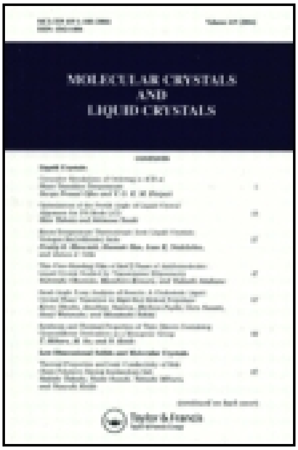

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Simulations of Flow-Induced Director Patterns in Nematic Liquid Crystals Through Leslie-Ericksen Equations in Two Dimensions

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A methodology for solving Leslie-Eriksen hydrodynamical equations in two dimensions is presented; applications to different geometries corresponding to common experimental set-ups are discussed. The non-linear system of partial differential equations, which describe the time evolution of the director field and of the velocity field for a nematic liquid crystal, are solved numerically. Time dependent distributions of the director orientations, influenced by competitive magnetic and mechanical torques are calculated to intepret rheological experiments.

Keywords: nematic liquid crystals; Leslie-Ericksen equations; rheology; hydrodynamics

Introduction by Professor David Dunmur[†]

In this last lecture of today we are honouring the memory of an outstanding scientist, Professor Pier Luigi Nordio from the Department of Physical Chemistry, University of Padova, who tragically died last October.

More than eighty percent of the scientists the world has known are alive and working today. Good science is immortal, but regretfully

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good scientists are not; the loss of any good person is a source of grief to family and friends, but the untimely death of an outstanding scientist who still had much to contribute to science is a greater loss.

Many here will be acquainted with the scientific work of Professor Nordio in the areas of esr, rotational diffusion, molecular dynamics and liquid crystals. For those who are perhaps not so familiar with Professor Nordio's seminal contributions, I would refer them to the web-site of theoretical chemistry at Padova. The scientific works of P L Nordio will live for ever, and will be a lasting memorial to his outstanding achievements as a scientist. But he was more than a great scientist, and I would like to say a few words about Pier Luigi Nordio the man.

Almost from the beginning of my interest in liquid crystals I was aware of the scientific work of Pier Luigi, and I formed a deep admiration for his work long before I met him. Indeed the power of his science was awe-inspiring, so meeting him for the first time in the late 1970's was something of a surprise. He was the most charming, approachable and communicative of men. Whoever he was speaking to would immediately feel relaxed in his presence, and to Pier Luigi everyone's opinion was valuable.

It was not until relatively recently that I became privileged to count myself as a friend of Pier Luigi and his family. In pushing forward the area of molecular design of liquid crystals, Pier Luigi and I combined two European Human Capital and Mobility Networks into a new European Training and Mobility of Researchers Network, of which he was the coordinator at the time of his death. This activity meant, for me, many weeks working with Pier Luigi, and a number of visits to Padova. It was during this period that I really came to appreciate Pier Luigi as more than a scientist.

No doubt like many other scientific visitors to Padova, I was treated to a guided tour of Venice, during which Pier Luigi revealed his origins as a proud Venetian. I also learnt of his other wide interests, he was a collector of ancient maps and old scientific texts, and I spent a number of happy hours with him searching through antique book fairs for new gems for him to purchase. Pier Luigi's breadth of interests and knowledge was daunting: history, geography, art, literature, philology, and he was something of an expert on North American Indian culture, an interest he shared with the Queen of Spain. He was a fount of knowledge about many things, but this knowledge was always revealed in a modest and humble fashion. Pier Luigi was a true scholar and teacher who could communicate with everyone.

Pier Luigi Nordio was a great man: an outstanding scientist certainly, but he was more than that. He can rightly claim the description as a Renaissance Man, but he was a Venetian as well, thus combining the very best of Italian culture and heritage. He is greatly missed by his family, friends and colleagues.

It is entirely appropriate that this evening's lecture in memory of Pier Luigi Nordio should be given by one of his more recent students, Dr Antonino Polimeno, who will present the lecture entitled "Simulations of Flow-induced Director Patterns in Nematic Liquid Crystals through Leslie-Ericksen Equations in Two Dimensions".

