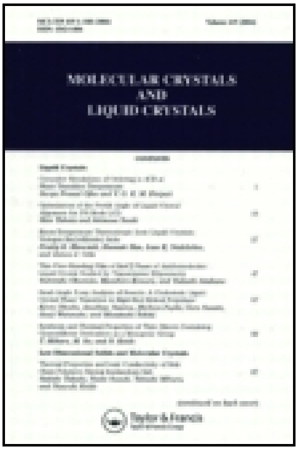

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

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Antonino Polimeno [a], Assis F. Martins [b] & Pier Luigi Nordio [a]

[a] Dipartimento di Chimica Fisica, Università di Padova, Via Loredan 2, 35131, Padova, Italy

[b] Departamento de Ciĕncia dos Materiais, FCT, Universidade Nova de Lisboa, 2825, Monte de Caparica, PORTUGAL

Version of record first published: 24 Sep 2006

Mol. Cryst. Liq. Cryst., 1999, Vol. 328, pp. 541-548
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Flow Patterns of the Nematic Director in a Rotating Cylindrical Sample

ANTONINO POLIMENO[a], ASSIS F. MARTINS[b] and PIER LUIGI NORDIO[a]

[a]*Dipartimento di Chimica Fisica, Università di Padova, Via Loredan 2, 35131 Padova, Italy; and* [b]*Departamento de Ciência dos Materiais, FCT, Universidade Nova de Lisboa, 2825 Monte de Caparica, PORTUGAL*

The nematic liquid crystal dynamics in a rotating cylindrical container, subjected to a constant magnetic field, has been considered in the past assuming a spatially homogeneous response of the director. In this communication, the formation and dynamics of flow-induced patterns of the director orientation field are investigated by numerical techniques, within different degrees of approximation. Nematodynamics equations are simplified by constraining the director to lie in a planar section of the cylinder, and the time and space dependence of the velocity field in the plane is taken into account. Patterns of the director orientation are calculated and discussed for different velocity profiles.

Keywords: nematics; hydrodynamics; viscoelastic properties

INTRODUCTION

The purpose of this study is to illustrate the dynamical behaviour of the director field of a nematic liquid crystalline sample, contained in a cylinder subjected to rotation, and under the influence of a constant magnetic field. Basic equations for determining flow patterns in time and space are obtained directly from the constitutive nematodynamics description based on Leslie-Ericksen formalism [1], under suitable simplifying hypotheses, namely constraint to the director and velocity field to lie on the plane of rotation, simplified forms for the elastic energy and stress tensors, ideal treatment of the velocity field and pure strong anchoring boundary conditions at the cylinder walls. The time evolution of the director field is then calculated numerically, for different time-dependent velocity profiles imposed to the cylindrical sample.

Nematics have been and are currently studied in spinning cylindrical vessels both in the course of rheological, electron spin resonance (ESR) and nuclear magnetic resonance (NMR) stationary experiments, i.e. with constant spinning velocity, and non-stationary experiments, e.g. by applying a sudden acceleration to the sample and a subsequent sudden deceleration, as a way to determine with a high degree of accuracy viscosity and elasticity parameters [2]. Standard interpretations [3] usually neglect any dependence of the director field from position and oversimplify the time behaviour. Director dynamics as predicted by nematodynamics equations is however a relatively complex phenomenon, and spatial dependence, boundary conditions and acceleration-deceleration effects can affect strongly the experimental outcomes. Numerical and analytical studies of the director dynamics, even in the absence of any time-dependent behaviour of the velocity field, reveal a significant complexity [4].

Here we intend to give an additional contribution to the interpretation of transient director patterns in a cylindrical two-dimensional geometry by taking into account explicitly non-stationary conditions of the velocity, following a methodology recently applied to stationary experiments[5]. The paper is organised as follows: in the next Section the model equations are summarised. In the last Section examples corresponding to different velocity profiles are shown and briefly discussed.

