Numerical Simulation of Flows of Liquid Crystalline Polymers through Parallel Plates Containing a Cylinder*

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Flows through parallel plates containing a cylinder are numerically calculated for nematic liquid crystalline polymers using a simplified model of the Leslie-Ericksen theory. A tensor expression for the orientation of the director is used in the basic equations in order to avoid the difficulty in calculation due to the tumbling of the director. The orientation of the director is affected by the contraction and expansion flows, and tumbling occurs. An area where the molecule aligns in the direction of the flow exists behind the cylinder. It extends downstream as the parameter λ approaches the value one. The flow field does not change significantly from that of Newtonian fluids.

Key Words: Liquid Crystalline Polymers, Complex Flow Geometry, Numerical Simulation, Director Orientation, Tumbling

1. Introduction

The behavior of nematic liquid crystals is well described by the Leslie-Ericksen model. These liquid crystals have both elastic and viscous properties, and their molecular orientation is affected by flows. Many studies on the flow analysis of nematic liquid crystals have been performed using the LE model⁽¹⁾⁻⁽⁵⁾. In the low-molecular-weight liquid crystals which are used as the materials for displays, however, the flows seem to be insignificant. On the other hand, the analysis of the flow and the orientation during processing is significant for liquid crystalline polymers (LCPs), which are used as the materials for polymer processing, because the molecular orientation dominates the mechanical properties of moldings.

The LCPs have polydomain structure and show complicated behavior in their rheological properties⁽⁶⁾⁻⁽⁹⁾. The constitutive equations of the

LCPs have been developed by many researchers⁽¹⁰⁾⁻⁽¹²⁾, but these are insufficient because of the complexity in rheological properties. The viscous force is much higher than the elastic force in the LCPs, in contrast with the case of low-molecular-weight liquid crystals. Vanderheyden and Ryskin⁽¹³⁾ applied the high-viscosity approximation to the Leslie-Ericksen model and derived an equation identical to that of Ericksen's transversely isotropic fluid (TIF) model. They also computed the flow of LCPs in a contracted channel and a dimpled channel. Baleo et al.⁽¹⁴⁾ also used the same constitutive equation as Vanderheyden and Ryskin and computed the director alignment for flows in various axial geometries. However, a difficulty arises in computation including the director tumbling because the governing equations are described in terms of the orientation vector. The occurrence of the director tumbling is expected in the present calculation because the flow through parallel plates containing a cylinder includes the converging and diverging flows and the flow around a cylinder. Therefore we transformed the vectorial expression of the governing equation to the tensorial one to avoid the difficulty in the calculation.

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Since the molecular alignment behind a cylinder is usually considered in the polymer processing, we focused on the relation between the flow and the molecular alignment in the present calculation. We mapped the flow domain onto the square one by using a boundary-fitted curvilinear coordinate system and solved the flow problem by using a finite difference method.

2. Governing Equation

The equation of continuity for incompressible fluids is given by

$$v_{i,i} = 0, \quad (1)$$

where v_i is a component of a velocity vector. Since the viscosity of LCPs is high, the Reynolds number is small enough that we can ignore the inertia. Therefore, the equation of motion is

$$-p_{,i} + \sigma_{ji,j} = 0. \quad (2)$$

For the analysis of the flow of nematic liquid crystals the Leslie-Ericksen constitutive equation in the form of the following equation has been used.

$$\begin{aligned} \sigma_{ij} = & -\frac{\partial F}{\partial n_{k,i}} n_{k,j} + \alpha_1 n_i n_j n_k n_l D_{kl} + \alpha_2 n_j N_i \\ & + \alpha_3 n_j N_i + \alpha_4 D_{ij} + \alpha_5 n_i n_k D_{kj} \\ & + \alpha_6 n_j n_k D_{ki}, \end{aligned} \quad (3)$$

where F is the Frank free energy, and n_i is the unit vector which is called the director and indicates the direction of molecular orientation. D_{ij} is the rate-of-deformation tensor defined by

$$D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}), \quad (4)$$

and N_i is given by

$$N_i = \frac{\partial n_i}{\partial t} + v_j n_{i,j} - W_{ij} n_j, \quad (5)$$

where W_{ij} is the vorticity tensor,

$$W_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}). \quad (6)$$

The six coefficients in Eq. (3) are called the Leslie coefficients. The torque balance equation for the director is

$$-\frac{\partial F}{\partial n_i} + \left(\frac{\partial F}{\partial n_{i,j}} \right)_{,j} = -\gamma n_i + \gamma_1 N_i + \gamma_2 n_k D_{ki}. \quad (7)$$

