Shear-Driven Mechanism of Temperature Gradient Formation in Microfluidic Nematic Devices: Theory and Numerical Studies †

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† Dedicated to the memory of Prof. W. Jeżewski.

Abstract: The purpose of this paper is to show some routes in describing the mechanism responsible for the formation of the temperature difference $\Delta T$ at the boundaries of the microfluidic hybrid aligned nematic (HAN) channel, initially equal to zero, if one sets up the stationary hydrodynamic flow $v_{st}$ or under the effect of an externally applied shear stress (SS) to the bounding surfaces. Calculations based on the nonlinear extension of the classical Ericksen–Leslie theory, supplemented by thermomechanical correction of the SS $\sigma_{zx}$ and Rayleigh dissipation function while accounting for the entropy balance equation, show that the $\Delta T$ is proportional to the heat flux $q$ across the HAN channel and grows by up to several degrees under the influence of the externally applied SS. The role of $v_{st} = u_{st}(z)\hat{n}$ with a sharp triangular profile $u_{st}(z)$ across the HAN in the production of the highest $\Delta T$ is also investigated.

Keywords: liquid crystals; microfluidics; hydrodynamics of anisotropic fluids

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1. Introduction

Consisting of anisotropic molecules, liquid crystal (LC) materials were called curious soft matter until their impressive impact on modern technology. The primary technological revolution was brought by these LC materials in the field of displays. With the development of the LC display market, the question arises about the following areas of application of LC materials. Perhaps there is no more suitable direction for the application of LC materials than LC sensors (LCSs) and LC actuators (LCAs) [1]. They have various advantages in comparison with other types of microsensors and microactuators; simple structure, high shape adaptability, easy downsizing, and low driving voltages. This is because LC materials are extremely sensitive to external disturbances and can be used for the construction of stimuli-responsive devices, such as LCSs or LCAs [1]. Nematic liquid crystal (NLC) channels or capillaries of appropriate size are microdevices in which the molecular orientations can be manipulated by forces applied macroscopically or can be generated locally within the microfluidic nematic channel [2] or capillary [3]. A challenging problem in all such systems is the precise handling of nematic microvolume, which in turn requires self-contained micropumps with small package sizes exhibiting either a very small displacement volume (displacement pumps) or a continuous volume flow (dynamic pumps). One of the pumping principle in the microsized LC channel confined between two infinitely long boundaries is based on the coupling between the tangential component of the shear stress (SS) $\sigma_{zx}$ and the director field $\hat{n}$, which describes the preferred orientation of the molecules, together with accounting the effect of the temperature gradient $\nabla T$ [4,5].
It has been shown that, due to the temperature gradient $\nabla T$, the horizontal hybrid aligned nematic (HAN) microfluidic channel, being initially at rest, starts moving in the horizontal direction if heated from below or above [6–8]. In the case when the director $\hat{n}$ is anchored homeotropically to the cooler ($T_{\text{lw}}$), lower boundaries and homogeneously to the hotter ($T_{\text{up}}$) upper boundaries, due to coupling between $\nabla T \sim \Delta T$ and $\nabla \hat{n}$, the hydrodynamic flow $v = v_x \hat{i} = u \hat{i}$ [7] in the horizontal direction is excited. Here, $\Delta T = T_{\text{up}} - T_{\text{lw}}$ is the temperature difference on the HAN boundaries, $d$ is the thickness of the HAN channel, and $\hat{i}$ is the unit vector taken parallel to the horizontal boundaries of the HAN channel (see Figure 1).

Figure 1. The geometry used for theoretical analysis.

The magnitude of the flow $v_x$ is proportional to $\sim \frac{d}{\eta} \sigma_{\text{tm}}^{\text{lm}}$ [6–8], where $\sigma_{\text{tm}}^{\text{lm}} \sim \xi \frac{\Delta T}{d^2}$ is the tangential component of the thermomechanical stress tensor $\sigma_{\text{tm}}$, $\eta$ is the viscosity, and $\xi$ is the thermomechanical constant [6]. The direction of the hydrodynamic flow $v$ is influenced by the character of the preferred anchoring of the average molecular direction $\hat{n}$ to the boundaries of the HAN channel and the heat flux $q$ across the bounding surface [7,8]. Measurements of the temperature of the induced flow were performed on the HAN cell [9], and the main result of that experimental study is the estimation of the thermomechanical constant $\xi \sim 10^{-12}$ J/K m [9].

Despite the fact that the possibility of formation of hydrodynamic flows in nematic channels under the influence of temperature gradients has been theoretically described since [6–8], only detailed numerical simulations performed within the framework of the extended Ericksen-Leslie theory [10,11] allowed us to recreate the complete picture of the formation of flows in nematic microchannels and capillaries. One of the aims of this paper is to describe the various regimes of hydrodynamic flow formation due to the interaction between the temperature and director field gradients obtained by numerical modeling of these processes. This paper is devoted to the possibilities of computational methods implemented in the framework of the nonlinear extension of the Ericksen–Leslie theory while accounting for the entropy balance equation [12]. Another purpose of our paper is to show some routes in describing the mechanism responsible for formation of the temperature difference $\Delta T$ on the boundaries of the HAN channel, being initially equal to zero, if one sets up the stationary hydrodynamic flow or under the effect of the externally applied shear stress to the bounding surfaces.

It should be noted that a whole class of confined active fluids under external shear stress [13–15] as well as the problem of thermomechanical coupling in cholesterics [16] are not included in the scope of our research interests. And this is despite the fact that research
in active matter has been fostered by many unexpected finding, ranging from spontaneous
flow to symmetry breaking in exotic active emulsions.

This is the first review to describe the role of thermomechanical force in the formation
of hydrodynamic flow in microsized nematic channels and capillaries in detail. It is based
on the nonlinear extension of the Ericksen–Leslie theory, supplemented by thermomechanical
-rotation of the director out from the

which the director rotates out from the

x

with respect to the direction of the flow velocity v

with the unit vector ̂\alpha

for two types of nematic phases: first, for the “laminar” case of nematic phase, when
the shear stress σ

strongly anchored to both boundaries under the influence of the tangential component of
the nematic flow

the director should be noted here [20]. In this case, there is a certain value of the shear rate, above
the director tumbles under the shear flow of the nematic.

in the shear flow. It is clear from Equation (1) that, if

|\gamma_2| > \gamma_1[17–19]. For

It has been thought that, in shear flows, the dynamics of nematics always produces an
alignment regime, where the director ̂n aligns at a stationary angle [17–19],

\theta_{st} = \frac{1}{2} \cos^{-1}(-\gamma_1/\gamma_2) = \frac{1}{2} \cos^{-1}\left(\frac{\gamma_1^{-1}}{\gamma_2}\right) = \tan^{-1}\left(\sqrt{\frac{a_3}{a_2}}\right),

with respect to the direction of the flow velocity v_{st} = \gamma y \hat{i}, when the hydrodynamic torque,