THE MODEL

The constitutive equations of nematodynamics for an incompressible nematic are a set of six non-linear coupled partial differential equations, for the velocity field $\underline{v}(t)$ and for the director field $\underline{n}(t)$. In the absence of external body forces and inertial effects, they assume the form:

$$\rho\frac{\partial \underline{v}}{\partial t} - [\hat{\nabla}\cdot\underline{\underline{\sigma}}] = 0 \tag{1}$$

$$\underline{G} + \underline{g} + [\hat{\nabla}\cdot\underline{\underline{\pi}}] = 0 \tag{2}$$

where ρ is the bulk density and $\underline{\underline{\sigma}}$ is the stress tensor, $\underline{G}$ and $\underline{g}$ are the external and internal force acting on the director, $[\hat{\nabla}\cdot\underline{\underline{\pi}}]$ is an elastic term. The stress matrix $\underline{\underline{\sigma}}$ depends upon the velocity and director components and their derivatives, and on the six viscosity coefficients α_i[1]. The internal director force $\underline{g}$ depends also upon the velocity and director field, and on the derivatives of the elastic energy W which we define in the spherical approximation as $W = \frac{1}{2}Kn_{i,j}n_{i,j}$. We shall consider the application to the experimental geometry sketched in Fig. 1a. A point in space is identified by vector $\underline{r}$, which is defined by the Cartesian coordinates (r_1, r_2) in the plane, or by the cylindrical coordinates (r, θ). The radius of the cylinder is R and the magnetic field is defined along the abscissas axis as $\underline{H} = H\underline{e}_1$; the external director body force is given by $\underline{G} = \chi_a H^2 n_1 \underline{e}_1$ where $\chi_a = \chi_{\|} - \chi_{\perp}$, $\chi_{\|}$ and $\chi_{\perp}$ being the principal diamagnetic susceptibilities per unit volume. The cylinder is subjected to rotation around the $\underline{e}_3$ axis at angular speed $\Omega R f(t)$ where $f(t)$ is a given function of time which specifies the rotation law of the cylinder walls. In the following we shall constrain both the velocity field and the director to lie in the plane of Fig. 1a. Moreover, we shall consider a simplified version of the velocity equation by neglecting any dependence upon the director orientation, i.e. by assuming an ideal Newtonian fluid behaviour. This approximation is justifiable under the hypothesis of a relatively fast relaxation of the velocity field with respect to the director, and leads to a considerable simplification of the numerical treatment. Notice that with this choice only the α_4 term in the stress tensor is taken into account. Standard boundary conditions are assumed for the velocity at the walls, namely that the fluid velocity coincides with walls velocity for $r = R$. Only the tangential component $v_\theta(r,t) \equiv v(r,t)$ depending upon r and t, is then left to be evaluated by the standard Navier-

Stokes equation

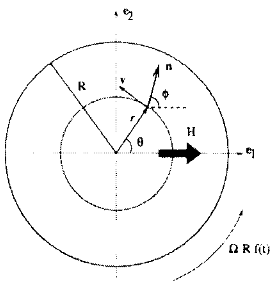
$$\rho\frac{\partial v}{\partial t}=\frac{\alpha_4}{2}\left(\frac{\partial^2 v}{\partial r^2}+\frac{1}{r}\frac{\partial v}{\partial r}-\frac{v}{r^2}\right) \tag{3}$$

with boundary and initial conditions $v(R,t)=\Omega Rf(t)$ and $v(r,0)=0$, i.e. at time $t=0$ the fluid and the cylinder are at rest ($v=0$). Next, let us consider the director equation. Since the director field vector is unitary, one can recover an equation in $\Phi(r,\theta,t)$, where $n_1=\cos\Phi$, $n_2=\sin\Phi$ (cfr. Fig. 1a). The time-dependence of the director angle Φ is affected by the velocity function $v(r,t)$, by the viscosity coefficients γ_1, γ_2, by the averaged elastic constant K and finally by the field intensity H:

