Research Orientation Distribution of Fiber Suspensions in Shear-ellipsoidal Extensional Flow

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Abstract

In this paper, an orientation distribution function is adopted to describe three-dimensional orientation distribution of short fibers suspensions in shear-ellipsoidal extensional flow field. A mathematical model of evolution process on fiber orientation distribution function is established by analytical method, namely specific form of Fokker-Plank partial differential equation and Jeffery equation. Numerical calculations method is used to describe three-dimensional and two-dimensional orientation distribution of fibers and made it visual. Therefore, analytical solution of differential equation on forecast fiber orientation distribution is obtained.

Keywords

Fiber orientation distribution; numerical simulation; fibers suspensions; polymer-fibers composites ;shear-ellipsoidal extensional force field.

1. Introduction

In recent years, fibers suspensions of polymer-fiber composites are attracted increasingly in many science and engineering fields, such materials science, paper-making industry, composites material production and so on. Furthermore, the orientation distribution and behavior of fibers is a hot issue increasingly in material processes, such as extrusion, injection, and compression molding. The reason of this phenomenon is the orientation distribution of fibers determines largely the mechanical properties of polymer-fiber composites. Namely, the final product has stiffer and stronger properties in the direction of greatest orientation; however, it has weaker and more compliant properties in the direction of least orientation.

There are some literatures dealing with the evolution of fiber orientation by experimental, numerical and analytical methods for decades. Lin et al. [1] obtained fiber orientation distribution in round turbulent jet of fiber suspension by numerical simulation methods. Najam [2] used a novel methodology in formulating a closure by employing an artificial neural network (ANN) to obtain model of fiber orientation in short fiber suspensions. Niskanen et al. [3] used flexible wood fibers in dilute suspension to investigate the development of fiber orientation distribution in a plane contracting channel flow by experiments and modeling. Parsheh et al. [4] investigated the influence of shape of planar contractions on the orientation distribution of stiff fibers suspended in turbulent flow. They demonstrate the shape effect by considering contraction with flat walls as well as three contractions with different mean rate of strain variation.

The research background of previous investigations has focused mainly on shear flow field, however, few articles studied extensional flow field with fiber suspension. Fiber has fast orientation in tensile direction in extensional flow. The biggest difference of fiber movement between shear flow and extensional flow is: fiber doesn’t turn over when fiber moves to the elongational direction in extensional

flow; however, even if fiber moves to shear direction, it continues to turn over in shear flow. Qu[5-6] designed a novel equipment and method which are completely different with conventional screw extruders and produce extensioal deformation in polymer processing, the vane extruder, which constituted by a certain groups of Vane Conveying and Plasticizing Unit(VCPU). Furthermore, Qu et al[7-10]has proved that vane extruder can make the material to produce large textensioal deformation and has better efficiency of disperse mixing through a lot of experiments. Luo et al. [11-12] investigate the orientation distribution of fiber suspensions based on planar extensional force field and shear-uniaxial extensional flow. Huang et al[13-14] investigate the orientation distribution of fiber suspensions based on equibiaxial and shear-planar extensional flow.

The objective in this article is to investigate the orientation distribution of fiber suspensions under the domination of shear-ellipsoidal extensional flow field. What is more, to establish the mathematical model on the evolution of fiber orientation in vane extruder, obtain three dimensional analytical solution, and make it visual.

2. Mathematical Model

2.1 Flow Field Control Equations

The fiber suspension is assumed to be stready, homogeneous and incompressible. Therefore, the basic governing equations of the flow field can be expressed as follows,

$$\nabla \cdot u = 0, \tag{1}$$

$$\frac{\partial u}{\partial t} + W \times u = -\nabla P + \frac{1}{\mathrm{Re}} \nabla^2 u. \tag{2}$$

Where, $W = \nabla \times u$ is vorticity, $P = p + \frac{|u|^2}{2}$ is total pressure in flow field, Re is Reynolds number.

