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THREE DIMENSIONAL SIMULATION OF SUSPENSION FLOW IN A MOLD CAVITY

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ABSTRACT

This paper presents three-dimensional simulation of fiber suspension flows in a cavity using the Finite Volume Method (FVM). The numerical simulation model described makes it possible to predict the propagation of the fiber-polymer solution and fiber orientation during the filling phase. Therefore, the objective of the work is to develop a Computational Fluid Dynamics (CFD) model to simulate and characterize the fiber suspension flow in three dimensional cavities. The model is intended to describe the fiber orientation distribution in three dimensional mold cavities. The continuity, momentum, energy and the fiber orientation equations are solved using the FVM. The flow is considered to be incompressible, non-isothermal, transient, and to behave as non-Newtonian fluid. A numerical analysis is presented to illustrate the application of the FVM to dilute suspension flows in injection molding processes. The volume-of-fluid method is employed to describe the flow of the two incompressible, immiscible phases, i.e., liquid suspension and air. Since the flow is a non-Newtonian, the Cross model is used to describe the shear-thinning behavior of the suspension. The governing equations of the flow and the fiber are implemented and solved by means of the open source code OpenFOAM. The evolution equation of the fiber orientation contains a fourth order orientation tensor which is approximated in terms of second order tensor through the use of appropriate closure rules. In this study the Hybrid closure model of Advani and Tucker is used to approximate the fourth order orientation tensor. To validate the numerical algorithm, test cases of suspension flow in a rectangular cavity are modeled for different fiber-polymer matrices. The numerical results are compared with available experimental findings and with those of Newtonian flows.

Key-Words: - Finite Volume Method, Fiber Suspension, Fiber Orientation, Non-Newtonian Fluid, Computational Fluid Dynamics, Hybrid Closure Model.

NOMENCLATURE

$\mathbf{A_2}$	Second order orientation tensor
$\mathbf{A_4}$	Fourth order orientation tensor
C_I	Interaction coefficient
C_p	Suspension Specific Heat
D	Fiber diameter
L	Fiber length
f	Scalar measure of orientation
k	Suspension thermal conductivity
p	Pressure
$\mathbf{p}$	Unit vector
$\mathbf{u}$	Flow velocity vector
x, y, z	Cartesian coordinates
$\psi(\mathbf{p})$	Orientation Distribution Function
$\dot{\gamma}$	Shear rate tensor
ξ	Volume fraction
$\boldsymbol{\omega}$	Vorticity tensor
$\boldsymbol{\delta}$	Unit tensor
ρ	Density
η_s	Viscosity of the suspension
r_e	Fiber aspect ratio

INTRODUCTION

Fiber suspension can occur in many engineering applications. In injection molding, for instance, it is a collection of solid fibers with different shape and size suspended in a liquid polymer. The mechanical, thermal and electrical properties and the thermal shrinkage of injection molded fiber reinforced products are highly dependent on the orientation of fibers. Simulation of fiber suspension can be used to improve the product quality in injection molding process. However, the study of the flow of fiber-filled polymers in injection molding process is quite complex due to the fact that the flow is modified by the presence of fibers and vice versa. This effect appears mainly in two things; the first is in the generation of the fluctuating stresses due to the liquid polymer movement and as a result the motion of the fibers is modified. The second is in the motion within the polymeric fluid that is induced by the motion of the fibers, as the polymeric fluid is assumed to remain in contact with the fibers without penetrating it. Therefore, it is very important to fully understand the flow behaviour of the fiber suspension inside injection mold cavities in order to be able to accurately predict the fiber orientation. Assuming that the fiber particles are rigid, neutrally buoyant, axisymmetric, and large enough so that Brownian motion can be negligible, Jeffery [1]) has studied the flow of fiber suspension and found a distribution function of the orientation angle of the particle. Following Jeffery, Lipscomb [2] has proposed a constitutive equation for dilute suspension of ellipsoidal particles with large aspect ratio. 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 the stress tensor in the flow field. In this case, the fiber stress is modelled by the constitutive equation of the fiber orientation tensor [3]. Instead of calculating the orientation distribution function directly, the orientation tensor method is used [4]. 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 [5-8]. In this paper, the hybrid closure approximation (HYB) which is developed by Advani and Tucker [7] is used. The flow of fiber suspension in injection molding be characterized as a multi-phase system consisting of the solid fiber, liquid polymer and air. However, modelling of individual fibers is computationally too expensive. Therefore, for this study, the fiber suspension is simulated as a single phase flow, either as Newtonian or non-Newtonian fluid.