Since the viscosity of LCPs is high, the Ericksen number, which represents the ratio of viscous force to elastic force, is likely to be extremely large, up to $O(10^{10})^{(13)}$, in the situations typical for industrial processing. This means that the term of the Frank free energy can be ignored in Eq. (3). Vanderheyden and Ryskin⁽¹³⁾ called this approximation the "high-viscosity approximation". Applying this approximation to the Leslie-Ericksen model, we obtained the stress tensor and the torque balance equation as follows:

$$\sigma_{ij} = \alpha_4 D_{ij} + \beta_1 n_i n_j n_k n_l D_{kl}$$

$$+ \beta_2 (n_i n_k D_{kj} + n_j n_k D_{ki}), \quad (8)$$

$$\frac{\partial n_i}{\partial t} + v_j n_{i,j} = W_{ij} n_j + \lambda (n_j D_{ij} - n_i n_k n_l D_{kl}), \quad (9)$$

where

$$\beta_1 = \alpha_1 - \lambda(\alpha_2 + \alpha_3) \quad (10)$$

$$\beta_2 = \alpha_5 + \lambda \alpha_2 \quad (11)$$

$$\lambda = \frac{\alpha_2 + \alpha_3}{\alpha_2 - \alpha_3}. \quad (12)$$

These equations are identical to the TIF model as shown by Vanderheyden and Ryskin⁽¹³⁾. The vectorial expression in Eqs. (8) and (9) gives rise to the difficulty in the calculation due to the molecular tumbling in the flow. In the present study, we introduced the orientation tensor defined by

$$S_{ij} = n_i n_j. \quad (13)$$

Equations (8) and (9) are transformed in terms of the orientation tensor as follows:

$$\sigma_{ij} = \alpha_4 D_{ij} + \beta_1 S_{ij} S_{kl} D_{kl} + \beta_2 (S_{ik} D_{kj} + S_{jk} D_{ki}) \quad (14)$$

$$\begin{aligned} \frac{\partial S_{ij}}{\partial t} + v_k S_{ij,k} = & W_{ik} S_{kj} + W_{jk} S_{ki} \\ & + \lambda (S_{ik} D_{kj} + S_{jk} D_{ki} - 2 S_{ij} S_{kl} D_{kl}). \end{aligned} \quad (15)$$

The governing equations are developed in the Cartesian coordinate system for calculations of two-dimensional flows. The stress tensor is transformed into a more convenient form for the numerical calculation:

$$\sigma_{ij} = \alpha_4 D_{ij} + \sigma'_{ij}. \quad (16)$$

Moreover, nondimensional variables are used in the development of the governing equations.

$$\begin{aligned} x^* = x/H, \quad y^* = y/H, \quad v_i^* = v_i/U, \\ p^* = p/(\alpha_4 U/H), \quad \sigma_{ij}^* = \sigma_{ij}/(\alpha_4 U/H), \\ \alpha_i^* = \alpha_i/\alpha_4 \end{aligned} \quad (17)$$

We omit the asterisk which means a nondimensional quantity for convenience although all the following equations are given in terms of the nondimensional quantities. Eliminating the pressure p in Eq. (2), we obtain the equation

$$\begin{aligned} \frac{1}{2} \left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) + \frac{\partial^2 \sigma'_{xx}}{\partial x \partial y} + \frac{\partial^2 \sigma'_{xy}}{\partial y^2} \\ - \frac{\partial^2 \sigma'_{xy}}{\partial x^2} - \frac{\partial^2 \sigma'_{yy}}{\partial x \partial y} = 0 \end{aligned} \quad (18)$$

where ω is the vorticity defined by

$$\omega = \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right). \quad (19)$$