The basic equations of nematodynamics

Nematic liquid crystals[1,2] (NLC) are an example of non-Newtonian fluids; their hydrodynamical behaviour can be described using augmented equations[3,4] governing the time evolution of field variables associated to complex viscoelastic properties. Existing treatments are usually limited to static systems or neglect partially or completely backflow effects related to the coupling of the director and velocity field dynamics[5]. A complete numerical treatment, despite its complications, is important not only for the comprehension of the dynamics of nematics themselves, but also for the possibility of being extended to more complex liquid crystalline phases, i.e. cholesterics and smectics.

The general expressions of Leslie-Ericksen equations for an incompressible nematic are:

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

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

where in the velocity equation (1) the vector $\mathbf{v}(\mathbf{r},t)$ is the velocity field of the fluid at a point $\mathbf{r}$ and time t, ρ is the bulk density, $\underline{\underline{\sigma}}$ is the stress tensor; in the director equation (2) the unitary vector $\mathbf{n}$ is the director field of the fluid at a point $\mathbf{r}$ and time t, $\mathbf{G}$ is the external body force acting on the director, $\mathbf{g}$ is the intrinsic director body force, $\underline{\underline{\pi}}$ is the director stress tensor, and d/dt is the material time derivative.

The stress matrix is written in explicit form, using Einstein summation convention, as:

$$\sigma_{ij} = -p\delta_{ij} - \pi_{jk}n_{k,i} + \sigma'_{ji} \tag{3}$$

$$\sigma'_{ji} = \alpha_1 n_k n_p A_{kp} n_j n_i + \alpha_2 n_j N_i + \alpha_3 n_i N_j + \\ + \alpha_4 A_{ji} + \alpha_5 n_j n_k A_{ki} + \alpha_6 n_i n_k A_{kj} \tag{4}$$

The internal director body force is defined in terms of derivatives of the velocity and director field and of derivatives of the elastic energy W which are written explicitly in the Appendix. If a static magnetic field is applied, the external force acting on the director is:

$$G_i = \chi_a H_j n_j H_i \tag{5}$$

where χ_a is the anisotropy of the principal magnetic susceptibilities per unit volume. Franck free energy density is given as:

$$W = \frac{1}{2}K_{11}(\hat{\nabla}\cdot\mathbf{n})^2 + \frac{1}{2}K_{22}(\mathbf{n}\cdot\hat{\nabla}\times\mathbf{n})^2 + \frac{1}{2}K_{33}(\mathbf{n}\times\hat{\nabla}\times\mathbf{n})^2 \tag{6}$$

The viscoelastic properties of the NLC are defined by the elastic constants K_{11}, K_{22}, K_{33} and by the viscosity coefficients α_i (i=1,...,6), γ_1 and γ_2 which appear in the expressions for the non-equilibrium parts of the stress tensor (3) and the internal director body force (cfr. Appendix).

The model

Simplified equations can be obtained after introducing the following conditions[6], which are valid for a nematic fluid confined to two dimensions:

- The dependence of **v** and **n** upon the displacement along e_3 is neglected
- Components of **v** and **n** along the e_3 axis are set to zero.

Reduced equations can be recovered after some algebraic manipulations, and they can be applied to a number of different geometrical setups. Explicit formulas are reported elsewhere[6]. In this work we shall discuss applications to two different geometries (cfr. Figure 1):

a) Two infinite plates at a distance 2d move at the same velocity, but in opposite directions. $\phi(\mathbf{r},t)$ is the angle between the director and the direction of the applied magnetic field **H** (e_1 axis). A point in space is identified only by its position along the e_1 direction, since translational invariance along e_2 is invoked. This is equivalent to a Couette geometry used in actual rheological experiments, where the plates correspond to the walls of two very close coaxial cylinders. Different profiles for the shear velocity can be chosen by changing the function f(t) (see Figure 1).

b) The circle represents a transverse section of a cylinder of radius R. Cylindrical coordinates (r, θ), or cartesian coordinates (r_1, r_2) can be employed. The magnetic field is applied along the e_1 axis. The time dependence of the rotational impulse imposed to the vessel is described by the function f(t) which assumes a constant value if the rotation is continuous. This setup is suitable to simulate NMR and ESR experiments[7,8].