Numerical implementation of the governing equations for fiber suspension and moving interface problem in injection molding has been performed using the Finite Difference Method (FDM) and the Finite Element Method (FEM). Bay [9] has studied filling and fiber orientation in simple injection moldings using the FDM method. Others, [10, 11] have used the FEM to predict the orientation of short fibers during the filling stage of injection molding. The FDM is used only for regular physical geometries even though it is simple and efficient. The FEM has no restriction in physical geometries, however it produces a large spares matrix in which it becomes inefficient and needs too much computer space for a large-scale system [12]. For modelling of fiber suspension, the FVM is more suitable in fluid flow studies. It is also computationally stable and utilizes computer space and time efficiently. The purpose of this study is to predict the fiber orientation for a Newtonian and a shear-thinning suspension behaviour using the FVM. Computational examples are given and the results are discussed in comparison with the experimental data.

THE BASIC GOVERNING EQUATIONS

Assuming that the flow is incompressible and non-isothermal, the instantaneous continuity, momentum and energy equations of fiber suspension [13] are:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

$$\rho \frac{\partial}{\partial t}(\mathbf{u}) + \rho \nabla \cdot (\mathbf{uu}) = -\nabla p \cdot I + \nabla \cdot \left[2\eta_s \dot{\boldsymbol{\gamma}} + 2\eta_s \phi\left(\mu_1 \dot{\boldsymbol{\gamma}} + \mu_2 \dot{\boldsymbol{\gamma}} : \mathbf{A_4}\right)\right] \tag{2}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) = k\nabla^2 T + \dot{\boldsymbol{\gamma}} \cdot \left[\nabla \cdot \left(2\eta_s \dot{\boldsymbol{\gamma}} + 2\eta_s \phi\left(\mu_1 \dot{\boldsymbol{\gamma}} + \mu_2 \dot{\boldsymbol{\gamma}} : \mathbf{A_4}\right)\right)\right] \tag{3}$$

where, t is the time; $\mathbf{u}$ is the velocity vector; ρ is the density; p is the hydrostatic pressure; C_p is the specific heat; T is the temperature, and k is the thermal conductivity. The suspension shear rate is $\dot{\boldsymbol{\gamma}}$; $\eta_{\mathbf{s}}$ is the viscosity of the suspension; $\mathbf{A_4}$ is the fourth order orientation tensor; μ_1 and μ_2 are rheological coefficients. The last expression on the right hand side of Eqs. (2) and (3) is the total stress tensor which is a combination of stresses from the contribution of the suspending fluid and the contribution of the fibers. It is assumed that the viscosity of the suspension is the same as the viscosity of the suspending fluid. The viscosity of the suspension η_s is dependent on the shear rate and temperature. For this study, the cross viscosity model [14] has been used.

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

The expression η_0 is given as

$$\eta_0 = \eta^* \exp\left(T_i / T\right) \tag{5}$$

where η^*, τ^*, m, and T_i are empirical constants.

Assuming that the fibers are rigid cylinders, uniform in length and diameter, and that the number of fibers per unit volume is uniform, the second- and fourth-orientation tensors [7] of the fiber can be defined respectively as:

$$\mathbf{A_2} \leftrightarrow A_{ij} = \int_p p_i p_j \psi(\mathbf{p}) d\mathbf{p} \qquad (6)$$

$$\mathbf{A_4} \leftrightarrow A_{ijkl} = \int_p p_i p_j p_k p_l \psi(\mathbf{p}) d\mathbf{p} \qquad (7)$$

where $\mathbf{p}$ is the unit vector parallel to the fiber's axis of symmetry, and $\psi(\mathbf{p})$ is the probability distribution function for fiber orientation at any position in the flow. The equation change for the second order orientation tensor proposed by Advani and Tucker [7] has been implemented.

