

Article

Electrically Induced Hydrodynamic Effect in Nematics Caused by Volume Reduction

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Abstract: A pressure gradient caused by the local field-induced reduction of the effective molecular volume results in a flow of the nematic liquid crystal (NLC). Here, the hydrodynamics of homeotropically aligned NLC molecules under the influence of this pressure gradient was studied theoretically. The equations describing the system were written and solved in the steady-state case using analytical methods, and the stationary velocity of the observed flow was found. We discussed the obtained results and compared them with existing experimental results.

Keywords: nematic liquid crystal; hydrodynamics; volume reduction

1. Introduction

Liquid crystals (LCs) offer a broad range of applications in the industry thanks to their unique anisotropic properties [1]. Namely, the ability of LCs to easily change the orientation of molecules in response to external influences (electric and magnetic fields, pressure gradients, etc.) has led to their use in displays [2], microfluidic devices [3], and light modulators [4]. These types of materials also have structural similarities with some biological structures [5–7] and are, therefore, actively studied to identify the potential for biomedical applications. Another point that has to be mentioned is that liquid crystal-based researches also provide a better understanding of some physical processes (such as cell signaling [8]).

The widely studied method of director reorientation in LCs is based on the coupling of director field and hydrodynamic flow. In nematics, the hydrodynamic movements may be initiated in a variety of ways, including the use of light [9,10], acoustic pressure [11], and electric field [12,13], to mention but a few. Different mechanisms of hydrodynamical flow in nematic liquid crystal (NLC) (Rayleigh–Bernard mechanism [14], thermocapillary (Marangoni) mechanism [15], backflow effect [16], and direct volume expansion mechanism [9]) have been extensively studied both theoretically and experimentally. In this work, the electric field-induced hydrodynamical motions are of particular interest, considering their promising applications in microfluidics, MEMS, and so on [17–20]. Here we will theoretically investigate the dynamics of the field-induced hydrodynamic flow caused by the effective volume reduction mechanism [17] in homeotropically aligned nematics. The mechanism involves the following: the applied electric field reduces the effective molecular volume in the applied zone, generating pressure gradients that result in a Poiseuille flow [21]. A complete understanding of this effect can be useful for applications requiring the transport of various types of microparticles.

The paper is organized as follows. In Section 2, the aforementioned changes in local volume have been estimated using a phenomenological approach. Then we constructed corresponding equations for the description of hydrodynamical effects in NLC, and we solved these equations analytically. In Section 3, some numerical estimations are discussed. Section 4 contains the conclusions and a brief description of the next steps.



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2. Theory

As mentioned, here we discuss nematic LC, in which the molecules are oriented predominantly in one direction, the unit vector of which is called the director $\mathbf{n}$. A cell is considered, such as that described in [17], which contains a homeotropically aligned nematic liquid crystal (Figure 1). The normal to the cell's walls is along the z -axis, while the x -axis is located in the cell plane.

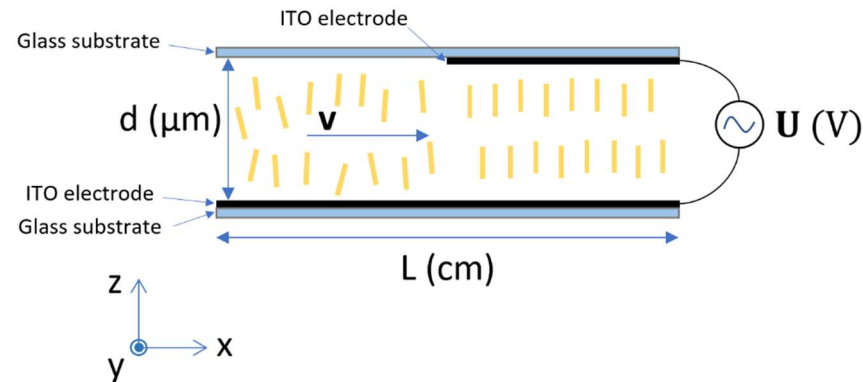


Figure 1. Schematic illustration of the considered cell: L is the length of the cell, and d is the distance between two substrates.

An electrical potential is applied to the right part of the LC cell. As a result, we have a higher orientation degree in the area of the applied field and, consequently, a reduction in the effective volume occupied by molecules. A pressure gradient, which in this case is caused by the local dielectric torque-induced reduction of the effective molecular volume, will result in a flow of the NLC. The authors in [17] observed the LC reorientation near the boundaries between two parts of the LC cell. This reorientation, in turn, can cause hydrodynamic flow; so-called backflow effects can be observed. As already explained by the authors in [17], this effect can support the observed material transport only at the early stage of the process since the characteristic relaxation time of the process is much shorter than the relaxation time of the director.