2.2 Constitutive Relation of the Fiber Suspension

A probability distribution function is proposed by Tucker et al [15-16] to describe orientation fiber proportion of general fiber along with the given orientation direction in the given small research space, namely:

$$P(\theta_1 \le \theta \le \theta_1 + \mathrm{d}\theta, \phi_1 \le \phi \le \phi_1 + \mathrm{d}\phi) = \psi(\theta_1, \phi_1) \sin\theta \mathrm{d}\theta \mathrm{d}\phi. \tag{3}$$

Where, $\psi(\theta, \phi)$ is the probability distribution function, which meets the conditions below:

Continuity condition

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -\frac{\partial}{\partial \theta}(\dot{\theta}\psi) - \frac{1}{\sin\theta}\frac{\partial}{\partial \phi}(\dot{\phi}\psi), \tag{4}$$

or

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -\frac{\partial}{\partial P}(\dot{P}\psi). \tag{5}$$

Where, Eq.(5) is Fokker-Planck equation[17]. $\dot{P}$ is the rotation component of fiber orientation vector, $\frac{\mathrm{d}\psi}{\mathrm{d}t}$ is material derivative, $\frac{\partial}{\partial P}$ is partial derivative in spherical coordinate system.

2.3 Regularization Condition

Due to any fiber must follows one direction orientation in the system, all orientation direction of all fiber correspond to one unit sphere in the whole system, namely:

$$\oint \psi(P)\mathrm{d}P = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \psi(\theta, \psi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi = 1. \tag{6}$$

2.4 Periodicity Condition

Due to head of fiber is no difference with tail in the process of it moving along with flow field, the angular orientation in (θ,ϕ) is also consistent, namely:

$$\psi(\theta,\phi)=\psi(\pi-\theta,\pi+\phi). \tag{7}$$

2.5 Orientation Equation for a Single Fiber

The evolution equation of P for a single fiber immersed in a Newtonian flow without external torque was firsty developed by Jeffery[18] in 1922, which can be expressed as follows:

$$\dot{P}=W\cdot P+\lambda(E\cdot P-E:PPP). \tag{8}$$

Where, W is vorticity tensor of fiber, E is deformation rate of fiber, $\lambda=\left(\beta^2-1\right)/\left(\beta^2+1\right)$ is the fiber shape factor, $\beta=L/d$ is the fiber aspect ratio.

Assuming the fiber internal influence is neglected and the fiber has free orientation in initial conditions[19-20]. Three dimensional orientation equation can be simplified in this condition:

$$\psi(P,t)=\frac{1}{4\pi}\left(\Delta^T\cdot\Delta:PP\right)^{-\frac{3}{2}}. \tag{9}$$

And two dimensional orientation equation also can be expressed below:

$$\psi(P,t)=\frac{1}{\pi}\left(\Delta^T\cdot\Delta:PP\right)^{-1}. \tag{10}$$

Where, Δ_{ij} is displacement tensor and its expression is written below:

$$\Delta_{ij}=\left(\partial X_i/\partial x_j\right), \tag{11}$$

where, X_i is the position vector at $\hat{t}=0$, x_j is the position vector at the present moment.

Displacement tensor Δ_{ij} must meet the special conditions below:

$$\frac{\mathrm{d}\Delta_{ij}}{\mathrm{d}\hat{t}}=-\Delta_{ik}\left(W_{kj}+\lambda E_{kj}\right). \tag{12}$$

Where, W_{kj} is vorticity tensor , E_{kj} is deformation rate tensor and when it is initial conditions, $\Delta_{ij}=\delta_{ij}$, namely:

$$\Delta_{ij}=\delta_{ij}=\begin{cases}1, & i=j\\ 0. & i\neq j\end{cases} \tag{13}$$

2.6 Analytical Solution of Orientation Distribution Equation

To obtain the analytical solution of the mathematical model for orientation distribution of fiber, several assumptions are made in this paper:

1, The flow field of plant fiber composite materials is incompressible, steady state, isothermal, three dimensional, equibiaxial elongational flow.

2, Gravity and inertia force can be ignored.

