Numerical Simulation of Emergence of Textures in Flows of Liquid Crystalline Polymers using a Constitutive Model with Long-Range Elasticity

Takehiro YAMAMOTO† and Michihiro KIMURA

Department of Mechanical Engineering, Graduate School of Engineering, Osaka University, 2-1, Yamadaoka, Suita, Osaka 565-0871, Japan
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Simple shear and Poiseuille flows of liquid crystalline polymers between parallel plates were numerically simulated using the Marrucci-Greco model, which is a constitutive equation that includes long-range elasticity effects. Homogeneous, inhomogeneous decoupled, and inhomogeneous full coupled models [Kupferman et al., J Non-Newtonian Fluid Mech, 91, 255 (2000)] were considered in the present simulation. In the simulation of Poiseuille flows, the relation between the long-range elasticity and the emergence of textures caused by the distribution of orientation angle of directors was investigated. The molecular orientation on the channel plate restricts rotation of directors near the plate through the long-range elasticity, and irregular rotation motions of directors were observed in the inhomogeneous full coupled simulation. Full coupled computations of the velocity field and the director motion predicted the emergence of textures during flows. In addition, the simulation results suggested that a director rotation and the molecular interaction due to the long-range elasticity are necessary for the emergence of textures.

Key Words: Liquid crystalline polymers / Long-range elasticity / Marrucci-Greco model / Texture / Numerical simulation

1. INTRODUCTION

Liquid crystalline polymers (LCPs) are important engineering materials because of the wide range of their applications. When LCPs are utilized for industrial products, the molecular orientation inside the product is important because characteristics of products of LCPs highly depend on it. In polymer processing such as injection molding, molecules of LCPs are easily aligned by the flow and keep the alignment until solidification. The distribution of molecular orientation is mainly determined by the flow. Consequently, the flow-induced molecular orientation is an important issue in studies of LCP flows. The flow-induced molecular orientation is often investigated numerically.

In numerical studies of flows in complex geometries, many researchers have performed numerical simulations using constitutive equations based on the Doi model with a quadratic closure to analyze the molecular orientation induced by complex flow fields. This model, however, has disadvantages caused by the closure approximation, e.g. it cannot predict the tumbling motion of director in shear flows. In spite of such disadvantages, this model is often applied for numerical simulations of the flow of LCPs because of its relatively simple formulation. For example, Mori et al. have numerically simulated the steady flow between parallel plates containing a cylinder and the spinning flow of LCPs using a modified Doi model. The simulation of spinning flow predicted a concave profile of velocity in a filament, which was found in the experimental study using aqueous solutions of hydroxypropylcellulose (HPC). Feng and Leaf have numerically simulated the startup flow of LCPs in eccentric cylinder geometry using the Doi model with a quadratic closure and showed that director tumbling occurred in the rotational regions of the flow field for strong nematic strength. Feng and Leaf also computed channel flows of LCPs to examine how contractions and expansions in a channel affect molecular orientation, using the Doi model with the Bingham closure. Furthermore, they found instability of molecular orientation similar to wavy patterns in an expansion channel. The distribution of molecular orientation in a fluid derives textures in observations with transmitted light. Because of the optical anisotropy caused by the molecular orientation, light through a fluid polarized and hence the distribution of molecular orientation causes patterns in the fluid. Yamamoto et al. have performed three-dimensional simulation of LCP
flows in a rectangular contraction channel and a rectangular expansion channel using the modified Doi model. They predicted highly three-dimensional structure near the expansion and discussed the relation between the orientation field and the velocity field. In this simulation, however, the emergence of textures was not predicted.

In several experimental studies, the emergence of wavy texture has been observed in LCP flows through a channel. An example of wavy texture is shown in Fig. 1, which indicates a texture observed in a startup flow of an aqueous solution of HPC through a slit cell. The texture was visualized with light through the cell between crossed polarizers. Mori et al. investigated the emergence of wavy texture in a slit channel and revealed that the emergence of the wavy texture requires a relatively long induction time and the long-range elasticity is involved in the emergence of wavy texture. They also suggested that full simulations including the long-range elasticity and flow modification should be performed for understanding their experimental results.

