Thermally excited vortical flow in a microsized liquid crystal volume

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Abstract. The thermally excited vortical flow in a microsized liquid crystal (LC) volume has been investigated theoretically based on the nonlinear extension of the Ericksen-Leslie theory, with accounting the entropy balance equation. Analysis of the numerical results show that due to interaction between the gradients of the director field $\nabla \hat{n}$ and temperature $\nabla T$, caused by the focused laser radiation, the thermally excited vortical fluid flow is maintained in the vicinity of the heat source. Calculations have shown that the features of the vortex flow is influenced not only by the power of the laser radiation, but also by duration of the energy injection into the microsized LC volume.

1. Introduction

The manipulation of tiny amounts of molecular liquids has become a paradigm in various fields of applied chemistry, physics and biotechnology related microfluidics. The development of future biodynamics applications requires complicated investigation of natural anisotropic soft materials with multicoupling interactions of inner fields initiated by external forces. The problem of motion of an ultra-thin (a few microliters) liquid crystal (LC) drops confined in the microsized volume, under the influence of the temperature gradient, caused, for instance, by the laser beam, has drawn considerable interest \cite{1, 2, 3, 4}. The understanding of how the temperature gradient $\nabla T$, caused by induced heating in the interior of the microsized hybrid- aligned liquid crystal (HALC) volume, can produce the hydrodynamic flow is a question of great fundamental interest, as well as essential piece of knowledge in soft material science. This problem will be treated in the framework of the appropriate nonlinear extension of the Ericksen-Leslie theory \cite{4}, with accounting the thermoconductivity equation for the temperature field $T$ \cite{5}.

2. Formulation of the relevant equations for nematic fluids

We are concerned here with describing the way how the temperature gradient, caused by induced heating in the interior of the microsized HALC volume can produce the vortical flow $\mathbf{v}$ inside the microsized LC cell. The HALC volume is delimited by two upper and lower horizontal solid surfaces, located at $z = \pm 2d$, and two lateral solid surfaces at distance $2L$ on scale on the order of micrometers ($d \ll L$), respectively. The coordinate system defined by our task assumes that

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the director \( \mathbf{n} = n_x \hat{i} + n_z \hat{k} \) is in the \( XZ \) plane, where \( \hat{i} \) is the unit vector directed parallel to the horizontal restricted surfaces, which, in turn, coincides with the planar director orientation on the lower restricted surface \((\hat{i} \parallel \mathbf{n}_{x=-d})\), whereas the unit vector \( \hat{k} \) is directed parallel to the lateral restricted surfaces, which coincides with the planar director orientation on these surfaces \((\hat{k} \parallel \mathbf{n}_{x=\pm L})\), and homeotropic director orientation on the upper restricted surface \((\hat{k} \parallel \mathbf{n}_{x=d})\), whereas \( \hat{j} = \hat{k} \times \hat{i} \). Therefore, the hybrid aligned nematic phase contains a gradient of \( \nabla \mathbf{n} \) from planar orientation on the lower and both lateral surfaces to homeotropic orientation on the upper restricted boundary, i.e.,

\[
(n_x)_{x=\pm L,-d<x<d} = 0, \quad (n_x)_{-L<x<L,z=-d} = 1, \quad (n_x)_{-L<x<L,z=d} = 0.
\]  

We consider the temperature regime with the heat source \( O \) in the interior of the LC sample, whereas on the boundaries the temperature is kept constant

\[
T_{-L<x<L,z=\pm d} = T_{x=\pm L,-d<x<d} = T_0,
\]

and we will assume the no-slip boundary conditions for the nematic molecules on these solid bounding surfaces, i.e.,

\[
\mathbf{v}_{-L<x<L,z=\pm d} = \mathbf{v}_{x=\pm L,-d<x<d} = 0,
\]

where \( \mathbf{v} = u \hat{i} + w \hat{k} \) is the velocity vector with the horizontal \( u \equiv v_x(x, z, t) \) and vertical \( w \equiv v_z(x, z, t) \) components. Taking into account the microsized HALC volume, one can assume the mass density \( \rho \) to be constant across the sample, and thus deal with an incompressible fluid. The incompressibility condition \( \nabla \cdot \mathbf{v} = 0 \) assumes that

\[
u_x + w_x = 0,
\]

where \( u_x = \frac{\partial u}{\partial x} \), and \( w_x = \frac{\partial w}{\partial x} \).

