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Steady Dynamics in Shearing Flows of Nematic Liquid Crystalline Polymers

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COLLEGE OF ARTS AND SCIENCES

**STEADY DYNAMICS IN SHEARING FLOWS OF
NEMATIC LIQUID CRYSTALLINE POLYMERS**

By
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ABSTRACT

The biaxiality of the steady state solutions and their stability to in-plane disturbances in shearing flows of nematic liquid crystalline polymers are studied by using simplified Wang (2002) model. We obtain all the steady states of Wang model exhibit biaxial symmetry in which two directors are confined to the shearing plane and analysis their stability with respect to in-plane disturbances at isolated Debra numbers and polymer concentration values.

CHAPTER 1

INTRODUCTION

Liquid crystals are materials exhibiting intermediate properties between crystalline solids and amorphous liquids. There are three main classes of liquid crystals: nematics (see Figure. 1), cholesterics and smectics (see Figure. 2). Nematics possess orientational but no positional order, i.e. on average they line up locally but their positions are still random. Both cholesterics and smectics show some position order. Here we only consider the nematic liquid crystals.

Although they were discovered more than one hundred years ago, the scientific principles that govern their transport and optical properties were established only recently (De Gennes, 1993). Since 1960s, the knowledge of liquid crystals has become very profitable: liquid crystals are now used in almost all lap-top computers, HD TVs and in many other applications such as high performance fibers, light valves and temperature sensors, etc. The microscopic structure order present in the liquid crystalline system is responsible for these properties. The distinguishing features of the mechanical behavior of liquid crystalline materials are their anisotropic, non-linear, viscoelastic behavior, quite distinct from Newtonian viscous fluids whose flow behavior is accurately described by the Navier-Stokes equation. These differences arise because liquid crystals display various degrees of orientational order and exhibit both long and short range elasticity effects.

Much of the fascination of flow phenomena in liquid crystals stems from the intimate coupling between fluid motion and the orientation of the anisotropic axis of these transversely isotropic liquids.

The earliest constitutive models were phenomenological. In the last several decades, the close relation between the internal microstructure and rheological properties has been recognized, and the more recent constitutive equations are based on micromechanical descriptions of macromolecular systems. This approach is referred to as *kinetic theory*, which is to develop descriptive equation at both macroscopic and mesoscale levels. Most of the hydrodynamic theories

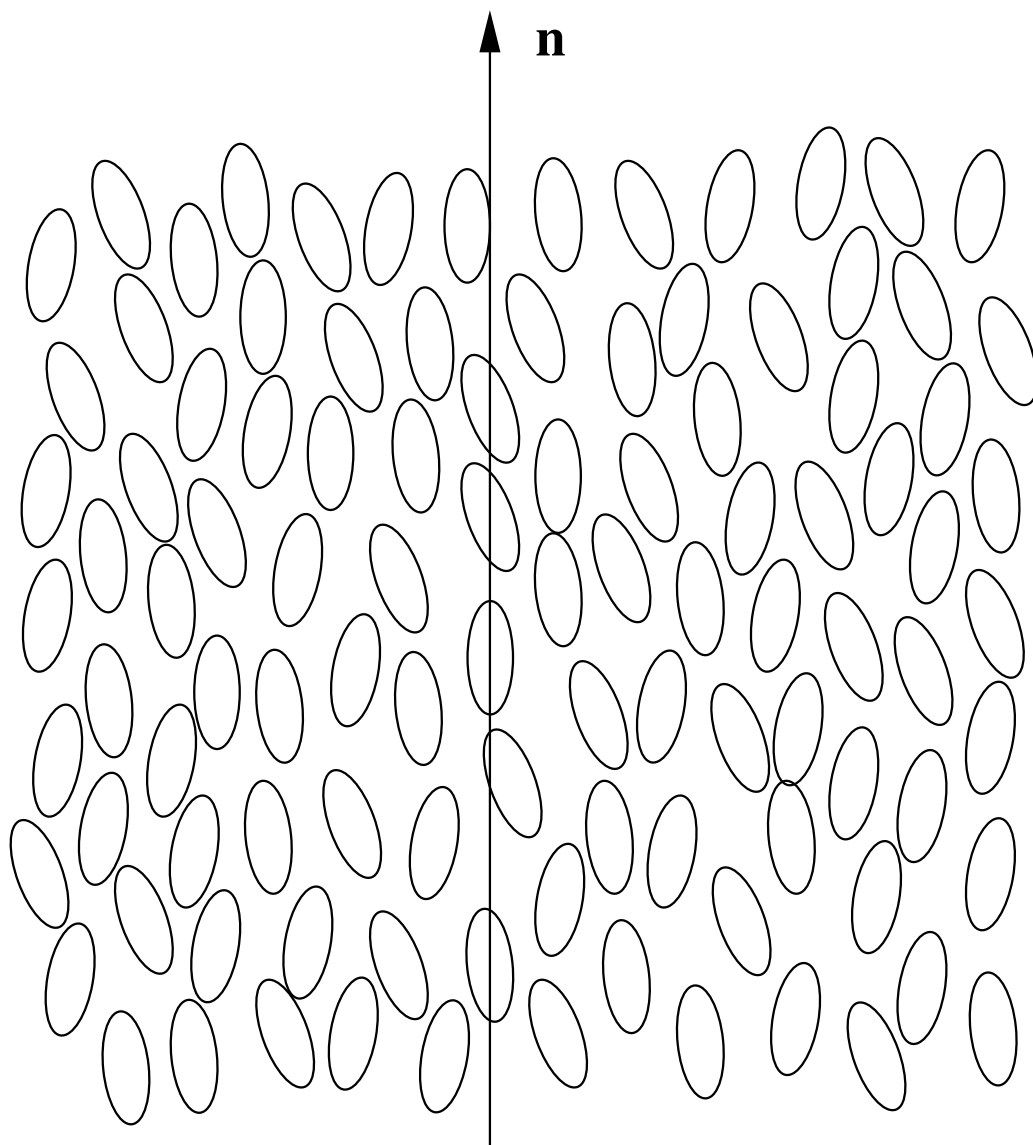


Figure 1: Molecules of Nematic Liquid Crystals.