$$\frac{DA_{ij}}{Dt} = \frac{\partial A_{ij}}{\partial t} + u_k \frac{\partial A_{ij}}{\partial x_k} = -(\omega_{ik} A_{kj} - A_{ik}\omega_{kj}) + \lambda(\dot{\gamma}_{ik} A_{kj} + A_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl} A_{ijkl}) + 2C_I \dot{\gamma}[\delta_{ij} - 3A_{ij}] \qquad (8)$$

where δ_{ij} is a unit tensor, and $\omega_{ij} = 0.5*(\nabla\mathbf{u} - (\nabla\mathbf{u})^T)$ and $\dot{\gamma}_{ij} = 0.5*(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ 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 introduced by Folgar and Tucker [15] and represents the degree of interaction between fibers. The fourth order orientation tensor evolved in Eq. (8) needs to be approximated in terms of the second order tensor in order to obtain a closed set of evolution equations for orientation tensors. In this paper, the hybrid closure approximation method proposed by Advani and Tucker [13] is used. Hybrid closure approximation is a combination of quadratic model, which gives exact result for perfectly aligned fibers, and linear model, which is exact for random alignment.

$$A_{ijkl} = fA_{ij}A_{kl} + (1-f)\left[-\frac{1}{35}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\right] + (1-f)\left[\frac{1}{7}(A_{ij}\delta_{kl} + A_{ik}\delta_{jl} + A_{il}\delta_{jk} + A_{kl}\delta_{ij} + A_{jl}\delta_{ik} + A_{jk}\delta_{il})\right] \qquad (9)$$

$$f = 1 - 27\det(A_{ij})$$

The volume of fluid method is used to track the flow front. It is to solve the following convective equation,

$$\frac{\partial \alpha}{\partial t} + \mathbf{u}\cdot\nabla\alpha = 0 \qquad (10)$$

where α is the suspension fraction in the cell and $\mathbf{u}$ is the velocity. The value of α in a cell should range between 0 and 1. If the cell is completely filled with suspension then α =1 and if it is filled with the void phase (air in this study) then its value should be 0. At the interface the value of α is between 0 and 1.

NUMERICAL IMPLEMENTAION

The FVM is implemented to solve the three-dimensional transient flow of the fiber suspension. The governing equations of the momentum and energy can be written in the following generic form [16, 17]:

$$\frac{\partial}{\partial}(\rho\phi) + \nabla\cdot(\rho\mathbf{u}\phi) = \nabla\cdot(\Gamma\nabla\phi) + S_\phi \qquad (11)$$

where S_ϕ , ϕ and Γ represent the source term, dependent variable and diffusivity respectively. After integrating Eq. (11) over the control volume Ω and converting the volume integrals to surface integrals according to the divergence theorem, we get:

$$\int_t^{t+\Delta t}\left(\frac{\partial(\rho\phi)}{\partial t}\Omega + \sum_{j=1}^{\mathbf{n}}(\rho\mathbf{u}\phi)_j\cdot\mathbf{A}_j - \sum_{j=1}^{\mathbf{n}}(\Gamma\nabla\phi)_j\cdot\mathbf{A}_j\right)dt = \int_t^{t+\Delta t}(S_\phi\,\Omega)dt \qquad (12)$$

where n is the number of cell-faces of the cell. In discretising the fiber orientation equation, the right hand side of Eq. (8) is considered as a source term, S_a. Then the differential equation will have the form:

$$\frac{\partial A_{ij}}{\partial t} + \mathbf{u}\frac{\partial A_{ij}}{\partial \mathbf{x}} = S_a \qquad (13)$$

Integrating Eq. (13) over a three dimensional control volume Ω and applying Gauss' theorem, we get:

$$\int_\Omega\left[\int_t^{t+\Delta t}\frac{\partial a_{ij}}{\partial t}dt\right]d\Omega + \int_t^{t+\Delta t}\left[\int_{\mathbf{A}}\mathbf{n}\cdot\left(\mathbf{u}\frac{\partial a_{ij}}{\partial \mathbf{x}}\right)dA\right]dt = \int_\Omega\int_t^{t+\Delta t}S_a\,dt\,d\Omega \qquad (14)$$