In numerical studies, some attempts have been done to investigate the effects of long-range elasticity. Constitutive equations including long-range elastic interactions in the nematic potential were successfully applied to describe defect textures. Tsuji and Rey have numerically analyzed the shear flow of LC materials using a nonlinear and nonequilibrium theory including the short- and long-range order elasticity and viscous effects. They classified the orientation mode in shear flow and analyzed the selection mechanism of mode. Kupferman et al. have numerically simulated shear flows of LCPs using the Marrucci-Greco model. They investigated flow-induced structures and reported that full coupling of the structure and momentum equations is required to observe a rich dynamics of LCPs. These results motivate us to perform the full simulation using a constitutive equation with the effect of long-range elasticity. Recently, microstructures of LCPs in plane shear flow were numerically analyzed with full kinematic model considering the kinematic-hydrodynamic coupling. In addition, Sgalari et al. have numerically simulated the evolution in LCP structures using the Marrucci-Greco model and successfully captured textures in LCPs. In this study, it is pointed out that three-dimensional flow computation is necessary for predicting textures that characterize the steady state of actual LCP materials. Zhou and Forest have investigated pressure-driven steady Poiseuille flows of nematic LCPs between parallel plates using the Marrucci-Greco model with both asymptotic analyses and numerical simulations. In their study, the flow was assumed to be fully developed in both the primary flow and the primary vorticity directions, and gapwise profiles of velocity and director orientation were considered. The boundary condition of orientation of director on the channel walls was varied to investigate effects of boundary anchoring. The analysis shows that the anchoring condition affects the orientation field and predicts that molecular elasticity is amplified in local boundary layers having length scales on the order of the inverse of square root of the Ericksen number.

In the present study, we numerically simulate flows of LCPs through a slit channel using the Marrucci-Greco model, which includes the effect of the long-range elasticity. We especially focus on the molecular orientation field and the emergence of textures. In the simulation, following a modeling method employed by Kupferman et al., we consider three kinds of model, i.e. homogeneous, inhomogeneous decoupled, and inhomogeneous full coupled models, to investigate effects of long-range elasticity on the molecular behavior.

2. NUMERICAL SCHEME

2.1 Basic Equations

In the present simulation, variables are scaled: The representative length and the representative velocity are expressed by $H$ and $V$, respectively. Time is scaled by $H/V$. The stress and the pressure are scaled by $ck_BT$, where $c$ is the number density of molecules, $k_B$ is the Boltzmann constant, and $T$ is the absolute temperature.

Basic equations of flow analysis of LCPs include the equation of continuity (1), the equation of motion (2), and a constitutive equation for LCPs, which is indicated later:

\[ \nabla \cdot \mathbf{v} = 0, \]

\[ Re \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\nabla p + \nabla \cdot \sigma, \]

where $Re$ is the Reynolds number defined by
\( Re = \frac{\rho V^2}{ck_s T}, \)  \hspace{1cm} (3)

which represents the ratio of the inertial force to the viscous force. \( v \) is the velocity vector, \( t \) is time, and \( p \) is the pressure. The stress tensor \( \sigma \) is described as a function of the orientation order parameter tensor \( S \), which is a second-order tensor defined by

\[
S = \int \psi(u, R, t) \left( uu - \frac{1}{d} \delta \right) d\Omega. \tag{4}
\]

Here \( \psi \) is an orientation distribution function, which is a function of a unit vector \( u \) parallel to a molecular orientation, the position vector \( R \), and \( t \). \( \delta \) is the unit tensor. \( d \) is the number of space dimension, i.e. \( d = 2 \) for a two-dimensional problem and \( d = 3 \) for a three-dimensional problem. The integral with respect to \( \Omega \) means the integral over all \( u \)-space.

The molecular orientation is often expressed by a director \( n \) and a scalar order parameter \( S \). The director is a unit vector whose direction coincides with the average molecular orientation. The degree of orientation is evaluated using the scalar order parameter \( S \) defined by

\[
S = \frac{3}{\sqrt{2}} S \cdot S, \tag{5}
\]

which takes a value between zero and unity, and \( S = 0 \) means a random state and \( S = 1 \) indicates that all molecules are oriented in the direction of \( n \).