The hydrodynamic equations describing the reorientation of the LC phase in 2D case, when the system is subjected to a temperature gradient \( \nabla T \), due to the heat source \( O \), can be derived from the torque balance equation

\[
\mathbf{T}_{el} + \mathbf{T}_{vis} + \mathbf{T}_{tm} = 0,
\]

where \([4] \mathbf{T}_{el} = \frac{\partial \mathbf{W}_{el}}{\partial \mathbf{n}} \times \mathbf{n} \) is the elastic, \( \mathbf{T}_{vis} = \frac{\partial \mathbf{R}_{vis}}{\partial \mathbf{v}} \times \mathbf{n} \) is the viscous, and \( \mathbf{T}_{tm} = \frac{\partial \mathbf{R}_{tm}}{\partial \mathbf{v}} \times \mathbf{n} \) is the thermomechanical torques, respectively (for details, see the Appendix in the Ref.[4]). The linear momentum equation for the velocity field \( \mathbf{v} \) can be written as

\[
\rho \frac{d \mathbf{v}}{dt} = \nabla \cdot \mathbf{\sigma},
\]

where \( \frac{d \mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + \mathbf{u} \times \mathbf{v} + \mathbf{w} \mathbf{v}_x \), \( \mathbf{\sigma} = \mathbf{\sigma}^{el} + \mathbf{\sigma}^{vis} + \mathbf{\sigma}^{tm} - \mathbf{P} \mathbf{E} \) is the full stress tensor (ST), and \( \mathbf{\sigma}^{el} = -\nabla \mathbf{W}_{el} \cdot (\nabla \mathbf{n})^T \), \( \mathbf{\sigma}^{vis} = \frac{\partial \mathbf{R}_{vis}}{\partial \mathbf{v}} \), and \( \mathbf{\sigma}^{tm} = \frac{\partial \mathbf{R}_{tm}}{\partial \mathbf{v}} \) are the ST components corresponding to the elastic, viscous, and thermomechanical forces, respectively (see the Appendix in the Ref.[4]). Here \( \mathbf{R} = \mathbf{R}^{vis} + \mathbf{R}^{tm} + \mathbf{R}^{th} \) is the full Rayleigh dissipation function, \( \mathbf{W}_{el} = \frac{1}{2} \left[ K_1 (\nabla \cdot \mathbf{n})^2 + K_3 (\mathbf{n} \times \nabla \times \mathbf{n})^2 \right] \) denotes the elastic energy density, \( K_1 \) and \( K_3 \) are splay and bend elastic coefficients, \( \mathbf{P} \) is the hydrostatic pressure in the HALC system, and \( \mathbf{E} \) is the unit tensor. When the temperature gradient \( \nabla T \) \(( \sim 1.0 \ [K/\mu m]) \) is set up, for instance, by means of the laser beam focused in the interior of the nematic volume, we expect that the temperature field \( T(x, z, t) \) satisfies the heat conduction equation \([4, 5]\)

\[
\rho C_P \frac{dT}{dt} = -\nabla \cdot \mathbf{q} + O(x, z),
\]
where $\mathbf{q} = -T \frac{\partial R}{\partial T}$ denotes the heat flow in the HALC system, $C_P$ is the heat capacity of the LC system, $\mathcal{O}(x, z) = \mathcal{O}_0 \exp \left[ -\frac{(x-x_0)^2 + (z-z_0)^2}{\Delta^2} \right] \mathcal{H}(t_{in} - t)$ is the heat source, $\mathcal{H}(t_{in} - t)$ is the Heaviside step function, $\mathcal{O}_0 = \frac{2}{3} \frac{\partial \psi}{\partial z}$ is the heat flow coefficient, $\alpha$ is the coefficient of absorption, $\mathcal{V}$ is the laser beam power, $\Delta$ is the Gaussian spot size, and $t_{in}$ is the duration of the energy injection into the LC sample.