T_{vis} = \frac{\gamma_1}{2} (1 + \gamma_2 \cos 2\theta_\gamma) \hat{j} = \left[(a_3 \cos^2 \theta - a_2 \sin^2 \theta) \gamma_1\right] \hat{j},

exerted per unit LC volume in a shear flow vanishes. Here, \gamma_1 = -\gamma_2/\gamma_1, \gamma_1 = a_3 - a_2 and
\gamma_2 = a_3 + a_2 are the rotational viscosity coefficients (RVCs), a_2 and a_3 are the Leslie
coefficients, and \gamma = \partial v_x/\partial z is the shear rate. However, it has been found that some LC
materials exhibit an unusual type of instability, when the director ̂n continuously rotates
in the shear flow. It is clear from Equation (1) that, if |\gamma_1| > |\gamma_2| or a_3 > 0 (because, in
practice, a_2 < 0), then no real solution for \theta_{st} exists. Physically, this means that, in this case,
the director tumbles under the shear flow of the nematic.

An interesting aspect of the tumbling rotation of the director’s field in the shearing
flow should be noted here [20]. In this case, there is a certain value of the shear rate, above
which the director rotates out from the x – z plane, and there is a steady-state solution
without tumbling.

Among the many questions that arise in this connection, we are interested in two.
First, how does the viscous torque T_{vis} = \frac{2}{\gamma^2}(1 + \gamma_2 \cos 2\theta_\gamma) \hat{j} affect the character of
the director field ̂n (or the polar angle \theta) evolution to its stationary orientation ̂n_{st} with
respect to the nematic flow v_{st} = u_{st} \hat{i} in the microsized HAN channel when the director is
strongly anchored to both boundaries under the influence of the tangential component of
the shear stress \sigma_{xz} while accounting for the temperature gradient \nabla T? This is investigated
for two types of nematic phases: first, for the “laminar” case of nematic phase, when
\gamma_2 > 1, and, second, for the “tumbling” case of nematic phase, when \gamma_2 < 1 [17–19]. For
instance, the liquid crystal composed of 4-\textit{cyano}-4'-\textit{pentylibiphenyl} (5CB) molecules belongs to the laminar nematic phase, whereas the liquid crystal composed of 4-\textit{cyano}-4'-\textit{octylibiphenyl} (8CB) molecules [21] belongs to the tumbling nematic phase. Second, is it possible to set up a temperature difference \( \Delta T \) across the HAN microfluidic channel, initially being equal to zero, under the action of the tangential component of the shear stress \( \sigma_{zx} \) applied to the boundary of the LC channel?

The answers to these questions are given within the framework of the nonlinear extension of the classical Ericksen–Leslie theory \([10,11]\), supplemented by thermomechanical correction of the shear stress and Rayleigh dissipation function while taking into account the entropy balance equation \([12]\). It has recently been shown, both experimentally \([22]\) and numerically \([23]\), that only stationary flow \( u_{st} \) with a triangular sharp profile and position of the maximum in the vicinity of the restricted boundaries may achieve the highest temperature difference \( \Delta T = T_{up} - T_{lw} \) in the HAN microfluidic channel of few degrees. By means of other hydrodynamic flow with profiles, which cannot demonstrate the sharp growth of \( u_{st} \) across the HAN channel, one can achieve the same result only by using of the “high-speed” hydrodynamic flow \( \sim 0.1 \text{\,µm/s} \) \([22]\). However, taking into account that some LC systems driven by external SS exhibit such non-equilibrium phenomena as a tumbling behavior \([7,8,23]\), the mechanical description can shed some light on the problem of temperature gradient formation; when under certain conditions, the thermomechanical force can overcome elastic, viscous, and anchor forces and cause a temperature gradient across the HAN channel.

2.1. Formulation of the Relevant Equations for Dynamical Reorientation in Microsized Nematic Fluids

First, we consider the description of the physical mechanism responsible for the shear-driven nematic flow in microfluidic hybrid aligned nematic (HAN) channels under the action of the external shear stress applied to the upper boundary of this channel (see Figure 1):

\[
(s_{zx}(z))_{z=d} = s_{zx}^0,
\tag{3}
\]

We consider a hybrid aligned channel composed of both the laminar and tumbling types nematics, which is bounded by two horizontal surfaces at a distance of \( d \) on a scale of the order of tens of micrometers. According to this geometry, the director is maintained in the \( xz \)-plane (or in the \( yz \)-plane), defined by the heat flux \( q = Q_0 \hat{k} \) normal to the horizontal boundaries of the LC channel. As we deal with the HAN channel under the influence of both the SS \( s_{zx}^0 \) and the heat flux \( q \) perpendicular to the HAN channel, taking into account the fact that the length of the channel \( L \) is much greater than the thickness \( d \), it can be assumed that the component of the director \( \hat{n} = n_x \hat{i} + n_z \hat{k} = \sin \theta(z,t) \hat{i} + \cos \theta(z,t) \hat{k} \) as well as the rest of the physical quantities depend only on the \( z \)-coordinate and time \( t \). Here, \( \theta \) denotes the angle between the director and the unit vector \( \hat{k} \) (see Figure 1). In order to understand how the viscous \( T_{vis} \), elastic \( T_{el} \) and thermomechanical \( T_{tm} \) torques as well as the tangential component of the shear stress \( \sigma_{zx} \) affect the character of the director field \( \hat{n} \) evolution to its stationary orientation with respect to the nematic flow \( \mathbf{v} \), we must formulate the boundary conditions for the temperature \( T(z,t) \), velocity \( \mathbf{v} \), and the director \( \hat{n} \) fields.

We consider a hydrodynamic regime where the HAN channel is subjected to uniform heating from above, for instance by the laser irradiation \([24]\), while director \( \hat{n} \) is strongly anchored to both solid surfaces, homeotropically to the lower cooler \( (T_1) \), and homogeneously to the upper bounding surfaces, where

\[
\theta(z)_{z=d} = \frac{\pi}{2}, \quad \theta(z)_{z=0} = 0,
\tag{4}
\]

whereas the boundary conditions for the temperature field are
Here, $\lambda_\perp$ is the heat conductivity coefficient perpendicular to the director $\hat{n}$ whereas $Q_0$ is the heat flux across the upper boundary. As a result, we obtain a picture where there is a balance between the heat flux $\mathbf{q}$; SS $c_{0,i}^{el}$; and the viscous, elastic, and anchoring forces, and in general, the LC fluid settles down to a stationary flow in the horizontal direction [7,8].

Under the assumption of an incompressible fluid, the hydrodynamic equations describing the orientation dynamics induced by both SS and $\mathbf{q}$ can be derived from the torque, linear momentum, and the entropy balance equations for such a LC system.