RESULTS AND DISCUSSION

In order to show that the method developed is suitable for the simulation of fiber suspension in injection mold cavities, a three-dimensional flow in a rectangular geometry is presented. The simulation results are compared with Bay's experimental measurements [18] of nylon 6/6 reinforced with 43% glass fibers. For the simulation, the open source software, OpenFOAM-1.5 [19] is used. The aspect ration of the nylon 6/6 fiber is assumed to be 19.1 so that λ equals 1. The rectangular cavity used for the computation is shown in Fig. 1 with dimensions 202mm x 3.18mm x 25.4 mm. the flow direction is along the x-axis, while y-axis is the thickness direction and z-axis is the width direction. Other parameters like thermal properties and viscosity constants are given in table 1. As initial conditions, an inlet volume flow rate of 4×10^4 mm^3/s, inlet temperature of 550^oC and random orientation state ($A_{xx} = 0.5,\ A_{yy} = 0.3,\ A_{zz} = 0.3,$ and $A_{xy} = A_{xz} = A_{yz} = 0.3$) are applied. At the cavity walls the temperature is assumed to be constant at a value of 297^oC.

TABLE 1. SUSPENSION PROPERTIES AND VISCOSITY CONSTANTS OF NYLON 6/6 [5]

m	0.549
η^*	4.37x10^{-9} Pa.s
T_i	1.68x10^{4o}C
C_I	0.001
τ^*	3.04x10^{4}pa
ρ	1.33x10^{3}kg/m^3
C_p	1.97x10^{3}J/kg.^{o}C
k	2.6x10^{-1}W/kg.^{o}C

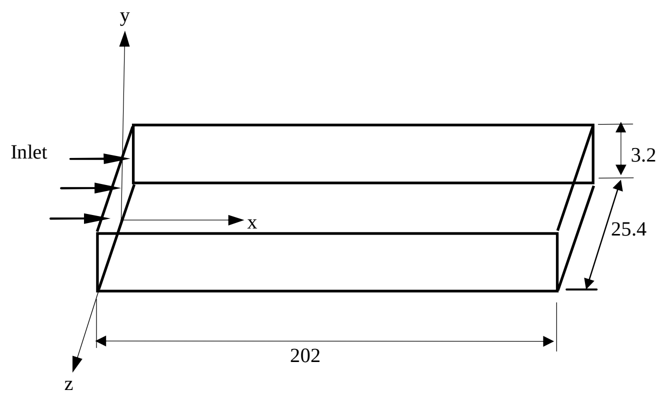
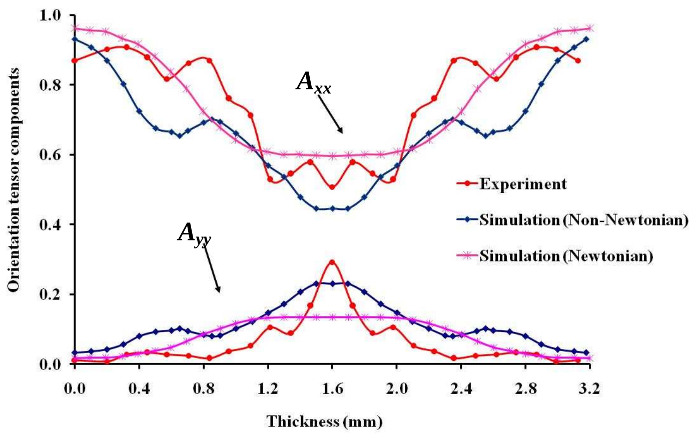


FIGURE 1. SCHEMATIC OF THE RECTANGULAR STRIP USED IN THE SIMULATION (ALL UNITS ARE IN mm).