The understanding of how the temperature gradient $\nabla T$, due to the heat source $\mathcal{O}$, can produce the vortical flow in the interior of the microsized HALC volume, will be provided by the solution of the dimensionless analog of balance equations (5), (6), and (7). The dimensionless torque balance has the form

$$n_x n_{x, \tau} - n_x n_{x, \tau} = \delta_1 [n_x M_{0, x} - n_x M_{0, z} + K_{31} (n_x f_{x, a} + n_x f_{z, a})]$$

$$+ \frac{1}{2} \psi_{xx} \left[ 1 + \gamma_21 \left( n_x^2 - n_z^2 \right) \right] - \frac{1}{2} \psi_{xz} \left[ 1 - \gamma_21 \left( n_x^2 - n_z^2 \right) \right]$$

$$+ 2 \gamma_21 \psi_{x, x} n_x n_z + \psi_{x} \bar{\mathcal{N}}_{x, z} + \bar{\mathcal{N}}_{x} \psi_{x, x} + \delta_2 \left( \chi_x \mathcal{L}_{x} + \chi_z \mathcal{L}_{z} \right). \quad (8)$$

The dimensionless linear momentum equation takes the form

$$\delta_3 \psi_{x, x} = a_1 \psi_{x, x, x, x} + a_2 \psi_{x, x, x, z} + a_3 \psi_{x, x, x, z} + a_4 \psi_{x, x, x, z} + a_5 \psi_{x, x, x, z} + a_6 \psi_{x, x, z} + a_7 \psi_{x, x, z} + a_7 \psi_{x, x, z} + a_7 \psi_{x, x, z} + a_7 \psi_{x, x, z} + a_1 \psi_{x, x} + a_2 \psi_{x, x}, \quad (9)$$

whereas the dimensionless entropy balance can be written as

$$\chi_{x, \tau} = \left[ \chi_x \left( \Lambda n_x^2 + n_x^2 \right) + (\Lambda - 1) n_x n_x - \chi_{x, \tau} \right]_{x, x}$$

$$+ \left[ \chi_z \left( \Lambda n_z^2 + n_z^2 \right) + (\Lambda - 1) n_z n_z - \chi_{x, \tau} \right]_{x, x}$$

$$+ \delta_4 \chi \left( \nabla \cdot \frac{\partial R_{1m}}{\partial \nabla \chi} \right) + \delta_5 \mathcal{O}(x, z, \tau) - \psi_{x} \chi_{x, x} + \psi_{x} \chi_{x, x}, \quad (10)$$

where $\tau = \frac{T}{T_1}$ is the dimensionless time, $t_T = \frac{\rho C_{p} d^2}{\Lambda}$, $\tilde{\psi} = \frac{t_T}{d} \psi$ is the scaled analog of the stream function $\psi$ for the velocity field $\mathbf{v} = \hat{u} \mathbf{i} + w \mathbf{k} = -\nabla \times \frac{1}{\tilde{\psi}} \tilde{\psi}$ (see the Appendix in the Ref.[4]), $\chi(x, z, \tau) = T(x, z, \tau) / T_{NI}$ is the dimensionless temperature, $T_{NI}$ is the temperature of the nematic-isotropic phase transition, $f = n_{x, x} - n_{x, z}, n_{x, \tau} = \frac{\partial n_x}{\partial T}, \mathcal{M}_0 = \nabla \cdot \mathbf{n}, \mathcal{N}_x = n_x n_{x, x} - n_x n_{x, z}, \mathcal{L}_x = n_x n_{x, x} - \frac{2}{3} n_x n_{x, z} + \frac{1}{2} n_x n_{x, z}, \mathcal{L}_z = -n_x n_{x, x} - \frac{2}{3} n_x n_{x, z} - \frac{1}{2} n_x n_{x, z}, \bar{x} = \frac{x}{\Lambda}$ and $\bar{z} = \frac{z}{\Lambda}$ are dimensionless space variables. Notice that the overbars in the space variables $x$ and $z$, as well as the stream function $\psi$ have been (and will be) eliminated in the last as well as in the following equations. The function $\mathcal{F} = \left( \sigma_{\xi x}^\tau + \sigma_{\xi x}^\tau - \sigma_{\xi x}^\tau - \sigma_{\xi x}^\tau \right)_{x, x} + \left( \sigma_{\xi x}^\tau + \sigma_{\xi x}^\tau \right)_{x, x} - \left( \sigma_{\xi x}^\tau + \sigma_{\xi x}^\tau \right)_{x, x},$ the coefficients $a_i (i = 1, ..., 12)$, the functions $\sigma_{ij}^\tau (i, j = x, z)$ and $\sigma_{ij} (i, j = x, z)$ are given in the Appendix of the Ref.[4]. The set of parameters of the LC system are: $K_{31} = \frac{K_{31}}{K_{11}}, \gamma_{21} = \frac{\gamma_{21}}{\gamma_{11}}, \Lambda = \frac{\gamma_{11}}{\gamma_{11}}, \delta_1 = \frac{\gamma_{11} K_{31}}{\gamma_{11}}, \delta_2 = \frac{\gamma_{11} T_{NI}}{\gamma_{11}}, \delta_3 = \frac{\rho C_{p} d^2}{\Lambda}, \delta_4 = \frac{\xi}{\Lambda, l_T},$ and $\delta_5 = \frac{2 \alpha}{\pi \sigma^2 \Lambda, l_T}.$