Taking into account the micro-size of the HAN channel, we can assume that the mass density $\rho$ is constant across the LC film, and thus, we deal with an incompressible liquid. The incompressibility $\nabla \cdot \mathbf{v} = 0$ implies that there is only one nonzero component of the vector $\mathbf{v}$, viz. $\mathbf{v}(z,t) = u(z,t)\hat{i}$.

If the director is disturbed by both the shear stress $c_{0,i}^{el}$ and the heat flux $\mathbf{q}$ generated by the uniform heating from above, the relaxation of $\hat{n}$ in the HAN channel is governed by elastic $\mathbf{T}_{\text{elast}} = \frac{\partial W_F}{\partial \hat{n}} \times \hat{n}$, viscous $\mathbf{T}_{\text{vis}} = \frac{\partial W_F}{\partial \hat{n}} \times \hat{n}$, and thermomechanical $\mathbf{T}_{\text{im}} = \frac{\partial R^{\text{im}}}{\partial \hat{n}} \times \hat{n}$ torques exerted per unit LC's volume. Here,$$
R^{\text{vis}} = \frac{1}{2} h(\theta) u_z^2 - \gamma_1 A(\theta) \theta_z u_z + \frac{1}{2} \gamma_1 \theta_2^2 \quad \text{is the viscous,} \quad R^{\text{im}} = \frac{\partial \theta}{\partial t} + \frac{1}{2} \sin^2 \theta \quad \text{is the thermomechanical,}\n$$and $R^{\text{th}} = \frac{1}{2} \left( \lambda_\parallel \cos^2 \theta + \lambda_\perp \sin^2 \theta \right)$ is the thermal contributions to the full Rayleigh dissipation function $R = R^{\text{vis}} + R^{\text{im}} + R^{\text{th}}$ [7,8]. The set of functions $h(\theta) = a_1 \sin^2 \theta \cos^2 \theta - \gamma_1 A(\theta) + \frac{1}{2} a_4 + g(\theta)$, $A(\theta) = \frac{1}{2} (1 + \gamma_2 \cos 2\theta)$, and $g(\theta) = \frac{1}{2} (a_6 \sin^2 \theta + a_8 \cos^2 \theta)$ are the hydrodynamic functions, $u_z = \partial u(z,t)/\partial z$, $\theta_z = \partial \theta(z,t)/\partial z$, $\gamma_1 = \partial \gamma(z,t)/\partial t$, and $T_z = \partial T(z,t)/\partial z$, whereas $a_i (i = 1, \ldots, 6)$ are six Leslie coefficients, and $\lambda_\parallel$ and $\lambda_\perp$ are the heat conductivity coefficients parallel and perpendicular to the director $\hat{n}$, respectively. In turn, $W_F = \frac{1}{2} \left[ K_1 (\nabla \cdot \hat{n})^2 + K_3 (\hat{n} \times \nabla \times \hat{n})^2 \right]$ denotes the elastic energy density, $K_1$ and $K_3$ are the splay and bend elastic constants, and $\hat{n}_J = \frac{\partial \hat{n}}{\partial t}$ is the material derivative of the director $\hat{n}$.

The hydrodynamic equations describing the reorientation dynamics in our case, when there is the heat flux $\mathbf{q}$ through the upper boundary of the HAN microfluidic channel and under the action of SS $c_{0,i}^{el}$, can be obtained from the torque balance equation [7,8]

$$\mathbf{T}_{\text{elast}} + \mathbf{T}_{\text{vis}} + \mathbf{T}_{\text{im}} = 0,$$}

whereas the Navier–Stokes equation can be written as [7,8]

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot \sigma.$$}

where $\rho$ is the mass density of the nematic phase; $\sigma = \sigma^{\text{elast}} + \sigma^{\text{vis}} + \sigma^{\text{im}} - \mathcal{P} \mathcal{I}$ is the full ST; and $\sigma^{\text{elast}} = -\frac{\partial W_F}{\partial \hat{n}} \cdot (\nabla \hat{n})$, $\sigma^{\text{vis}} = \frac{\partial W_F}{\partial \hat{n}}$, and $\sigma^{\text{im}} = \frac{\partial R^{\text{im}}}{\partial \hat{n}}$ are the ST components corresponding to the elastic, viscous, and thermomechanical forces, respectively, while $\mathcal{P}$ is the hydrostatic pressure in the HAN microsized channel and $\mathcal{I}$ is the unit tensor.

When the temperature gradient $\nabla T$ is set across the HAN channel, we expect that the temperature field $T(z,t)$ satisfies the entropy balance equation [7,8,12]

$$\rho C_P \frac{dT}{dt} = -\nabla \cdot \mathbf{Q},$$}

where $C_P$ is the specific heat at constant pressure, and $\mathbf{Q}$ is the heat flux.
where $Q = -T \frac{\partial P}{\partial T}$ is the heat flux and $C_P$ is the heat capacity of the liquid crystal phase.

To describe the evolution of the director field $\mathbf{n}$ (or the polar angle $\theta(z,t)$) to its stationary orientation $\mathbf{n}_0(z)$ and exciting the velocity field $v(z,t)$ caused by both the heat flux $q$ and the external SS $\sigma^0_{zz}$, we consider the dimensionless analog of the torque and linear momentum balance equations as well as the entropy balance equation.

The dimensionless torque balance equation describing the reorientation of the director field $\mathbf{n}$ (or the polar angle $\theta(z,t)$) to its stationary orientation $\mathbf{n}_0(z)$ can be written as [7,8]

$$\tau_1(\chi)\theta_{\tau} = \mathcal{A}(\theta)u_{zz} + (\mathcal{G}(\theta)\theta_{zz} - 1/2\mathcal{G}_\theta(\theta)\theta_{zz}^2 - \delta_1 \chi_{zz} \theta_z^2 \left( 1 + \sin^2 \theta \right)),$$

where $\mathcal{G}(\theta) = \sin^2 \theta + K_{31} \cos^2 \theta$, $\mathcal{G}_\theta(\theta)$ is the derivative of $\mathcal{G}(\theta)$ with respect to $\theta$, $\chi(z,t) = T(z,t)/T_{NI}$ is the nematic temperature, $T_{NI}$ is the nematic-isotropic (NI) transition temperature, $\theta_{zz} = \partial^2 \theta(z,t)/\partial z^2$, $\chi_{zz} = \partial^2 \chi(z,t)/\partial z^2$, $K_{31} = K_3/K_1$, $K_1$ and $K_3$ are the splay and bend elastic constants of the nematic phase, $\tau = (K_{10}/\gamma_{10}^2) t$ is the dimensionless time, $z = z/d$ denotes the dimensionless distance away from the lower solid surface, $\mathcal{A}(\theta) = \theta K_{10}$ is the dimensionless velocity, $\tau_1(\chi) = \gamma_1/\gamma_{10}$ is the dimensionless RVC, $\delta_1 = \xi T_{NI}/K_{10}$ is the parameter of the nematic system, and $\xi \sim 10^{-12} J/mK$ is the thermomechanical constant [9]. Notice that the overbars in the space variable $z$ and velocity $u$ have been eliminated and that $\gamma_{10}$ and $K_{10}$ are the highest values of the RVC $\gamma_1(\chi)$ and the splay constant $K_1(\chi)$ in the temperature interval $[\chi_1, \chi_2]$ belonging to the nematic phase. In the case of an incompressible fluid. The dimensionless Navier–Stokes equation reduces to [7,8]

