단섬유 보강 성형공정에서 텐서를 이용한 섬유배향 예측을 위한 최종적 근사모델에 대한 모델링

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Modeling of Closure Approximation for Fiber Orientation Tensor for Short Fiber Reinforced Plastic Processings

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Introduction

There are many examples of natural or man-made suspensions which contain several kinds of particles. Fiber suspension is one of the kind and its presence and orientation in polymer-based matrix greatly influences mechanical, thermal and rheological properties. Typically, anisotropic properties are induced. Therefore, numerical simulation or CAD/CAE system, which could be used for the systematic and efficient mold design to induce optimal properties, has been required. Recently, many researchers have developed several numerical simulation techniques. Theoretically, exact description of fiber orientation including multi-particle interactions can be achieved through the calculation of individual fiber. However, this necessitates formidable computation time and cannot be implemented in real industrial community. Another simulation method, which adopts orientation tensor to represent fiber orientation, is used in commercial software package for its compact representation and less computation time. But, in this method a significant deviation between predicted values and experimental ones still exists. It is mainly due to non-existence of an exact closure approximation which approximates 4th order tensor in terms of 2nd order tensor. In this regard, nowadays, developing an exact closure approximation is a crucial problem in this research field. We have developed closure approximations termed 'ORW', 'ORW3' and 'IBOF' which are more accurate than previous models. Also we have developed CAE system for the prediction of fiber orientation including coupling effect between fluid and fiber. Also, in-plane velocity gradient effect as well as usual shear effect has been included. Nowadays, we focus our research effort on the modeling of fiber-fiber interaction.

Theory

The most general description of fiber orientation state is the probability distribution function φ, which satisfies the following conservation equation [1]

$$\frac{D\varphi}{Dt} = -\frac{\partial}{\partial p} \cdot (\varphi \dot{p}) \qquad (1)$$

$$\dot{p} = -\frac{1}{2}\dot{\omega}_{ij} p_j + \frac{1}{2}\lambda(\dot{\gamma}_{ij} p_j - \dot{\gamma}_{kl} p_k p_l p_i) - \frac{C_I \dot{\gamma}}{\varphi}\frac{\partial \varphi}{\partial p_i} \qquad (2)$$

where $\dot{p}$ describes the fiber angular velocity. $\dot{\omega}$ and $\dot{\gamma}$ are the rate of rotation tensor and the rate of deformation tensor, respectively. λ is a parameter related to the aspect ratio of the fiber and C_I is a fiber-fiber interaction coefficient. We call the computation of φ using a finite difference method 'DFC' which stands for 'Distribution Function Calculation'. DFC, however, requires an extremely high computational cost, so we resort to the tensor representation, which in turn requires a closure approximation.

The evolution equation for the second-order orientation tensor a_{ij} can be expressed as follows:

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

Closure approximation which approximates 4th order orientation tensor in terms of 2nd order orientation tensor is inherently required. Many closure approximations have been developed. Especially, we developed models named 'ORW', 'ORW3' and 'IBOF'.

IBOF assumes the following function form, which is the same as NAT (Natural Closure Approximation) proposed by Verleye et al. [2,3].

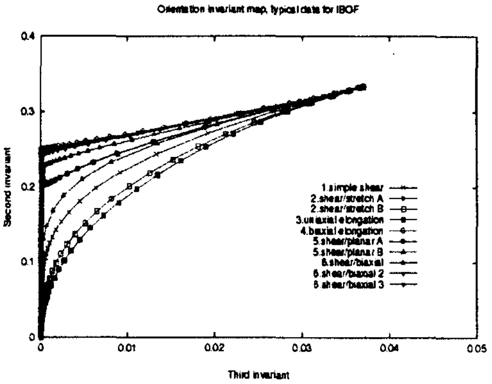


Fig 1. Typical fitting data of flow field for IBOF closure approximation

$$a_{ijkl}=\beta_1 S(\delta_{ij}\delta_{kl})+\beta_2 S(\delta_{ij}a_{kl})+\beta_3 S(a_{ij}a_{kl})$$
$$+\beta_4 S(\delta_{ij}a_{km}a_{ml})+\beta_5 S(a_{ij}a_{km}a_{ml})+\beta_6 S(a_{im}a_{mj}a_{kn}a_{nl}) \qquad (4)$$

where the operator S indicates the symmetric part of its argument. The coefficients β_1 - β_6 are polynomial functions of the second and third invariants of a_{ij} (Ⅱ and Ⅲ). Least-square optimization procedure was performed at eigenvector space of 2nd order orientation tensor. Flow data used are the same as ORW and represented by the following 'Orientation invariant map' (Fig.1)

For mold filling simulation, following models have been adopted for the coupled analysis of fiber suspension flow.

Constitutive equation (Dinh and Armstrong model [4])

$$\tau_{ij}=\eta\left(u_{i,j}+u_{j,i}\right)+\eta N u_{k,l}a_{ijkl} \qquad (5)$$

Pressure equation [5,6]

$$\frac{\partial}{\partial x}\left[\left(S-S^x\right)\frac{\partial P}{\partial x}-S^{xy}\frac{\partial P}{\partial y}-F^x\right]+\frac{\partial}{\partial y}\left[\left(S-S^y\right)\frac{\partial P}{\partial y}-S^{xy}\frac{\partial P}{\partial x}-F^y\right]=0 \qquad (6)$$

