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Nematic Liquid Crystal under Plane Oscillatory Flows

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We consider planarly oriented nematic liquid crystal subjected to plane, rectilinear, oscillatory Couette or Poiseuille flow in the case, when the director is initially perpendicular to the flow plane. Using the Galerkin method we found the critical amplitude of the flow at which the homogeneous instability develops. The analytical approximations for the frequency dependence of the critical amplitude for different types of flow are obtained. The results are compared with experimental data.

Keywords: nematic liquid crystal; oscillatory flow; instability

INTRODUCTION

The mean molecular orientation of a nematic liquid crystal (NLC) can be characterised by unit vector n (director). The strong coupling between the director and the velocity provides the setting of different types of flow instabilities^[1, 2]. A situation of particular interest is achieved when the director is perpendicular to the flow plane. The experiments with the steady shear flow in NLC^[3, 4] show, that at a certain value of shear rate S_h a homogeneous distortion of the director takes place. When a stabilising magnetic field H is applied along the initial director orientation, S_h increases. Furthermore, above a certain limiting magnetic field H_L , the nature of the instability changes: a pattern consisting of rolls parallel to the shear direction appears. The investigation of steady Poiseuille flow^[5] demonstrated the homogeneous instability, which appears at a certain value of the pressure gradient, but no roll instability was found. The mechanism of the homogeneous instability in steady flow was proposed in^[4] (Pieranski-Guyon mechanism). The theoretical description developed in [6, 7, 8] for the steady flow gives good agreement with the experimental results.

In the case of oscillatory Poiseuille flow both homogeneous and roll instabilities were found^[4, 5, 6, 7, 8, 9]. In nematics under oscillatory Couette flow only the rolls were observed. The simple model for the roll instability with square-wave excitation of the shear flow was proposed in^[4] with the threshold amplitudes is in good agreement with the experimental results. The same model has been analysed for instabilities under Poiseuille flow. The results agreed qualitatively with experimental data^[8].

In this work we present results of numerical stability analysis of the nematodynamic equations by a Galerkin method in the case of plane low-frequency oscillatory Couette and Poiseuille flow. The obtained approximate expressions for the critical flow amplitude for oscillatory shear and Poiseuille flow are compared with the results of direct numerical simulations. The influence of the shape of the flow excitation is analysed.

BASIC EQUATIONS

Consider the nematic layer of thickness d confined between two infinite parallel plates with strong planar anchoring. Oscillatory Couette flow can be produced by periodic motion of one of the plates in its plane. Oscillatory Poiseuille flow is obtained by applying an alternating pressure gradient at opposite ends of the cell. We choose the x axis along the flow direction and the z axis perpendicular to the confining plates. Thus, the director lies at the boundaries along the y axis. We use the dimesionless variables $\{\tilde{z}=z/d, \tilde{t}=t/\tau_d, \tilde{\omega}=\omega\tau_d, \tilde{\mathbf{v}}=\mathbf{v}\tau_d/d\}$, where $\tau_d=\gamma_1 d^2/K_{22}$ is the director relaxation time and ω is the circular frequency of the oscillations. In the frequency range $\omega \ll 1/\tau_v$ to be considered here (viscous damping time $\tau_v = \rho d^2/\gamma_1$ so that for $\rho \approx 10^3$ kg/m³, $d \approx 10^{-4}$ m and $\gamma_1 \approx 10^{-1} \, \mathrm{N \cdot s/m^2}$ one has $1/\tau_v \approx 10^4 \, \mathrm{s^{-1}})$ one can neglect the time derivative (inertia term) in the Navier-Stokes equation. When the director and the velocity depend only on z and t the nematodynamic equations^[1] have solution (basic state) $\{\mathbf{n^0} = (0,1,0), \mathbf{v^0} = (v_r^0,0,0), p^0\}$ for any flow amplitude, where the flow velocity satisfies

$$v_{x,x}^0 - p_{,x}^0 = 0. (1)$$

Here tildes are omitted and $\{v_r^0(z=1/2)=A\omega r_d/d\cos\omega t, v_x^0(z=-1/2)=0, p^0=0\}$ for Couette flow, $\{v_x^0(z=\pm 1/2)=0, p_{,x}^0=\frac{\Delta P}{\Delta x}\frac{r_dd}{\alpha_d/2}\cos\omega t\}$ for Poiseuille flow, A is the amplitude of the displacement of oscillating plate and $\Delta P/\Delta x$ is the amplitude of the pressure gradient along x axis. In order to test the stability of this solution we linearize the nematodynamic equations [1] around the basic state. We assume $\{\mathbf{n}=\mathbf{n}^0+\delta\mathbf{n},\ \mathbf{v}=0\}$