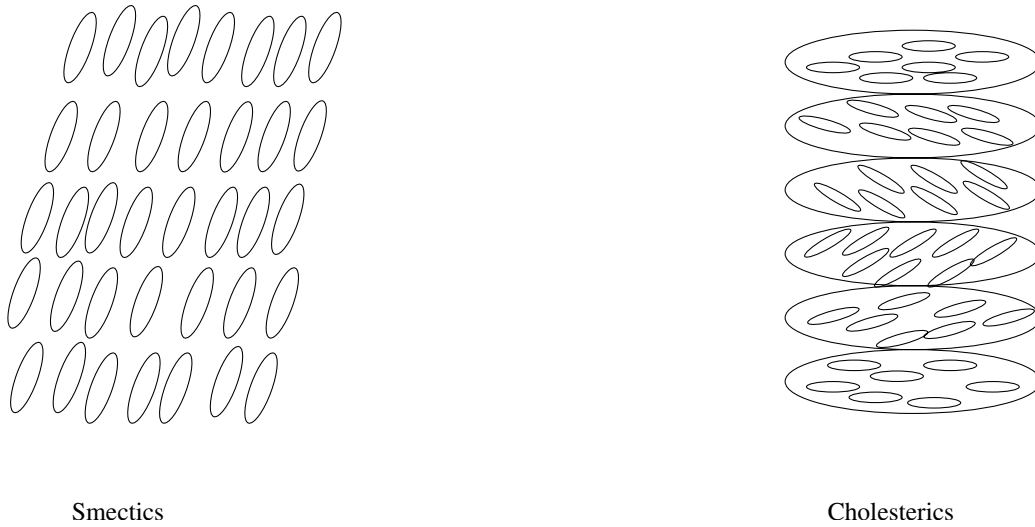


Figure 2: Molecules of Cholesteric and Smectic Liquid Crystals.

formulated for liquid crystals are based on two classical theories: the Leslie-Ericksen(LE)(1979) theory and the Doi theory(1986). The LE theory is a nonhomogeneous continuum theory that applies to low-molecular-weight nematics. It accounts for the effects of director distortion, but does not account for the molecular elasticity displayed by polymeric nematics nonlinear rheology. The original Doi theory (Doi, 1981) is a homogeneous molecular theory that is capable of predicting the isotropic-nematic(I-N) phase transition. The nonhomogeneous Doi theories were developed by several researchers (Marrucci and Greco, 1991; Wang, 2002). In the theory of Wang (Wang, 2002), molecular geometry is accounted for by its aspect ratio, which allows additional degree of freedom in the modeling of the liquid crystal polymer.

1.1 The LE Continuum Theory

The earliest constitutive equations were developed by Ericksen (1960 & 1961) and Leslie (1966 & 1968). The LE theory extends Frank's continuum theory of

elasticity (Frank, 1958) developed for liquid crystals at rest to model flow behavior and directly incorporates Frank's distortional free energy. It is a vector theory that uses the average of the molecular orientation, called the director (\mathbf{n} , $\mathbf{n} \cdot \mathbf{n} = 1$), to describe the intrinsic microstructure of liquid crystal materials. It was remarkably successful in describing the optical behavior of low molecular-weight LCs (Leslie, 1979; Rey and Denn, 1988) under imposed external field and linear viscoelastic regime, especially at low deformation rates. However, the theory still suffered from some drawbacks: The assumption of linear dependence of the viscous stress on shear rate in the development of the LE theory restricts it to low deformation rates, thus the model can not describe nonlinear rheological properties, such as shear-thinning of the viscosity and normal stresses which are observed in liquid crystalline polymers (LCPs) (Wissbrun, 1981). Moreover, one can not describe a biaxial LC (i.e., a LC with two characteristic directions of orientation) in terms of a single unit vector. These drawbacks made it impossible to predict some aspects of the complex behavior of liquid crystalline polymers (LCPs) such as phase transition and defect generation/annihilation. Although many improvements on the LE theory are reported when using the second order tensor theories (de Gennes, 1993), the proliferation of unknown phenomenological parameters limits the use of this type of formulation. The extensive work done using the LE theory to interpret experimental data has led to some effort in determining the different constants from molecular theories (Marrucci, 1982; Kuzuu and Doi, 1983 & 1984).

1.2 The Doi Molecular Theory

Doi (1981) made the first attempt at developing a molecular theory for liquid crystalline polymers. Doi theory overcomes a number of drawbacks present in the LE theory; primarily it accounts for the isotropic-nematic phase transition. It is also able to predict some nonlinear rheological properties exhibited by LCPs.

Doi's model is based on Onsager's expression for the free energy of a solution containing rod-like polymeric molecules (Onsager, 1949). Using Onsager's

expression for the free energy, Doi obtained a self-consistent mean field potential that accounted for the excluded volume interactions of a single test rod with the surrounding rigid rods. He simplified this expression for the potential to a form that is similar to the polymer-polymer interaction potential (Maier and Saupe, 1958 & 1959) which is later referred to as Maier-Saupe potential. Next, starting from the kinetic theory of Kirkwood and Auer (1951), Doi developed an expression for the orientational distribution function for the concentrated rigid rod solution, which included the Maier-Saupe potential.

Doi's model takes into account the effects of flow, Brownian motion, and intermolecular forces on the molecular orientation distribution. It employs the orientation distribution function which describes the probability density of molecular orientation, to capture the microscopic behavior. Subsequent to its establishment, the Doi theory was successfully applied for LCPs flows, and it could describe rudimentary phase-transition behavior. The probability density function can be expanded in terms of its moments, and the basis corresponding to the second moments is exactly the second order tensor mentioned above, and thus the Doi theory includes all the above description. As compared to the LE theory, it was applicable in a broader flow regime where the degree of orientation of the LC system can vary.

The original Doi theory is for spatially homogeneous flows of rodlike liquid crystal polymers. Doi, Shimada and Okano (1988) extended it to model flows of nonhomogeneous LCPs by introducing a long-range intermolecular potential. Marrucci and Greco (1991) further improved the extended Doi theory by incorporating the molecular anisotropy and the range of interaction into the theory. Wang (2002) extended the theories to model flows of spheroidal LCP molecules, in which the intermolecular potential developed ensures the second law of thermodynamics and showed the kinetic theory limits to the LE theory in the limit of weak flow as well as weak distortional elasticity.

CHAPTER 2

MODEL FORMULATION

We use the theory developed by Wang (2002) and assume all LCP molecules are of the same spheroidal configuration. Let $f(\mathbf{x}, \mathbf{m}, t)$ be the probability distribution function for the molecule in the configuration (\mathbf{x}, \mathbf{m}) at time t . In order to establish the kinetic equation, we need the intermolecular potential V_i which includes the following two parts:

1. Maier-Saupe potential: $-\frac{3NkT}{2}\mathbf{M} : \mathbf{mm}$;
2. Isotropic as well as anisotropic long range molecular interaction part:

$$\left(\frac{\mathcal{L}^2}{24}\Delta + \frac{L^2}{48}\mathbf{mm} : \nabla\nabla\right)\mathbf{M} : \mathbf{mm} + \frac{L^2}{48}\mathbf{mm}\nabla\nabla :: \mathbf{M}_4;$$

where \mathbf{mm} is the tensor product of \mathbf{m} with \mathbf{m} , \mathbf{M} is the second moment of \mathbf{m} with respect to the PDF f , $\mathbf{M} = \langle \mathbf{mm} \rangle$, “:” and “::” denote the contraction operation between the tensors over two and four pairs of indices, k is the Boltzmann constant, T is the absolute temperature, N is the dimensionless polymer number density.