Modified Cross Model

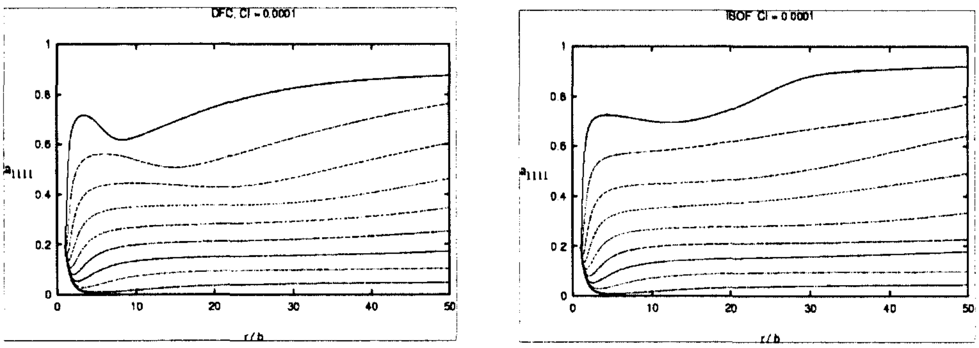
$$\eta(\dot{\gamma},T)=\frac{\eta_o}{1+C(\eta_o\dot{\gamma})^{1-m}} \quad , \quad \eta_o=B\exp\left(\frac{T_b}{T}\right) \tag{7}$$

Energy Equation

$$\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}\right)=k\frac{\partial^2 T}{\partial z^2}+\eta\dot{\gamma}^2 \tag{8}$$

Numerical tests

We will compare results from DFC and closure approximations via an isothermal, Newtonian radial diverging flow fields where material elements undergo non-homogeneous deformation during flow (Fig2).

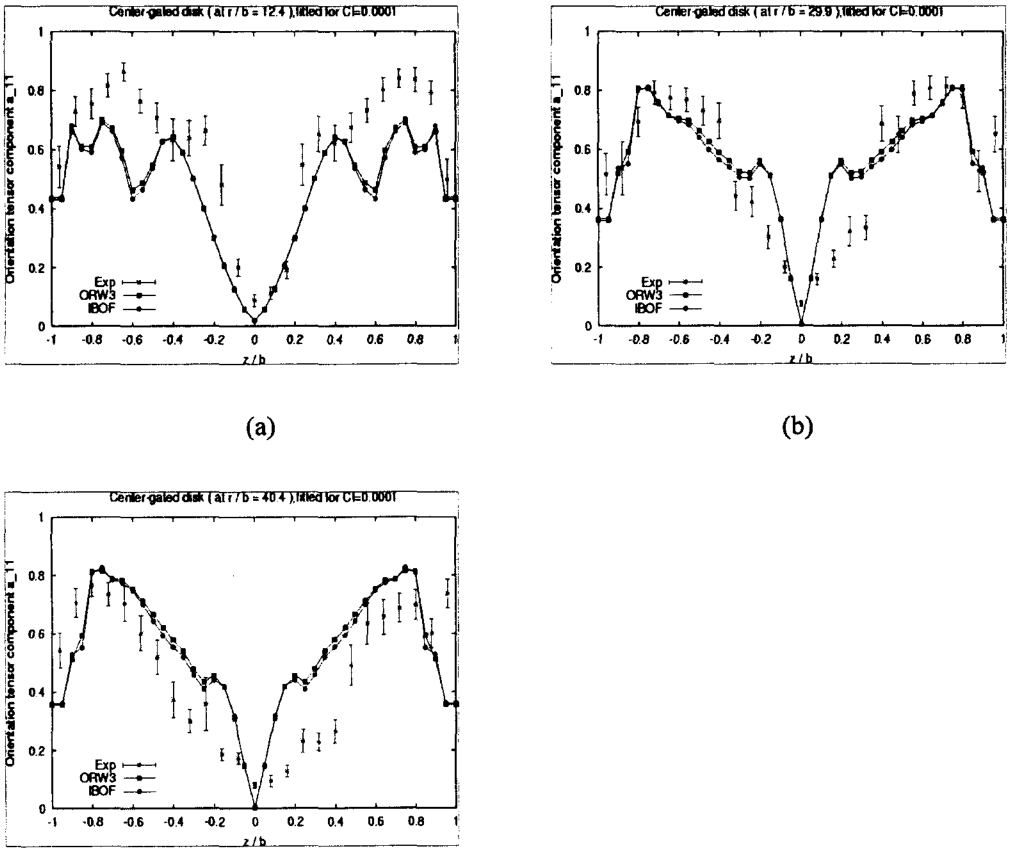


(a) (b)

Fig 2. a_{11} component in isothermal Newtonian radial diverging flow as a function of radial location (r/b) at several thickness positions (z/b) C_I=0.0001 : (a) DFC, (b) IBOF

Fig.2 shows that IBOF excellently matches with DFC results. IBOF does not show any non-physical oscillatory behaviors which previous Orthotropic closure approximation, ORF and ORL [7] frequently suffered from.

Also, we have performed non-isothermal non-Newtonian coupled simulation of fiber suspension adopting closure models 'ORW3' and 'IBOF' (Fig.3). Fig.3 shows that IBOF and ORW3 qualitatively match experimental data. However, some discrepancy still exists. More sophisticated modeling of fiber-fiber interaction term might be helpful.



(a) (b)

(c)

Fig 3. a_{11} component in non-isothermal non-Newtonian radial diverging flow as a function of several thickness positions (z/b) for C_I=0.0001 with ORW3 and IBOF: (a) r/b=12.4, (b) r/b=29.9, (c) r/b=40.4

Conclusion

We have presented new models of closure approximation and simulation program, which adopts coupling effect between fiber and fluid. Validation test cases are radial diverging flow. Both isothermal Newtonian and non-isothermal non-Newtonian cases have been examined. Some discrepancies still exist between predicted values and experimental cases even if excellent closure approximations have been implemented. It seems that more sophisticated model for fiber-fiber interaction term is necessary.

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