Exciting of the vortical flow in the HALC volume confined between two horizontal and two lateral solid surfaces, when the heating regime is produced by the tightly focused infrared laser heating, can be obtained by solving the system of nonlinear partial differential equations (8), (9), and (10) with the appropriate dimensionless boundary and initial conditions:

(i) Boundary conditions at the solid surfaces:

$$(n_x)_{x=\pm 10, -1 \leq x \leq 1} = 0, \quad (n_x)_{1 \leq x \leq 10, a = -1} = 0, \quad (n_x)_{-1 \leq x \leq 10, a = -1} = 1,$$

$$(\chi_{x})_{x=\pm 10, -1 \leq x \leq 1} = 0.97, \quad (\chi_{x})_{1 \leq x \leq 10, a = -1} = 0.97, \quad (\chi_{x})_{-1 \leq x \leq 10, a = -1} = 0,$$

$$(\psi_{x})_{x=\pm 10, -1 \leq x \leq 1} = (\psi_{x})_{1 \leq x \leq 10, a = -1} = (\psi_{x})_{-1 \leq x \leq 10, a = -1} = 0. \quad (11)$$
the parameters $\chi$ in Eqs. (8) - (10) has the following values [4]:

$$\chi \sim 10^{-3}, \chi_2 \sim 0.3, \chi_3 \sim 10^{-6}, \text{ and } \chi_4 \sim 10^{-4}.$$ 

Taking into account that the dimensionless temperature $\chi$ should be in the range of $[0.97 - 1.0]$, the parameters $\chi_5$ can be estimated as $\chi_5 \sim 7.0$. This estimation of $\chi_5 = \frac{2a_0}{\pi d_0^2} \frac{d^2}{\chi_0}$ was made taking into account the fact that the duration of the laser pulse of power $Q_0 \sim 0.05 \text{ W}$, for the infrared laser with the wavelength of 1061 $[\text{nm}]$, was $\tau_{in} \sim 3.2 \text{ ms}$. 

Using the fact that $\chi_3 \ll 1$, the equation Eq.(9) can be considerably simplified and takes the form

$$a_1 \psi_{xxxz} + a_2 \psi_{xxzz} + a_3 \psi_{xxxx} + a_4 \psi_{xxzz} + a_5 \psi_{xxxx} + a_6 \psi_{xxxz} + a_7 \psi_{xxzz} + a_8 \psi_{xxzz} + a_9 \psi_{xxxz} + a_{10} \psi_{xxxz} + a_{11} \psi_{xxzz} + a_{12} \psi_{zzzz} + F = 0,$$ (13)

where $a_i$ ($i = 1, \ldots, 12$) and $F$ are functions which have been defined in the Appendix of the Ref.[4].

3. Evolution of the velocity field under the influence of the temperature gradient

The calculations have been carried out by using both the relaxation [6] and the sweep [7] methods. Having obtained the initial distributions of the director and the temperature fields, as well as the function $F$, which is involved in Eq.(13), one can calculate, using the Eq.(13), the initial distribution of the stream function $\psi(x, z, \Delta \tau)$, corresponding to the first time step $\Delta \tau$. The next time step $\Delta \tau$ for the velocity and temperature fields, as well as for the director’s distribution across the LC sample is initiated by the sweep method. The stability of the numerical procedure for Eqs. (8), (9), and (13) was defined by the conditions [7]:

$$\frac{\Delta \tau}{\Delta \tau_0} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta z^2}\right) \leq \frac{3}{2}, \frac{3a_0}{(\Delta z)^2} - \frac{2a_0}{(\Delta x)^2} > 0,$$

where $\Delta x$ and $\Delta z$ are the space steps in the $x$ and $z$ directions, and $a_1$ and $a_5$ are the coefficients defined in Eq.(13). In the calculations, the relaxation criterion $\epsilon = |(\chi_{m+1}(x, z, \tau) - \chi_{m}(x, z, \tau))/\chi_{m}(x, z, \tau)|$ was chosen to be equal to $10^{-4}$, and the numerical procedure was then carried out until a prescribed accuracy has been achieved. Here $m$ is the iteration number.