The orientational properties of liquid crystals can be characterized by a second order, symmetric and traceless orientation tensor

$$\mathbf{Q} = \langle \mathbf{mm} \rangle - \mathbf{I}/3, \quad (1)$$

$$\text{where} \quad \langle (\cdot) \rangle = \int_{|\mathbf{m}|=1} (\cdot) f(\mathbf{m}, t, \mathbf{x}) d\mathbf{m}, \quad (2)$$

The probability density function $f(\mathbf{m}, t, \mathbf{x})$ corresponds to the probability that an arbitrary rodlike liquid crystal polymer molecule is in direction \mathbf{m} at location \mathbf{x} and time t .

Following the development of the Smoluchowski equation for polymer solution (Doi and Edwards, 1986), we obtain *kinetic(Smoluchowski) equation*:

$$\frac{Df}{Dt} = \mathcal{R} \cdot [D_r(\mathbf{m}, a)(\mathcal{R}f + \frac{1}{kT}f\mathcal{R}V_i)] - \mathcal{R} \cdot [\dot{\mathbf{m}}f], \quad (3)$$

where $D_r(\mathbf{m}, a)$ is the rotary diffusivity, inversely proportional to the relaxation time due to molecular rotation, $\mathcal{R} = \mathbf{m} \times \frac{\partial}{\partial \mathbf{m}}$ is the rotational gradient operator, and $\frac{D}{Dt}(\bullet)$ denotes the material derivative $\frac{\partial}{\partial t}(\bullet) + \mathbf{v} \cdot \nabla(\bullet)$, a is a shape parameter: $a = 1$: rod; $a = 0$: sphere; $a = -1$: disk.

Like in most kinetic theories, the macroscopic, or average, internal orientation properties of nematic liquid crystals are defined in terms of the moments of \mathbf{m} with respect to the probability density function f (Doi, 1986).

Taking the second moment of \mathbf{m} with respect to the PDF f , we obtain *the orientation tensor equation*

$$\left\{ \begin{array}{l} \frac{d}{dt} \mathbf{M} - \Omega \cdot \mathbf{M} + \mathbf{M} \cdot \Omega - a[\mathbf{D} \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{D}] = -2a\mathbf{D} : \mathbf{M}_4 - \\ 6D_r^0[\mathbf{M} - \frac{\mathbf{I}}{3} - \frac{1}{6kT}(\langle \mathbf{m} \times \mathcal{R}V_i \mathbf{m} \rangle + \langle \mathbf{m} \mathbf{m} \times \mathcal{R}V_i \rangle)] = \\ -2a\mathbf{D} : \mathbf{M}_4 - 6D_r^0[\mathbf{M} - \frac{\mathbf{I}}{3} - \frac{N}{2}((\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \cdot \mathbf{M} + \mathbf{M} \cdot (\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M}) + \\ N(\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} : \mathbf{M}_4 - \frac{NL^2}{96}((\nabla \nabla \mathbf{M}) : \mathbf{M}_4 + ((\nabla \nabla \mathbf{M}) : \mathbf{M}_4)^T + \\ \mathbf{M}_4 : \nabla \nabla \mathbf{M} + (\mathbf{M}_4 : \nabla \nabla \mathbf{M})^T + \mathbf{M} \nabla \nabla : \mathbf{M}_4 + \\ (\mathbf{M} \nabla \nabla : \mathbf{M}_4)^T - 4\mathbf{M}_6 :: \nabla \nabla \mathbf{M} - 2\mathbf{M}_4 \nabla \nabla :: \mathbf{M}_4]. \end{array} \right. \quad (4)$$

where D_r^0 is an averaged rotary diffusivity resulted from the averaging process (Doi and Edwards, 1986) which is assumed a shape dependent constant in this study. V_i is the intermolecular potential. And we have $\Omega = \frac{1}{2}(\nabla \mathbf{v} - \nabla \mathbf{v}^T)$, $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$.

The total extra stress

$$\begin{aligned}
\tau = & 2\eta_s \mathbf{D} + 3akT[\mathbf{M} - \frac{\mathbf{I}}{3} - \frac{N}{2}((\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \cdot \mathbf{M} + \mathbf{M} \cdot (\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \\
& - 2(\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} : \mathbf{M}_4)] - \frac{kTN\mathcal{L}^2}{16}(\Delta\mathbf{M} \cdot \mathbf{M} - \mathbf{M} \cdot \Delta\mathbf{M}) \\
& - \frac{NkT\mathcal{L}^2}{32}[\nabla\mathbf{M} : \nabla\mathbf{M} - (\nabla\nabla\mathbf{M}) : \mathbf{M}] + \\
& \frac{akTN\mathcal{L}^2}{32}[4\mathbf{M}_6 :: \nabla\nabla\mathbf{M} + 2\mathbf{M}_4\nabla\nabla :: \mathbf{M}_4 - \nabla\nabla\mathbf{M}:\mathbf{M}_4 - (\nabla\nabla\mathbf{M}:\mathbf{M}_4)^T - \\
& \mathbf{M}_4:\nabla\nabla\mathbf{M} - (\mathbf{M}_4:\nabla\nabla\mathbf{M})^T - (\mathbf{M}\nabla\nabla:\mathbf{M}_4)^T - \mathbf{M}\nabla\nabla:\mathbf{M}_4] - \frac{kTN\mathcal{L}^2}{32}[\nabla\nabla\mathbf{M}:\mathbf{M}_4 - \\
& (\nabla\nabla\mathbf{M}:\mathbf{M}_4)^T - \mathbf{M}_4:\nabla\nabla\mathbf{M} + (\mathbf{M}_4:\nabla\nabla\mathbf{M})^T - \mathbf{M}\nabla\nabla:\mathbf{M}_4 + (\mathbf{M}\nabla\nabla:\mathbf{M}_4)^T] \\
& + 3kT[\zeta_1(a)(\mathbf{D}\mathbf{M} + \mathbf{M}\mathbf{D}) + \zeta_2(a)\mathbf{D} : \mathbf{M}_4].
\end{aligned} \tag{5}$$

Balance of linear momentum

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (-p\mathbf{I} + \tau) \tag{6}$$

where ρ is the fluid density, p is the scalar pressure. *Continuity equation*

$$\nabla \cdot \mathbf{v} = 0 \tag{7}$$

The kinetic equation, orientation tensor equation, constitutive equation for the extra stress, balance of linear momentum and the continuity equation constitute the hydrodynamical model for nematic liquid crystalline polymers (NLCPs). The results from Wang(2002) show many new features which are not shown by the LE theory.

CHAPTER 3

SIMPLIFIED MODEL AND STABILITY

We consider the shear flow between two parallel plates located at $y = 0$ and h , in Cartesian coordinates (x, y, z) . Figure. 3 depicts the cross section of the shear flow on the (x, y) plane. In this chapter, we will study the dynamics in shearing flows of nematic LCP.