$$\delta_2 u_{\tau}(z,t) = \sigma_{zz} = \left[ \hbar(\theta)u_{zz} - \mathcal{A}(\theta)\theta_{\tau} - \delta_1 \chi_{zz} \theta_z \sin^2 \theta \left( 1 + \frac{1}{2} \sin^2 \theta \right) \right]_{zz},$$

$$\mathcal{P}_{zz}(z,t) + \frac{\partial \mathcal{R}(z,t)}{\partial \theta_{\tau}} \theta_{zz} = 0,$$

where $\hbar(\theta) = h(\theta)/\gamma_{10}$ and $\mathcal{A}(\theta) = \mathcal{A}(\theta)/\gamma_{10}$; $\mathcal{R}(z,t) = \frac{\gamma_{10}^2}{K_{10}}R(z,t)$ is the full dimensionless Rayleigh dissipation function; and $\mathcal{P}(z,t) = \frac{\partial^2 \mathcal{R}(z,t)}{\partial \theta^2}$ is the dimensionless hydrostatic pressure in the HAN channel, whereas $\delta_2 = \rho K_{10}/\gamma_{10}^2$ is an extra one parameter of the nematic system. The ST component $\sigma_{zz}$ is given by [7] $\sigma_{zz}(z,t) = \frac{\delta R(z,t)}{\delta u_{zz}} = \hbar(\theta)u_{zz} - \mathcal{A}(\theta)\theta_{\tau} - \delta_1 \chi_{zz} \theta_z \sin^2 \theta \left( 1 + \frac{1}{2} \sin^2 \theta \right)$.

When the temperature gradient $\nabla \chi$ is set across the HAN channel, we expect that the temperature field $\chi(z,t)$ satisfies the dimensionless entropy balance equation: [7,8]

$$\delta_3 \chi_{zz}(z,t) = \left[ \chi_{zz} \left( \lambda \cos^2 \theta + \sin^2 \theta \right) \right]_{zz} +$$
$$\delta_4 \left[ \chi_{zz} \left( \theta_{\tau} \frac{1}{2} \sin^2 \theta - u_{zz} \sin^2 \theta (1 + \frac{1}{2} \sin^2 \theta) \right) \right]_{zz},$$

where $\lambda = \lambda_{||}/\lambda_\perp$, and $\delta_3 = \frac{\rho c_p K_{10}}{\lambda_\perp T_{NI}^2}$ and $\delta_4 = \frac{\xi K_{10}}{\gamma_{10}^2 \lambda_{||} T_{NI}}$ are two extra parameters of the nematic system. Note that the overbars in the $z$ space variable and in the last four Equations (9)–(12) have also been eliminated.

In order to elucidate the role of both the heat flux $q = q_0 \mathbf{k}$ and the external SS $\sigma_{zz}^0$ on the reorientation process in the microsized HAN channel, we consider the hydrodynamic regime when the director $\mathbf{n}$ is strongly anchored to both solid surfaces, homeotropically to the lower, cooler boundary $(\chi_1)$, whereas on the upper boundary, it is assumed that the
heat flux is vanished or restricted. In this case, the boundary conditions must satisfy the following equations

\[ \theta(z)_{z=0} = 0, \theta(z)_{z=1} = \frac{\pi}{2}, \]
\[ \chi(z)_{z=0} = \chi_1, \chi(z)_{z=1} = \eta_0, \]  

(13)

where \( q_0 = -\frac{Q_0 dT}{N_1 \lambda_z} \) is the dimensionless heat flux across the upper boundary of the HAN channel.

The velocity on the lower boundary must satisfy the no-slip boundary condition,

\[ u(z)_{z=0} = 0, \]  

(14)

whereas on the upper boundary the SS is applied as

\[ (\sigma_{zx}(z))_{z=1} = \sigma_0. \]  

(15)

Now, the reorientation of the director in the microsized HAN channel confined between two solid surfaces, when the relaxation mode is governed by viscous, elastic, thermomechanical forces and the SS \( \sigma_0 \) with accounting for the heat flux \( q_0 \hat{k} \), can be obtained by solving the system of nonlinear partial differential Equations (9), (10), and (12), with the appropriate boundary conditions for the polar angle \( \theta(z, \tau) \), temperature \( \chi(z, \tau) \) (Equation (13)), and the velocity \( u(z, \tau) \) (Equations (14) and (15)) as well as with the initial condition

\[ \theta(z, \tau = 0) = \frac{\pi}{2}. \]  

(16)

2.2. Numerical Results for the Relaxation Modes in the HAN Channel

First, we focus on the problem of how much the viscous torque \( T_{\text{vis}} = T_1(\chi)\theta_{,z} - \mathcal{A}(\theta)u_{,z} = T_1(\chi)\theta_{,z} - \frac{1}{2}(1 + \gamma_{21})\cos 2\theta)u_{,z} \) influences the evolution of the director field \( \hat{n}(z, \tau) \) (or the polar angle \( \theta(z, \tau) \)) to its stationary \( \hat{n}_{\text{st}}(z) \) distribution across the microfluidic HAN channel with the temperature gradient. In our case, the \( \nabla \chi \) is set by the heat flux \( q \) (see Equation (13)) directed across the microfluidic HAN channel.

Calculations of the temperature dependence \( \gamma_{21} = -\gamma_2/\gamma_1 \) as well as a comparison of the RVCs values \( \gamma_1 \) and \( \gamma_2 \), both for 5CB and 8CB, at temperatures corresponding to the nematic phase, are given in Table 1.

