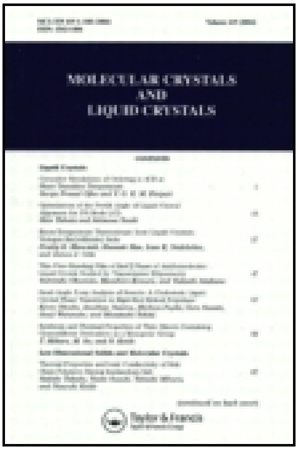

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Analysis of the Steady Director of Nematic Polymers in Hele–Shaw Flow

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In this article, a theory analysis of the steady director of nematic polymers in Hele–Shaw flow was given. The Ericksen's Transversely Isotropic Fluid equations are used for modeling the motion of the director. There is a singular point for the steady state of director in expanding Hele–Shaw flows. If the shear rate in the direction perpendicular to the flow plane is larger than a switch value, which is a function of velocity derivatives in the flow plane, the steady director will align with the flow direction; otherwise, it will tend to be perpendicular to the flow direction. Under this result, the Leslie–Ericksen (L–E) theory may explain the widely recognized phenomenon in the molding process of nematic polymers, which is that the molecular chains in the skin regions are largely aligned along the injection direction while the chain orientation in the central core is more or less random.

Keywords: director, Hele-Shaw, LCPs, nematic

INTRODUCTION

Liquid crystalline polymers (LCPs) have a high degree of long-range molecular orientation order, thereby being referred as anisotropic fluids. When such LCPs are processed, the resulting solid polymer maintains the high molecular orientation order of LCPs and consequently exhibits special properties in comparison with traditional polymers. Therefore, it is very valuable to predict the development of the molecular orientations during the processing of the LCPs.

At present, the Leslie–Ericksen (L–E) theory and Doi's theory are the two popular constitutive theories for liquid crystals [1]. The L–E theory, which is based on macroscopic continuum mechanics, is suitable for describing the rheological properties of low molecular weight

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nematics. The Doi's theory, derived from microscopic molecular theory, is a kinetic model for rod-like polymers. Usually the Doi's model is too complicated to be used in the simulation of complex flows. As mentioned by Rong-Yen Chang *et al.* in [2], Marrucci, Kuzuu, and Doi have demonstrated that the Doi's theory could be reduced to the L–E theory in the limit of low shear ratess. Many researchers have used the L–E theory in analyzing flow-induced behavior of LCPs. For example, Shigeomi CHONO and Tomohiro TSUJI in [1], Rong-Yen Chang *et al.* in [2], Marifi Güler in [3], Baleo *et al.* in [4], and Vanderheyden and Ryskin in [5].

In this article, the steady state director of nematic polymers in Hele-Shaw flow was analyzed by using the L–E theory, which was approximated by the Ericksen's Transversely Isotropic Fluid equations for nematic polymers of high viscosities [5]. There is a singular point for the steady state of director in expanding Hele-Shaw flows. If the shear rate in the direction perpendicular to the flow plane is larger than a switch value, which is a function of velocity derivatives in the flow plane, the steady director will align with the flow direction; otherwise, it will tend to be perpendicular to the flow direction. Under this result, the L–E theory may explain the widely recognized phenomenon in the molding process of nematic polymers, which is that the molecular chains in the skin regions are largely aligned along the injection direction while the chain orientation in the central core is more or less random.

GOVERNING EQUATIONS

In this section, the center of a fully developed symmetric expanding Hele-Shaw flow, shown in Fig. 1, was considered. In this flow, z is the gapwise direction, and the velocities in x–y plain are symmetric over a centerline, therefore, at the center, the following equations are tenable:

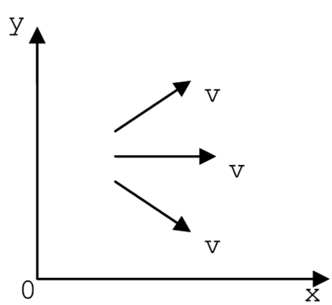

FIGURE 1 Velocity directions of a symmetric expansion flow.