3.1 Simplified Model

For simplicity, we set $L = 0$, then the governing equation becomes:

Orientation tensor equation,

$$\begin{aligned} & \frac{d}{dt} \mathbf{M} - \boldsymbol{\Omega} \cdot \mathbf{M} + \mathbf{M} \cdot \boldsymbol{\Omega} - a[\mathbf{D} \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{D}] \\ &= -2a\mathbf{D} : \mathbf{M}\mathbf{M} - 6D_r^0[Q - \frac{N}{2}((\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \cdot \mathbf{M} \\ & \quad + \mathbf{M} \cdot (\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M}) + N(\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} : \mathbf{M}_4 \end{aligned} \quad (8)$$

Balance of linear momentum,

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (-p\mathbf{I} + \boldsymbol{\tau}) \quad (9)$$

Constitutive equation for the *extra stress*,

$$\begin{aligned} \boldsymbol{\tau} = & 2\eta_s \mathbf{D} + 3ackT[\mathbf{M} - \frac{\mathbf{I}}{3} - \frac{N}{2}((\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \cdot \mathbf{M} + \mathbf{M} \cdot (\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} \\ & - 2(\mathbf{I} + \frac{\mathcal{L}^2}{24}\Delta)\mathbf{M} : \mathbf{M}_4)] - \frac{ckTN\mathcal{L}^2}{16}(\Delta\mathbf{M} \cdot \mathbf{M} - \mathbf{M} \cdot \Delta\mathbf{M}) \\ & - \frac{cNkT\mathcal{L}^2}{32}[\nabla\mathbf{M} : \nabla\mathbf{M} - (\nabla\nabla\mathbf{M}) : \mathbf{M}]. \end{aligned} \quad (10)$$

Corresponding to the incompressibility, \mathbf{v} satisfies the divergence-free equation,

$$\nabla \cdot \mathbf{v} = 0 \quad (11)$$

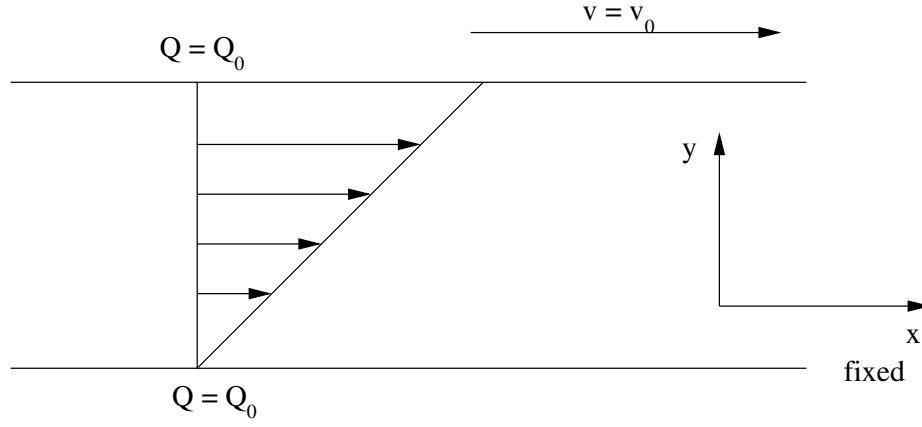


Figure 3: Geometry of the shear flow. The gap width is h . The LCP is sheared by moving the upper plate with a constant speed v_0 and the lower one is fixed. At the bounding surfaces, the orientation tensor is equal to its equilibrium value.

3.2 Dimensionless Form

To get nondimensional form of the above model, we use the length scale h and the LCP relaxation time scale $t_0 = t_n$. And we denote the position vector by \mathbf{x} , the velocity vector by \mathbf{v} , the extra stress tensor by τ , and the pressure by p , respectively. The dimensionless flow and stress variables are:

$$\begin{aligned}\tilde{\mathbf{v}} &= \frac{t_0}{h} \mathbf{v}, \tilde{\mathbf{x}} = \frac{1}{h} \mathbf{x} \\ \tilde{t} &= \frac{t}{t_0}, \tilde{\tau} = \frac{h^2}{f_0} \tau, \tilde{p} = \frac{h^2}{f_0} p,\end{aligned}\tag{12}$$

where $f_0 = \rho h^4 / t_0^2$ is an inertial force and ρ is the LCP density. Let c be the LCP number density, k the Boltzmann constant, T absolute temperature, N a dimensionless concentration, η the solvent viscosity, and $\zeta_i, i = 1, 2, 3$ three friction coefficients related to LCP-solvent interaction. The following seven dimensionless parameters arise:

$$\begin{aligned}Re &= \frac{\rho h^2}{t_0 \eta}, \alpha = \frac{3ckTt_0^2}{h^2 \rho}, Er = \frac{8h^2}{ND_r^0 t_0 L^2}, \\ \mu_i &= \frac{3ckT\zeta_i t_0}{h^2 \rho}, \quad i = 1, 2, 3\end{aligned}\tag{13}$$

α measures the strength of elastic energy relative to kinetic energy; Re is the solvent Reynolds number; Er is the Ericksen number which measures the strength of the short-range nematic potential relative to that of the isotropic distortional elastic energy; $\mu_i, i = 1, 2, 3$ are three nematic Reynolds numbers. Then we have the nondimensional equation as follows:

$$\begin{aligned}\frac{d}{dt} \mathbf{M} - \Omega \cdot \mathbf{M} + \mathbf{M} \cdot \Omega - a[\mathbf{D} \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{D}] &= \\ -2a\mathbf{D} : \mathbf{M}_4 - \frac{6}{De}[Q - N(\mathbf{M} \cdot \mathbf{M} - \mathbf{M} : \mathbf{M}_4)] & \\ + \frac{1}{Er}[\Delta \mathbf{M} \cdot \mathbf{M} + \mathbf{M} \cdot \Delta \mathbf{M} - 2\Delta \mathbf{M} : \mathbf{M}_4] &\end{aligned}\tag{14}$$

$$\begin{aligned}
\tau = & (2/\mathcal{R}] + \mu_3(a))\mathbf{D} + a\alpha[\mathbf{M} - \frac{\mathbf{I}}{3} - \frac{N}{2}((\mathbf{I} + \frac{1}{3NEr}\Delta)\mathbf{M} \cdot \mathbf{M} \\
& + \mathbf{M} \cdot (\mathbf{I} + \frac{1}{3NEr}\Delta)\mathbf{M} - 2(\mathbf{I} + \frac{1}{3NEr}\Delta)\mathbf{M} : \mathbf{M}_4)] \\
& - \frac{\alpha}{6Er}(\Delta\mathbf{M} \cdot \mathbf{M} - \mathbf{M} \cdot \Delta\mathbf{M}) - \frac{\alpha}{12Er}[\nabla\mathbf{M} : \nabla\mathbf{M} - (\nabla\nabla\mathbf{M}) : \mathbf{M}] \quad (15)
\end{aligned}$$