Here ϕ is the stream function. Stress components are

$$\begin{aligned} \sigma'_{xx} = & \beta_1 S_{xx} \left\{ (S_{xx} - S_{yy}) \frac{\partial^2 \phi}{\partial x \partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\} \\ & + \beta_2 \left\{ 2 S_{xx} \frac{\partial^2 \phi}{\partial x \partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\} \end{aligned} \quad (20)$$

$$\begin{aligned} \sigma'_{xy} = & \beta_1 S_{xy} \left\{ (S_{xx} - S_{yy}) \frac{\partial^2 \phi}{\partial x \partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\} \\ & + \frac{1}{2} \beta_2 \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \end{aligned} \quad (21)$$

$$\sigma'_{yy} = \beta_1 S_{yy} \left\{ (S_{xx} - S_{yy}) \frac{\partial^2 \phi}{\partial x \partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\}$$

$$+ \beta_2 \left\{ -2S_{yy} \frac{\partial^2 \phi}{\partial x \partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\}. \quad (22)$$

The torque balance equations are given by

$$\begin{aligned} \frac{\partial S_{xx}}{\partial t} = & -v_x \frac{\partial S_{xx}}{\partial x} - v_y \frac{\partial S_{xx}}{\partial y} + S_{xy} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \\ & + \lambda \left\{ 2S_{xx}(1 - S_{xx} + S_{yy}) \frac{\partial^2 \phi}{\partial x \partial y} \right. \\ & \left. + S_{xy}(1 - 2S_{xx}) \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\} \end{aligned} \quad (23)$$

$$\begin{aligned} \frac{\partial S_{xy}}{\partial t} = & -v_x \frac{\partial S_{xy}}{\partial x} - v_y \frac{\partial S_{xy}}{\partial y} + \frac{1}{2}(S_{yy} - S_{xx}) \\ & \times \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + \lambda \left\{ 2S_{xy}(S_{yy} - S_{xx}) \right. \\ & \times \frac{\partial^2 \phi}{\partial x \partial y} + \frac{1}{2}(S_{xx} + S_{yy} - 4S_{xy}^2) \left(\frac{\partial^2 \phi}{\partial y^2} \right. \\ & \left. \left. - \frac{\partial^2 \phi}{\partial x^2} \right) \right\} \end{aligned} \quad (24)$$

$$\begin{aligned} \frac{\partial S_{yy}}{\partial t} = & -v_x \frac{\partial S_{yy}}{\partial x} - v_y \frac{\partial S_{yy}}{\partial y} - S_{xy} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \\ & + \lambda \left\{ 2S_{yy}(-1 - S_{xx} + S_{yy}) \frac{\partial^2 \phi}{\partial x \partial y} \right. \\ & \left. + S_{xy}(1 - 2S_{yy}) \left(\frac{\partial^2 \phi}{\partial y^2} - \frac{\partial^2 \phi}{\partial x^2} \right) \right\}. \end{aligned} \quad (25)$$

3. Computation Method and Conditions

3.1 Computation method

The governing equations are solved by using the finite difference method. It is hard to impose boundary conditions in the Cartesian coordinate system since the domain has a curved boundary. Therefore, we transformed the governing equations by using a boundary-fitted curvilinear coordinate system $(\xi, \eta)^{(18)-(20)}$. The governing equations must be transformed to the (ξ, η) coordinate system using

$$\frac{\partial}{\partial x} = \frac{1}{J} \left(y_\eta \frac{\partial}{\partial \xi} - y_\xi \frac{\partial}{\partial \eta} \right) \quad (26)$$

$$\frac{\partial}{\partial y} = \frac{1}{J} \left(-x_\eta \frac{\partial}{\partial \xi} + x_\xi \frac{\partial}{\partial \eta} \right) \quad (27)$$

where indices denote the partial derivative with respect to ξ and η and J is the Jacobian defined by

$$J = x_\xi y_\eta - x_\eta y_\xi. \quad (28)$$

The governing equations transformed to the (ξ, η) coordinate system are discretized by the finite difference method. The equations of motion are discretized using a central difference. The mapping functions $x(\xi, \eta)$ and $y(\xi, \eta)$ are obtained by solving Poisson's equations for ξ and η . We solved the torque balance equations using the Euler forward difference scheme for the time derivatives and a method of characteristics for the convective terms in the same way as Baleo et al.⁽¹⁴⁾ The convective term is given by