We employed the Marrucci-Greco model\(^\text{17})\) as a constitutive equation of LCPs. In this model, the evolution equation of \( S \) is described by the following equations:

\[
\left( \frac{\partial}{\partial t} + v \cdot \nabla \right) S = F(S) + G(S), \tag{6}
\]

\[
F(S) = F^h(S) + F^{ih}(S), \tag{7}
\]

\[
F^h(S) = -\frac{1}{De} \left[ 2(1 - \delta) \right] S \cdot S + \frac{2}{3} U S : S + 6 U (S : S) \left( S + \frac{1}{d} \delta \right), \tag{8}
\]

\[
F^{ih}(S) = \frac{1}{Er} \left[ (\nabla^2 S) \cdot S + S \cdot (\nabla^2 S) \right] + \frac{2}{3} \nabla^2 S - 2(\nabla^2 S) : S \left( S + \frac{1}{d} \delta \right), \tag{9}
\]

\[
G(S) = \frac{1}{2} (\kappa + \kappa^T) + S \cdot \kappa^T + \kappa \cdot S - 2(\kappa : S) \left( S + \frac{1}{d} \delta \right), \tag{10}
\]

\[
\kappa = \omega + \lambda D. \tag{11}
\]

In Eq. (10), \( \kappa^T \) indicates the transpose of tensor \( \kappa \). The Deborah number \( De \) and the Ericksen number \( Er \) are defined by

\[
De = \frac{V}{D_k H}, \tag{12}
\]

and

\[
Er = \frac{8VH}{UD_k R^2} = \frac{8}{U} \left( \frac{H}{R} \right)^2 De, \tag{13}
\]

where \( D_k \) is an averaged rotational diffusion coefficient\(^{20})\), the parameter \( U \) is the nematic strength, and \( R \) is a characteristic interaction distance between molecules. The Deborah number indicates the ratio of the molecular time scale to the characteristic time of flow. The Ericksen number indicates the ratio of the strength of the short range nematic potential to that of the long range Marrucci-Greco elastic potential.\(^{17})\) The term of \( F \) in Eq. (6) represents the inter-molecular kinetics and consists of a homogeneous part \( F^h \) and an inhomogeneous one \( F^{ih} \) as shown in Eqs. (8) and (9). The term of \( G(S) \) represents the molecular advection as shown in Eq. (10). \( \omega \) and \( D \) are the vorticity tensor and the rate of deformation tensor, respectively. \( \lambda \) is a parameter which relates the molecular aspect ratio \( r \) as \( \lambda = (r^2 - 1)/(r^2 + 1) \). When a parameter \( \lambda \) is set to unity and \( F^{ih} \) is neglected, this model reduces to the Doi model with the quadratic closure approximation.\(^{25})\)

In addition, the stress tensor \( \sigma \) is described as a function of \( S \) by

\[
\sigma = -\frac{1}{2} De F(S) + \frac{1}{2} \frac{De}{Er} \left[ (\nabla^2 S) \cdot S + S \cdot (\nabla^2 S) \right] + 2\nu_s D, \tag{14}
\]

where \( \nu_s \) defined by

\[
\nu_s = \frac{\eta_s (V/H)}{ck_s T}, \tag{15}
\]

means the ratio of the solvent viscosity \( \eta_s \) to the characteristic polymer viscosity \( ck_s T(V/H) \).

### 2.2 Numerical Method

In the present study, we basically applied a numerical method used in the previous study.\(^9\) The basic equations are discretized with a finite difference method and are numerically solved. In the present simulation, the flow field is assumed to be two-dimensional, while the orientation field is three-dimensional. We considered both shear and Poiseuille flows between parallel plates.

We apply the MAC method to decouple pressure and velocity.
calculations for the equation of motion (2). The pressure field is obtained by solving a Poisson equation for \( p \) derived by taking the gradient of Eq. (2), and the velocity field is determined from Eq. (2). A staggered grid is used and variables are defined at points in a control volume as shown in Fig. 2. The pressure and the orientational order parameter tensor \( S \) are defined at the center of the control volume and the \( x \)- and \( z \)-components of \( v \), \( v_x \) and \( v_z \), are defined at the center of faces.