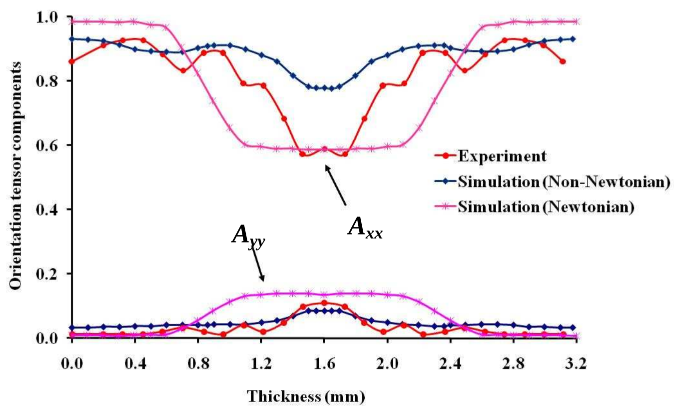
Figure 2 shows a comparison between the simulation and experimental results of A_{xx} and A_{yy} orientation components across the mold at different distance from the inlet. Two types of simulations, Non-Newtonian and Newtonian, are compared with the experimental results. For the Non-Newtonian suspension, the viscosity depends on the shear rate and temperature, whereas for the Newtonian the viscosity is taken as constant. The value of the anisotropy parameters vary between 0 and 1 which means that the perfect alignment of the fibers to the reference direction is indicated by 1 and that 0 indicates that the fibers are aligned perpendicular to the reference direction. As shown in Fig. 2, the two simulations predict values of A_{xx} close to the experimental data. However, the Non-Newtonian simulation shows the random nature of the orientation component while the Newtonian simulation shows smooth change in A_{xx}. Close to the walls, big values of A_{xx} show that the fibers are perfectly aligned to the flow direction due to the shear effect whereas they orient randomly near to the mid plane region of the cavity. It can also be clearly seen that the simulated fiber suspension results coincide well with the experimental measurements. Although the Non-Newtonian simulation shows a closer trend to the experiment than the Newtonian simulation, over-predicted values for A_{xx} appear at positions far from the inlet, showing perfect alignment to the flow direction. This deviation might be due to the fact that the packing and cooling stages of the injection molding process were not simulated. Further adjustment on different coefficients (such as C_I), using other closure methods, and using other Non-Newtonian viscosity models might improve the results. The fibers near the walls generate high stresses and slow down the streamwise velocity, and increase the transverse velocity. As for the orientation component A_{yy}, the predicted values are of the same range of the experiment for both simulations. The small values of A_{yy} show that fibers are aligned more to the flow direction. The values of A_{yy} are always maximum at mid plane and they keeps decreasing towards the mold walls. Non-Newtonian simulation shows better agreement with the experiment in all locations along the axial direction.

For the orientation component A_{xy}, the Newtonian simulation results are compared with experimental data at locations 9mm, 54mm, and 167mm from the inlet, as shown in Fig. 3. Non zero values for A_{xy} indicate that the fibers orients at certain angle from the x-y plane which means that the principal axes of the fibers are not aligned exactly to the flow or thickness direction. Figure 3a shows the comparison of the orientation component A_{xy} close to the inlet. Along the vertical direction (y), the fibers tend to orient out of the plane positively in the first half of the thickness, while they tend to orient negatively for the second half. It is also seen in the experiment that A_{xy} is skew-symmetric about the thickness mid plane. Simulation results could predict the skew-symmetry nature of the experiment as well as the orientation direction in both thickness halves. Figure 3b shows the comparison at a distance of 54mm from the inlet. The experimental values of A_{xy} show the same behavior observed at the location close to the inlet. The simulated values are close to the measured ones; however no negative orientation was predicted. At a distance of 167mm from the inlet, most of the A_{xy} values were measured to be positive as shown in Fig. 3c. The simulated values are also close to the measured ones, and no negative orientation could be predicted. However, orientation values close to zero were predicted in locations where the experimental values were negative.

These three-dimensional simulation results indicate that the Finite Volume Method for three-dimensional suspension simulations gives accurate results.



(a)