$$v_y = 0,\ v_z = 0,\ \frac{\partial v_x}{\partial y} = 0 \tag{1}$$

The Ericksen's Transversely Isotropic Fluid equations are used for modeling the motion of the director:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0 \tag{2}$$

$$\left(\frac{Dn_i}{Dt} = W_{ij}n_j + \ddot{e}(A_{ij}n_j - n_i n_k n_l A_{kl}\right) \tag{3}$$

$$(n_x^2 + n_y^2 + n_z^2) = 1 \tag{4}$$

where

$$W_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial_j} - \frac{\partial v_j}{\partial_i}\right) \tag{5}$$

$$A_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial_j} + \frac{\partial v_j}{\partial_i}\right) \tag{6}$$

$$i, j = x, y, z.$$

Due to $v_y = 0$ and $v_z = 0$,

$$\frac{\partial v_y}{\partial x} = \frac{\partial v_y}{\partial z} = \frac{\partial v_z}{\partial x} = \frac{\partial v_z}{\partial y} = \frac{\partial v_z}{\partial z} = 0. \tag{7}$$

Then

$$W = \frac{1}{2}\begin{bmatrix} 0 & 0 & \frac{\partial v_x}{\partial z} \\ 0 & 0 & 0 \\ -\frac{\partial v_x}{\partial z} & 0 & 0 \end{bmatrix} \tag{8}$$

$$A = \frac{1}{2}\begin{bmatrix} 2\frac{\partial v_x}{\partial x} & 0 & \frac{\partial v_x}{\partial z} \\ 0 & 2\frac{\partial v_y}{\partial y} & 0 \\ \frac{\partial v_x}{\partial z} & 0 & 0 \end{bmatrix}. \tag{9}$$

Equation (3) turns to

$$\frac{Dn_x}{Dt} = \frac{1 + \ddot{e}}{2}\frac{\partial v_x}{\partial z} n_z + \ddot{e} \cdot n_x\left(\frac{\partial v_x}{\partial x} - m\right) \tag{10a}$$

$$\frac{Dn_y}{Dt} = \ddot{e} \cdot n_y \left(\frac{\partial v_y}{\partial y} - m \right) \tag{10b}$$

$$\frac{Dn_z}{Dt} = \frac{\ddot{e} - 1}{2} \frac{\partial v_x}{\partial z} n_x - \ddot{e} \cdot m \cdot n_z \tag{10c}$$

$$m = \frac{\partial v_x}{\partial x} n_x^2 + \frac{\partial v_y}{\partial y} n_y^2 + \frac{\partial v_x}{\partial z} n_x n_z \tag{11}$$

STEADY STATE ANALYSIS

At steady state of a fluid particle, $\frac{Dn_x}{Dt} = \frac{Dn_y}{Dt} = \frac{Dn_z}{Dt} = 0$, Eq. (10a)–(10c) become:

$$\frac{1 + \ddot{e}}{2} \frac{\partial v_x}{\partial z} n_z + \ddot{e} \cdot n_x \left(\frac{\partial v_x}{\partial x} - m \right) = 0 \tag{12a}$$

$$\ddot{e} \cdot n_y \left(\frac{\partial v_y}{\partial y} - m \right) = 0 \tag{12b}$$

$$\frac{\ddot{e} - 1}{2} \frac{\partial v_x}{\partial z} n_x - \ddot{e} \cdot m \cdot n_z = 0 \tag{12c}$$

When $n_y \neq 0$

Equation (12b) becomes

$$m = \frac{\partial v_y}{\partial y}. \tag{13}$$

And Eq. (12a) and (12c) becomes

$$\frac{1 + \ddot{e}}{2} \frac{\partial v_x}{\partial z} n_z + 2\ddot{e} \frac{\partial v_x}{\partial x} n_x = 0 \tag{14a}$$

$$\frac{\ddot{e} - 1}{2} \frac{\partial v_x}{\partial z} n_x + \ddot{e} \frac{\partial v_x}{\partial x} n_z = 0. \tag{14b}$$

The solution of the above equations is: $n_x = n_z = 0$. Obviously, the point with $n_x = n_z = 0$ and $n_y = 1$ satisfies Eq. (4) and (12a)–(12c). Therefore, $n_x = n_z = 0$ and $n_y = 1$ is a balance point of director.