The basic equations are discretized by the central difference method in space except for the convective term in Eq. (6), which is discretized with the third-order upwind difference. The Poisson equation for \( p \) is solved with the SOR method. Both the equation of motion and the evolution equation of \( S \) are integrated with respect to time using the Euler explicit scheme.

In addition, because \( S \) is a symmetric traceless tensor, the relations that \( S^{n+1}_{ij} = -(S^{n+1}_{ji}+S^{n+1}_{ij}) \), i.e. \( \text{tr} S = 0 \), and that \( S^0 = S^x \) are applied for the computation of \( S \). Consequently, the independent components of \( S \) are \( S_{xx}, S_{yy}, S_{zz}, S_{xy}, S_{xz}, \) and \( S_{yz} \).

### 2.3 Model Classification

We considered three types of computational models, which were employed in the numerical simulation of shear flows by Kupferman et al.\(^{20}\) The first model is a homogeneous model, in which the inhomogeneous term \( F^\phi \) is neglected. Consequently, this model does not describe the effect of the long-range elasticity. In addition, the velocity field is fixed and the motion of director at each point is determined independently by the shear rate at a point considered. The second model is an inhomogeneous decoupled model. In this model, all the terms of \( F^\phi, F^\theta, \) and \( G \) are considered and hence the effect of long-range elasticity is included. However, the computation of velocity field is decoupled with the orientation field. That is, the velocity field is fixed and only the evolution of \( S \) is computed. Finally, an inhomogeneous full coupled model is considered. In this model, the effect of long-range elasticity is included and the velocity field is computed coupling with the orientation field.

### 3. RESULTS AND DISCUSSION

#### 3.1 Shear Flow

We consider two types of flow between parallel plates: shear flows and Poiseuille flows. Shear flows of LCPs have been well analyzed.\(^{17-20}\) However, we first computed the shear flow to confirm the accuracy of the present scheme and to obtain data useful for the analysis of the flow behavior in the Poiseuille flow. The shear flow considered is schematically depicted in Fig. 3. The plates place at \( z = \pm 1/2 \) and move in the counter direction to each other at the representative velocity \( V \).

The flow direction is \( x \) and the direction of velocity gradient is \( z \). Furthermore, the motion of directors is represented in terms of the orientation angle of director \( \theta \) defined in Fig. 3. Although three-dimensional orientation fields are computed, we focus the motion of orientation angle in the \( x-z \) plane.

The fluid is at rest at the initial condition. Moreover, as for the boundary conditions, the non-slip condition is given on the walls, and the directors on the plates are set to be aligned in the flow direction with the scalar order at equilibrium. The flow is assumed to be fully developed in the \( x \)-direction.

In the present study, the homogeneous and the inhomogeneous decoupled models are considered; the inhomogeneous full coupled model is not simulated. The results of the full coupled model in shear flows are available in a literature\(^{20}\), where a rich set of dynamics is reported.

The value of \( \lambda \) is fixed to 0.8 for each simulation. Fig. 4 shows the results for the homogeneous model at three Deborah numbers. The value of \( U \) is fixed to 6. This figure indicates the motion of director in terms of the orientation angle \( \theta \). Under the condition considered in the simulation by Kupferman et al. (\( \lambda = 0.8, U = 6, \) and \( De = 10 \)), we obtained the same results of director motion predicted in their simulation.

In each case in Fig. 4, the directors show transient behavior in the early stage of flow and reach a steady motion. The director motion shows tumbling at \( De = 0.1 \), wagging at...
$De = 7$, and flow aligning at $De = 10$. In general, this model predicts the change in director motion from tumbling to aligning with increasing the Deborah number. When $\lambda = 1$, this model corresponds to the Doi model with the quadratic closure approximation. The period of rotation becomes long as $\lambda$ increases and the model with $\lambda = 1$ does not predict the tumbling motion. In the homogeneous model, because the motion of a director depends on the shear rate only and the shear rate is constant in the channel, each director behaves in the same manner with keeping the phase difference at the initial condition.