3, The constitutive equation adopt the Newton constitutive equation.

4, The orientation of fiber is free orientation in the initial conditions, namely, the initial orientation of fiber is $1/4\pi$ at $t=0$ moment in all position.

5, Ignore internal interactions of fiber.

6, Fiber shape factor $\lambda=1$.

The velocity gradient tensor ∇v, vorticity tensor W and rate of deformation tensor of fiber E can be written as:

$$\nabla v = \begin{pmatrix} 2\dot{\varepsilon} & \dot{\gamma} & 0 \\ \dot{\gamma} & \dot{\varepsilon} & 0 \\ 0 & 0 & -3\dot{\varepsilon} \end{pmatrix}, \quad E = \begin{pmatrix} 2\dot{\varepsilon} & \dot{\gamma} & 0 \\ \dot{\gamma} & \dot{\varepsilon} & 0 \\ 0 & 0 & -3\dot{\varepsilon} \end{pmatrix}, \quad W = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{14a,b,c}$$

Where, v is flow velocity, $\dot{\gamma}$ is scalar rate of shear deformation and $\dot{\varepsilon}$ is scalar rate of extensional deformation. Eq.(14c) can be split into two tensor below:

$$E = \dot{\varepsilon}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -3 \end{pmatrix} + \dot{\gamma}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = E' + E''. \tag{15}$$

Therefore, displacement tensor Δ_{ij} can be expressed below:

$$\frac{\mathrm{d}\Delta_{ij}}{\mathrm{d}\hat{t}} = -\Delta'_{ik}E'_{kj} - \Delta''_{ik}E''_{kj}. \tag{16}$$

Through Eq.(16) can be shown:

$$\frac{\mathrm{d}\Delta'_{11}}{\mathrm{d}\hat{t}} = -\left(\Delta'_{11}E'_{11} + \Delta'_{12}E'_{21} + \Delta'_{31}E'_{31}\right) = -2\Delta'_{11}$$

$$\Delta'_{11} = e^{-2t}. \tag{17}$$

The other components of Δ' can be acquired by the above similar method. Therefore, deformation tensor Δ' can be shown below:

$$\Delta' = \begin{pmatrix} e^{-2t} & 0 & 0 \\ 0 & e^{-t} & 0 \\ 0 & 0 & e^{3t} \end{pmatrix}. \tag{18}$$

Similarly, Through Eq.(18) can be also shown:

$$\frac{\mathrm{d}\Delta''_{11}}{\mathrm{d}\hat{t}} = -\left(\Delta''_{11}E''_{11} + \Delta''_{12}E''_{21} + \Delta''_{31}E''_{31}\right) = 0, \ \Delta''_{11} = 1. \tag{19}$$

$$\frac{\mathrm{d}\Delta''_{12}}{\mathrm{d}\hat{t}} = -\left(\Delta''_{11}E''_{12} + \Delta''_{12}E''_{22} + \Delta''_{13}E''_{32}\right) = -\dot{\gamma}, \ \Delta''_{12} = -\dot{\gamma}T. \tag{20}$$

The other components of Δ'' can be acquired by the above similar method. Therefore, deformation tensor Δ'' can be shown below:

$$\Delta'' = \begin{pmatrix} 1 & -\dot{\gamma}T & 0 \\ -\dot{\gamma}T & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

The last deformation tensor Δ can be shown below：

$$\Delta = \lambda_1\Delta' + \lambda_2\Delta'' = \begin{pmatrix} 0.8e^{-2t} + 0.2 & -0.2\dot{\gamma}T & 0 \\ -0.2\dot{\gamma}T & 0.8e^{-t} + 0.2 & 0 \\ 0 & 0 & 0.8e^{3t} + 0.2 \end{pmatrix}. \tag{22}$$

Where, $\lambda_1 = 0.8$ and $\lambda_2 = 0.2$ is the weight parameter, respectively.