Let $q_1 = n_x$, $q_2 = n_z$, then at the above balance point, $q_1 = q_2 = 0$.

$$\frac{Dq}{Dt} = Q \cdot q + O(\|q\|^2) \tag{15}$$

where

$$\mathbf{Q} = \begin{bmatrix} 2\ddot{e} \cdot \frac{\partial v_x}{\partial x} & \frac{1}{2}\frac{\partial v_x}{\partial z}(\ddot{e}+1) \\ \frac{1}{2}\frac{\partial v_x}{\partial z}(\ddot{e}-1) & \ddot{e} \cdot \frac{\partial v_x}{\partial x} \end{bmatrix}. \tag{16}$$

The condition for local stable of Eq. (15) at $\mathbf{q} = 0$ is that all the eigenvalues of $\mathbf{Q}$ have a minus real part. It means all the roots of Eq. (17) should have minus real part. That requires all its coefficients are positive.

$$s^2 - 3\lambda \cdot \frac{\partial v_x}{\partial x} s + 2\lambda^2 \left(\frac{\partial v_x}{\partial x}\right)^2 - \frac{1}{4}\left(\frac{\partial v_x}{\partial z}\right)^2 (\lambda^2 - 1) = 0. \tag{17}$$

Conclusion 1: At the center of a fully developed symmetric expansion flow shown in Figure 1, the condition for local stable of the director of a fluid particle with $n_x = n_z = 0$ and $n_y = 1$ is:

$$\left(\frac{\partial v_x}{\partial z}\right)^2 < \frac{8\lambda^2}{\lambda^2 - 1}\left(\frac{\partial v_x}{\partial x}\right)^2 \quad \text{and} \quad \frac{\partial v_x}{\partial x} < 0. \tag{18}$$

When $n_y = 0$

Equation (4) becomes

$$n_x^2 + n_z^2 = 1 \tag{19}$$

Obviously, $n_x = n_z = 0$ violates Eq. (19). Then Eq. (20) must be tenable for the solutions of Eq. (12a) and (12c) other than $n_x = n_z = 0$.

$$4\lambda^2 m^2 - 4\lambda^2 \frac{\partial v_x}{\partial x} m - \left(\frac{\partial v_x}{\partial z}\right)^2 (\lambda^2 - 1) = 0. \tag{20}$$

The roots are

$$m_1 = \frac{1}{2}\frac{\partial v_x}{\partial x} + \frac{\sqrt{\lambda^2 \left(\frac{\partial v_x}{\partial x}\right)^2 + \left(\frac{\partial v_x}{\partial z}\right)^2 (\lambda^2 - 1)}}{2\lambda} \tag{21a}$$

and

$$m_2 = \frac{1}{2}\frac{\partial v_x}{\partial x} - \frac{\sqrt{\lambda^2 \left(\frac{\partial v_x}{\partial x}\right)^2 + \left(\frac{\partial v_x}{\partial z}\right)^2 (\lambda^2 - 1)}}{2\lambda}. \tag{21b}$$

From Eq. (12c), (19), and (20), we can get the steady director with $n_{y0} = 0$

$$n_{x0} = \frac{\lambda \cdot m}{\sqrt{\lambda^2 m^2 + (\frac{\lambda-1}{2})^2 (\frac{\partial v_x}{\partial z})^2}} \tag{22a}$$

$$n_{z0} = \frac{(\lambda - 1)}{2\lambda m} \frac{\partial v_x}{\partial z} n_{x0} \tag{22b}$$

It can be proved that this solution also satisfies Eqs. (11), (12a), and (12b). Therefore, it is a balance point of the director.