3.3 Steady States

Let σ_i be the eigenvalues and \mathbf{n}_i the corresponding orthonormal eigenvectors of the orientation tensor \mathbf{Q} , where $i=1,2,3$. Then \mathbf{Q} has a spectral representation,

$$\mathbf{Q} = \sum_{i=1}^3 \sigma_i \mathbf{n}_i \mathbf{n}_i, \quad (16)$$

from which we can define the specific nematic symmetries and their representations. It follows from (1)

$$tr(\mathbf{Q}) = \sum_{i=1}^3 \sigma_i = 0, \quad -\frac{1}{3} \leq \sigma_i \leq \frac{2}{3}, \quad i = 1, 2, 3. \quad (17)$$

Then it follows that

$$\sigma_i = \langle (\mathbf{m} \cdot \mathbf{n}_i)^2 \rangle - \frac{1}{3}, \quad i = 1, 2, 3. \quad (18)$$

This reveals that each eigenvalue of \mathbf{Q} is a measure for the degree of orientation with the corresponding eigenvector direction. If we knew the eigenvalues and the corresponding eigenvectors, we would be able to explore fully the macroscopic orientational information provided by the orientation tensor. Therefore, we should look for the degrees of orientation that can readily and accurately yield the eigenvalues and the eigenvectors of \mathbf{Q} . If all eigenvalues of \mathbf{Q} are distinct, the nematic liquid crystal is called biaxial, in which the triad of orthonormal eigenvectors of \mathbf{Q} , \mathbf{n}_i , $i=1,2,3$, are equally important and therefore all called directors.

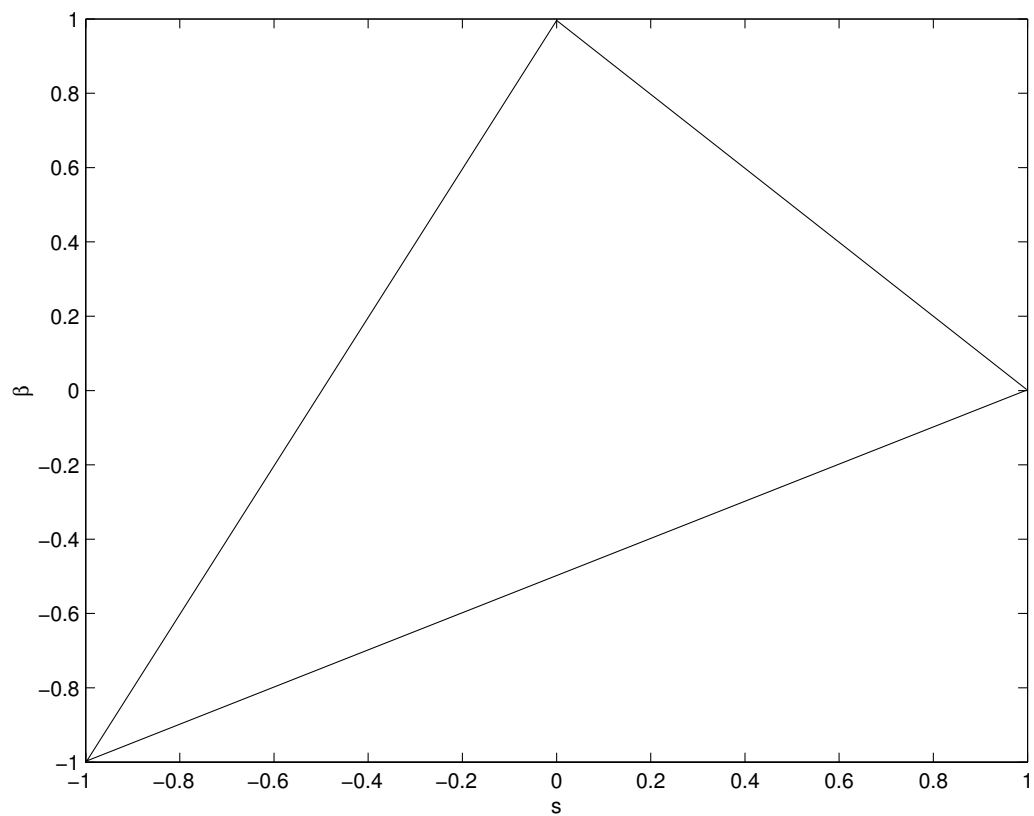


Figure 4: The range of values for the pair of order parameters (s, β) is the closed triangular region.

Defining

$$s = \langle (\mathbf{n}_3 \cdot \mathbf{m})^2 \rangle - \langle (\mathbf{n}_1 \cdot \mathbf{m})^2 \rangle, \beta = \langle (\mathbf{n}_2 \cdot \mathbf{m})^2 \rangle - \langle (\mathbf{n}_1 \cdot \mathbf{m})^2 \rangle, \quad (19)$$

we transform (16) into a biaxial representation

$$\mathbf{Q} = s(\mathbf{n}_3\mathbf{n}_3 - \frac{\mathbf{I}}{3}) + \beta(\mathbf{n}_2\mathbf{n}_2 - \frac{\mathbf{I}}{3}). \quad (20)$$

The degree of orientation variable with respect to each director can be represented as a function of s and β :

$$\begin{aligned} d_1 &= \langle (\mathbf{n}_1 \cdot \mathbf{m})^2 \rangle = \frac{1 - s - \beta}{3}, \\ d_2 &= \langle (\mathbf{n}_2 \cdot \mathbf{m})^2 \rangle = \frac{2\beta - s + 1}{3}, \\ d_3 &= \langle (\mathbf{n}_3 \cdot \mathbf{m})^2 \rangle = \frac{2s - \beta + 1}{3}. \end{aligned} \quad (21)$$

We thus adopt (s, β) as the orientation variables and define (s, β) as the order parameters. In simple shear flows, we are interested in the steady states where the directors \mathbf{n}_2 and \mathbf{n}_3 are confined to the shearing plane(i.e., the plane orthogonal to the shearing plate or surface).

3.3.1 Biaxial Steady States

We consider the simple shear flows of liquid crystal polymers in Cartesian coordinates (x, y, z) , the velocity field is $\mathbf{v} = (vy, 0, 0)$ where v is a constant shear rate. The dimensionless form of the space variables,

$$\tilde{\mathbf{v}} = (De\tilde{y}, 0, 0), \quad (22)$$

where $De = \frac{t_0 v}{h}$ is the Debra number or the dimensionless shear rate and \tilde{y} is the dimensionless spatial variable. We will seek the steady states of the orientation tensor \mathbf{Q} . Let the orientation tensor \mathbf{Q} as

$$s(\mathbf{e}_z\mathbf{e}_z - \mathbf{I}/3) + \beta(\mathbf{nn} - \mathbf{I}/3) \quad (23)$$

where s, β are two order parameters

$$\begin{aligned}\mathbf{n} &= (\cos \phi, \sin \phi, 0) \\ \mathbf{n}^\perp &= (-\sin \phi, \cos \phi, 0)\end{aligned}\tag{24}$$

are directors in the shearing plane (x, y) , where $0 \leq \phi < \pi$.

For biaxial nematic liquid crystals, there are three distinct directors. The degrees of orientation with respect to the directors are, in general, distinct. We define the unit eigenvector corresponding to the largest eigenvalue (or degree of orientation) as the major director (or major optical axis).