Therefore:

$$\Delta^T\Delta = \begin{pmatrix} 0.64e^{-4t} + 0.32e^{-2t} + 0.04t^2 + 0.04 & -0.16te^{-2t} - 0.16te^{-t} - 0.08t & 0 \\ -0.16te^{-2t} - 0.16te^{-t} - 0.08t & 0.64e^{-2t} + 0.32e^{-t} + 0.04t^2 + 0.04 & 0 \\ 0 & 0 & 0.64e^{6t} + 0.32e^{3t} + 0.04 \end{pmatrix}. \tag{23}$$

Eq.(22) are substituted into Eq.(9) and shown below:

$$\psi(P,t)=\frac{1}{4\pi}\left(\Delta^T\cdot\Delta:PP\right)^{-\frac{3}{2}}$$

$$=\frac{1}{4\pi}\left[\left(\Delta_{ik}^T\Delta_{kj}e_ie_j\right):P_se_sP_te_t\right]^{-\frac{3}{2}}$$

$$=\frac{1}{4\pi}\left(\Delta_{sk}^T\Delta_{ks}P_sP_t\right)^{-\frac{3}{2}}$$

$$=\frac{1}{4\pi}\left(\Delta_{11}^T\Delta_{11}P_1P_1+\Delta_{22}^TP_2P_2+\Delta_{33}^T\Delta_{33}P_3P_3+\Delta_{12}^T\Delta_{12}P_1P_2+\Delta_{21}^T\Delta_{21}P_2P_1\right)^{-\frac{3}{2}}$$

$$=\frac{1}{4\pi}[(0.64e^{-4t}+0.32e^{-2t}+0.04t^2+0.04)\sin^2\theta\cos^2\phi$$

$$+(0.64e^{-2t}+0.32e^{-t}+0.04t^2+0.04)\sin^2\theta\sin^2\phi+(0.64e^{6t}+0.32e^{3t}+0.04)\cos^2\theta$$

$$+2(-0.16te^{-2t}-0.16te^{-t}-0.08t)\sin^2\theta\sin2\phi]^{-\frac{3}{2}}. \tag{24}$$

Where, $t=\dot{\gamma}T_0$ expresses dimensionless cumulant along with time, T_0 means current time.

3. Results and Discussion

Interval $\theta\in(0,\pi)$ and interval $\phi\in(0,2\pi)$ are divided 100 nodes respectively. According to Eq.(24) of analytical solution of orientation distribution function of fiber in shear-ellipsoidal extensional flow, several pictures can be shown by numerical simulation in Fig. 1 and Fig. 2.

The evolution characteristics of the fiber dimensional orientation each extensional segment can be shown obviously from $T=0.1$ to $T=4.0$ in Fig. 1. The orientation of fiber is clutter at initial moments. However, there are more fibers at the directions of $(\theta,\phi)=(\frac{\pi}{2},0)$, $(\theta,\phi)=(\frac{\pi}{2},\pi)$, $(\theta,\phi)=(\pi/2,3\pi/2)$ and $(\theta,\phi)=(\frac{\pi}{2},2\pi)$. Furthermore, the plant fibers have a tendency obviously to gather in the three directions with the passage of time in the flow field. In general, there are four peaks. There is an obvious gather trend at the above three directions along with time increasingly. Therefore, the orientation of fiber at the above three directions is higher greatly than other directions. Furthermore, the extensional deformation accumulates and the orientation of fiber is more and more obvious along with time increasingly. Therefore, the slope of orientation is more and more sharp and the maximum value of orientation distribution function $\psi(\theta,\phi,t)$ is close to the position of $\phi=0$.

From figure 2, it can reflect the orientation change characteristics of plant fiber at the surface $\theta=\pi/2$ clearly. At the beginning, the slope of orientation distribution of plant fiber is slower and wider, it also means that the orientation distribution of plant fiber is relatively clutter. The slope of fiber orientation distribution is relatively gentle and the fiber distribution is relatively clutter in the short time interval. The orientation of fiber at the direction of $\phi=\pi/2,3\pi/2$ achieves maximum and minimum values respectively. However, gathered trend of fiber can be seen clearly, orientation is more and more obvious and the degree of orientation is sharp increasingly at angle of orientation $\phi=\pi/2,3\pi/2$ along with increasing time. Finally, fiber orientation exists only at angle of orientation $\phi=\pi/2,3\pi/2$. In fact, fiber orientation is along with the direction of extend, due to fiber has no difference between head and tail.

