Orienting properties of discotic nematic liquid crystals in Jeffrey-Hamel flows

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Abstract: The orienting properties of incompressible discotic nematic liquid crystals for creeping flows between converging and diverging planar walls (Jeffrey-Hamel) are analyzed using the Leslie-Ericksen theory. The dependence of director orientation on the reactive parameter \( \lambda \) and the flow kinematics is presented. Closed form stationary solutions for the director orientation are found when elastic effects are neglected. Stationary numerical solutions for the velocity and director fields using the full Leslie-Ericksen theory are presented. The director field in converging flow is characterized by azimuthal (radial) centerline orientation, by being asymmetric with respect to the azimuthal (radial) direction, and by having an allowed orientation range that spans two half-quadrants (full quadrants). In the limiting case of perfectly flat disk \( \lambda = -\infty \) the flow-induced director orientation in converging flow is the azimuthal direction, while in diverging flow the director rotates by a full \( \pi \) radians. By reducing the vertex angle between the walls to vanishingly small values, converging flow solutions properly reduce to those of flow between parallel plates, but diverging flows are expected to lead to a new instability.

Key words: Discotic-nematic liquid crystals; Jeffrey-Hamel flows; orienting properties; reactive parameter

1. Introduction

Discotic nematic liquid crystals are found in petroleum and coal mesophase pitches [1], and are synthesized from plane aromatic compounds [2, 3]. Advances in the spinning of carbonaceous mesophases into fibers [4, 5] make the understanding of the flow behavior of discotic liquid crystals to be of considerable practical value. For general reviews see [6, 7].

In discotic nematic phases, the director or preferred average molecular orientation lies along the short molecular axis, resulting in optical and diamagnetically negative uniaxial phases. Mechanical manifestations of this molecular arrangement also show up in the estimated backflow effects [8], in the calculated ordering of the Miesowicz viscosities \( (\eta_2 < \eta_3 < \eta_1) \) [9], and in the predicted sign and magnitude of the reactive parameter \( (\lambda < -1) \) [10 - 13]. The contrasting behavior between rod-like and disc-like nematics follows from their different ordering. Assuming the nematic molecules to be ellipsoids of revolution with aspect ratio \( p = a/b \), where \( a \) is the polar radius and \( b \) is the equatorial radius, the two possible ordering modes are: 1) rod-like (oblate ellipsoid, \( p > 1 \)) molecules orient their long molecular axis along the director, and 2) disc-like (prolate ellipsoid, \( p < 1 \)) molecules orient their short axis along the director.

The analysis of discotic nematic flow behavior has been restricted to inelastic simple shear flows, that is, to find the stationary stable director orientation in the absence of elastic effects [12 - 14] and the viscosity of the flow-aligned material [13].

The aim of this paper is to predict the effects of the shape anisotropy \( (p < 1) \) on the orienting properties of discotic nematics, and to extend the analysis of their flow behavior to pressure-driven creeping flows between planar, non-parallel walls (Jeffrey-Hamel flows) by solving numerically the governing Leslie-Ericksen (LE) equations of uniaxial nematics [15]. The present paper extends the study of rod-like nematics in Jeffrey-Hamel flows [16, 17]. We present stable, in-plane, stationary solutions for the director orientation and the velocity field. In this paper we on-
ly consider flow-aligning discotics \((\lambda < -1)\) [12]. The chosen nonviscometric flow allows for the study of the orienting properties of discotic nematic phases in the presence of combined inhomogeneous shear and elongation deformations. The orienting effect of shear can be singled out by letting the angle between the walls be close to zero. The orienting effect of elongation is found from the centerline director orientation since shear vanishes there. The geometry also allows to study the case in which the two orienting effects cooperate (converging flow) or compete (diverging flow) with each other. We expect that the degree of “universality” found in the mechanical properties of low-molar mass rod-like nematic liquid crystals [18] is also present in discotic nematic liquid crystals, and that the results of this work are generally applicable to discotic nematics in Jeffrey-Hamel creeping flows.

2. Balance equations, boundary conditions, and physical constants

A detailed derivation of the LE equations for converging and diverging flows of uniaxial, incompressible nematics has been given in [16]. Jeffrey-Hamel flows are best described with a cylindrical \((r, \psi, z)\) coordinate system; see Fig. 1. The vertex angle is \(2\psi_0\). In this paper all angles are given in units of radians. We take the velocity \(v\), director \(n\), and pressure \(p\) fields to be of the following form:

\[
\begin{align*}
  v &= \left( \frac{u(\psi)}{r}, 0, 0 \right) \quad (1a) \\
  n &= (\cos W(\psi), \sin W(\psi), 0) \quad (1b) \\
  p &= \frac{\sigma(\psi)}{r^2} + \text{constant} \quad (1c)
\end{align*}
\]

In Sect. 3 we show that for flow-aligning discotic nematics \(\lambda < -1\) and for the initial (prior to flow) director orientations considered in this paper, the director lies in the shear plane. Therefore, there is no out-of-plane director component \((n_z = 0)\) and, consequently, there is no transverse flow \((v_z = 0)\). Equation \((1a)\) then follows from the incompressibility assumption \((\nabla \cdot v = 0)\). The form of the pressure \((1c)\) follows from consistency requirements.

The governing equations for the conservation of linear and angular momentum are [16]

\[
\begin{align*}
g(1 + W')^2 + a_1 u + a_2 u W' + a_3 u' + a_4 u' W' + a_5 u'' + 2\sigma &= 0 \quad (2a) \\
g' - \frac{3}{2} g' W^2 - g' W^3 - 2g W'' - 2g W' W'' + a_6 u' + a_7 u W' + a_8 u' W' + a_9 u'' + a_{10} u - \sigma &= 0 \quad (2b) \\
g' (W^2 - 1) + g W'' - [g_2 \cos 2 W + \gamma_1] \frac{u'}{2} - [g_2 \sin 2 W] u &= 0 \quad (2c) \\
g(W) &= K_{11} \cos^2 W + K_{33} \sin^2 W \quad (2d) \\
g' (W) &= (K_{33} - K_{11}) \sin 2 W \quad (2e) \\
\gamma_1 &= a_3 - a_2 \quad (2f) \\
\gamma_2 &= a_6 - a_5 = a_3 + a_2 \quad (2g)
\end{align*}
\]

The coefficients \(\{a_i\}, i = 1, \ldots, 10\), tabulated in Appendix 1, are functions of the Leslie coefficients \(\{a_{ij}\}, i = 1, \ldots, 6\) and the director angle \(W(\psi)\); the constants \(\{K_{ij}\}, i = 1, 3\) are the splay and bend Frank elasticity coefficients, respectively; \(\gamma_1\) and \(\gamma_2\) are the rotational and irrotational viscosities, respectively. The equality in \((2g)\) is due to Parodi [19]. The reactive parameter \(\lambda\) is defined as [19]:

![Fig. 1. Jeffrey-Hamel flow geometry. \(W(\psi)\) is the angle of the director (director orientation) with respect to the radial direction, measured counterclockwise from the ray at \(\psi\). \(2\psi_0\) is the vertex angle.](image-url)