We can get the equations for the order parameters (s, β) and the angle parameter ϕ for our model, then the orientation tensor becomes:

$$\begin{aligned}s_{,t} &= -U(s) + \frac{2N\beta s}{3}(s - \beta - 1) \\ &+ \frac{aDe}{3} \sin(2\phi)(1 - \beta - s - 3\beta s) = f(s, \beta, \phi)\end{aligned}\tag{25}$$

$$\begin{aligned}\beta_{,t} &= -U(\beta) + \frac{2N\beta s}{3}(\beta - s - 1) \\ &+ \frac{aDe}{3} \sin(2\phi)(2 - 2s + \beta - 3\beta^2) = g(s, \beta, \phi)\end{aligned}\tag{26}$$

$$\phi_{,t} = \frac{De}{6\beta}(a \cos(2\phi)(2 + \beta - 2s) - 3\beta) = h(s, \beta, \phi)\tag{27}$$

where $(\cdot)_{,t}$ denotes the time derivative and

$$U(s) = s(1 - \frac{N}{3}(1 - s)(2s + 1))\tag{28}$$

In steady states, the angle parameter equation in (7-9) yields

$$\cos(2\phi) = \frac{3\beta}{a(2 + \beta - 2s)}\tag{29}$$

Using the biaxial representation of \mathbf{Q} along with the constraints in (1), the orientation tensor equation transforms into three equations for order and angle

parameters. Here we choose $a = 0.9$, then we can get the equilibria by using Maple to solve the three equations (25)-(27). After we obtain a steady state in terms of order and angle parameters, the Jacobian of the above system will be:

$$\mathbf{A} = \begin{pmatrix} \frac{\partial f(s,\beta,\phi)}{\partial s} & \frac{\partial f(s,\beta,\phi)}{\partial \beta} & \frac{\partial f(s,\beta,\phi)}{\partial \phi} \\ \frac{\partial g(s,\beta,\phi)}{\partial s} & \frac{\partial g(s,\beta,\phi)}{\partial \beta} & \frac{\partial g(s,\beta,\phi)}{\partial \phi} \\ \frac{\partial h(s,\beta,\phi)}{\partial s} & \frac{\partial h(s,\beta,\phi)}{\partial \beta} & \frac{\partial h(s,\beta,\phi)}{\partial \phi} \end{pmatrix}, \quad (30)$$

Then we put equilibria into the Jacobian matrix \mathbf{A} to calculate the eigenvalues. Let e_i , $i = 1, 2, 3$ be the eigenvalues. Then the steady state is said to be stable if $Re(e_{max}) < 0$, where $e_{max} = \max_{1 \leq i \leq 3} e_i$, neutrally stable if $Re(e_{max}) = 0$, and unstable if $Re(e_{max}) > 0$.

3.3.2 Steady States for Small Debra Number

We now study the orientation patterns and their stability of the biaxial steady state solutions in phase spaces (N, s) , (N, β) , (N, ϕ) , and (s, β) at given Debra numbers. If $De = 0$, the equilibria are uniaxial which has been studied a lot (Doi and Edwards, 1986) and is thus ignored here.

Firstly, we consider shear flows with nonzero small Debra numbers, say $De = 0.1$. From Figure.5, we can find there exist seven steady state solution families. Among all these seven steady state solution families, only one family exists for all N . This family is referred to as the flow-aligning family. All the other six families come into existence in pairs at three distinct critical values of N . In these six steady state families, five are unstable to in-plane disturbances. The remaining family with two positive order parameters is stable to in-plane disturbances. The major director in this family is parallel to the direction neutral to the flow (i.e., the e_z direction) since the two positive order parameters in the family yield a relatively high degree of orientation with that direction. It is referred to as the log-rolling family.

Figure.5 (a)-(d) depict the phase diagrams of the steady state families in the (N, s) , (N, β) , (s, β) and (N, ϕ) for $De = 0.1$, respectively.

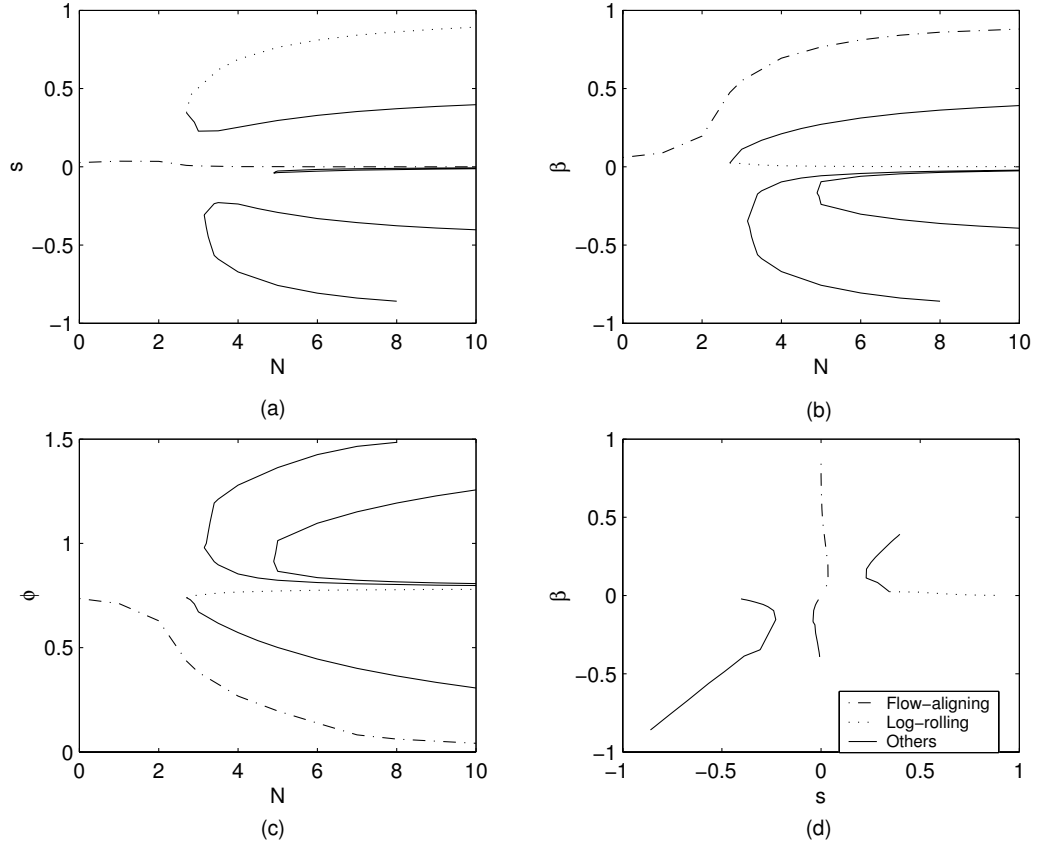


Figure 5: Variations of steady state solutions of Wang model as functions of polymer concentration N for $N \in [0, 10]$. The Debra number is $De = 0.1$. The legend in (d) applies to (a)-(c) as well. (a) The order parameter s vs N . (b) The order parameter β vs N . (c) The angle parameter ϕ vs N . (d) The order parameter s vs β for $N \in [0, 10]$.

