Numerical Simulation of Polymer-fiber Composites Based on Ellipsoidal Extensional Force Field

Zan Huang

School of Marine engineering, Guangzhou Maritime Institute, Guangzhou 510725, China

zhuanggz@aliyun.com

Keywords: numerical simulation; dynamics analysis; fibers suspensions; ellipsoidal extensional force field

Abstract. In this paper, a mathematical model is established to simulate orientation distribution of plant fibers suspensions in ellipsoid extensional force field. Furthermore, the analytical solutions of differential equations on plant fibers orientation can be acquired in complex flow field.

Introduction

The orientation distribution and behavior of polymer-fiber composites is attracted increasingly in material processes in recent years, such as extrusion, injection, and compression molding, and so on. Furthermore, fibers suspensions are hot issue in many science and engineering fields, such materials science, paper-making industry, composites material production and so on. The mechanical properties of polymer-fiber composites are determined largely by the orientation distribution of fibers.

There are some literatures dealing with the dynamics of polymer-fiber composites by experimental, numerical and analytical methods for decades. Zhang et al. [1] predicted the fiber orientation distribution and rheological properties through a curved expansion and rotating duct in dilute fiber suspensions. Najam et al. [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. Huang et al. [3-4] investigate the orientation distribution of fiber suspensions based on shear-planar extensional force field and equibiaxial extensional flow. Lin et al. [5] obtained fiber orientation distribution in round turbulent jet of fiber suspension by numerical simulation methods. The above research has focused mainly in shear force field, however, few articles studied extensional force field with polymer-fiber composites.

The objective in this article is to establish the mathematical model and obtain analytical solutions on orientation distribution of polymer-fiber composites based on ellipsoidal extensional force field.

Mathematical model

Many years ago, Jeffery[6] developed firstly the evolution equation of P for a single fiber immersed in a Newtonian flow without external torque. Furthermore, the expression is shown below:

$$\dot{P} = W \cdot P + \lambda(E \cdot P - E : PPP). \tag{1}$$

Where, E is deformation rate of fiber, W is vorticity tensor 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 [7]. Three dimensional orientation equation can be simplified at this condition:

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

And two dimensional orientation equation also can be expressed $\psi(P,t) = \frac{1}{\pi}\left(\Delta^T \cdot \Delta : PP\right)^{-1}$. Where,

Δ_{ij} is displacement tensor and its expression is written $\Delta_{ij} = (\partial X_i / \partial x_j)$, 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:

$$\frac{\mathrm{d}\Delta_{ij}}{\mathrm{d}\hat{t}} = -\Delta_{ik}\left(W_{kj} + \lambda E_{kj}\right). \tag{3}$$

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

$$\Delta_{ij} = \delta_{ij} = \begin{cases} 1, & i = j \\ 0. & i \neq j \end{cases}. \tag{4}$$

To obtain the analytical solution of the mathematical model for orientation distribution of fiber, several assumptions are made in this paper: The flow field of plant fiber composite materials is incompressible, steady state, isothermal, three dimensional, ellipsoidal extensional force field. Gravity and inertia force can be ignored. The constitutive equation adopt the Newtonian constitutive equation. The orientation of fiber is free orientation in the initial conditions, i.e., the initial orientation of fiber is $1/4\pi$ at $t = 0$ moment in all position. Ignore internal interactions of fiber. 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:

$$\nabla v = \dot{\varepsilon}\begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -3 \end{bmatrix},\ E = \dot{\varepsilon}\begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -3 \end{bmatrix},\ W = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{5a,b,c}$$

Where, v is flow velocity, $\dot{\varepsilon}$ is scalar rate of extensional deformation.

Eq. (4)-(5) are substituted into Eq. (3) and it can be rewritten as:

$$\frac{\mathrm{d}\Delta_{ij}}{\mathrm{d}\hat{t}} = -\Delta_{ik}E_{kj}. \tag{6}$$

Some results can be obtained from Eq. (6) and shown below:

$$\frac{\mathrm{d}\Delta_{11}}{\mathrm{d}\hat{t}} = -\left(\Delta_{11}E_{11} + \Delta_{12}E_{21} + \Delta_{31}E_{31}\right) = -2\Delta_{11}$$

$$\Delta_{11} = e^{-2t}. \tag{7}$$

The other components can be acquired by the above similar method. Therefore, displacement tensor can be shown below:

$$\Delta = \begin{pmatrix} e^{-2t} & 0 & 0 \\ 0 & e^{-t} & 0 \\ 0 & 0 & e^{3t} \end{pmatrix}. \tag{8}$$