**Table 1.** The RVC values \( \gamma_1 \) and \( \gamma_2 \) and their ratio \( \gamma_{21} = -\gamma_2/\gamma_1 \) for 5CB and 8CB nematic liquid crystals. The values of the phase transition temperatures NI are \( T_{NI} \sim 307 \text{ K} \) and \( \sim 313 \text{ K} \), for 5CB and 8CB, respectively. All data for the RVCs are given in Pa s [21].

| \( T/T_{NI} \) | 0.964 | 0.974 | 0.98 | 0.984 | 0.99 | 0.993 |
|----------------|-------|-------|------|-------|------|-------|
| \( \gamma_1(5CB) \) | 0.968 | 0.78  | 0.61 | 0.984 | 0.99 | 0.45  |
| \( -\gamma_2(5CB) \) | 1.01 | 0.80  | 0.67 | 0.56  |      |       |
| \( \gamma_{21}(5CB) \) | 1.04 | 1.03  | 1.1  | 1.24  |      |       |
| \( \gamma_1(8CB) \) |      | 0.86  | 0.73 |       |      |       |
| \( -\gamma_2(8CB) \) | 0.52 | 0.47  |      |       |      |       |
| \( \gamma_{21}(8CB) \) | 0.60 | 0.64  |      |       |      |       |

The rest material parameters of these 5CB and 8CB nematic crystals are the mass density \( \sim 10^3 \text{ kg/m}^3 \) and the experimental data for elastic constants [25] \( K_1(T) \) and \( K_3(T) \) varying between 6 and 13 pN, and 7 and 14 pN, respectively. Therefore, the highest values are \( K_{10} \sim 13 \text{ pN} \), \( K_{30} \sim 14 \text{ pN} \), \( \gamma_{10}(5CB) \sim 0.968 \text{ Pa s} \), and \( \gamma_{10}(8CB) \sim 0.86 \text{ Pa s} \),
respectively. Next, we use the measured values obtained by adiabatic screening calorimetry and photopyroelectric methods for the specific heat $C_p \sim 10^3$ J/kg K [26], the thermal conductivity coefficients $\lambda_\| \sim 0.24$ and $\lambda_\perp \sim 0.13$ W/m K [27], the calculated value of the thermomechanical constant $\xi \sim 10^{-12}$ J/m K [9], and measured values of the Leslie coefficients $\alpha(T)$ ($i = 1, \ldots, 6$) [21].

The set of parameter values involved in Equations (9), (10), and (12) is $\delta_1 = 24$, $\delta_2 = 2 \times 10^{-6}$, $\delta_3 = 6 \times 10^{-4}$, and $\delta_4 = 10^{-10}$. Using the fact that $\delta_2 \ll 1$, the Navier–Stokes Equation (10) can be considerably simplified as velocity adiabatically follows the motion of the director. Thus, the whole left-hand side of Equation (10) can be neglected, reducing it to

$$\sigma_{xz} = \bar{\tau}(\theta)u_z - \mathcal{A}(\theta)\theta, - \delta_1 \chi_{xz} \sin^2 \theta \left(1 + \frac{1}{2} \sin^2 \theta\right) = \sigma_{xz}^0,$$  

(17)

while Equation (12) can also be significantly simplified. Since both parameters $\delta_3$ and $\delta_4 \ll 1$, and the entire left part of Equation (12) and the second term can be neglected, so the Equation (12) takes the form:

$$\left[\chi_{xz} \left(\lambda \cos^2 \theta + \sin^2 \theta\right)\right]_{\tau} = 0.$$  

(18)

The last equation has a solution

$$\chi_{xz}(z, \tau) = \frac{q_0}{\lambda \cos^2 \theta + \sin^2 \theta}.$$  

(19)

From a physical point of view, this means that the temperature field $\chi(z, \tau)$ across the HAN cell under the above conditions is proportional to the heat flux $q_0$ across the upper bounded surface when the temperature on the lower surface is kept constant.

In the case when the SS $\sigma_{xz}^0$ is equal to 10 (~5 Pa) and there is the heat flux $q_0 = 0.02$ (Q$_0 \sim 200$ nW/µm$^2$) directed to the bulk of the nematic channel, the evolution of the director field $\mathbf{\hat{n}}$ to its stationary orientation $\mathbf{\hat{n}}_{st}$ in the microsized HAN channel, which is described by the polar angle $\theta(z, \tau)$ for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.4$ (~0.07 s) (curve 7) for both cases 5CB (see Figure 2a) and 8CB (Figure 2b), is shown in Figure 2.

![Figure 2](image_url)

**Figure 2.** (a) The evolution of the polar angle $\theta(z, \tau)(5CB)$ to its stationary distribution across the HAN microfluidic channel under the effect of SS $\sigma_{xz}^0$ = 10 (~5 Pa) for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.4$ (~0.07 s) (curve 7). Here, $\tau_k = 0.067 \times (k - 1)$ ($k = 2, \ldots, 7$). (b) The same as in (a) but for the evolution of $\theta(z, \tau)(8CB)$ to its stationary distribution across the HAN microfluidic channel. Here, $q_0$ is equal to 0.02.

All calculations in this paper were carried out by the numerical relaxation method [28], whereas the relaxation criterion $\varepsilon = |(\theta_{(m+1)}(z, \tau) - \theta_{(m)}(z, \tau))/\theta_{(m)}(z, \tau)|$ was chosen to
be equal to $10^{-4}$ and, then, the numerical procedure was carried out until a prescribed accuracy was achieved. Here $m$ is the iteration number.

In turn, the relaxation of the velocity field $u(z, \tau_k)$ to its stationary distribution across the HAN microfluidic channel under the effect of the same SS $\sigma_{2x}^0 = 10$ ($\sim 5$ Pa) for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.4$ ($\sim 0.07$ s) (curve 7) both for 5CB (see Figure 3a) and 8CB (see Figure 3b) nematics, is shown in Figure 3.

![Figure 3.](image)

**Figure 3.** (a) The relaxation of the velocity field $u(z, \tau_k)(5CB)$ to its stationary distribution across the HAN microfluidic channel under the effect of SS $\sigma_{2x}^0 = 10$ ($\sim 5$ Pa) for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.4$ ($\sim 0.07$ s) (curve 7). Here, $\tau_k = 0.067 \times (k - 1)$ ($k = 2, \ldots, 7$). (b) The same as in (a) but for the relaxation of the velocity field $u(z, \tau_k)(8CB)$ to its stationary distribution through the HAN microfluidic channel. Here, $q_0$ is equal to 0.02.