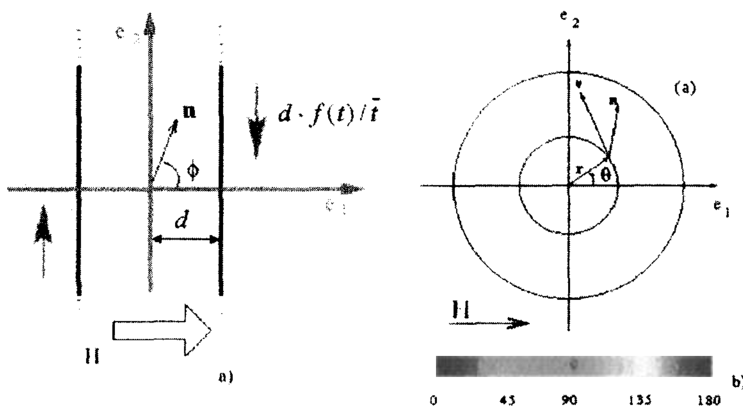


FIGURE 1. Geometrical setups
See Color Plate V at the back of this issue.

After a suitable scaling, the nematodynamics equations are specified in a convenient form for each geometry. Their solution requires a specification of boundary and initial conditions, though a precise definition of the behaviour of the fluid at the nematic-solid interface is difficult and dependent upon the experimental situation. Since the main purpose of this study is to outline an efficient methodology for treating nematics and interpret the main phenomena observed in magnetic resonance and in rheological experiments, very simple descriptions of the director and velocity fields at the interface have been considered. Newtonian behaviour is assumed for the velocity in the vicinity of the internal walls and simplified boundary conditions for the director can be imposed essentially in two ways: a) constant orientation of the director in the proximity of the walls (*strong anchoring*) or b) on the other extreme the effects of the walls on the director orientation are neglected (*weak anchoring*). Moreover at the beginning of each simulation, we assume that the system is at rest and fully aligned to the magnetic field.

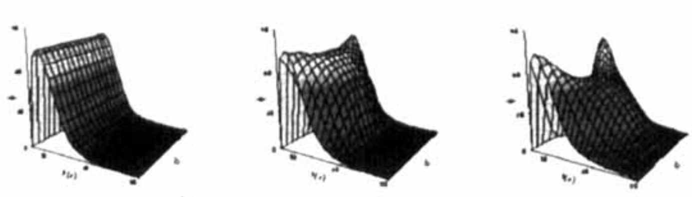
Results

Three examples are given below in order to illustrate the versatility of this approach. We have considered MBBA (4-Methoxybenzylidene-4'-n-butylaniline) as a typical nematogen for which viscoelastic parameters have been measured (Table 1).

Density [Kg / dm^3]	1.0
Magnetic susceptibility	10^{-7}
Leslie coefficients [Pa s]	-0.0087 -0.052 -0.002 0.058 0.038 -0.016
Elastic constants [N]	$5.3\ 10^{-12}$, $2.2\ 10^{-12}$, $7.45\ 10^{-12}$

TABLE. 1 Parameters used in the simulations for MBBA, 10 K below the clearing point

In the shearing flow experiment, sketched in Figure 1a, a pulsed velocity profile is applied: the plates shift at a constant scaled speed v/d 1.0 s^{-1} (d is the distance between the plates) for 5 s and then stop, while a constant magnetic field of 0.1T is applied. The director, as expected, relaxes towards aligning again with the field and its reorientation process can be explored through three dimensional plots (Figure 2), for sample thicknesses of 200 μm (a), 1000 μm (b), 20000 μm (c). Time, distance and ϕ are represented on the three axes. In the thinnest sample the response is quick and the system behaves rigidly. By increasing the distance between the plates, only in proximity of the walls one finds a rapid alignment along the shear direction, while in the core the response is slow. The threshold value of the angle reached by the director under the competitive effects of the applied field and the induced shear flow deformation has been estimated theoretically with a good agreement in the comparison with the numerical values.



a) b) c)

FIGURE 2 Time evolution of director orientation for infinite planar cells of thickness a) 200 μm, b) 1000 μm, c) 20000 μm
See Color Plate VI at the back of this issue.

From the analysis of the calculated results reported in Figure 2, one can infer the dependence of the director dynamics upon the thickness of the planar cell: the director tends to lag behind in the bulk of the sample for larger thicknesses, as an effect of the delay in adjusting to the velocity flux.