Figure 5 shows the motion of director for the inhomogeneous decoupled model in the same way in Fig. 4. In these computations, $\lambda = 0.8$, $U = 6$, and $Er = 1000$. In general, the motion of director changes from tumbling through wagging to aligning with increasing the Deborah number. However, the long-range elasticity originates in $F^{ik}$ affects the director motion and generates differences from the results of the homogeneous model. In Fig. 5b, the director shows a wagging motion at $z = -0.4875$ and $-0.2875$, where directors show a tumbling motion under the corresponding homogeneous condition. Because the orientation of director is fixed to the flow direction on the plates, the motion of director is restricted near the plates by the effect of the long range elasticity. Consequently, at these points, the director can not rotate in the same manner as directors far from the wall where the effect of fixed orientation on the plates is weak. This tendency agrees

![Fig. 4. Time evolution of orientation angle $\theta$ of directors in simple shear flows for homogeneous decoupled model at $\lambda = 0.8$, $U = 6$, and $De = 0.1$ (a), $7$ (b), and $10$ (c).](image)

![Fig. 5. Time evolution of orientation angle $\theta$ of directors in simple shear flows for inhomogeneous decoupled model at $\lambda = 0.8$, $U = 6$, $Er = 1000$, and $De = 0.1$ (a), $5$ (b), and $10$ (c).](image)
with results of simulation by Kapferman et al.\(^{20}\) that molecular orientation is governed by the homogeneous dynamics with a boundary layer connecting it to the anchoring at the walls.

In addition, in Fig. 5a, the initial phase difference decreases with time because molecules interact each other through the long-range elasticity and hence motion of one director affects other directors' motion. As a result, the motions of each director are synchronized and hence the phase difference decreases.

3.2 Poiseuille Flow between Parallel Plates

We next consider Poiseuille flows between parallel plates shown in Fig. 6. In this problem, the representative length \(H\) and velocity \(V\) are the channel width and the mean velocity, respectively. The flow direction is \(x\) and the channel walls place at \(z = \pm 1/2\). In Poiseuille flows, the velocity gradient varies with \(z\) and its magnitude is larger nearer the wall. The computations were carried out using the symmetrical condition and the computational domain is the half channel of \(z < 0\). We chose the size of computational domain as 5 in length and 1/2 in height after preliminary computations. We give initial conditions that the velocity is zero and the directors are aligned in the \(x\)-direction. The fluid begins to flow at \(t = 0\). As for the boundary condition on the parallel plates, the non-slip condition is applied and the directors are parallel to the plates. The value of \(S\) at equilibrium is given on the plates.

In the computations of both homogeneous model and inhomogeneous decoupled model, the velocity field is fixed to the Newtonian velocity profile whose mean velocity is \(V\) because preliminary computations confirmed that the velocity profile for the Marrucci-Greco model is not largely different from the counterpart of Newtonian fluids under the present computational conditions. On the other hand, in the simulation of inhomogeneous full coupled model, computations of the velocity field and the orientation field are coupled. Consequently the boundary condition of velocity is necessary for the simulation of the full coupled model. We considered the following boundary conditions at both the entrance and the exit of the channel: The velocity profile is fixed to the fully developed Newtonian Poiseuille velocity profile at the entrance and the natural boundary condition, i.e. the velocity field does not change in the flow direction, is given at the exit.

For both homogeneous and inhomogeneous decoupled models, we indicate the results at \(x = 1.75\). Fig. 7 shows the results for the homogeneous model at \(\lambda = 0.8, \text{De} = 5\), and \(U = 6\) and 10. This figure shows the orientation behavior of directors in terms of \(\theta\). The out-of-plane orientation, i.e. the orientation angle in the \(y\)-direction, is enough small to neglect in the analysis of orientation behavior. Also for simulations of the inhomogeneous decoupled and the full models, the orientation in the \(y\)-direction is much small.

For \(U = 6\), the director shows tumbling near the channel center and wagging near the wall. These results coincide with the results of the shear rate dependence of director motion in the simple shear flow because the long-range elasticity is not included in this model and hence the director motion is governed by local shear rates. For \(U = 10\) in Fig. 7b, the effect of shear rate is weak and the tumbling motion appears at each \(z\) position.