$$\frac{\partial S_{ij}}{\partial s} = v_x \frac{\partial S_{ij}}{\partial x} + v_y \frac{\partial S_{ij}}{\partial y}, \quad (29)$$

where s is a time variable and its value at the point A shown in Fig. 1 is calculated by

$$\frac{\partial S_{ij}^A}{\partial s} = \{S_{ij}^A - S_{ij}^B\} / \left\{ \left(\frac{\Delta d_x}{v_x} \right)^2 + \left(\frac{\Delta d_y}{v_y} \right)^2 \right\}^{1/2}. \quad (30)$$

Therefore, the orientation tensor at the time $(n+1)\Delta t$ is calculated by

$$S_{ij}^{(n+1)} = S_{ij}^{(n)} + \frac{\partial S_{ij}}{\partial t} \Delta t, \quad (31)$$

where Δt is a virtual time increment.

The convergent solution was obtained by the iteration of the two subproblems of the velocity and the orientation tensor. The convergence criterion used was $\varepsilon \leq 10^{-4}$ for ϕ and all components of S_{ij} .

3.2 Computational conditions

Figure 2 shows the schematic description of the flow geometry. We need only consider the flow in the upper half of the flow domain due to symmetry. The lengths of the parallel plates before and after the cylinder are 2.25 times the length of the gap between parallel plates H . The cylinder diameters used are $0.5H$ and $0.25H$. Figure 3 shows the finite difference grids. The numbers of grids are 190×20 for the geometry (a) and 180×20 for the geometry (b).

Fig. 1 Calculation of the director convective terms along the streamline

Fig. 2 Flow geometry

(a) $d = 0.5H$

(b) $d = 0.25H$

Fig. 3 Finite difference meshes

The velocity profile for Newtonian fluids given by Eq. (32) was imposed at the inlet and the outlet of the parallel plates.

$$v_x = \frac{3}{2}(1-4y^2), \quad v_y = 0 \quad (32)$$

The symmetry condition for the velocity was given along the centerline and the no-slip condition at the wall. For the orientation tensor, the orientational angle ϕ_0 , which is called the Leslie angle, defined by the following equation is given at the inlet.

$$\cos 2\phi_0 = \frac{1}{\lambda} \quad (33)$$

Nondimensional constants β_1 and β_2 in Eqs. (17)–(19) are phenomenological parameters to be determined from the experiment. However, they have not been obtained yet because their measurement is very difficult. We used the values; $\beta_1=0.5$ and $\beta_2=-0.5$ to compare our results with those of Vanderheyden and Ryskin⁽¹³⁾ and Baleo et al.⁽¹⁴⁾ From Eq. (33), we used various values of λ larger than one and examined the effect of λ on the director field in the present study.

4. Results and Discussions

Figure 4 shows the results of the calculation for $\lambda=5.0$ and $d=0.5H$. The molecules uniformly align upstream far from the cylinder. As a molecule approaches the cylinder, it aligns its long axis in the direction parallel to the streamline due to the converging flow. This tendency is marked in the middle between the plate and the centerline. Then it starts rotating just before the narrowest part and its axis

Fig. 4 Profiles of (a) director alignment, (b) streamlines and (c) normal stress difference. $\lambda=5.0$ and $d=0.5H$. Flow is from left to right

becomes aligned perpendicular to the streamline due to the diverging flow after passing through the narrowest part. The situation is reversed near the centerline: the direction of the molecular axis is perpendicular to the streamline in front of the cylinder and is parallel to that behind the cylinder. At the outlet the molecules align uniformly again. Since the director pattern in Fig. 4(a) agrees well with the results of Baleo et al.⁽¹⁴⁾, the present calculations seem to be correct. Figure 4(b) represents the pattern of the streamlines. The pattern of LCPs is similar to that of Newtonian fluids although the streamlines of LCPs slightly approach the cylinder compared to the streamlines of the Newtonian fluids. Figure 4(c) shows the stress distribution. An unsymmetrical pattern due to the molecular alignment is obtained in contrast with the symmetrical pattern for the Newtonian fluids.