A different experimental setup is sketched in Figure 1b, for a cylindrical sample of a nematic liquid crystal. In Figure 3 director patterns at different times are shown for a tube rotating continuously; the radius of the cylinder is 5 mm and the intensity of the applied field is 0.3349 T. We use an extended colour map to describe the local orientations: values of ϕ range from 0°(blue), 45°(cyan), 135°(yellow), to 180°(red).

Complex patterns characterized by director vortices form and rapidly change. A thorough investigation is currently being performed to characterize the dynamical behaviour of the director patterns in dependence of the rotation speed, the radius of the cylinder, the boundary conditions imposed to the system[6]. Some general features can be already outlined: i) the system seems always to exhibit homogeneous director alignment with respect to the magnetic field for low values of the rotation speed; ii) unstable inhomogeneous patterns start to appear for rotation speeds close to the so called *critical speed*[1], $\chi_a H^2/2\gamma_1$, which discriminates in simplified treatments the regime of homogeneous alignment from the dynamical director regime; iii) for high rotation speeds the pattern dynamics is significantly changed and the director assumes a powder-pattern-like distribution with small fluctuations in time and space. In Figure 3 we show a typical example of the intermediate dynamical regime patterns for a rotation speed close to twice the value of the critical speed, i.e. 2.24 s^{-1}.

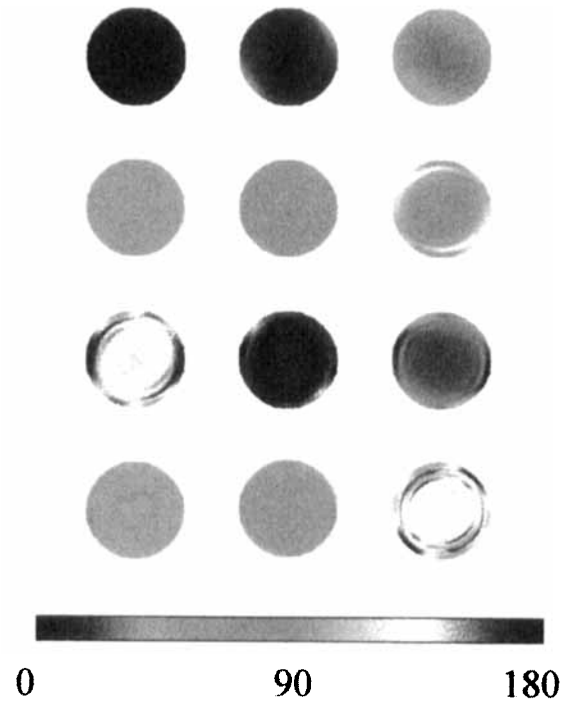


FIGURE 3 Time evolution of director patterns for a cylinder of radius 5 mm, rotating continuously with a rotation speed equal to 2.24 s^{-1}, at 0, 0.25, 0.5, 0.75, 1, 1.25, 1.5, 1.75, 2, 2.25, 2.5, 2.75, 3 s.
See Color Plate VII at the back of this issue.

Final remarks

The effort of working out a complete treatment of Leslie-Ericksen equations, at least in two dimensions, is rewarded by the abundance of informations obtained about director dynamics of nematic liquid crystals. Our aim is to go further in developing this methodology by taking into account the full spatial dependence in three dimensions, different boundary conditions and refining the geometrical and "mechanical" setups to compare directly with rheological experiments and to simulate transient behaviours of common devices based on the dynamical behaviours of nematics, like cells in liquid crystal displays.

Appendix

Quantities appearing in equations (2), (3) and (4) are written explicitly here in terms of spatial derivatives of the velocity and director fields [1,2].

$$\pi_{ji} = \partial W / \partial n_{i,j} \tag{7}$$

$$g_i = \lambda n_i - \partial W / \partial n_i + g_i' \tag{8}$$

$$g_i' = -\gamma_1 N_i - \gamma_2 n_j A_{ji} \tag{9}$$

$$N_i = dn_i/dt + \frac{1}{2}(v_{k,i} - v_{i,k}) n_k \tag{10}$$

$$A_{ji} = \frac{1}{2}(v_{j,i} + v_{i,j}) \tag{11}$$

Viscosity coefficients γ_1 and γ_2 are related to Leslie-Ericksen viscosities by the following expressions:

$$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_3 + \alpha_2 = \alpha_6 - \alpha_5 \tag{12}$$

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