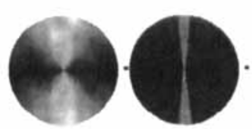
$$\gamma_1\left[\frac{\partial\Phi}{\partial t}+\frac{v}{r}\frac{\partial\Phi}{\partial\theta}-\frac{1}{2}\left(\frac{\partial v}{\partial r}+\frac{v}{r}\right)\right]+$$

$$\gamma_2\left(\frac{\partial v}{\partial r}-\frac{v}{r}\right)\cos 2(\Phi-\theta)-K\hat{\nabla}^2\Phi+\frac{\chi_a H^2}{2}\sin 2\Phi=0 \tag{4}$$

with boundary and initial conditions $\Phi(R,\theta,t)=\theta$ and $\Phi(r,\theta,0)=\Phi_{\rm st}(r,\theta)$, i.e. the director is supposed to be perpendicular to the walls at all times (rigid radial anchoring), and at time $t=0$ the system is prepared in a stationary configuration $\Phi_{\rm st}(r,\theta)$, obtained in the absence of rotation, $\Omega=0$, but in the presence of the field. The choice of a perfectly rigid radial align-



(a)



(b)

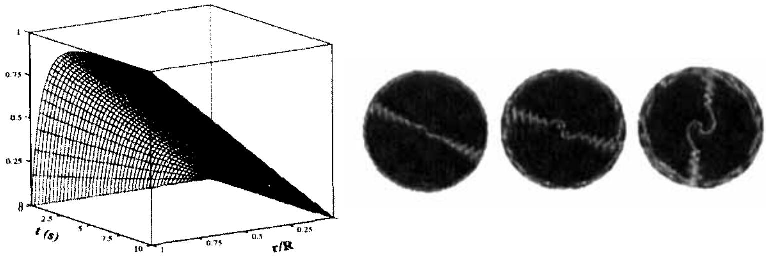
Figure 1: Standard cylindrical geometry for a nematic sample in a cylindral vessel (a); snapshots of distribution $\Phi(r,\theta,t)$ for a still sample at times 0 and 5 s (b).

ment of the director to the internal walls of the cylinder is mainly dictated by the necessity of keeping simple the geometry of the problem, at the cost of possible significant departure from realistic conditions in actual experiments. Perfect rigid radial alignment is however a permitted mode in two dimensions, especially for small values (≤ 1 mm) of the cylinder radius[4].

The numerical treatment of both the velocity equation (3) and the director orientation equation (4) can be performed using an expansion in terms of basis functions in θ and r, with time-dependent coefficients. The methodology, based on Galerkin variational principle, takes advantage from the cylindrical geometry using Bessel functions for the radial coordinate, and it has been illustrated elsewhere [5], for stationary conditions, i.e. $f(t)$ constant.

RESULTS AND DISCUSSION

We analyse here just three cases, with no pretense of completeness. We choose, quite arbitrarily, as physical parameters $\chi_a = 10^{-7}$, $K = 5 \times 10^{-6}$ dyne, $\gamma_1 = 1$ P, $\gamma_2 = 0.5$ P, $\alpha_4 = 1$ P, $\rho = 1$ g/cm^3, $H = 3360$ G. We show in Fig. 1b the case of a still cylinder, $\Omega = 0$. The starting configuration is assumed to be a perfect radial distribution, i.e. at $t = 0$ $\Phi = \theta$ in the whole sample. We use a false color representation, where light gray means that the director is perpendicular to the field and dark gray means that the director is parallel to the field. After 5 seconds the system has reached a stationary state, and the director is aligned to the field in most of the sample, with a thin layer perpendicular which is forced on the system by boundary conditions. This is the stationary distribution $\Phi_{st}(r, t)$ which we shall take as starting condition for all other cases. Next in Figg. 2a and 2b we show the calculated velocity profile and three snapshots of the director patterns for the case of a continuous acceleration till a constant velocity of rotation is reached of 0.5 s^{-1}. In Fig. 2a we can see the velocity profile, which reaches rapidly a stationary condition within the sample (i.e. $v = \Omega r$). The director patterns are shown in Fig. 2b: a stationary state is not reached by the director within the calculation time, and spiraliform patterns are formed. In Figg. 3a and 3b we show results for the case of