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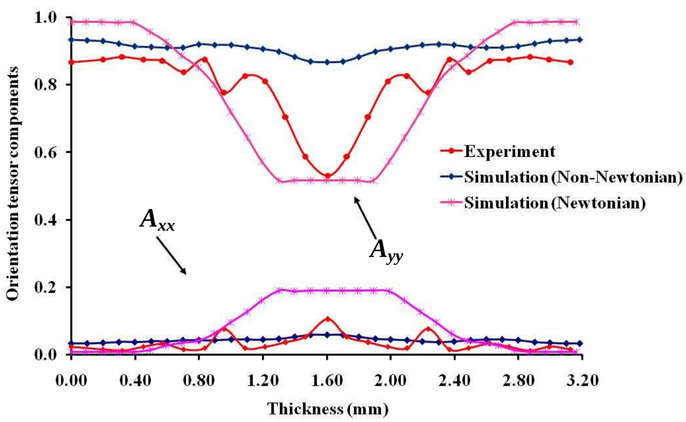
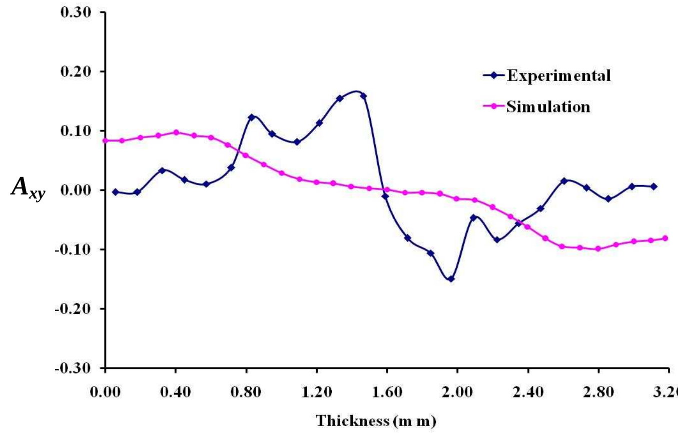
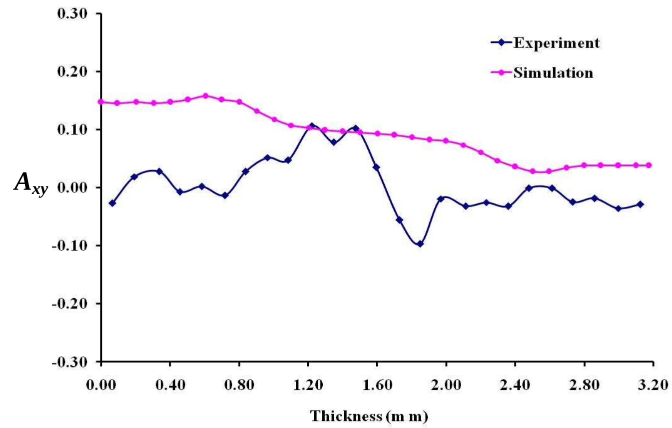


(c)

FIGURE 2. COMPARISON OF THE SIMULATED AND EXPERIMENTAL [18] RESULTS OF ORIENTATION COMPONENTS A_{xx} AND A_{yy} AT THE END OF FILLING AT (a) x=9mm, (b) x=54mm, and (c) x=167mm.



(a)



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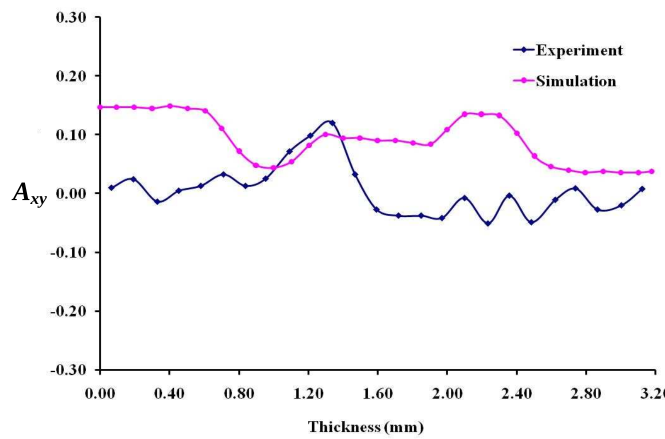

(c)

FIGURE 3. COMPARISON OF THE SIMULATED AND EXPERIMENTAL [18] RESULTS OF ORIENTATION COMPONENT A_{xy} AT THE END OF FILLING AT (a) x=9mm, (b) x=54mm, and (c) x=167mm.

CONCLUSION

Simulation of fiber orientation using the Finite Volume Method has been carried out and correlated with the results of Bay's experimental measurements [18]. Combining the Finite Volume Method and the volume of fluid method provides good results for studying the fiber suspension problems in three dimensional cavities. It is observed that the simulated fiber orientation results in the rectangular plate coincide well with the experimental data. The fiber orientation equation is solved using second order tensor method to represent the important statistics of the distribution function. The fibers tend to align perfectly to the flow direction at the walls due to formation of shear layer near the wall. However, since there is little shearing at the midplane, the orientation component A_{xx} is not changed significantly near the midplane. In general, the simulation results obtained indicate that implementation of the Finite Volume Method for a three-dimensional suspension simulation is important. The current model is tested only on rectangular cavities. The capability of the present model for cylindrical geometries and for complex mold cavities will be dealt in later publications.

