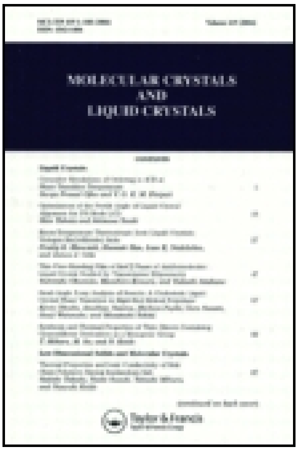

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Dynamical Regimes of Nematic Infinite Planar Samples

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Abstract A computational treatment of Leslie-Ericksen constitutive equations of nematodynamics, is applied to an infinite planar sample, in the presence of mechanical stresses and magnetic torques. Dynamical regimes are explored in order to investigate the competing effects of magnetic and mechanical torques and backflow effects resulting from coupling of velocity and director fields and to understand the transient behaviour of the nematic director, when the magnetic field is parallel or perpendicular to the shear direction.

Keywords nematic liquid crystals; Leslie-Ericksen equations; rheology of complex fluids.

INTRODUCTION

It is well known that, in the absence of external magnetic or electric fields, shear flow induces the alignment of nematic liquid crystals, characterised by a positive product of the second and third Leslie coefficient $\alpha_2 \cdot \alpha_3 > 0$ (aligning), in a preferential direction in the plane of shear[1]. Under the influence of viscous torque, the director forms a constant angle with flow direction. In the case of nematic liquid crystal characterised by Leslie coefficients product $\alpha_2 \cdot \alpha_3 < 0$ (non-aligning), the director can exhibit tumbling non-stationary distributions[2].

Shear flow studies in the absence of any aligning field are experimentally difficult since excellent surface conditions are required; the most common experimental situation is the competition of two applied torques, the magnetic one, due to the presence of a static magnetic field, and the mechanical one, due to the shear stress[3,4]. For a given geometry, i.e. for a given set of initial conditions, boundary conditions and field angle with respect to the shear plane, a number of situations can be explored. For instance, different stationary and transient behaviours are expected and observed applying a field perpendicular to the shear plane and changing the velocity profiles to simulate continuous, oscillatory or *start and stop* shear. Standard predictions based on analytical or numerical solutions of constitutive Leslie-Ericksen (LE) nematodynamics equations are based on the assumption that i) the velocity flow of the fluid is stationary and uncoupled from the director flow and ii) that the director lies in the shear plane, unless a strong magnetic field is applied. Evidences that the director may come out of the shear plane are nevertheless observed[5], and only by taking into account, in the solution of nematodynamics equations, all the director components and velocity components, we can rationalize in a systematic way both the dynamic and static behaviour of the nematic fluid.

In this paper we shall discuss some selected results, which can be obtained by numerically solving LE equations for the idealised configuration, made of a sample of nematic sandwiched between two sliding parallel plates. Our basic approximation will be to invoke spatial translational invariance in the two direction parallel to the plates, i.e. to assume that the director field, the velocity field and the stress tensor of the liquid crystal depend only upon the relative distance between the plates. This geometry can be thought as the simplified equivalent of a rheological Couette setup, made of two coaxial rotating cylinders, when the internal distance is sufficiently small compared to the radii of the cylinders, i.e. in the case of negligible curvature effects.

Let us briefly summarise LE equations[1,6-8] for an incompressible nematic. The velocity and director time evolution equations are given by the expressions:

$$[\hat{\nabla} \cdot \sigma] = \rho \frac{d\mathbf{v}}{dt} \tag{1}$$

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

In the *velocity equation* (1) vector $\mathbf{v}(\mathbf{r},t) \equiv (v_x, v_y, v_z)$ is the velocity field of the fluid at a point $\mathbf{r}$ and time t, ρ is the bulk density, σ is the stress tensor; all the terms in the *director equation* (2) are function of the unitary vector $\mathbf{n} \equiv (n_x, n_y, n_z)$, which is the director field of the fluid at a point $\mathbf{r}$ and time t: $\mathbf{G}$ is the external force acting on the sample, $\mathbf{g}$ is the intrinsic director body force, π is the elastic tensor[9,10]. The stress matrix σ is given by the sum of an elastic term and a viscous term, which are rather complex functions of the viscoelastic properties of the nematic liquid crystal, defined by the elastic constants K_{11}, K_{22}, K_{33} and by Leslie coefficients $\alpha_i (i = 1,...6)$, and of the director and velocity components. The internal director body force $\mathbf{g}$ is defined in terms of derivatives of the velocity and director field and of derivatives of the elastic Frank free energy:

$$W = \frac{1}{2} K_{11} (\hat{\nabla} \cdot \mathbf{n})^2 + \frac{1}{2} K_{22} (\mathbf{n} \cdot \hat{\nabla} \times \mathbf{n})^2 + \frac{1}{2} K_{33} (\mathbf{n} \times \hat{\nabla} \times \mathbf{n})^2 \tag{3}$$

If a static magnetic field is applied, as in our case, the external force $\mathbf{G}$ acting on the director is $\mathbf{G} = \chi_a (\mathbf{H} \cdot \mathbf{n}) \mathbf{H}$, where χ_a is the anisotropy of the principal magnetic susceptibilities per unit volume[9,10].

THE MODEL

A Cartesian frame of reference $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ is identified. A point in space is $\mathbf{r} \equiv (x, y, z)$. The shear plane is coincident with the yz plane, and the shear flow is imposed along the $\mathbf{y}$ direction; the magnetic field $\mathbf{H}$ can be oriented along any arbitrary direction, and we shall discuss the case of parallel field (along $\mathbf{z}$)[11] and perpendicular field (along $\mathbf{x}$); the two parallel plates are arranged as shown in Figure 1 at a distance d, perpendicularly to the $\mathbf{z}$ directWe shall assume in the following that only dependence upon z is retained, i.e. that all components of director and velocity fields are functions of z and time only. From the condition of incompressibility, $v_{x,x}+v_{y,y}+v_{z,z}=0$, it follows that v_z is constant and uncoupled, so that it will be put equal to zero. Strong anchoring boundary conditions are chosen[11], for sake of simplicity, assuming that the director is aligned along $\mathbf{x}$ at all times at the boundaries:

$$\mathbf{n}(\pm d/2,t)=\mathbf{x} \tag{4}$$

whereas the velocity flow is controlled at boundaries by standard non-slip conditions:

$$\begin{aligned} &v_x(\pm d/2,t)=0 \\ &v_y(d/2,t)=vf(t),\ v_y(-d/2,t)=0 \end{aligned} \tag{5}$$

Different shear modes can be implemented by changing function $f(t)$ that defines the profile in time of the imposed motion. The shear rate parameter $\gamma = v/d$ will be used in the following to specify the order of magnitude, in s^{-1}, of the imposed shear.

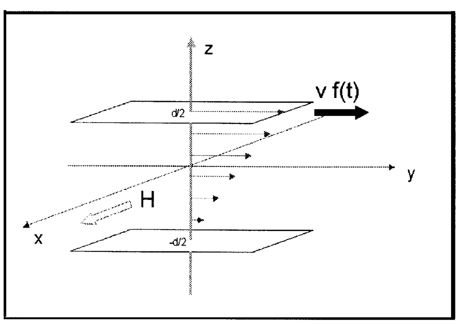


FIGURE 1 Geometrical setup with magnetic field along $\mathbf{x}$.