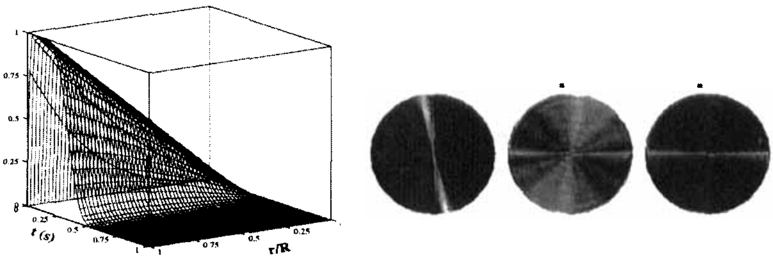
(a) (b)

Figure 2: Acceleration and steady rotation: normalised velocity profile $v(r,t)/\Omega R$ as a function of r/R and t (a) and snapshots of distribution $\Phi(r,\theta,t)$ at times 10, 50 and 100 s (b).

sudden acceleration followed by sudden deceleration. In Fig. 3a the calculated velocity profile is shown for a function $f(t)$ which produces a sudden acceleration in less than 0.15 s from zero velocity to 5 s^{-1}, followed by a fast deceleration to zero, for a total of 0.5 s which corresponds roughly to a $\pi/2$ rotation. Fig. 3b shows the corresponding director patterns. During the acceleration pulse the director rapidly becomes perpendicular to the field in most of the sample, and then it relaxes, less rapidly, to a stationary state which is equivalent to the initial one, with a dominant orientation parallel to the field, except that the remaining area perpendicular to the field is now switched of 90 degrees.

Further comments

Director flow patterns in two dimensions, for a cylindrical nematic sample, have been presented in the previous Section under the influence of three different motional regimes (still geometry, acceleration-steady rota-



(a) (b)

Figure 3: Acceleration-deceleration: normalised velocity profile $v(r,t)/\Omega R$ as a function of r/R and t (a) and snapshots of distribution $\Phi(r,\theta,t)$ at times 0.05, 0.5 and 2 s (b).

tion, acceleration followed by sudden deceleration). The time dependence of the velocity field, treated as a radial-dependent quantity predicted by a standard Navier-Stokes description, has been taken into account in the evolution equation for the director orientation, obtained from Leslie-Ericksen equations. In the case of an accelerating and then steady rotating cylinder a steady-state director flow is not reached, and spiraliform patterns are formed, as it was already observed in simulations with no explicit coupling with a time-dependent velocity field [5]. In the case of a sudden acceleration followed by a sudden deceleration the director first undergoes during the acceleration phase a fast relaxing reorganization (almost, but not completely reorienting itself perpendicularly to the imposed magnetic field), and then it reaches a new stationary state which is equivalent to the initial state. Rigid anchoring at the walls has been assumed in all the cases analysed here and further work is certainly required to understand the effect of slip at the boundaries, which is likely to be responsible for relaxing twisted configurations. The effect of the director dynamics on the velocity field has also been neglected, and a more advanced analysys will have to take it into account explicitly. Nevertheless time-dependent patterns as predicted by the present model are likely to be already applicable to the interpretation of actual rheo-NMR and ESR experiments in stationary and non-stationary conditions for measuring viscoelastic constants.

Acknowledgements

This work has been supported by the E.C. TMR Contract N. FMRX-CT97-0121. Support has been provided also by the Italian Ministry for Universities and Scientific and Technological Research and in part by the Italian National Research Council through its Centro Studi sugli Stati Molecolari and the Committee for Information Science and Technology.

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