Determination of Director Angle for Flow Aligning Nematic Liquid Crystals under Couette Geometry

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Abstract: We consider steady state flow of nematic liquid crystals in a Couette geometry driven by the relative rotation of the two concentric cylinders. We use the standard Ericksen-Leslie continuum model. The director, a unit vector, represents the average molecular orientation. We assume strong anchoring conditions at the walls of the flow which fixes the director orientation, and find an explicit expression of the director angle as a function of its distance from the common axis of the rotating cylinders.

Keywords: Nematic liquid crystals, couette two, ericksen-leslie model.

1. INTRODUCTION

Nematic liquid crystals consist of elongated and rigid rod-like molecules. In the absence of flow and external fields they tend to follow a preferred direction of alignment. The hydrodynamic theory for liquid crystals, developed by Ericksen [8] and Leslie [9, 10], uses the director, n, and the velocity, v, as fundamental unknowns. Imposed boundary conditions and the balance between viscous and elastic forces in response to external stimuli determine stable flow configurations in various regimes. In the Couette geometry that we consider for this article, the external stimulus is provided by the relative rotation of the bounding cylinders.

In this article, we consider flow-aligning nematic liquid crystals. At a steady state of the flow between two concentric cylinders, we find an explicit expression of the director angle as a function of the distance from the common axis of the two rotating cylinders. In Section 2, we introduce the model, discuss the constitutive relations leading to constraints. We also define the flow alignment angle (equation 8) for flow-aligning nematics. Section 3 describes the equations of motion for the Couette geometry. The liquid crystal sample is confined between two concentric cylinders and the flow is driven by the relative rotation of the cylinders. In Section 4, we solve the system of equations that arising from balance of linear and angular momentum. Section 5 provides a summary and discusses possibilities for future research.

2. ERICKSEN-LESLIE MODEL AND CONSTITUTIVE EQUATIONS

Let $\mathrm{v}=(v_1,v_2,v_3)$ and $\mathrm{n}=(n_1,n_2,n_3)$ represent the velocity and director fields. We assume that the director is a unit vector, $\mathrm{n}\cdot\mathrm{n}=1$, and the flow is incompressible, which gives $\nabla\cdot\mathrm{v}=0$. The Ericksen-Leslie model uses the Frank-Oseen elastic energy, $F(n,\nabla n)$, a function of the director and its gradients defined by:

$$F(\mathrm{n},\nabla\mathrm{n})=\frac{1}{2}K_1\left|\nabla\mathrm{n}\right|^2+\frac{1}{2}K_2\left|\mathrm{n}.(\nabla\times\mathrm{n})\right|^2+\frac{1}{2}\left|\mathrm{n}\times(\nabla\times\mathrm{n})\right|^2,\quad(1)$$

where the constants K_1, K_2, and K_3 correspond to splay, twist, and bend deformations. The Cauchy stress tensor σ is:

$$\sigma=-p\mathrm{I}-(\nabla n)^T\frac{\partial F}{\partial\nabla n}+\sigma_{v,}\quad(2)$$

where p is the pressure and σ_v is the viscous part of the stress tensor [6, 7, 9, 12]. We assume that the viscous part of the stress tensor has a linear relationship to the velocity gradient:

$$\begin{aligned}\sigma_v &=(\alpha_1\mathrm{n}\ .\ \mathrm{An})\mathrm{n}\otimes\mathrm{n}+\alpha_2\mathrm{N}\otimes\mathrm{n}+\alpha_3\mathrm{n}\otimes\mathrm{N}\\&+\alpha_4\mathrm{A}+\alpha_5\mathrm{An}\otimes\mathrm{n}+\alpha_6\mathrm{n}\otimes\mathrm{An}\end{aligned}\quad(3)$$

where $2A=\nabla v+(\nabla v)^T$ T is the symmetric part of the velocity gradient, $2\Omega=\nabla v-(\nabla v)^T$ represents the skew-symmetric part of the velocity gradient, and $\mathrm{N}=\mathrm{n}_t+(v.\nabla)\mathrm{n}-\Omega\mathrm{n}$ measures relative rate of change of the director. The coefficients α_i in equation (3) are the Leslie coefficients and their values depend on the underlying liquid crystal.