 $\mathbf{v}^0 + \delta \mathbf{v}, p = p^0 + \delta p\}$, where all perturbations δf are small with boundary conditions $\delta f(z=\pm 1/2)=0$. Solving the equation (1) and introducing the shear rate $S\equiv v_{x,z}^0$ one obtains $\{S=S^0\cos\omega t, S^0=\frac{\tau_d}{d}A\omega\}$ for Couette flow and $\{S=8S^0z\cos\omega t, S^0=\frac{\Delta P}{\Delta x}\frac{\tau_d}{\alpha_4}\frac{d}{4}\}$ for Poiseuille flow.

The linearized nematodynamic equations read

$$n_{x,t} - n_{x,zz} = \beta_1 S n_z n_{z,t} - k n_{z,zz} = -\beta_2 (S n_x + u_{,z}) -\mu u_{,zz} = \partial_z (\beta_2 n_{z,z} + \xi S n_x) - p_{,y}$$
(2)

where

$$n_x \equiv \delta n_x, \quad n_z \equiv \delta n_z, \quad u \equiv \delta v_y, \quad \beta_1 = -\alpha_2/\gamma_1,$$

$$\beta_2 = \alpha_3/\gamma_1, \quad k = K_{11}/K_{22}, \quad \gamma_1 = \alpha_3 - \alpha_2,$$

$$2\mu = (\alpha_3 + \alpha_4 + \alpha_6)/\gamma_1, \quad 2\xi = (\alpha_3 + \alpha_6)/\gamma_1.$$

Here α_i are the viscosity coefficients, K_{ii} are the elastic constants and the notation $f_{,i} \equiv \partial f/\partial i$ has been used throughout.

Let us collect all functions in vector $\mathbf{v} = (n_x, n_z, u)^T$. From the Floquet-theorem one can write the solution of Eqs.(2) in the general form

$$\mathbf{v} = e^{\sigma t} \sum_{n=1}^{\infty} \sum_{k=-\infty}^{\infty} \mathbf{v}_{nk} \phi_n(z) e^{ki\omega t}, \tag{3}$$

where σ is the growth rate and $\{\phi_n(z)\}$ is a set of orthogonal functions, such that $\phi_n(z=\pm 1/2)=0$ for every n. Substituting (3) into Eqs.(2) one obtain after projection and truncation a linear system for the expansion coefficients \mathbf{v}_{nk} in Eq.(3) of the form

$$(\mathbf{A} + S^{0}\mathbf{B})\mathbf{v} = \sigma \mathbf{C}\mathbf{v}. \tag{4}$$

If one assumes a stationary bifurcation i.e. $\Re(\sigma) = \Im(\sigma) = 0$ at the threshold, one has to solve the eigenvalue problem for $\sigma = 0$

$$\mathbf{A}^{-1}\mathbf{B}\mathbf{v} = -\frac{1}{S^0}\mathbf{v}.\tag{5}$$

The determination of S^0 using Eq.(5) is technically more convenient than using (4). We have always checked the consistency of the results obtained from (5) with the results of (4).

Calculations were performed for the MBBA material parameters (see Appendix) with z-modes n = 4..16 and time harmonics |k| = 3..7 for

frequency range 0.01 - 100 Hz. The relative error turned out to be smaller than $\sim 0.5\%$.

OSCILLATORY COUETTE FLOW

In this case the Eqs.(2) have two types of solutions with different z symmetry:

$$\{n_x(z) \text{ even/odd}, n_z(z) \text{ even/odd}, u(z) \text{ odd/even}\}$$

The solution corresponding to the first class [where $n_x(z)$ an even function of z] is following Manneville^[8] associated with an average twist. The second one [where $n_x(z)$ an odd function of z] is associated with an average splay. In additional the solutions of the Eqs.(2) can be splitted into two classes of time symmetry according to the different types of the parity of the time-harmonics in the Fourier expansion (3)

$$\{n_x(t) \text{ odd/even}, n_z(t) \text{ even/odd}, u(t) \text{ even/odd}\}$$

The corresponding solutions we call odd - time and even - time solutions, respectively. In the case of Couette flow the coefficients Eqs.(2) are independent of z. We used the set of trigonometric functions $\phi_n = \cos([2n-1]\pi z)$ for even functions and $\psi_n = \sin(2n\pi z)$ for odd functions in (3).