However, due to the gradient of fiber orientation is very cliffy, the step length $\delta\theta, \delta\phi$ has great influence to the result of accuracy. Furthermore, it can be seen gathered trend at $\phi = \pi/2, 3\pi/2$ and the orientation changes obviously increasingly, the degree of orientation is becoming more and more sharp.

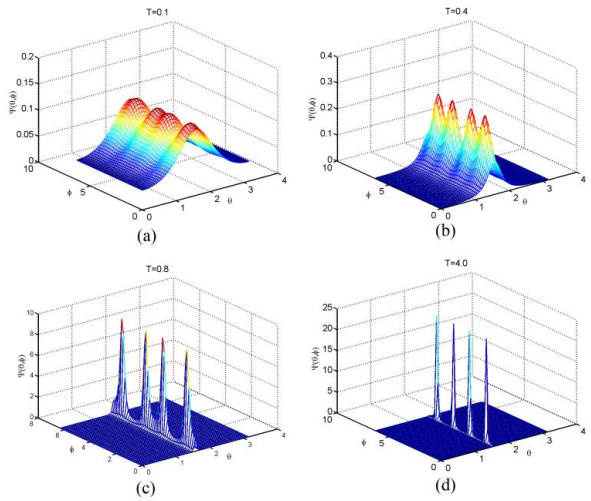

Fig. 1 The fiber orientation distribution function evolves for shear-ellipsoidal extensional flow field

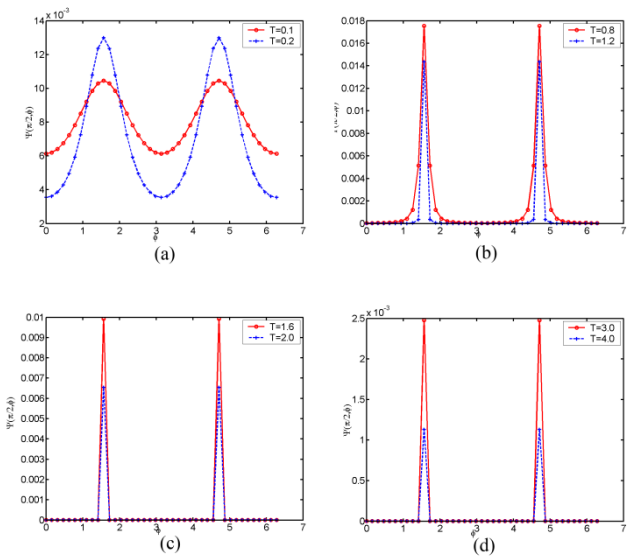

Fig.2 The fiber orientation distribution changing for shear-ellipsoidal extensional flow field at $\theta = \pi/2$

4. Conclusions

1, The period of motion of short fiber is relevant with extensional flow field and length to diameter ratio. The greater of extensional deformation rate, the shorter of period of motion; the bigger of length to diameter ratio, the longer of period of motion.

2, The motion of fiber is not constant periodic, but it is sometimes fast and sometimes slow.

3, The value of fiber orientation distribution function is relevant with initial angle and cumulative deformation in shear-ellipsoidal extensional flow field.

4, The numerical distribution of fiber orientation distribution function has great variation in extensional flow field. When shear-ellipsoidal extensional deformation rate is small, its numerical distribution is wide. However, the orientation distribution of fiber is more and more narrow along with shear-ellipsoidal extensional deformation increasingly. It tends to the direction of shear-ellipsoidal extensional flow gradually.

Acknowledgements

The authors wish to acknowledge the Guangzhou Science and Technology Plan Project (201541) and the "Innovation and Strengthen University" Project of Guangzhou Maritime Institute (A330106, B510647) for financial support.

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