Let $q_1 = n_x - n_{x0}$, $q_2 = n_y$-n_{y0}, then at balance point $q_1 = q_2 = 0$

According to $n_x^2 + n_y^2 + n_z^2 = 1$, we can get

$$\frac{\partial n_z}{\partial n_x} = -\frac{n_x}{n_z} \quad \text{and} \quad \frac{\partial n_z}{\partial n_y} = -\frac{n_y}{n_z}. \tag{23}$$

Then near the balance points, we have

$$n_z = n_{z0} + \frac{\partial n_z}{\partial n_x}\bigg|_{\text{balance - point}} q_1 + \frac{\partial n_z}{\partial n_y}\bigg|_{\text{balance - point}} q_2 + o(\|q\|^2). \tag{24}$$

Eq. (10a) and (10b) turn to

$$\frac{D\mathbf{q}}{Dt} = \mathbf{Q} \cdot \mathbf{q} + \mathbf{B} + O(\|q\|^2), \tag{25}$$

where

$$\mathbf{Q} = \begin{bmatrix} \ddot{e}\left(\frac{\partial v_x}{\partial x} - m\right) - \frac{\ddot{e}+1}{2}\frac{\partial v_x}{\partial z}\frac{n_{x0}}{n_{z0}} & -\frac{\ddot{e}+1}{2}\frac{\partial v_x}{\partial z}\frac{n_{y0}}{n_{z0}} \\ 0 & -\lambda\left(m + \frac{\partial v_x}{\partial x}\right) \end{bmatrix} \tag{26a}$$

$$\mathbf{B} = \begin{bmatrix} \frac{\ddot{e}+1}{2}\frac{\partial v_x}{\partial z} n_{z0} + \ddot{e}\left(\frac{\partial v_x}{\partial x} - m\right) n_{x0} \\ -\lambda\left(m + \frac{\partial v_x}{\partial x}\right) n_{y0} \end{bmatrix} = 0. \tag{26b}$$

The local stable conditions are

$$\ddot{e}\left(\frac{\partial v_x}{\partial x} - m\right) - \frac{\ddot{e}+1}{2}\frac{\partial v_x}{\partial z}\frac{n_{x0}}{n_{z0}} < 0 \tag{27a}$$

and

$$-\lambda\left(m + \frac{\partial v_x}{\partial x}\right) < 0. \tag{27b}$$

Equation (25) is unstable for $m = m_2$. When $m = m_1$, the condition for local stable of Eqs. (4)–(25) is

$$\left(\frac{\partial v_x}{\partial z}\right)^2 > \frac{8\ddot{e}^2}{\ddot{e}^2 - 1}\left(\frac{\partial v_x}{\partial x}\right)^2. \tag{28}$$

Conclusion 2: At the center of the symmetric expansion flow shown in Fig. 1, the condition for local stable of the director of a fluid particle with $n_y = 0$ is Eq. (28).

DISCUSSIONS

It can be seen from conclusions 1 and 2 that, in expansion Hele–Shaw flows of nematics, there is a singular point for the steady state of director. If the shear rate in z direction is larger than a switch value, which is given by Eq. (29), the steady director will align with the flow direction:

$$\left(\frac{\partial v_x}{\partial z}\right)^2 = \frac{8\ddot{e}^2}{\ddot{e}^2 - 1}\left(\frac{\partial v_x}{\partial x}\right)^2. \tag{29}$$

Otherwise, if the shear rate in z direction is less than the switch value, the director will tend to be perpendicular to the flow direction. In Hele–Shaw flows, there exist two kinds of singular layers near the center. The small position changing of the singular layers during the injection process will produce director oscillations around the two singular layers. In the central core between the two singular layers, there is no strong shear rate to align the directors. Therefore, the director orientation will tend to be random due to the director oscillations around the two singular layers. In most injection moulds, the flows near inlets are expanding flows. The phenomenon of random directors in the central core may be kept with the flow due to the lack of strong shear rate to align the directors in the central core. In the skin layers, the strong shear rate in the gapwise direction will guarantee the director aligning along the flow directions.

Under this result, the L–E theory may explain the widely recognized phenomenon in the molding process of nematic polymers, which is that the molecular chains in the skin regions are largely aligned along the injection direction while the chain orientation in the central core is more or less random.

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