For rather small frequencies the threshold amplitude for homogeneous even-twist instability sets in first. When the flow frequency increased then at some point there is a crossover to an even-splay instability. The numerical analysis shows, that the odd-time solution does not become relevant at any frequency. The homogeneous instability was found only for the case $\alpha_3 < 0$. When α_3 goes to zero the critical amplitude goes to infinity. This agrees with the instability mechanism proposed by Pieranski and Guyon^[4].

To get an analytic estimate of the frequency dependence of the critical amplitude we truncate the expansion (3) at lowest order time- and z-harmonics. One obtains for the $\epsilon ven-twist$ solution, using $\phi_1(z) = \cos \pi z$, $\psi_1(z) = \sin 2\pi z$

$$S_{twist}^{osc} = \sqrt{2} S_{twist}^{st} \sqrt{1 + \left\{1 + \frac{32}{81} \frac{\beta_2^2 (8\beta_2^2 - 9\pi^2 \mu)}{\mu^2 \pi^2}\right\} \frac{\omega^2}{k^2 \pi^4}}$$
 (6)

with the critical shear rate for the steady flow instability

$$S_{twist}^{st} = 3\pi^3 \sqrt{\frac{k\mu}{\beta_1 \beta_2 (-9\mu\pi^2 + 16\xi)}}.$$

For the even-splay solution, using $\phi_1(z) = \sin 2\pi z$, $\psi_1(z) = \cos \pi z$ one obtains

$$S_{splay}^{osc} = \sqrt{2} S_{splay}^{st} \sqrt{1 + \left\{ \frac{1}{16} + \frac{8}{81} \frac{\beta_2^2 (32\beta_2^2 - 9\pi^2 \mu)}{\mu^2 \pi^2} \right\} \frac{\omega^2}{k^2 \pi^4}}$$
 (7)

with the critical shear rate for the steady flow instability

$$S_{splay}^{st} = 12\pi^3 \sqrt{\frac{k\mu}{\beta_1\beta_2(-9\mu\pi^2 + 64\xi)}}.$$

In Fig. 1 the frequency dependence for the critical flow amplitude $S_c^{osc}/(\omega\tau_d)=A/d$, obtained from numerical calculations and approximate expressions (6)-(7) for both *twist* and *splay z*-symmetry are plotted. In

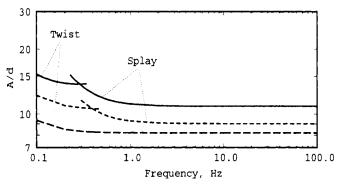


Figure 1: Critical amplitude for homogeneous instability in oscillatory Couette flow. Solid lines - numerical solutions. Dashed lines - approximation for even-twist (6), and even-splay (7) solutions. Long-dashed line - critical amplitude for the square-wave excitation (see text).

order to analyse the influence of the shape of Couette flow on the threshold of homogeneous instability the calculations for square-wave exitation $\{S=+S^0 \text{ for } 0<\omega t<\pi, S=-S^0 \text{ for } \pi<\omega t<2\pi\}$ were performed by direct simulations of Eqs.(2). The resulting curve (long-dashed) also presented in Fig. 1 lies lower than the curve corresponding to the sinusoidal excitation. A similar situation appears in the case of oscillatory Poiseuille flow and will be discussed in the Sec. Conclusion.

