -\nabla p + \nabla \cdot \tau \tag{2}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T \right) = k \nabla^2 T + \dot{\gamma} \cdot \tau \tag{3}$$

where $\boldsymbol{u}$ is the velocity vector, ρ is the density with T being the temperature and p the hydrostatic pressure. The terms C_p, k, τ and $\dot{\gamma}$ represent the specific heat, the thermal conductivity, the total extra stress tensor, and the shear rate of the suspension, respectively.

For this study, the density, thermal conductivity and specific heat capacity values are assumed to be constant. Moreover, the melt is assumed to be a non-Newtonian fluid exhibiting a shear thinning behavior with increasing shear rate and also its viscosity depends on the shear rate and temperature. To account for the dependence of the viscosity on the shear rate, the cross model is used.

$$\eta = \frac{\eta_0}{1 + \left(\eta_0 \dot{\gamma} \middle/ \tau^* \right)^{1-n}} \tag{4}$$

where η_o, τ^*, and n are empirical constants.

The total stress for the suspension can be obtained by combining the contribution of the suspending fluid τ^s and the contribution of the fiber τ^f to the total extra stress. The fiber contribution to the total stress is [12],

$$\boldsymbol{\tau}^f = \eta \xi N \frac{\partial u_k}{\partial x_l} A_{ijkl} \tag{5}$$

where η_s, and A_{ijkl} represent the suspension viscosity and the fourth order orientation tensor respectively. The coefficient N is a dimensionless number, called the particle number, which can be described in terms of the volume fraction and fiber aspect ratio. Physically, it represents the magnitude by which the suspension resists elongation parallel to the fiber axial direction. Similarly, the suspending fluid contribution to the total stress is,

$$\boldsymbol{\tau}^s = 2\eta\dot{\gamma} = \frac{1}{2}\eta\left(\boldsymbol{u} - \boldsymbol{u}^{\mathbf{T}}\right) \tag{6}$$

Therefore the total stress becomes

$$\boldsymbol{\tau} = \boldsymbol{\tau}^s + \boldsymbol{\tau}^f \tag{7}$$

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In addition to the flow governing equation, one additional equation for the fiber orientation to be coupled with the flow equations is required. Assuming that the fibers are rigid cylinders, uniform in length and diameter, and that the number of fibers per unit volume is uniform, the equation change for the second order orientation tensor proposed by Advani and Tucker [13] is used.

$$\frac{Da_{ij}}{Dt} = \frac{\partial a_{ij}}{\partial t} + u_k \frac{\partial a_{ij}}{\partial x_k} = -\left(\omega_{ik}a_{kj} - a_{ik}\omega_{kj}\right) + \\ \lambda\left(\dot{\gamma}_{ik}a_{kj} + a_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl}A_{ijkl}\right) + 2C_I\dot{\gamma}\left[\delta_{ij} - 3a_{ij}\right]$$

(8)

where u_k is the velocity component, δ_{ij} is a unit tensor, and ω_{ij} and $\dot{\gamma}_{ij}$ are the rotation rate and rate of deformation tensors respectively. λ is a constant that depends on the geometry of the fibers, defined as $\lambda = (r_e^2 - 1)/(r_e^2 + 1)$ with r_e being fiber aspect ratio. C_I is a dimensionless interaction coefficient which represents the degree of interaction between short fibers. The fourth order orientation tensor evolved in Equations (5 and 8) needs to be approximated in terms of the second order tensor. In this paper, the hybrid closure approximation method proposed by Advani and Tucker is used [11].

For the numerical simulation, MoldFlow software is used. All the data required for the simulation, such as the type of polymer suspension to be used, glass fiber content and others parameters are provided as an input.