Figure 5 shows the results of the director pattern for $\lambda=50$ and $d=0.25H$. In spite of the smallness of the cylinder, the director field is disturbed over a wide area by the presence of the cylinder. The molecules near the centerline are subject to the elongational flow just behind the cylinder and align parallel to the centerline. This behavior of the molecules is seen downstream far from the cylinder. Figures 6(a), 6(b) and 6(c) show the director patterns for $\lambda=2.0$,

Fig. 5 Profile of director alignment for the geometry with the small cylinder. $\lambda=5.0$ and $d=0.25H$. Flow is from left to right

Fig. 6 Profiles of director alignment for various values of λ . $d=0.5H$. Flow is from left to right

Fig. 7 Tumbling of director; (a) changes of director along the streamlines; and (b) changes of orientation angle. $\lambda=5.0$ and $d=0.5H$

1.5 and 1.2, respectively. The main feature of the pattern is almost the same in spite of the difference in λ . The area where the director is disturbed becomes smaller before the cylinder and wider after the cylinder with decreasing λ .

The rotation of the molecule called "tumbling" can be seen in Fig. 6. The tumbling behavior along the streamline is shown in Fig. 7. The molecule on the streamline far from the cylinder changes the direction of its axis, which becomes parallel to the streamline due to the converging flow and perpendicular to the streamline due to the diverging flow. Then, it returns to the Leslie angle ϕ_0 . Thus, the molecule on the streamline far from the cylinder does not tumble although the direction of its axis changes due to the converging and diverging flows. On the other hand, the molecule which flows near the cylinder tumbles when it returns to the Leslie angle from the direction in which its axis is parallel to the streamline which is brought about by the elongational flow behind the cylinder. Vanderheyden and Ryskin⁽¹³⁾ reported that the tumbling occurred at $\lambda < 5.0$ for the flow in a slightly dimpled channel. Their calculations are limited to the case of $\lambda=5.0$ because of the difficulty in the calculation induced by the molecular tumbling. No problem due to the tumbling occurred in the present calculation since the orientation tensor was used.

In the processing of fiber-reinforced plastics, the fibers align in the direction parallel to the streamline

Fig. 8 Changes of orientation angle behind the cylinder for various values of λ

behind the cylinder. This is a serious problem that decreases the strength of moldings. Figure 8 shows the change of orientation angle ϕ behind the cylinder at $y^*=0.05$. The orientation angle quickly returns to ϕ_0 behind the cylinder for $\lambda=5.0$. However, for other results the orientation angle does not return to ϕ_0 at the outlet of the flow domain and in particular it hardly changes for $\lambda=1.2$. It is difficult to determine an accurate value of λ for LCPs in general. Taratuta et al.⁽²¹⁾ measured the Leslie coefficients for PBG (poly (γ -benzylglutamate)) and found $\alpha_2 = -3.84 \text{ Pa}\cdot\text{s}$ and $\alpha_3 = -0.14 \text{ Pa}\cdot\text{s}$. From this result, we find λ to be 1.08. It is not clear whether the values of λ for all LCPs are near one. It is, however, expected that the area where the molecules align parallel to the streamline extends downstream behind the cylinder as λ approaches one and that this causes a serious problem in the processing. The abrupt change from a positive value to a negative value of the orientation angle, which indicates the occurrence of the tumbling, is found in the results in Fig. 8 except for $\lambda=1.2$.

5. Conclusions

In this work, we calculated the flow of LCPs between parallel plates containing a cylinder using the simplified model of the Leslie-Ericksen theory derived by applying the high-viscosity approximation. We transformed the governing equation into a tensorial form to avoid the problem in numerical calculation due to the molecular tumbling. As a result, we succeeded in solving the flow problem with molecular tumbling. The molecular alignment is largely affected by the converging and diverging flows. In the vicinity of the centerline behind the cylinder, an area where the molecule aligns in the direction of the streamline exists, which extends downstream as λ approaches one. This area gives rise to a problem in the processing of LCPs.

The constitutive equation used in the present calculation is identical to that of the TIF model and

corresponds to the Doi theory⁽¹⁰⁾ in the limit of a weak velocity gradient. Therefore, we need to use the Doi theory in the prediction of molecular orientation in the flow at high shear rates as observed in injection molding.

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