For nematic liquid crystals in motion, the balance of linear and angular momentum are:

$$\rho[vt+(v\,.\nabla)v]=\nabla.\sigma\ \text{and}\quad(4)$$

$$\gamma_1\left[\mathrm{n}_t+(v.\nabla)\mathrm{n}\right]\times\mathrm{n}=\left[\nabla.\frac{\partial F}{\partial\nabla\mathrm{n}}\right]\times\mathrm{n}+\gamma_1\Omega\mathrm{n}\times\mathrm{n}-\gamma_2A\mathrm{n}\times\mathrm{n},\quad(5)$$

where $\rho>0$ denotes the constant density of the material, γ_1 represents the rotational viscosity and γ_2

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the torsion. Both γ_1 and γ_2 are linear combinations of Leslie coefficients. The six Leslie coefficients are not independent and they satisfy certain constraints. For a detailed derivation and discussion of the constitutive properties for nematic liquid crystals, see [1, 2, 9, 14]. In particular, the coefficients satisfy a linear constraint and the rotational viscosity is positive:

$$\alpha_6-\alpha_5=\alpha_2+\alpha_3, \text{ and} \tag{6}$$

$$\gamma_1=\alpha_3-\alpha_2>0, \gamma_2=\alpha_6-\alpha_5 \tag{7}$$

In addition to the trivial stable states possible for nematic liquid crystals without the infuence of flow or external fields, when $\alpha_2\alpha_3>0$, the sample can attain a non-trivial stable state where the director aligns itself at a specific angle. Nematic liquid crystals possessing this property are called flow-aligning and the angle at which the director orients itself is the flow-alignment angle and it satisfies the following condition:

$$\cos 2\phi = -\frac{\gamma_1}{\gamma_2} \tag{8}$$

where ϕ is the flow-alignmnet angle and a detailed discussion on flow-aligning nematics and the flow-alignment condition can be found in [5, 14].

3. GOVERNING EQUATIONS FOR COUETTE FLOW

We consider flow between two concentric cylinders of radii R_1 and R_2 ($R_2 > R_1$), rotating with angular velocities Ω_1 *and* Ω_2 respectively. Assuming a cylindrical polar coordinate system (r, θ, z) with z along the common axis of the cylinders and considering in-plane velocity components only, we examine solutions of the form:

$$\begin{aligned} \mathrm{v} &= (v_1;\ v_2;\ v_3) = (0,\ r\omega,\ 0) \text{ and} \\ n &= (n_1;\ n_2;\ n_3) = (\sin\phi,\ \cos\phi,\ 0), \end{aligned} \tag{9}$$

where $\omega=\omega(r,t)$ and $\phi=\phi(r,t)$. These choices automatically satisfy the requirements that n is a unit vector and the flow is incompressible. One component of the vector equation (4) determines the pressure while the other component relevant in this geometry yields:

$$\rho r\omega t=\frac{K_1}{r}\left(\frac{\phi_r}{r}+\phi_{rr}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\hat{\sigma}_{21}\right)+\frac{1}{r}\hat{\sigma}_{12}, \tag{10}$$

where $\hat{\sigma}_{12}$ and $\hat{\sigma}_{21}$ are components of the viscous part of the stress tensor σ_v. Similarly, The balance of angular momentum (5) for the director reduces to:

$$\gamma_1\phi_t=\frac{K_1}{r}\left(\phi_r+r\phi_{rr}\right)-\frac{r\omega_r}{2}\left(\gamma_1+\gamma_2\cos 2\phi\right) \tag{11}$$

Using equation (11) to replace the term containing the radial derivatives of ϕ in (10) and evaluating the remaining terms using (3), we obtain:

$$\begin{aligned} \rho r\omega t &= \frac{1}{r}\gamma_1\phi_t+\frac{1}{2}\left\{\frac{\partial}{\partial r}\left[g(\phi)r\omega_r\right]+2g(\phi)\omega_r\right\} \\ &+\frac{1}{r}\frac{\partial}{\partial r}\left[\phi_t\left(\alpha_3\cos^2\phi-\alpha_2\sin^2\phi\right)\right] \\ &+\frac{\phi_t}{r}\left[\alpha_2\cos^2\phi-\alpha_3\sin^2\phi\right] \end{aligned} \tag{12}$$

where $g(\phi)$ is a generalized measure of viscous effects in the liquid crystal and equals:

$$\begin{aligned} g(\phi) &= 2\alpha_1 sin^2\phi\ cos^2\phi-\alpha_2 sin^2\phi \\ &+\alpha_3 cos^2\phi+\alpha_4+\alpha_5 sin^2\phi+\alpha_6 cos^2\phi \end{aligned} \tag{13}$$