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REFERENCES

1. Jeffery, G.B., *The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid* Proceedings of the Royal Society of London. Series A, , 1922. Vol. 102(No. 715): p. 161-179
2. Lipscomb, G.G., *Analysis of Suspension Rheology in Complex Flows*, in *PhD Dissertation in Department of Chemical Engineering* 1981, University of California, Berkley
3. Reddy, B.D. and G.P. Mitchell, *Finite element Analysis of Fibre Suspension Flows.* Computer Methods in Applied Mechanics and Engineering, 2001. 190: p. 2349-2367.
4. Azaiez, J., K. Chiba, and F. Chinesta, *State-of-the-Art on Numerical Simulation of Fiber- Reinforced Thermoplastic Forming Processes.* Archive of Computational Methods in Engnineering, 2002. 9(2): p. 141-198.
5. Chung, D.H. and T.H. Kwon, *Applications of Recently Proposed Closure Approximations to Injection Molding Filling Simulation of Short-Fiber Reinforced Plastics.* Korea-Australia Rheology Journal, 2000. 12(2): p. 125-133.
6. Greene, J.P. and J.O. Wilkes, *Numerical analysis of injection molding of glass fiber reinforced thermodynamics. Part2: fiber orientation.* Journal of Polymer Engineering and Science, 1997. 3**7**(5).
7. Advanin, S.G. and C.L.T. III, *The Use Tesor to Describe and Predict fiber Orientation in Short Fiber Composites.* Journal of Rheology, 1987. 31(8): p. 751-784.
8. Chung, D.H. and T.H. Kwon, *Fiber Orientation in the Processing of Polymer Composites.* Korea-Australia Rheology Journal, 2002. 14(4): p. 175-188.
9. Bay, R.S. and C.L. Tucker, *Fiber Orientatoin in Simple Injection Moldings. Part I: Theory and Numerical Methods.* Journal of Polymer Composites 1992. 13(4): p. 15.
10. Vincent, M., E. Devilers, and J.-F. Agassant, *Fibre Orientation Calculation in Injection Molding of Reinforced Thermoplastics.* Journal of Non-Newtonian Fluid Mechanics, 1997. 73: p. 317-326.
11. Wang, J., *Improved Fiber Orientation Perdictions for Injecion Molding Composites*, in *PhD Dissertation in Mechanical Enigineering*. 2007, Illinois: Urbana-Champaign. p. 161.
12. Chang, R.-Y. and W.-H. Yang, *Numerical Simulation of Mold Filling in Injection Molding Using a Three-Dimensional Finite Volume Approach.* International Journal for Numerical Methods in Fluids, 2001. 37: p. 125-148.
13. Ausias, G., X.J. Fan, and R.I. Tanner, *Direct Simulation for Concentrated Fibre Suspensions in Transient and Steady State Shear Flows.* Journal of Non-Newtonian Fluid Mechanics, 2006. 135: p. 46-57.
14. Hieber, C.A., *melt viscosity characterization and its application to injection molding* Injection and Compression Moding Foundamentals, ed. A.I. Isayev. 1987, New York: Marcel Dekker.
15. Folgar, F. and C.L.T. III, *Orientation Behavior of Fibers in Concentrated Suspensions.* Journal of Reniforced Plastics and Composites, 1984. 3.
16. Versteeg, H.K. and W. Malalasekera, *An Introduction to Computational Fluid Dynamics: the Finite Volume Method*. 1995: Longman Scientific and Technical.
17. J.H.Ferziger and M.Peric, *Computational Methods for Fluid Dynamics*. 2002: Springer
18. Bay, R.S., *Fiber orientation in injection molded composites: A comparison of theory and experiment*, in *PhD Dissertation in Mechanical Engineering* 1991, University of Illinois at Urbana-Champaign.
19. OpenFOAM. http://www.openfoam.com.