The flow-aligning family exists for all De and N . And it is the unique steady state solution family in $0 < N < \frac{8}{3}$. The order parameter β maintains monotonically increasing for all N . The value of order parameter s is much smaller than that of the order parameter β , but it won't be zero. We observe a rapid growth for the order parameter β when N is slightly larger than the critical value. For the angle parameter ϕ , it experiences a rapid decline to zero when N is slightly larger than the critical value. It can be shown all the eigenvalues of the flow-aligning family are negative which shows that the flow-aligning family is stable for all De and N .

Both order parameters s and β in the log-rolling family are positive. The positive order parameter s maintains monotonically increasing as N increases. The positive parameter β is much smaller than the order parameter s . β approaches zero, but it won't be zero. For the angle parameter ϕ , the scope of its change is small, which is between 0.75 and 0.78. This family is stable to in-plane disturbances.

Comparing these two families, we can find for the flow-aligning family the variation of order parameter β is much bigger than that of order parameter s , and for the log-rolling family, the situation is reversed. And the variation of angle parameter ϕ in the flow-aligning family is much bigger than that in the log-rolling family.

3.3.3 Steady States for Large Debra Number

Now we consider shear flows with nonzero large Debra numbers, say $De = 10$. There are three families of steady states for $De = 10$ which include the flow-aligning and log-rolling families. The third family is unstable and is ignored in the following discussion.

Figure.6 (a)-(d) depict the phase diagrams of the steady state families in the (N, s) , (N, β) , (s, β) and (N, ϕ) for $De = 10$, respectively.

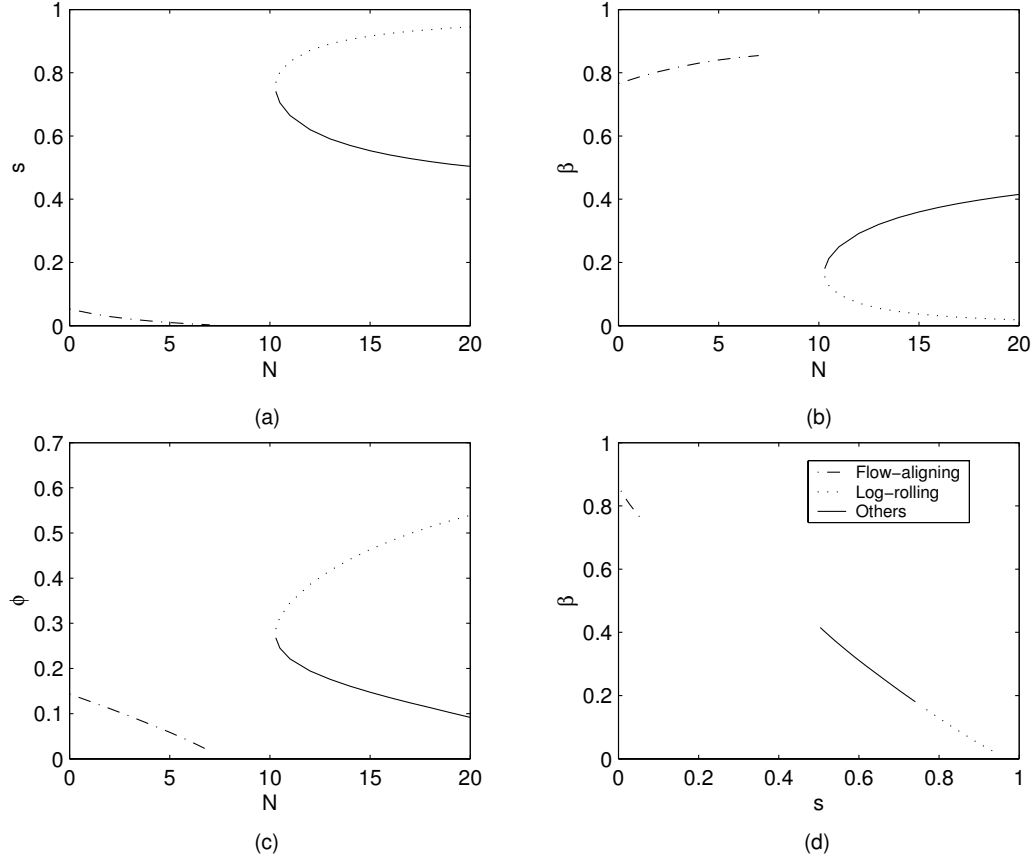


Figure 6: Variations of steady state solutions of Wang model as functions of polymer concentration N for $N \in [0, 20]$. The Debra number is $De = 10$. The legend in (d) applies to (a)-(c) as well. (a) The order parameter s vs N . (b) The order parameter β vs N . (c) The angle parameter ϕ vs N . (d) The order parameter s vs β for $N \in [0, 20]$.

The flow-aligning family is the unique steady state solution family in $0 < N < 8$. Both the order parameters s and β are positive. The order parameter s decreases as N increasing. And the order parameter β increases as N increases. The angle parameter ϕ decreases and approaches zero with relatively high speed.

For the log-rolling family, the order parameter s and angle parameter ϕ increase as N increases. And the order parameter β decreases as N increases. Also these two families experience the similar circumstances. The variation of angle parameter ϕ in the flow-aligning family is much bigger than that in the log-rolling family, etc.

3.3.4 Steady States for Different Polymer Concentration Values

Now we come to study the orientation patterns and their stability of the biaxial steady state solutions in phase spaces (De, s) , (De, β) , (De, ϕ) , and (s, β) at given polymer concentration N .

First, we consider shear flows with $N = 6$. There exist five steady state families. Among all these five steady state solution families, only flow-aligning family exists for all De , and this family is stable to in-plane disturbances. The variations of the order parameters s, β and the angle parameter ϕ are small. That is the reason why there is only one point exists in Figure. 7(d) for the flow-aligning family.

The other stable steady state solution family is the log-rolling family. It exists for $De \in (0, 3.2)$, and there is a local maximum for the order parameter s around $De = 0.7$. The order parameter β increases as De increases. And the angle parameter ϕ decreases at the same time.

Secondly, we consider shear flows with $N = 3$. There exists only one steady state family, which is the flow-aligning family. It exists for all De from 0 to 10. For De from 0 to 2, we observe a rapid growth in positive order parameter s . And it becomes stable around 0.21 for the rest of De . The order parameter β experiences the similar situation with s . We also can observe a rapid decay for the

angle parameter ϕ . In Figure. 8 (d), the order parameters s and β maintain a rapid growth simultaneously with respect to De from 0 to 2.