In this study, we assume the pressure gradient in the cell to be constant. We also make the simplifying assumptions that NLC is incompressible and that a Poiseuille flow with $\mathbf{v} = v\mathbf{e}_x$ will be created as the pressure gradient is along the x -axis, where $\mathbf{v}$ is the hydrodynamic velocity of the fluid in the cell. It is important to note that the incompressibility approximation is considered a good approximation when the flow velocities are well below the velocity of the sound [1]. Since, in this case, we only have very slow motions, this approximation can be used to describe the system.

Firstly, let us estimate the local volume change rate generated by the spatially non-uniform electric field by applying a phenomenological approach. It is possible to estimate the dependence of the LC density on the order parameter using the approach developed in [22]. The volume is proportional to the average distances of molecules along the x , y , and z directions. Therefore, using mean field theory, the following expression can be derived for the volume as a function of the order parameter [22,23]:

$$V(S) = \frac{4\pi R_0^3}{81h} N \left[\left(\frac{R_{\parallel}}{R_{\perp}} + 2 \right) - \left(\frac{R_{\parallel}}{R_{\perp}} - 1 \right) S \right]^2 \left[\left(\frac{R_{\parallel}}{R_{\perp}} + 2 \right) + 2 \left(\frac{R_{\parallel}}{R_{\perp}} - 1 \right) S \right], \quad (1)$$

where R_0 is effective hard sphere radius, $R_{\parallel}/R_{\perp}$ is the length to breadth ratio, h is the packing fraction, which is equal to the relation of the volume occupied by particles to the total volume, N is the number of molecules, and S is the order parameter.

The changes of the order parameter induced by electric fields in nematic liquid crystals are discussed in detail in [24]. In [24], it was reported that S is significantly increased by

applying an electric field E . For moderate values of E , that dependence is expected to be linear

$$\Delta S = aE \quad (2)$$

where a is the coefficient of linear dependence, which is given in the following form [24]:

$$a = \frac{k_B T S_0^{\frac{1}{2}} L_0^{\frac{1}{2}}}{4\pi K_3^{\frac{1}{2}} R_{\parallel}} \left(\frac{1}{K_1} + \frac{1}{K_2} \right) \frac{1}{|E_0|} \quad (3)$$

where k_B is Boltzmann constant, T is the temperature, S_0 is the non-zero order parameter in the absence of the electric field, K_i ($i = 1, 2, 3$) are the curvature elastic constants, $R_{\parallel}$ is the molecule length, E_0 is the molecular electric field and estimated as $\sim 1.7 \times 10^6$ V/cm, and $L_0 = (L_1 + L_2(1 + 3 \cos^2 \phi)/6)$, where L_1, L_2 are elastic constants and $\cos \phi = (\nabla S \cdot \mathbf{n})/|\nabla S|$ [24,25].

So, considering that the application of the electric field is expected to increase the order parameter S , from Equations (1) and (2), we can obtain the volume change induced by the field

$$\Delta V = V(S) - V(S_0) = -6V_0 S_0 \left(\frac{\frac{R_{\parallel}}{R_{\perp}} - 1}{\frac{R_{\parallel}}{R_{\perp}} + 2} \right)^2 \Delta S(E) \quad (4)$$

where V_0 is the volume in the isotropic phase, and S_0 is the order parameter in the absence of electric field. Thus, the rate of the volume change will be

$$\frac{\partial V}{\partial t} \approx \frac{\Delta V}{\tau} = -6V_0 S_0 \left(\frac{\frac{R_{\parallel}}{R_{\perp}} - 1}{\frac{R_{\parallel}}{R_{\perp}} + 2} \right)^2 \frac{aE}{\tau} \quad (5)$$

where τ is time characterizing the volume reduction process.

To describe the observed hydrodynamic effects in experiments, we need to write correct and fundamental equations to describe the system under study. Let us start with writing the Navier-Stokes equation for the hydrodynamic flow velocity $v(r, t)$ of an incompressible NLC. With the presence of the above-mentioned pressure, the equation has the following form [26]:

$$\rho \frac{\partial v}{\partial t} = -\frac{\Delta p}{L/2} + \eta \frac{\partial^2 v}{\partial z^2} \quad (6)$$

here ρ is the density of NLC, $\Delta p/(L/2)$ is the hydrodynamic pressure gradient, η is the viscosity constant, and L is the length of the cell (Figure 1). In turn, the hydrodynamic pressure gradient is caused by the incompressibility of NLC, which simply means that the decrease in liquid volume in one part of the cell is compensated for by the flow to the free volume.

$$l \int_0^d v(z, t) dz = \frac{\partial V}{\partial t} \approx \frac{\Delta V}{\tau} \quad (7)$$

where d is thickness of the cell, and l is its width.