Recently, the laser-induced heating has been used to inject the energy $O(x, z, \tau) = \delta_5 \exp \left[-\frac{(x-x_0)^2 + (z-z_0)^2}{2\Delta^2}\right]H(\tau_m - \tau)$ in the interior of the LC sample [4], where $\delta_5$ is the dimensionless heat flow coefficient, $\Delta$ is the Gaussian spot size, and $\tau_m$ is the duration of the energy injection into the LC sample. Note that the magnitude $\delta_5$ and duration $\tau_m$ of the heat injection are restricted only by the nematic phase stability condition. In the following the heating regime with $\delta_5 = 7$ will be considered.

Figure 1 shows the beginning of the vortex formation in the centre of the microsized LC volume during the first two time terms of the heating regime (Fig.1(a) $\tau_1 = 10^{-4}$ ($\sim 0.2 \text{ ms}$) and Fig.1(b) $\tau_2 = 2 \times \tau_1$) after switching on the laser irradiation focused in the interior ($x = 0.0$ and $z = -0.25$) of the LC sample.

The thermally excited flow in that case is characterized by maintaining two vortices, one biggest vortical flow in the vicinity of the heat source initiated by the laser beam and directed...
Figure 1. The evolution of the vortical flow inside the LC sample during the first two time terms of the heating regime (a) $\tau_1 = 10^{-4}$ ($\sim 0.2 \mu s$) and (b) $\tau_2 = 2 \times \tau_1$, respectively, after switching on the laser irradiation focused in the interior ($x = 0.0$ and $z = -0.25$) of the LC sample. Here 1 mm of the arrow length is equal to 1.3 nm/s, $O_0 = 0.05 \, W$, and the ratio $L/d$ is equal to 10.

in the negative sense (anticlockwise) around their center $x = 0.0$, $z \sim -0.25$, and one smallest vortical flow, which is settled down close to the upper restricted surface, around their center $x = 0.1$ and $z \sim 0.625$, respectively (see Figs.1(a)). According to our calculations the highest value of $v$ in the microsized HALC volume is reached in the vicinity of two points, first, $x = 0.0$ and $z = 0.25$ (directed in the negative sense) and second, $x = 0.0$ and $z = -0.75$ (directed in the positive sense), respectively. In that case there is the biggest horizontal flow $u \sim 0.048 \, [\mu m/s]$, directed both in the negative and positive senses (see Fig.1(a)). Our calculations also show that the laser beam with $O_0 = 0.05 \, W$ and $t_{in} \sim 3.2 \, \mu s$ can disturb the full HALC microvolume. Further calculations show that vortical flow in the vicinity of the heat source is gradually increased during the next few time terms of the heating regime $\tau_2 = 2 \times 10^{-4}$ ($\sim 0.4 \, \mu s$) (see Fig.1(b)), $\tau_3 = 4 \times 10^{-4}$ ($\sim 0.8 \, \mu s$) (see Fig.2(a)), and $\tau_4 = 8 \times 10^{-4}$ ($\sim 1.6 \, \mu s$) (see Fig.2(b)), until it reached maximum, after the time term of the heating regime $\tau_5 = \tau_{in} = 16 \times 10^{-4}$ ($\sim 3.2 \, \mu s$) (see Fig.3).

Figure 2. Same as in Fig.1, but for the next two time terms of the heating regime (a) $\tau_2 = 4 \times \tau_1$ and (b) $\tau_2 = 8 \times \tau_1$, respectively.

4. Conclusion
In summary, we have investigated the thermally excited vortical flow in a microsized HALC volume based on the nonlinear extension of the Ericksen-Leslie theory, with accounting the
Figure 3. Same as in Fig.1, but for the time term of the heating regime $\tau_5 = \tau_{in} = 16 \times \tau_1 (t_{in} \sim 3.2 \mu s)$.

The entropy balance equation. Analysis of the numerical results show that due to interaction between the gradients of the director field $\nabla \hat{n}$ and temperature $\nabla T$, caused by the focused laser radiation, the thermally excited vortical fluid flow is maintained in the vicinity of the heat source. Calculations have shown that the features of the vortex flow is influenced not only by the power of the laser radiation, but also by duration of the energy injection into the microsized LC volume.

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