MODEL VALIDATION

The numerical model is validated by comparing the simulation results with qualitative experimental data. The materials used for the experiment is nylon polymer reinforced with 30% short glass fibers. Once the test samples are produced, small sections are cut out from the final molded specimens at three different positions along its length to examine the orientation states of the fibers. The three positions considered are near the mold inlet (10 mm from inlet), at the middle section of the specimen (82 mm from inlet) and far from inlet (150 mm from inlet) as shown in Figure 2. Then the fibers distribution on the cut surfaces are examined by taking pictures using a Scanning Electron Microscope (SEM).
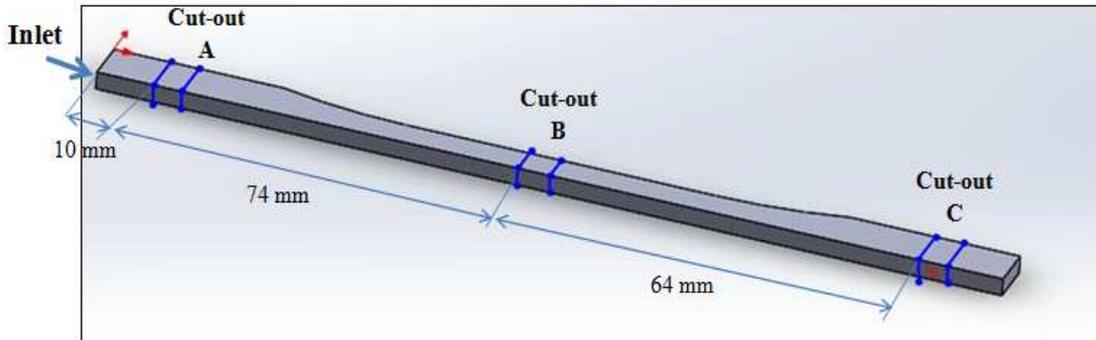

Figure 2. Cut out locations on the final molded sample for SEM observation

RESULTS AND DISCUSSION

Figure 3 shows the fiber orientation across the sample thickness for the cut out position B which is at the middle of the sample. As can be clearly seen from the SEM image, two different regions (or three layers of orientation structures) across the thickness of the sample part can be found: a shell region which is near to the mold cavity wall, and a core region at the middle of the cross section. The figure shows that there are grooves and holes (circular sections) visible in the region close to the wall, which indicates that the fibers are oriented in random fashion. On the other hand there are more grooves than holes in the shell region. This indicates that most of the fibers in this region are oriented in the flow direction (x-direction). In the core region, circular sections are dominant indicating that the fibers are predominantly oriented perpendicular to the flow direction.
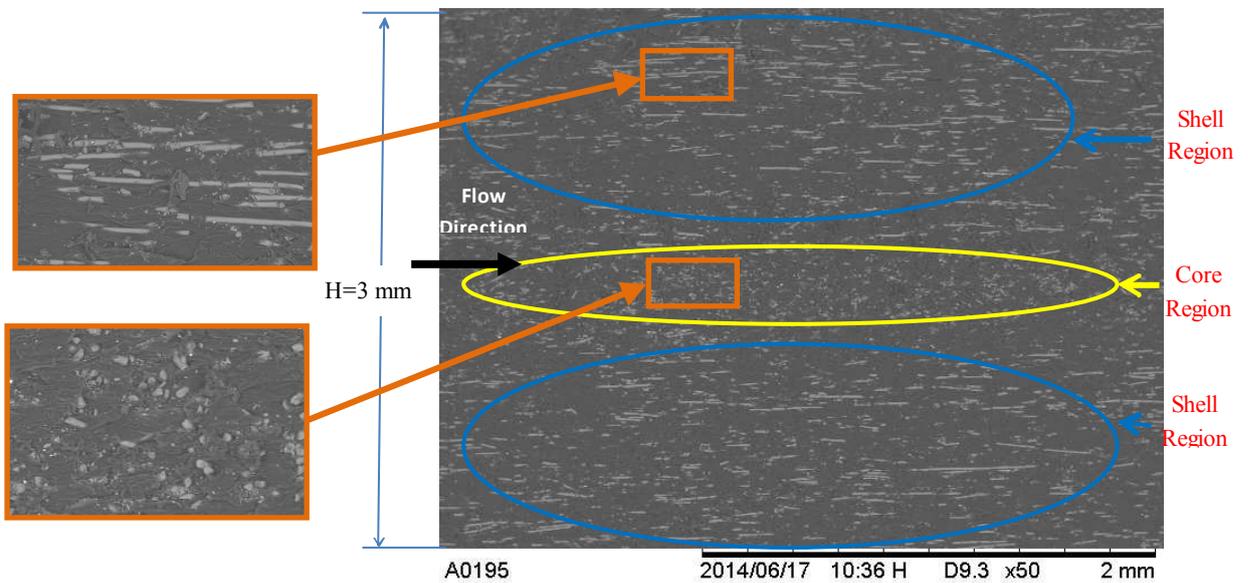

Figure 3. SEM micrograph of cut out B in the molded dog-bone shaped sample.