Next, we consider the flow of inhomogeneous decoupled model for \(U = 10\), which is suitable for investigating the effects of the long-range order because the dependence of director motion on the shear rate is weak in the flow of \(U = 10\)
as compared to that of $U=6$ and no wagging motion is seen even near the plate as shown in Fig. 7b.

We performed simulations at three Deborah numbers to investigate the effect of long-range order on the molecular orientation. Fig. 8 shows the motion of directors in terms of $\theta$ for the inhomogeneous decoupled model at $\lambda = 0.8$, $U = 10$, $Er = 1000$, and $De = 0.1$, 1, and 20.

Directors show complex flow behaviors as compared to the results for the homogeneous model. At $De = 0.1$ in Fig. 8a, the long-range elastic effect is relatively weak. However, a wagging motion is seen near the center, at $z = -0.0375$, where directors show tumbling for the inhomogeneous decoupled model. The following is a possible mechanism of this phenomenon: Near the center, the shear rate is small. Thus directors tend to rotate slowly and the driving force of rotation is not strong. Consequently, the director has a tendency to be restricted by neighboring directors’ motion in process of a rotation and can not continue to rotate against the restriction. At other positions of $z$ in this figure, tumbling motions are observed. However, the motion is irregular and the rotational speed changes during the rotation. This phenomenon appears remarkably at larger $De$ in Figs. 8b and 8c. Basically the period of director rotation in a shear flow depends on the shear rate and is long at low shear rates. When effects of long-range elasticity exist, a rotation of director is affected by neighboring directors’ motion. Thus, the rotational speed changes during the rotation and an irregular tumbling motion is induced.

At higher Deborah numbers, $De = 1$ (Fig. 8b) and $De = 20$ (Fig. 8c), wagging motions appear at positions of $z = -0.4875$, where directors are tumbling at $De = 0.1$. Near the plate, the shear rate is relatively large and the driving force of rotation is also relatively strong. As a result, the tumbling occurs if the director can rotate against the restriction by neighboring director’s motion. However, when the long-range order exceeds, the motion of directors is restricted near the plate and hence the directors can not rotate and show wagging motion around $0^\circ$.

Figure 9 shows the change in the scalar order parameter $S$ with time for $U=10$, $De=1$, and $Er=1000$. The order parameter keeps relatively large values except when a director rotates. In general, $S$ rapidly decreases when the director changes its orientation largely and the value of $S$ quickly falls when a director rotates. The value of $S$ at local minimum fluctuates with time, which means the dynamics of director is very complex.

Next, we analyze the flow behavior of the inhomogeneous full model. $Re$ and $\nu_s$ are set to unity for this computation. In the results of this model, it can be observed that director motions similar to those of inhomogeneous decoupled model. Hence we do not repeat the analysis of director motion discussed for the decoupled model. Here, we focus on the emergence of textures during a flow and analyze its relation with the orientation field. In the simulation of Poiseuille flows by Zhou and Forest, the change in velocity and orientation fields was not considered and hence the streamwise evolution in textures was not investigated.

Figure 10 shows the time evolution of the distribution of orientation angle $\theta$ at $\lambda = 0.9$, $U = 10$, $De = 0.1$, and $Er = 600$ for the full model. The results in the lower half region of the channel ($z \leq 0$) is indicated in the figure. Time $t$ means the elapsed time from the startup of flow. In this computation, the orientation of directors at the entrance is fixed to be parallel to the flow. Furthermore, the directors are initially aligned to the flow direction everywhere in the channel (Fig. 10a). After the
startup of flow, the directors change their direction largely near
the entrance as shown in Fig.10b and the molecular distribution
parallel to the plate appears all over the channel. This
distribution is due to the difference in shear rate. After that,
another type of disturbance occurs as shown in Fig.10c, and it
spreads with time. The spread of distribution pattern is not
only due to the advection but also due to the long-range order
because the moving speed of texture is much faster than the
mean velocity.