First, the effect of the viscous torque $T_{vis}$, or $\gamma_{21} = \gamma_2 / \gamma_1$, on the evolution of the velocity field $u(z, \tau)$ is manifested in the qualitative difference in the velocity profiles for 5CB and 8CB nematics. In the case of 5CB, we have concave profiles (see Figure 3a), while in the case of 8CB, these profiles represent almost linear dependencies at the final stage of evolution, where the velocity $u(z, \tau_k)$ increases from zero ($u(z = 0, \tau_k) = 0$) at the lower boundary of the channel to the value $u(z = 1, \tau_k) \sim 22$ ($\sim 0.7$ mm/s) at the upper boundary. In the case of 5CB, the value of velocity $u(z = 1, \tau_k)(5CB)$ at the upper boundary is equal to $\sim 23$ ($\sim 0.73$ mm/s). Second, the main effect of the viscous torque $T_{vis}$, or $\gamma_{21} = \gamma_2 / \gamma_1$, is manifested in the character of evolution of the director field $\hat{n}$ to its stationary orientation $\hat{n}_{st}$ in the microsized HAN channel, which is described by the polar angle $\theta(z, \tau_k)$. Indeed, in the case of 5CB, the polar angle $\theta(z, \tau_k)(5CB)$ increases monotonically from 0 to $\sim 1.57$ ($\pi / 2$), whereas in the case of 8CB, the polar angle $\theta(z, \tau_k)(8CB)$ increases monotonically from 0 to $\theta(z = 0.64, \tau_k)(8CB) \sim 2.48$ in the vicinity of the center of the HAN channel, with a subsequent decrease to the value of $\sim 1.57$ ($\pi / 2$) at the upper boundary of the HAN channel. Thus, the main effect of $\gamma_{21} = \gamma_2 / \gamma_1$ is to influence the nature of the reorientation of the director field $\hat{n}$ to its stationary orientation $\hat{n}_{st}$ in the microsized HAN channel, which is described by the polar angle $\theta(z, \tau_k)$. In the case of the tumbling type nematic phase, composed of 8CB molecules, when $|\gamma_1| > |\gamma_2|$, the director tumbles under shear flow of the nematic, whereas in the case of the lamellar type nematic phase, composed of 5CB molecules, when $|\gamma_1| < |\gamma_2|$, the dynamics of nematic liquid crystals produces the alignment regime.

In turn, when the SS $\sigma_{2x}^0$ is increased and equal to 20 ($\sim 10$ Pa) (see Figure 4a) and 30 ($\sim 15$ Pa) (see Figure 4b) and there is a heat flux at 0.02 ($Q_0 \sim 200$ nW/$\mu m^2$) in the case of the tumbling type nematic phase composed of 8CB molecules, when $|\gamma_1| > |\gamma_2|$, the evolution of the directors field $\hat{n}$ to its stationary orientation $\hat{n}_{st}$ in the vicinity of the center of the HAN channel undergoes a qualitative change.
Figure 4. (a) The evolution of the polar angle $\theta(z, \tau_i)$ to its stationary distribution across the HAN microfluidic channel in the case of the tumbling type nematic phase composed of 8CB molecules and under the effect of SS $\sigma_{zx}^0 = 20$ (10 Pa) for different times starting from $\tau_i = 0.001$ (curve 1) to $\tau_R = \tau_T \sim 0.4$ (~0.07 s) (curve 7). Here, $\tau_k = 0.067 \times (k - 1)$ ($k = 2, ..., 7$). (b) The same as in (a) but with $\sigma_{zx}^0 = 30$ (~15 Pa) and $\tau_R = \tau_T \sim 0.6$ (~0.1 s). Here, $\tau_k = 0.1 \times (k - 1)$ ($k = 2, ..., 7$), and $\sigma_0$ is equal to 0.02.

Figure 5. (a) The relaxation of the velocity field $u(z, \tau_i)$ to its stationary distribution across the HAN microfluidic channel in the case of the tumbling type nematic phase composed of 8CB molecules and under the effect of SS $\sigma_{zx}^0 = 20$ (10 Pa) for different times starting from $\tau_i = 0.001$ (curve 1) to $\tau_R = \tau_T \sim 0.4$ (~0.07 s) (curve 7). Here, $\tau_k = 0.067 \times (k - 1)$ ($k = 2, ..., 7$). (b) The same as in (a) but with SS $\sigma_{zx}^0 = 30$ (~15 Pa) and $\tau_R = \tau_T \sim 0.6$ (~0.1 s). Here, $\tau_k = 0.1 \times (k - 1)$ ($k = 2, ..., 7$), and $\sigma_0$ is equal to 0.02.

According to our calculations, the shear stress $\sigma_{zx}^0$ produces the velocity field $u(z, \tau)$ directed in the positive direction (see Figure 5) and its effect on the director distribution across the HAN microfluidic channel is so strong that, in the middle part of the nematic channel, the biggest value of the polar angle $\theta(z, \tau)$ is equal to $5.5$ (~315°) at $\sigma_{zx}^0 = 30$ (~15 Pa) and the director practically executes a full cycle of rotation (see Figure 4b). That influence decreases with a further decrease in $\sigma_{zx}^0$. However, taking into account that the director field is strongly anchored to both boundaries of the HAN channel, homeotropically to the lower and homogeneously to the upper, the balance of the viscous, elastic, thermomechanical, and anchoring forces and the SS $\sigma_{zx}$ applied to the upper restricted surface leads to rotation of the director field mainly in the middle part of the HAN microfluidic channel.

The maximum absolute value of the dimensionless velocity $u_{sd}(z) = \frac{\tau_{mad} \omega_{ref}}{\Delta \mu_0}$ in the microsized HAN channel at the final stage of the relaxation process is equal to ~75 (2.266 mm/s) at $\sigma_{zx}^0 = 20$ (~10 Pa) (see Figure 5a) and is ~95 (2.871 mm/s) at $\sigma_{zx}^0 = 30$ (~15 Pa) (see Figure 5b).

In the case when the heat flux $q_0 = 0.02$ ($Q_0 \sim 200$ nW/µm²) across the upper boundary is directed to the bulk of the tumbling type nematic phase composed of 8CB
molecules whereas the SS $\sigma_{zx}$ is applied to the upper restricted surface, the relaxation of the temperature field $\chi(z, \tau)$ to its stationary distribution $\chi_{st}(z)$ across the HAN channel is characterized by an almost linear dependence $\chi(z, \tau)$ from the temperature at the lower boundary $\chi_{z=0} = 0.98$ ($\sim 307$ K) to the temperature at the upper boundary $\chi_{z=1} = \chi_{up}$ (see Figure 6).

Figure 6. Plot of relaxation of the dimensionless temperature at the upper boundary of the tumbling type nematic phase $\chi_{up}(\tau)$ to its stationary value $\chi_{stup}$ for three values of SS: $\sigma^{0}_{zx} = 10$ (curve 1), 20 (curve 2), and 30 (curve 3). The curves correspond to the heat flux $q_0 = 0.02$ ($Q_0 \sim 200$ nW/µm²), directed across the upper boundary.