The second law of thermodynamics applied in the form of the Calusius-Duhem inequality implies that $g(\phi)>0$. The orientation of the molecules (and hence the value of n) at the boundary depends on the preparation and treatment of the boundary material. Without loss of generality, we will assume that the walls are crystalline which leads to strong anchoring boundary conditions for the director. Under this assumption:

$$\phi\ (R_1,\ 0)\ = (R_2,\ 0)\ = \phi_0 \tag{14}$$

where homogenous and homeotropic boundary conditions are given by,

$$\phi_0 = 0, \phi_0 = \pm/2 \tag{15}$$

respectively.

An analysis leading to the existence of weak solutions for the Leslie-Ericksen system in the Couette geometry follows from the corresponding theory for more general systems by Calderer and Liu [3] and Lin and Liu [11].

4. DETERMINATION OF DIRECTOR ANGLE AT STEADY STATE

We seek steady state solutions of the system of equations (11) and (12). For time-independent velocity and director fields, $\omega(r,t)=\omega(r)$ *and* $\phi(r,t)=\phi(r)$, all time derivative terms vanish and the right hand side of (12) reduces to:

$$\frac{d}{dr}\left[g(\phi)r\omega_r\right]+2g(\phi)\omega_r=0 \tag{16}$$

Similarly, dividing both sides of (11) by γ_1 and assuming a time independent field for the director, we arrive at:

$$0=\frac{K_1}{\gamma_1}\left(\frac{\phi_r}{r}+\phi_{rr}\right)-\frac{r\omega_r}{2}\left(1+\frac{\gamma_2}{\gamma_1}\cos 2\phi\right). \quad (17)$$

Main Result: In the flow aligning regime, the director angle ϕ at a distance r from the common rotational axis of the cylinders can be expressed explicitly by the function $\phi(r)=-A\ln r+B$ where the constants are given by $A=\frac{\pi}{\ln R_2-\ln R_1}$ *and* $B=\frac{\pi}{2}\frac{\ln(R_1R_2)}{\ln R_1-\ln R_2}$ where R_1 and R_2 are radii of the inner and outer cylinders respectively.

Proof: Integrating (16) yields the relationship $r^3\omega_r(r)g(\phi)=C$, where the constant C may be interpreted as the magnitude of the moment per unit length of a cylinder with radius r. When $(\omega_r(r)=0)$, ($equivalently$, $\omega = constant$), the motion corresponds to a rigid body rotation. We may conceptualize incompressible isotropic viscous fluids as a special case of anisotropic liquid crystals where the director $\phi(r)$ is independent of the radial coordinate. Under these assumptions, all terms involving derivatives of ϕ in equation (17) are zero. Thus, for non-rigid body motions $(\omega_r(r)\neq 0)$, and for flow-aligning nematic liquid crystals using equation (8), equation (17) reduces to;

$$\frac{\phi_r}{r}+\phi_{rr}=0 \quad (18)$$

After integrating equation (18), we get

$$\phi(r)=A\ln r+B \quad (19)$$

where A and B are constants of integration. Using homeotropic boundary conditions (15), we evaluate the constants as:

$$A=\frac{\pi}{\ln R_2-\ln R_1}, B=\frac{\pi}{2}\left\{\frac{\ln R_1+\ln R_2}{\ln R_1-\ln R_2}\right\} \quad (20)$$

Remark: We use homeotropic boundary conditions because homogeneous boundary conditions give only the trivial solution.

5. SUMMARY AND FUTURE RESEARCH

In this paper we have found an explicit expression of the director angle ϕ at a distance r from the common axis of the rotating cylinders. To study stability, there are many experimental [4, 13] and numerical [15] work are done involving director angles in the Couette flow of nematic liquid crystals. Our future work will involve the comparison between this analytical work and the existing experimental and numerical work.

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