From the initial complete form of LE equations we can now develop a reduced system of five coupled partial differential equations for the three components of the director, subjected to the constraint $\mathbf{n}^2=1$, and the two components of velocity v_x and v_y [12]:

$$\gamma_1 \frac{\partial n_x}{\partial t} = \chi_a H^2 n_x + \lambda n_x - \alpha_2 \frac{\partial v_x}{\partial z} n_z + K_{22} \frac{\partial^2 n_x}{\partial z^2} + \\ + (K_{33} - K_{22}) \left(\frac{\partial^2 n_x}{\partial z^2} n_z^2 + 2 n_z \frac{\partial n_z}{\partial z} \frac{\partial n_x}{\partial z} \right) \tag{6}$$

$$\gamma_1 \frac{\partial n_y}{\partial t} = \chi_a H^2 n_y + \lambda n_y - \alpha_2 \frac{\partial v_y}{\partial z} n_z + K_{22} \frac{\partial^2 n_y}{\partial z^2} + \\ + (K_{33} - K_{22}) \left(\frac{\partial^2 n_y}{\partial z^2} n_z^2 + 2 n_z \frac{\partial n_z}{\partial z} \frac{\partial n_y}{\partial z} \right) \tag{7}$$

$$\gamma_1 \frac{\partial n_z}{\partial t} = \chi_a H^2 n_z + \lambda n_z - 2\alpha_3 \left(\frac{\partial v_x}{\partial z} n_x + \frac{\partial v_y}{\partial z} n_y \right) + \\ - (K_{33} - K_{22}) n_z \left[\left(\frac{\partial n_x}{\partial z} \right)^2 + \left(\frac{\partial n_y}{\partial z} \right)^2 \right] + K_{11} \frac{\partial^2 n_z}{\partial z^2} + \\ + (K_{33} - K_{22}) \left[\frac{\partial^2 n_z}{\partial z^2} n_z^2 + n_z \left(\frac{\partial n_z}{\partial z} \right)^2 \right] \tag{8}$$

$$\rho \frac{\partial v_x}{\partial t} = \frac{\partial}{\partial z} \left\{ \frac{1}{2} \frac{\partial v_x}{\partial z} \left[2\alpha_1 n_x^2 n_z^2 + (\alpha_3 + \alpha_6) n_x^2 + \alpha_4 + (\alpha_5 - \alpha_2) n_z^2 \right] + \\ + \frac{1}{2} \frac{\partial v_y}{\partial z} (2\alpha_1 n_z^2 + \alpha_3 + \alpha_6) n_x n_y + \alpha_2 n_z \frac{\partial n_x}{\partial t} + \\ + \alpha_3 n_x \frac{\partial n_z}{\partial t} \right\} \tag{9}$$

$$\rho \frac{\partial v_y}{\partial t} = \frac{\partial}{\partial z} \left\{ \frac{1}{2} \frac{\partial v_y}{\partial z} \left[2\alpha_1 n_y^2 n_z^2 + (\alpha_3 + \alpha_6) n_y^2 + \alpha_4 + (\alpha_5 - \alpha_2) n_z^2 \right] + \\ + \frac{1}{2} \frac{\partial v_x}{\partial z} (2\alpha_1 n_z^2 + \alpha_3 + \alpha_6) n_x n_y + \alpha_2 n_z \frac{\partial n_y}{\partial t} + \\ + \alpha_3 n_y \frac{\partial n_z}{\partial t} \right\} \tag{10}$$

For the cases explicitly discussed in the following sections, initial conditions are chosen *i)* aligning at time equal zero the director to $\mathbf{x}$ direction, $\mathbf{n}(z,0)=\mathbf{x}$, and *ii)* assuming that the initial velocity of the fluid is zero, $v_x(z,0)=v_y(z,0)=0$. The system of equations can be solved numerically, using a simple finite difference scheme in space combined with an accurate explicit solver in time.