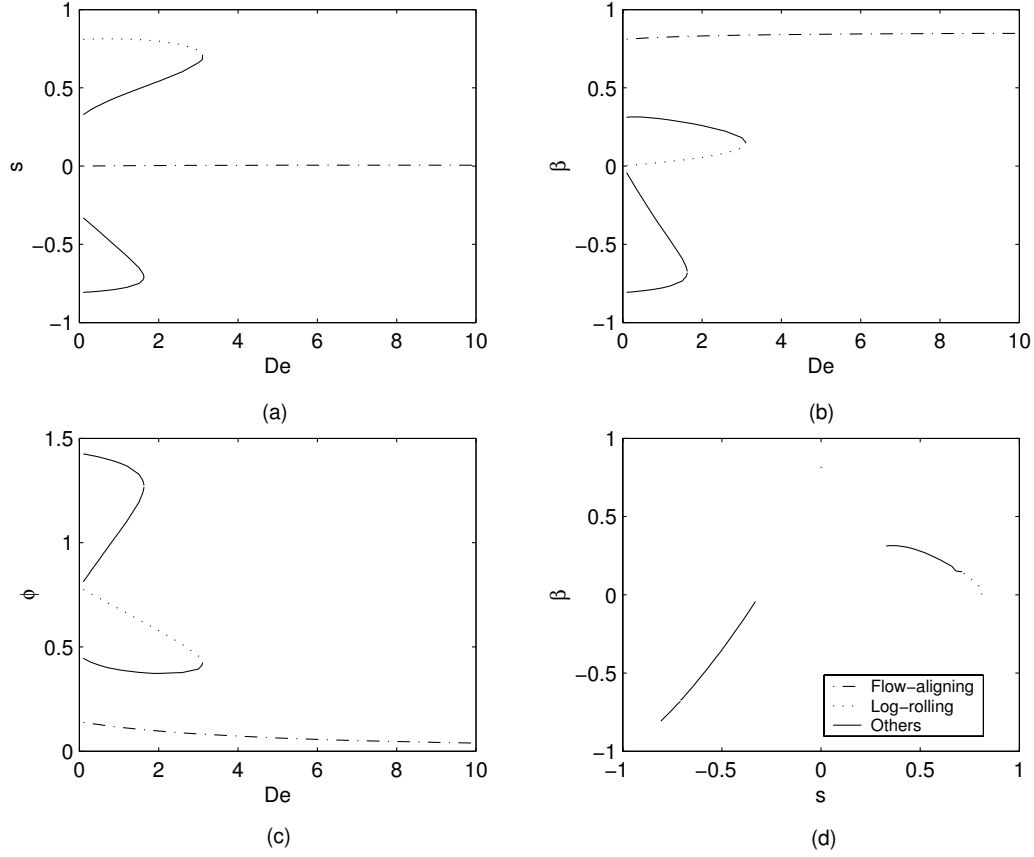


Figure 7: Variations of steady state solutions of Wang model as functions of polymer concentration De for $De \in (0, 10]$. The polymer concentration N is $N = 6$. (a) The order parameter s vs De . (b) The order parameter β vs De . (c) The angle parameter ϕ vs De . (d) The order parameter s vs β for $De \in (0, 10]$.

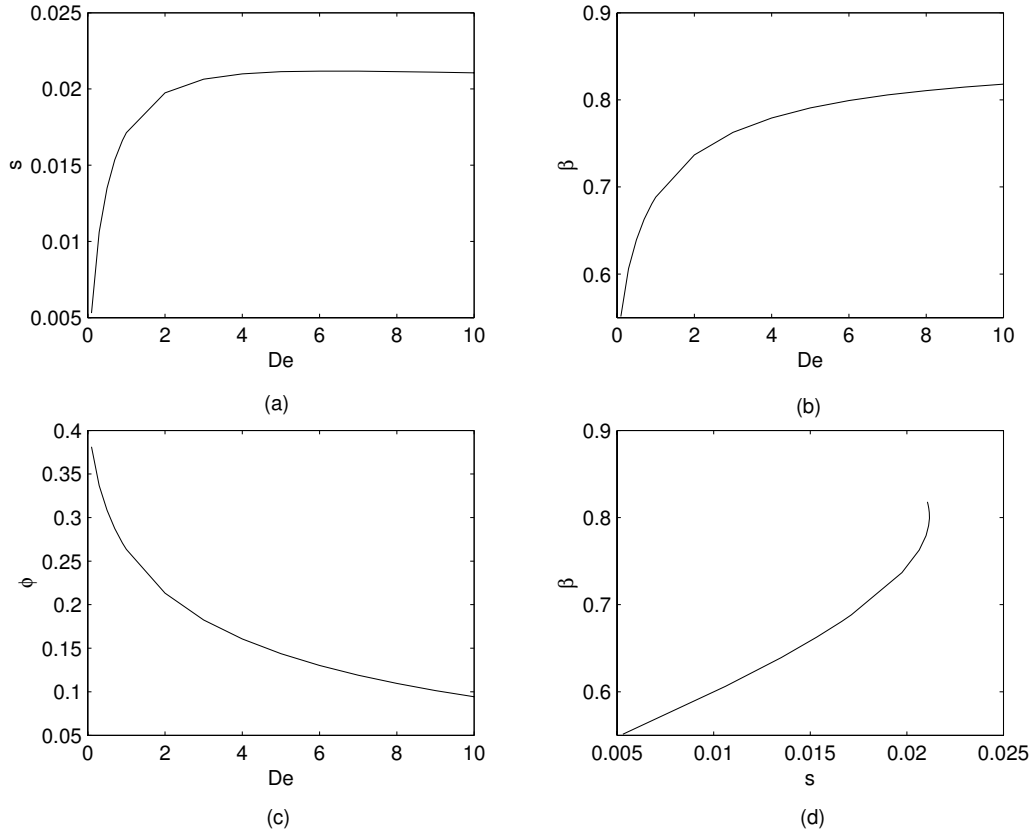


Figure 8: Variations of steady state solutions of Wang model as functions of polymer concentration De for $De \in (0, 10]$. The polymer concentration N is $N = 3$. (a) The order parameter s vs De . (b) The order parameter β vs De . (c) The angle parameter ϕ vs De . (d) The order parameter s vs β for $De \in (0, 10]$.

CHAPTER 4

CONCLUSION

We have discussed in detail the orientation tensor \mathbf{Q} and its symmetry using a biaxial representation. We have used biaxial liquid crystal's two order parameters and one angle parameter to give a complete description of the orientation. Our results show that our model admits multiple steady state solution families, all of which exhibit biaxial symmetry in simple shear flows. And we have investigated the stability of the steady state solutions subject to the in-plane disturbances. Flow-aligning family and log-rolling family are stable to in-plane disturbances. The flow-aligning family is the unique stable steady state family for all Debra numbers and polymer concentration values, for example, it is the only steady state solution family for $N = 3$.

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BIOGRAPHICAL SKETCH

Fangyu Liu was born in 1980, and interested in simple logic and math at very young age. He graduated from Nanchang University in four years with Bachelor of Science degrees in Mathematics. Then he entered the master's degree program in Applied Mathematics at the Department of Mathematics in 2002.