Figure 4 shows comparison of experimental and simulation results of fibers orientation across the thickness of the specimen near the mold inlet. From Eq. (8), the first principal values of the fiber orientation tensor, a_{xx}, are used to show the probability of fibers alignment in the flow direction. In this case a value of a_{xx} close to 1 indicates that there is high probability of fibers alignment in the flow direction whereas a value close to 0 indicates a high probability of fibers alignment perpendicular to the flow direction or offset orientation. Therefore, as can be seen from the simulation results in Figure 4(b), the flow direction orientation component (a_{xx}) is maximum near the mold cavity walls whereas minimum at the mid-plane of the thickness. The minimum values of the flow direction orientation component are around 0.1 indicating that most of the fibers are oriented perpendicular to the flow direction in this region. On the other hand, the maximum value of a_{xx} near the mold cavity walls is 0.84 indicating that the probability of fibers alignment the flow direction is high in the shell region. The SEM image shown in Figure 4(a) shows similar behavior indicating that the simulations results are in good agreement with the experimental data. Moreover, these arguments are in line with other similar research works [11, 14].
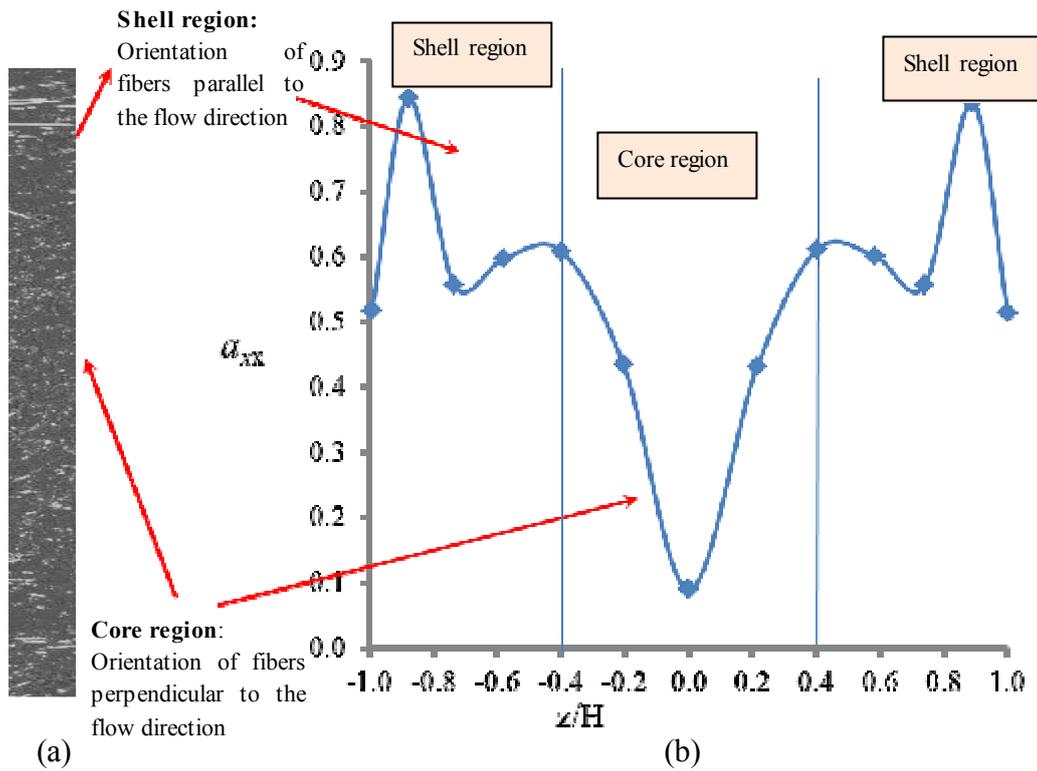
Figure 4. (a) SEM image for fibers orientation and (b) simulation results of flow directional orientation tensor component (a_{xx}) across the thickness of the specimen near the mold inlet.