Eq. (8) are substituted into Eq. (2) and shown below:

$$\begin{aligned} \psi(P,t) &= \frac{1}{4\pi}\left(\Delta^T \cdot \Delta : PP\right)^{-\frac{3}{2}} \\ &= \frac{1}{4\pi}\left[\left(\Delta_{ik}^T \Delta_{kj} e_i e_j\right) : P_s e_s P_t e_t\right]^{-\frac{3}{2}} \\ &= \frac{1}{4\pi}\left(\Delta_{sk}^T \Delta_{ks} P_s P_t\right)^{-\frac{3}{2}} \\ &= \frac{1}{4\pi}\left(\Delta_{11}^T \Delta_{11} P_1 P_1 + \Delta_{22}^T P_2 P_2 + \Delta_{33}^T \Delta_{33} P_3 P_3\right)^{-\frac{3}{2}} \\ &= \frac{1}{4\pi}\left(e^{-2t}e^{-2t}\sin^2\theta\cos^2\phi + e^{-t}e^{-t}\sin^2\theta\sin^2\phi + e^{3t}e^{3t}\cos^2\theta\right)^{-\frac{3}{2}} \end{aligned}$$

$$=\frac{1}{4\pi}\left(e^{-4t}\sin^2\theta\cos^2\phi+e^{-2t}\sin^2\theta\sin^2\phi+e^{6t}\cos^2\theta\right)^{-\frac{3}{2}}. \tag{9}$$

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

Results and discussion

Interval $\theta\in(0,\pi)$ and interval $\phi\in(0,2\pi)$ are divided 50 nodes respectively. According to Eq.(9) of analytical solution of orientation distribution function of fiber in ellipsoidal extensional force field, several pictures can be shown by numerical simulation in Fig. 1 and Fig. 2.

Figure 1 reflects the evolution characteristics of the fibers dimensional orientation each extensional segment can be shown obviously from $T=0.1$ to $T=4.0$. The orientation of fiber is clutter at initial moments. However, there are more fibers at the directions of $(\theta,\phi)=(\frac{\pi}{2},0)$, $(\theta,\phi)=(\frac{\pi}{2},\pi)$ and $(\theta,\phi)=(\frac{\pi}{2},2\pi)$. There is an obvious gather trend at the above three directions along with time increasingly. The degree of orientation for plant fibers in these three directions was significantly higher than other directions orientation. 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 $\phi=0$. With the passage of time, the orientation of these situations is obvious especially, but the fiber orientation in the direction $\theta=0,\pi$ is less and less, finally the basic tending to zero, zero can be ignored.

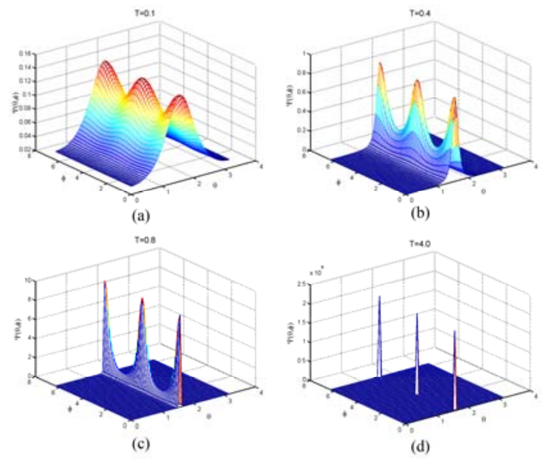

Fig. 1 The fiber orientation distribution function evolves for ellipsoidal extensional force field

Figure 2 can reflect clearly the evolution characteristics of fiber orientation at the surface $\theta=\pi/2$. The slope of fiber orientation distribution is relatively gentle and the fiber distribution is relatively clutter in the short time interval. At the beginning, the orientation distribution of plant fiber slope is slower, wide distribution, also means that plant fiber distribution is relatively clutter. The orientation of fiber at the direction of $\phi=0,\pi,2\pi$ 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 $\phi=0,\pi,2\pi$ along with increasing time. Finally, fiber orientation exists only at angle of orientation $\phi=0,\pi,2\pi$. 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.

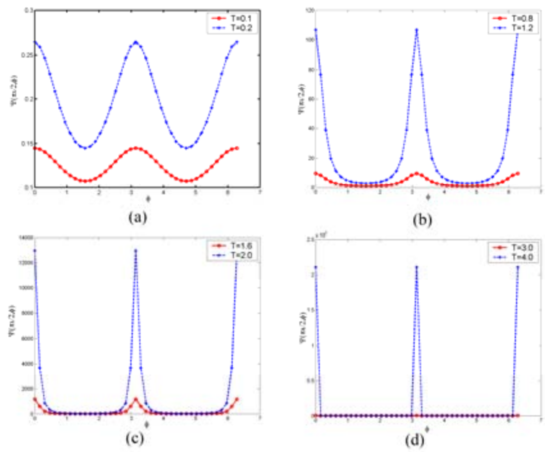

Fig.2 The fiber orientation distribution changing for ellipsoidal extensional force field at $\theta = \pi / 2$

Conclusions

The motion of fiber is not the uniform periodic motion, but it is sometimes fast and sometimes slow. The numerical distribution of fiber orientation distribution function has great variation in ellipsoidal extensional force field. When extensional deformation rate is small, its numerical distribution is wide. However, the orientation distribution of fiber is more and more narrow along with tensile deformation increasingly. It tends to the direction of extend 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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