Calculations show that, under the effect of the lower SS $\sigma^{0}_{zx} = 10$ (see Figure 6 (curve 1)) and higher $\sigma^{0}_{zx} = 30$ (see Figure 6 (curve 3)), the heating of the upper boundary is characterized practically by the same value of $\chi_{stup}$: $\chi_{stup}(\sigma^{0}_{zx} = 10) \sim 0.995$ ($\sim 311.5$ K) and $\chi_{stup}(\sigma^{0}_{zx} = 30) \sim 0.9946$ ($\sim 311.3$ K) but not for $\chi_{stup}(\sigma^{0}_{zx} = 20) \sim 0.9924$ ($\sim 310.6$ K). Note that, in all of these cases, the dimensionless temperature at the lower boundary is kept constant $\chi_{stlw} \sim 0.98$ ($\sim 307$ K) and the vertical temperature gradient $\nabla \chi$ is created across the HAN microfluidic channel, directed towards the warmer upper boundary. Thus, the highest temperature difference $\Delta \chi = \chi_{stup} - \chi_{stlw} = 0.015$ ($\sim 4.5$ K), which was initially equal to 0, is built up in the HAN microfluidic channel under the effect of the lower SS $\sigma^{0}_{zx} = 10$ and after time $\tau_R \sim 0.4$ ($\sim 0.07$ s).

The effects of SS $\sigma^{0}_{zx}$ directed in the negative direction both on the evolution of director field $\hat{n}$ to its stationary orientation $\hat{n}_{st}$ in the microsized HAN channel composed of 8CB molecules, which is described by the polar angle $\theta(z, \tau_k)$ (see Figure 7) and the velocity field $u(z, \tau_k)$ (see Figure 8) for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.4$ ($\sim 0.07$ s) (curve 7), are shown in Figures 7 and 8, respectively.
The relaxation process of the velocity field is characterized by the growth of $|u(z, \tau)|$ upon increasing $\tau$, before achieving the stationary distribution $u_{st}(z) = u(z, \tau = \tau_f)$. This distribution is characterized by the maximum value of $u_{st}(z = 1)$ on the upper bounding surface ($z = 1$), and the hydrodynamic flow $u_{st}(z = 1)$ is directed parallel to both bounding surfaces in the negative direction. The maximum value of the non-dimensional velocity $|u_{st}(z = 1)| = \frac{\tau_f}{K_m} |v_{st}^0(z = 1)|$ in the HAN channel on the upper bounding surface at the final stage of the relaxation process is equal to $\sim 60.4 (\sim 1.9 \text{ mm/s})$ at $v_{st}^0 = -20 (\sim 10 \text{ Pa})$ (see Figure 8a) and $\sim 102 (\sim 3.14 \text{ mm/s})$ at $v_{st}^0 = -30 (\sim 15 \text{ Pa})$ (see Figure 8b). In the case when the heat flux across the upper surface is restricted ($q_0 = 0.02 (Q_0 \sim 200 \text{ nW/\mu m}^2)$), we deal with the almost linear increase of $\chi(z, \tau)$ across the HAN channel from the temperature at the lower ($\chi_{z=0} = 0.98 (\sim 307 \text{ K})$) to the value at the upper boundary $\chi(z = 1)$. The relaxation
of the dimensionless temperature at the upper boundary of the HAN microfluidic channel $\chi_{z=1}(\tau)$ consisting of $5CB$ molecules to its stationary value $\chi_{z=1}^{st}$ for three values of SS, $\sigma_{z=1}^{0} = -10$ (curve 1), $-20$ (curve 2), and $-30$ (curve 3), is shown in Figure 9.

![Plot of relaxation of the dimensionless temperature on the upper boundary of the HAN microfluidic channel](image)

**Figure 9.** Plot of relaxation of the dimensionless temperature on the upper boundary of the HAN microfluidic channel $\chi_{up}(\tau)$ to its stationary value $\chi_{up}^{st}$ for three values of SS $\sigma_{z=1}^{0} = -10$ (curve 1), $-20$ (curve 2), and $-30$ (curve 3). The curves correspond to the heat flux $q_0 = 0.02$ ($Q_0 \sim 200$ nW/µm²), directed across the upper boundary.

The calculations show that the relaxation process $\chi_{z=1}(\tau)$ up to its stationary value $\chi_{z=1}^{st}$ at both lower values of SS $\sigma_{z=1}^{0} = -20$ ($\sim -10$ Pa) and $-30$ ($\sim -15$ Pa) is characterized by the oscillatory behavior of $\chi_{z=1}(\tau)$, before achieving $\chi_{z=1}^{st}(\sigma_{z=1}^{0} = -20) = 0.9945$ ($\sim -311.3$ K) and $\chi_{z=1}^{st}(\sigma_{z=1}^{0} = -30) = 0.993$ ($\sim -310.8$ K), respectively, whereas $\chi_{z=1}^{st}(\sigma_{z=1}^{0} = -10)$ is equal to $\sim 0.992$ ($\sim -310.4$ K). Thus, the highest temperature difference $\Delta \chi = 0.0145$ ($\sim -4.3$ K), which initially was equal to zero, is built in the HAN channel under the influence of SS $\sigma_{z=1}^{0} = -20$ ($\sim -10$ Pa). Note that, in all these cases, the dimensionless temperature at the lower boundary is kept constant $\chi_{z=0} = 0.98$ ($\sim 307$ K), and the vertical temperature gradient $\nabla \chi$ is created over the HAN channel, directed towards the warmer upper boundary.

The effect of SS $\sigma_{z=1}^{0}$ applied both in the positive $10$ ($\sim 5$ Pa) (see Figure 10a) (case I) and negative $-10$ ($\sim -5$ Pa) (see Figure 10b) (case II) directions on the evolution of the director field $\hat{n}$ to its stationary orientation $\hat{n}_{st}$ in the microsized HAN channel, composed of laminar type nematic (5CB), is shown in Figure 10. This evolution is described by the polar angle $\theta(z, \tau_k)$, and the calculations are given for different times starting from $\tau_1 = 0.001$ (curve 1) to $\tau_k = \tau_2 \sim 0.47$ ($\sim 0.08$ s) (curve 7).

First, the effect of SS on the evolution of the director field $\hat{n}$ is manifested in the qualitative difference in the polar angle profiles for cases I (see Figure 10a) and II (see Figure 10b). In case I, we have convex profiles, when the polar angle $\theta(z, \tau_k)(5CB)$ increases monotonically from 0 to $\sim 1.57 (\pi / 2)$, whereas in case II, the polar angle $\theta(z, \tau_k)(5CB)$ decreases monotonically from 0 to $\theta(z = 0.3, \tau_k)(5CB) \sim -0.28$, with a subsequent increase in the value of $\sim 1.57 (\pi / 2)$ at the upper boundary of the HAN channel.