Similarly, the simulation results of the flow orientation component a_{xx} for the cut-out positions A, B, and C across the sample thickness are shown in Figure 5. The results show that the value of a_{xx} at the middle section (84 mm from inlet) of the specimen is 0.9 in the shell region and 0.84 in the core region which indicates that the fibers orient entirely to the flow direction at the middle position of the sample. This might be due to the reason that the cross section at the middle section is smaller than that of near inlet. During the mold filling stage, as the molten nylon/fiber mixture approaches the other end of the mold cavity (far from inlet), the probability of fibers alignment to the flow direction is higher than near inlet position. This is due to the reason that the initial orientation value given for the simulation is random orientation. Therefore, the fibers will need to travel longer distance in order to be aligned to the flow direction.
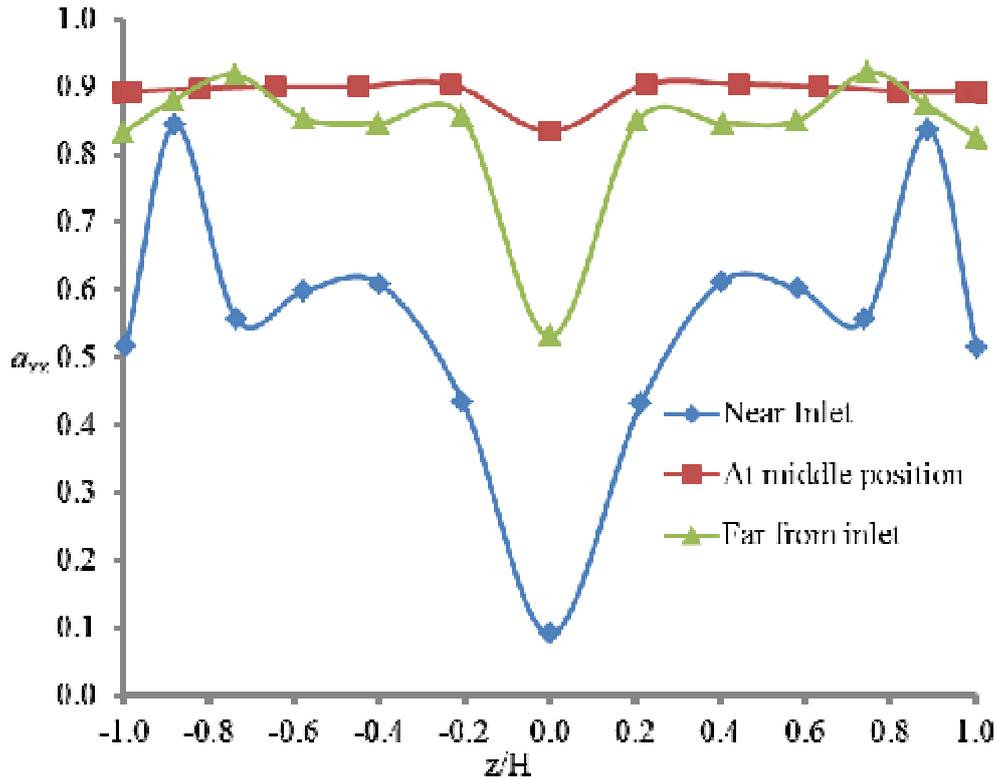
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Figure 5. Simulation results for Flow directional orientation tensor component (a_{xx}) at various cut-out positions across the thickness of the specimen.

CONCLUSION

In this paper the numerical formulation used to simulate the degree of flow induced fiber orientation in dog-bone shaped specimen during injection molding has been presented. The simulation model has been validated by performing experiments and compared the experiments qualitative data with quantitative simulation results. Both the experiment and simulation results have showed that three layer fiber orientation structures (two shell regions and one core region) formed during mold filling. The simulation results support the experiment that for thin plates the probability of fiber alignment to the flow direction near the mold cavity walls is high. On the other hand the probability of fibers alignment to the flow direction is low at the core region. From the simulation and experimental results it can be concluded that (since the flow is parallel to the length of the specimen) the final dog-bone shaped product can withstand both tensile and compression force. The shell layer which has high probability of fibers alignment in the flow direction is strong along the length whereas the core region is strong across the length. In general, the results of this study could assist in decisions regarding the short fiber reinforced polymer composites.

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