RESULTS

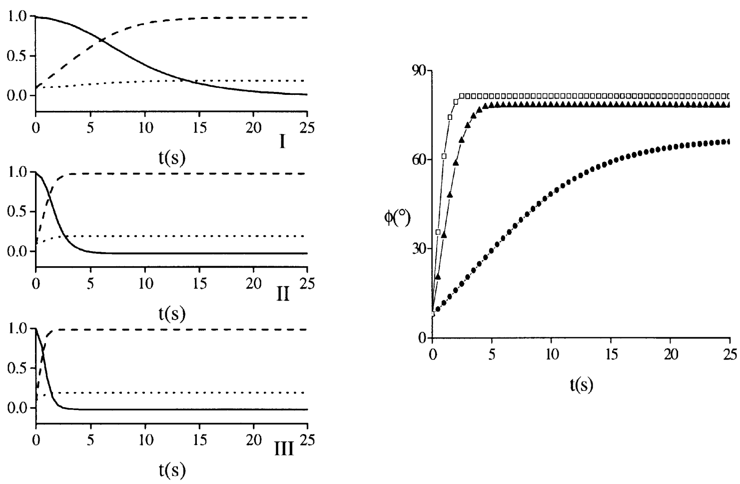
Several dynamical behaviours and cases of interest can be studied, in connection with interpretation of rheological and combined rheological and magnetic resonance experiments [13,14]. Here we shall present a necessarily limited overview of some general characteristics of the director and velocity fields dynamic in a prototype aligning nematic, MBBA (4-Methoxybenzylidene-4'-n-butylaniline) 10°C below the clearing point T_{NI} (viscoelastic coefficients are reported in Table 1), for a sample 50 μm thick; the intensity of the imposed magnetic field is specified in each case.

ρ (g/cm^3)	1.0
χ_a	10^{-7}
K_{11}, K_{22}, K_{33} (dyne)	5.3×10^{-7} 2.2×10^{-7} 7.45×10^{-7}
$\alpha_i\,(i=1,\ldots6)$ (poise)	-0.087 –0.052 –0.002 0.058 0.038 –0.016

TABLE 1 Viscoelastic parameters for MBBA (10° below T_{NI}).

We shall first analyse in some detail three cases of continuous shear, $f(t)=1$, in the absence of magnetic field, in the presence of a magnetic field along the $\mathbf{z}$ direction, i.e. in the shear plane, and in the presence of a magnetic field in the $\mathbf{x}$ direction, i.e. perpendicular to the shear plane.

If no magnetic field is applied, the steady alignment configuration depends only on the viscosity coefficients, mainly α_2 and α_3 [1]. The transient behaviour and the steady state of the director are shown in Figure 2, by representing the director components in the middle of the sample ($z = 0$) versus time (a) and the average angle $\phi = \int_{-d/2}^{d/2} dz \left| n_x(z,t) \right|$ formed by the director with the $\mathbf{x}$ axis in the whole sample (b).



(a) (b)

FIGURE 2 In absence of magnetic field: (a) Time evolution of director components n_x (straight line), n_y (dashed line), n_z (dotted line) at shear rate 1 s^{-1} (I), 5 s^{-1} (II), 10 s^{-1} (III). (b) Value of the average angle between $\mathbf{n}$ and the x direction at shear rate 1 s^{-1} (circles), 5 s^{-1} (triangles), 10 s^{-1} (squares).

Different shear rates are responsible for the time scale of the transient regime shown by the director, Figure 2(a): since the system is initially aligned to the $\mathbf{x}$ axis, the director rotates, aligning in the shear plane in a time which is roughly inversely proportional to the shear rate. In the steady state the director component along the initial x direction is negligible, as it is clear from Figure 2(b).

When a magnetic field is present, either aligned along $\mathbf{z}$ or $\mathbf{x}$, the final state depends also on the relative magnitude of the field itself and the shear rate[15,16]. In Figure 3(a) and 3(b), we show the director dynamic and steady state for the case of a pplane, and the final alignment is in agreement with simple analytical predictions[10].