OSCILLATORY POISEUILLE FLOW

In the case of oscillatory Poiseuille flow the solutions of Eqs. (2) have the following types of z symmetry

$$\{n_x \text{ even/odd}, n_z \text{ odd/even}, u \text{ even/odd}\}$$

The time symmetry types are the same as in the case of oscillatory shear flow. Because of linear z-dependence of the coefficients in Eqs.(2) from

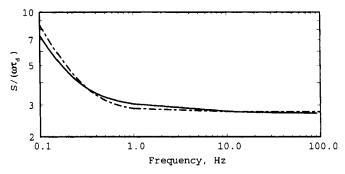


Figure 2: Critical amplitude for homogeneous instability in oscillatory Poiseuille flow. Solid line - numerical solution, corresponding to *even-twist* symmetry, dash-dotted line - approximate solution (8).

the basic flow we used the combination of Chebyshev polynomials $\{T_n(z) - T_0(z)\}$ for even n and $\{T_n(z) - T_1(z)\}$ for odd n as trial functions in (3). In contrast to the case of Couette flow, under Poiseuille flow only the even-twist homogeneous instability develops (Fig. 2). At a certain frequency ($\omega \tau_d \approx 10^6$), when the influence of the boundaries vanish, the time symmetry of the orientational instability changes from even to odd.

In order to obtain an approximate expression for the critical value of shear rate S we truncate the expansion (3) using $\phi_1(z) = -8z^2 + 2$, $\psi_1(z) = 32z^3 - 8z$. Then one has

$$S_{twist}^{osc} = \sqrt{2} S_{twist}^{st} \sqrt{1 + \left\{ \frac{1}{2} + \frac{\beta_2^2 \pi (4\mu - \beta_2^2)}{\mu^2} \right\} \frac{\omega^2}{1152k^2}},$$
 (8)

with the stationary Poiseuile flow threshold amplitude

$$S_{twist}^{st} = 8\sqrt{6}\sqrt{\frac{k\mu}{\beta_1\beta_2(-2\mu+\xi)}}.$$

In Fig. 3 the comparison between experimental data^[9] and our numerical results is presented. We used the MBBA material parameters, cell thickness $d=200\mu\mathrm{m}$ and $\Delta x=108$ mm were taken from^[9]. Since the

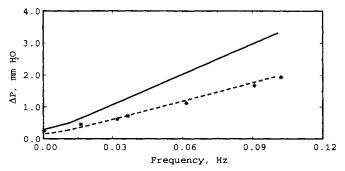


Figure 3: Critical amplitude of Poiseuille flow for different shapes of excitation. Stars are experimental points, solid line - numerical solution for the sinusoidal excitation, dashed line - square-wave excitation.

shape of excitation in^[9] was not controlled we performed the calculations of the critical amplitude for both sinusoidal and square-wave oscillatory Poiseuille flow.

CONCLUSION

We have studied the orientational instabilities in a nematic layer with the director oriented perpendicular to both the velocity and the velocity gradient under low-frequency oscillatory Couette and Poiseuille flow. For the flow-aligning nematics ($\alpha_3 < 0$) the basic state looses stability via a stationary bifurcation and the threshold amplitude decreases with increasing flow frequency. The obtained analytical approximation for the frequency dependence of the critical amplitude is in a good agreement with the results of direct numerical calculations.

The critical amplitude for the square-wave shape of excitation was found to be in $\approx \sqrt{2}$ smaller than for the sinusoidal one for both Couette and Poiseuille flow in agreement with the lowest order time Fourier expansion of Eqs.(2). One can see that in this case the square of the critical shear rate S^2 proportional to the time-average $< f^2(t) >$, where f(t) is the shape of excitation.

For oscillatory Poiseuille flow at the increasing of flow frequency the changing of the time symmetry of the unstable solution from even [with time-average $\langle n_x \rangle \neq 0$] to odd [$\langle n_x \rangle = 0$] was observed at $\omega \tau_d \approx 10^6$.

This is in agreement with the results of analysis developed in [10], where the preferred stable time-average director orientation in the bulk was found in the y-z plane at some angle with respect to the y axis.

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Appendix: Material parameters

Numerical simulations were performed for the following values of the MBBA material parameters at 25 °C [11, 12]:

$$K_{11} = 6.66, K_{22} = 4.2, K_{33} = 8.61$$
 (in units 10^{-12} N); $\alpha_1 = -18.1, \alpha_2 = -110.4, \alpha_3 = -1.1, \alpha_4 = 82.6, \alpha_5 = 77.9, \alpha_6 = -33.6$ (in units 10^{-3} N·s/m²).

We used the cell thickness $d = 40 \mu \text{m}$

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