Computations at other Ericksen numbers are carried out to
investigate the effects of $Er$ on the emergence of textures.
Fig. 11 shows the distribution of orientation angle at $\lambda = 0.9$,
$U = 10$, $De = 0.1$, and $Er = 90$ and 120. Textures are observed
in both cases and the interval of texture tends to widen at
smaller $Er$. In addition, computations at smaller $Er$, which is
not shown in the present paper, predicts that no texture
emerges at $Er$ smaller than a critical value. These results imply
that long-range elasticity affects the emergence of textures and
their patterns. However, in the present simulations, we can not
clearly find $Er$ scaling property in the interval of textures.

These textures are not observed in the simulation of the
decoupled model. Thus, it can be considered that coupling of
the orientation field with the velocity field is a key of this
phenomenon. In the velocity field, small disturbance occurs as
shown in Fig. 12, which shows the distribution of velocity in
the $x$-direction, $v_x$, in a Poiseuille flow for the full model at
$\lambda = 0.9$, $U = 10$, $De = 0.1$, and $Er = 600$. We can see small
distribution in the velocity field, which is not seen in the
decoupled model because the velocity field is fixed. We think
that such a disturbance in the velocity field accelerates the

![Figure 9. Time evolution of scalar order parameter $S$ in Poiseuille flows for the inhomogeneous decoupled model at $\lambda = 0.8$, $U = 10$, $Er = 1000$, and $De = 1$.](image)

![Figure 10. Time evolution of distribution of orientation angle $\theta$ of directors in a Poiseuille flow for full model at $\lambda = 0.9$, $U = 10$, $De = 0.1$, and $Er = 600$: $t = 0$ (a), 50 (b), 80 (c), 150 (d), 300 (e), 450 (f), and 750 (g). The upper side and the lower side in each figure indicate the channel center and the lower plate, respectively.](image)

![Figure 11. Distributions of orientation angle $\theta$ of directors in a Poiseuille flow for full model at $\lambda = 0.9$, $U = 10$, $De = 0.1$, and $Er = 90$ (a) and 120 (b). The upper side and the lower side in each figure indicate the channel center and the lower plate, respectively.](image)

![Figure 12. Distribution of velocity in the $x$ direction, $v_x$, in a Poiseuille flow for the full model at $\lambda = 0.9$, $U = 10$, $De = 0.1$, and $Er = 600$. Lines indicate contours of $v_x$. The dashed line indicates the center line of channel.](image)
disturbance in the molecular orientation and contributes to the promotion of emergence of textures.

Furthermore, we investigated the effect of $\lambda$ on the orientation field. Fig. 13 shows the effect of $\lambda$ on the director motion. The computations were carried out under the same condition as the computation in Fig. 10 except for the value of $\lambda$. It is known that in simple shear flows directors rotate at longer period for larger $\lambda$ and do not show the tumbling at $\lambda = 1.26$. In other words, directors are more difficult to rotate at larger $\lambda$. Consequently, the interval of textures is shorter at $\lambda = 0.8$ (Fig. 13a) than $\lambda = 0.9$ (Fig. 10g). Furthermore, at $\lambda = 0.95$ (Fig. 13b), directors do not rotate and no texture is observed in this case. These results suggest that it requires director rotation, molecular interactions due to the long-range order, and a certain degree of disturbance in the velocity field for the emergence of textures.

4. CONCLUSION

We numerically simulated the orientation behavior of LCPs in Poiseuille flows. In the simulations, the Marrucci-Greco model was employed as a constitutive equation to investigate the effect of the long-range order on the orientation field. The results of simulation for inhomogeneous decoupled model indicate that the director motion is highly affected by neighboring directors’ motion through the long-range elasticity. In the coupled simulation, textures emerged and their intervals depended on the Ericksen number. Furthermore, the coupled simulation predicted that the director rotation and the molecular interaction due to the long-range elasticity are necessary for the emergence of textures and that a small disturbance in velocity field is a possible accelerator of the texture emergence.

Although it is difficult to directly compare the results of the present simulation with experimental results such as shown in Fig. 1 because the picture in the figure shows a texture that includes effects of molecular orientation across the cell thickness, the present results give information for analyzing the emergence of textures in LCPs. In future studies, three-dimensional analysis is necessary for elucidating the mechanism of emergence of textures during flow.

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