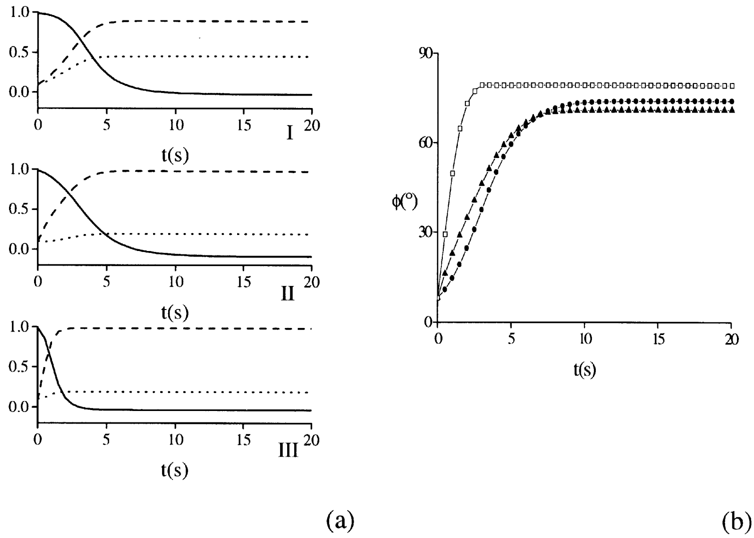


FIGURE 3 In presence of a magnetic field in the shear plane $H_z = 500G$: (a) Time evolution of director components n_x (straight line), n_y (dashed line), n_z (dotted line) at shear rate 1 s^{-1} (I), 5 s^{-1}(II), 10 s^{-1}(III). (b) Value of the average angle between **n** and the **x** direction at shear rate 1 s^{-1} (circles), 5 s^{-1} (triangles), 10 s^{-1} (squares).

If the field is aligned perpendicularly to the shear plane, different regimes can be observed, which depend upon the shear rate γ. In the first case, corresponding to low shear rates, the director remains aligned with the field. For high shear rates, on the contrary, the system aligns in the shear plane with the flow direction. An intermediate regime is shown corresponding to moderate shear rates, in which the balance of magnetic and mechanical torques induces the director to align out of the shear plane at some finite angle with the field, as shown in Figure 4(a) and (b). Predictions based on stability analysis[11] allow to estimate approximately the magnitude of critical shear rates above which the director starts to leave his initially preferred orientation with the magnetic field: a full dynamical calculation allows to estimate the transient director behaviour.

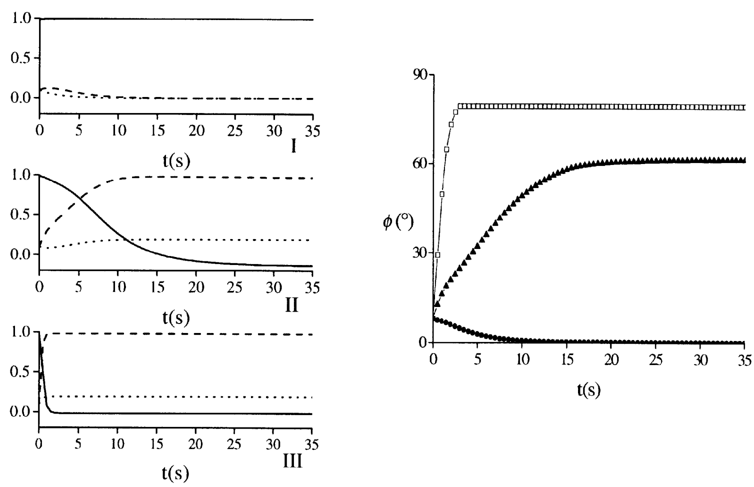
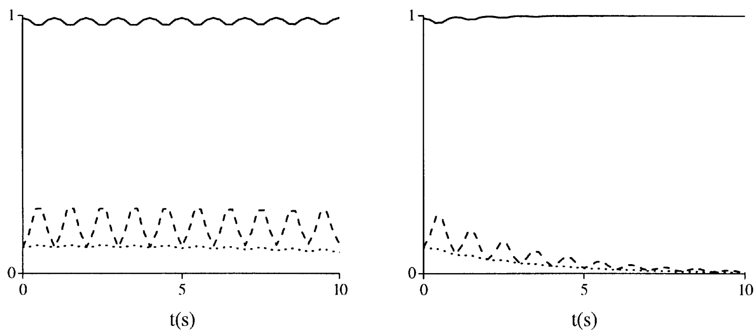


FIGURE 4 In presence of a magnetic field perpendicular to the shear plane $H_x = 500G$: (a) Time evolution of director components n_x (straight line), n_y (dashed line), n_z (dotted line) at shear rate 1 s^{-1} (I), 3.5 s^{-1}(II), 10 s^{-1}(III). (b) Value of the average angle between $\mathbf{n}$ and the $\mathbf{x}$ direction at shear rate 1 s^{-1} (circles), 3.5 s^{-1} (triangles), 10 s^{-1} (squares).