By Solving Equation (6) in the steady-state case and substituting in Equation (7), we will have for stationary velocity

$$v(z) = -\frac{6}{ld^3} \frac{\Delta V}{\tau} (z^2 - zd) \quad (8)$$

The maximum velocity occurs at the middle plane of the cell, and it will be

$$v\left(\frac{d}{2}\right) \approx -\frac{6}{ld^3} \frac{\Delta V}{\Delta t} \left(\frac{d^2}{4} - \frac{d^2}{2} \right) = \frac{24\pi R_0^3}{h} N \frac{S_0 a E}{\tau l d} \quad (9)$$

3. Numerical Estimates

We can numerically estimate the stationary velocity of the flow using Equation (9). One can compare the theoretical and experimental results using experimental data from the [17]. Thus, we have a NLC cell with $L = 1.6$ cm and $d = 20$ μm ; $E = 2.5 \times 10^4$ V/cm. R_0 is the effective hard-sphere radius, and for 5CB it is $R_0 = 2.5 \times 10^{-8}$ cm. The length of the molecules of 5CB is 20 Å, and the width is 5 Å. So, for these molecules $R_{\parallel}/R_{\perp} = 4$. In Equation (9), h is the packing fraction, and for 5CB it is 0.3–0.8 [27].

From Equation (3) we can estimate the coefficient a considering that $R_{\parallel} = 20$ Å; $E_0 \sim 1.7 \times 10^6$ V/cm; $T = 293$ K; $L_0 \sim 10^{-6}$ dyn [24]; $S_0 \approx 0.5$; $k_B = 1.38 \times 10^{-16} \frac{\text{erg}}{\text{K}}$; $K_1 = 7 \times 10^{-7}$ dyn; $K_2 = 4 \times 10^{-7}$ dyn; $K_3 = 10^{-6}$ dyn [28]. So, for a we will have: $a \approx 8 \cdot 10^{-6} \text{ cgs} = 2.7 \times 10^{-8} \text{ cm/V}$.

We also need to estimate the number of molecules in the right part of the LC cell. The number of molecules per unit volume is $N_0 = \frac{\rho N_A}{M}$, where ρ is density and for 5CB, $\rho = 1.025 \frac{\text{g}}{\text{cm}^3}$; $N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$; $M = 249.3 \text{ g/mol}$. So, for N_0 we have $N_0 \sim 2.5 \times 10^{21} \text{ cm}^{-3}$ and for $N = N_0 \cdot \frac{L^2 d}{2} \approx 6.4 \times 10^{18}$.

The pressure difference ΔP , created by the change in the volume, can be estimated using the van der Waals equation. Given the accuracy that meets our purposes, one can roughly estimate it with a simpler equation $\Delta P \sim \frac{\rho R T}{M} \frac{\Delta V}{V}$, where $R = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ is the universal gas constant. The estimated value of ΔP is ~ 16.6 kPa. Using the Navier–Stokes equation, one can determine the flow velocity at the middle of the LC cell

$$v\left(\frac{d}{2}\right) = \frac{1}{2\eta} \frac{\Delta p}{L/2} \frac{d^2}{4} \quad (10)$$

Using the involved parameter values for velocity of flow we obtain $v\left(\frac{d}{2}\right) \approx 10.4 \mu\text{m/s}$.

In this case, the characteristic time of the process is the stabilization time, when the final volume change is established in the part of the LC cell where the field is applied. So, this characteristic volume reduction time should be the orientational relaxation time, which can be theoretically estimated by $\tau \approx \frac{\gamma d^2}{K_1 \pi^2} \approx 0.58 \text{ s}$ [29], where viscosity is $\gamma \approx 1$ P. So, using these estimations, the maximum stationary velocity during the relaxation process (when the electrical potential is abruptly switched off) will be $v\left(\frac{d}{2}\right) \approx \frac{24\pi R_0^3 N S_0 a E}{h \tau d} \approx 22.7 \mu\text{m/s}$. In the experiments [17], the recorded speed of movement of microparticles was $\sim 0.2 \mu\text{m/s}$ for an electrical potential of 50 V_{RMS} applied to the right area of the LC cell at 1 kHz. The difference between our theoretical calculations and experimental results can be explained by considering that we solved the Navier–Stokes equation in a steady-state case with a simple approximation without considering the effects associated with the various dissipations. For an accurate estimation of the speed of movement of microparticles (also considering their sizes), it is necessary to consider the viscosity of liquid crystals and those other dissipation effects.

4. Conclusions and Next Steps

It was shown that the volume reduction caused by the application of a spatially non-uniform electric field leads to a pressure gradient. Consequently, this pressure gradient induces material flow. The effective molecular volume changes induced by this external stimulus have been evaluated. The fundamental equations describing the system have been written. We solved these equations in the steady state case and estimated the stationary velocity of the flow induced by that volume reduction. The obtained results were compared with existing experimental results. However, there was a marked difference between our theoretical calculations and experimental results.

Nevertheless, this difference is understandable, considering that we solved the Navier–Stokes equation in a simplified steady-state case. In the future, we need to solve the Navier–Stokes equation, including the viscosity of LCs and the contributions of some

dissipation effects. Thus, the improvement of the theoretical model is one of the topics of our ongoing research.

As has already been mentioned, the characteristic relaxation time was of the order of seconds, but in experiments [17] the authors observed that the movement of particles continued during the entire time of the application of the electrical field (about half an hour). This problem is another interesting topic for us and will be part of future studies.

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