A second case of interest is given by a pulsed or oscillatory shear profile, $f(t) = sin(\omega t)$, where ω is a given frequency of oscillation[15]. We shall consider here only the case of sinusoidal shear in absence and in presence of a perpendicular field, for a moderate shear rate γ. In the first case, the director, initially aligned along $\mathbf{x}$ direction, will be subjected to a continuously changing velocity field. In Figure 5(a) the director components in the centre of the sample are shown again: the director oscillates in and out of the shear plane with a typical delay in phases and with frequencies which can be determined exactly from the numerical simulation. In Figure 5(b) the effect of the magnetic field does not allow the periodical motion of the director, but damps it forcing the re-establishment of the initial alignment.



(a) (b)

FIGURE 5 Oscillatory stress of frequency $\omega = 2\pi/5$ at shear rate 5 s^{-1}: time evolution of director components n_x (straight line), n_y (dashed line), n_z (dotted line) in absence of magnetic field (a) and in presence of a perpendicular magnetic field $H_x = 400G$.

CONCLUSIONS

A computational treatment of the hydrodynamical behaviour of an infinite planar sample of an aligning nematic liquid crystal in the presence of a magnetic field and shear has been presented.

The full dimensionality of both the director and velocity fields has been taken into account, to simulate orientations of the nematic director intermediate between the direction of alignment imposed by the field and the preferential direction of flow due to the shear.

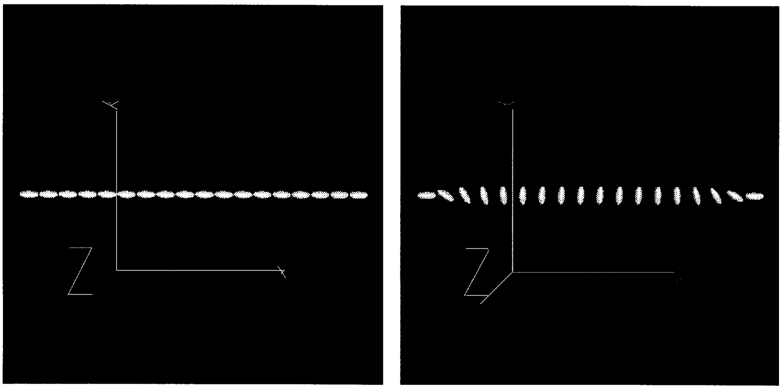


FIGURE 6 Snapshots at time 0 s and 5 s, in absence of magnetic field and at shear rate 10 s^{-1}, evidencing the homogeneous director distortion due to the shear stress in the nematic sample.

Two cases of shear have been analysed, continuous and oscillatory: in the first case the transient and stationary behaviour of the director has been shown to be dependent on the relative orientation field-shear, as the system attempts to compromise between competing magnetic and magnetical stresses; in the second case, it has been shown that the presence of a magnetic field perpendicular to the director of the oscillatory shear acts as a '*damping*' effect upon the periodical time evolution of the director. It should be stressed that since the analysis presented here is poised to consider truly infinite systems, with translational invariance along $\mathbf{x}$ and $\mathbf{y}$ directions, perpendicular to the direction $\mathbf{z}$ between plates, only a limited number of dynamic instabilities are allowed to the director. Transient and stationary periodic patterns, like the so-called 'rolling instabilities'[15,16], which are known to develop in finite sample with continuous or periodic shear and perpendicular magnetic field, cannot be predicted.

The generalization of the numerical technique presented here is possible, and preliminary results based of fully tridimensional treatments of Leslie-Ericksen nematodynamics equations show that periodic patterns are easily developed, together with several other director patterns, depending upon the shear time profile, intensity of magnetic field and viscoelastic parameters[17].

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