Second, the effect of SS applied both in the positive (case I) and negative (case II) directions on the evolution of the velocity field $u(z, \tau)$ is mainly quantitative (see Figure 11a,b), where the velocity $u(z, \tau_k)$ increases from zero $u(z = 0, \tau_k) = 0$ at the lower boundary of the channel to the value $u(z = 1, \tau_k) \sim 22$ ($\sim 0.7$ mm/s) at the upper boundary in case I and from zero $u(z = 0, \tau_k) = 0$ at the lower boundary of the channel to the value $u(z = 1, \tau_k) \sim -10$ ($\sim -0.32$ mm/s) at the upper boundary in case II.
negative field $\mathbf{\hat{\tau}}$ profiles, when the polar angle $\theta_{CB}$ of the director field $\mathbf{\hat{\tau}}$ the upper boundary of the HAN channel.

As a result, the temperature difference, being initially equal to zero, grows by up to the maximum possible value $\Delta \chi = \chi_{up} - \chi_{low}$, corresponding to the nematic phase. The answer to the question of which restricted surfaces are cooler or warmer depends on the direction of the hydrodynamic flow $\mathbf{v} = u(z)\mathbf{\hat{z}}$.

As a result, the temperature difference, being initially equal to zero, grows by up to the maximum possible value $\Delta \chi = \chi_{up} - \chi_{low}$, corresponding to the nematic phase. The answer to the question of which restricted surfaces are cooler or warmer depends on the direction of the hydrodynamic flow $\mathbf{v} = u(z)\mathbf{\hat{z}}$.

We consider a nematic system consisting of asymmetric polar molecules, such as cyanobiphenyl, which are confined between two solid surfaces that impose a preferred orientation of the average molecular direction $\mathbf{\hat{n}}$ on the restricted surfaces, for instance, homeotropic on the lower boundary surfaces and planar on the upper bounding surfaces. Therefore, we describe the HAN channel under the influence of the temperature gradient.

**Figure 10.** (a) The evolution of the polar angle $\theta(z, \tau_k)$ to its stationary distribution across the HAN microfluidic channel composed of 5CB molecules and under the effect of two values of SS $\varepsilon_{x,y,\gamma}$: (a) the first is equal to 10 ($\sim 5$ Pa), whereas (b) the second is equal to $-10$ ($\sim 5$ Pa). The different times started from $\tau_1 = 0.001$ (curve 1) to $\tau_R = \tau_7 \sim 0.47$ ($\sim 0.08$ s) (curve 7), whereas $\phi_0$ is equal to 0.02. Here, $\tau_k = 0.078 \times (k - 1) \ (k = \text{2,...,7})$.

**Figure 11.** The evolution of the velocity field $u(z, \tau_k)$ to its stationary distribution across the HAN microfluidic channel composed of 5CB molecules and under the effect of two values of SS $\varepsilon_{x,y,\gamma}$: (a) the first is equal to 10 ($\sim 5$ Pa), whereas (b) the second is equal to $-10$ ($\sim -5$ Pa), respectively. Different times the same as in Figure 10.

3. A Role of a Flow in a Temperature Gradient Formation across a HAN Channel

The purpose of this paragraph is to show the simple way the temperature gradient can be built up across the HAN channel under the action of the hydrodynamic flow in the framework of the classical Ericksen–Leslie theory \cite{10,11} while accounting for the entropy balance equation \cite{12}. We consider the thermal conductivity regime, which assumes that the temperature at the lower boundary is kept constant whereas, at the upper boundary, where it was assumed that the heat flux is vanished, it must satisfy the boundary conditions

$$\chi(z)_{z=0} = \chi_{1\nu}, \quad (\chi_z(z))_{z=1} = 0. \quad (20)$$

The effect of SS applied both in the positive (case I) and negative (case II) of the HAN microfluidic channel, composed of 5CB molecules and under the effect of two values of SS $\varepsilon_{x,y,\gamma}$: (a) the first is equal to 10 ($\sim 5$ Pa), whereas (b) the second is equal to $-10$ ($\sim -5$ Pa), respectively. Different times the same as in Figure 10.

As a result, the temperature difference, being initially equal to zero, grows by up to the maximum possible value $\Delta \chi = \chi_{up} - \chi_{low}$, corresponding to the nematic phase. The answer to the question of which restricted surfaces are cooler or warmer depends on the direction of the hydrodynamic flow $\mathbf{v} = u(z)\mathbf{\hat{z}}$.

We consider a nematic system consisting of asymmetric polar molecules, such as cyanobiphenyl, which are confined between two solid surfaces that impose a preferred orientation of the average molecular direction $\mathbf{\hat{n}}$ on the restricted surfaces, for instance, homeotropic on the lower boundary surfaces and planar on the upper bounding surfaces.
\( \nabla \chi \) parallel to the unit vector \( \hat{k} \). Here, \( \hat{k} \) is a unit vector directed from the lower substrate to the upper one (see Figure 1). The coordinate system defined by this task assumes that the director \( \hat{n}(r,t) \) lies in the \( xz \) plane (or in the \( yz \) plane) (see Figure 1).

Assuming that the temperature gradient is \( \nabla \chi = \frac{\delta \chi(z,r)}{\delta z} \hat{k} \) due to the growth of the temperature difference at the HAN boundaries under the action of the hydrodynamic flow changes only in the direction \( z \), we can assume that the components of the director \( \hat{n} = \sin \theta(z,t) \hat{i} + \cos \theta(z,t) \hat{k} \) as well as other physical quantities depend only on the \( z \) coordinate. Here, \( \theta \) denotes the polar angle, i.e., the angle between the direction of the director \( \hat{n} \) and the normal \( \hat{k} \) to the bounding surfaces.

Assuming that we deal with an incompressible fluid, the dimensionless hydrodynamic equations corresponding to the torque balance (see Equation (9)) and the linear moment balance (see Equation (10)) equations as well as the entropy balance equation (see Equation (12)) take the following form [23],

\[
\theta_r = \mathcal{A}(\theta) u_x + \mathcal{G}(\theta) \theta_{zz} + \frac{1}{2} \mathcal{G} \rho(\theta) \theta^2_{zz} - \delta_6 \chi \theta z \left( \frac{1}{2} + \sin^2 \theta \right), \tag{21}
\]

\[
\delta_7 u_r(z, \tau) = (\sigma_{\tau z})_{zz}, \tag{22}
\]

\[
\delta_8 \chi_r(z, \tau) = \left[ \chi \left( 1 \cos^2 \theta + \sin^2 \theta \right) \right]_{zz} + \\
\delta_9 \left[ \chi \theta z \left( \theta \left( \frac{1}{2} + \sin^2 \theta \right) - u_z \sin \theta (1 + \frac{1}{2} \sin^2 \theta) \right) \right]_{zz}, \tag{23}
\]

where \( \mathcal{A}(\theta) = \frac{1}{2} (1 - \gamma_{21} \cos 2\theta) \) and \( \mathcal{G}(\theta) = \sin^2 \theta + K_{31} \cos^2 \theta \) are the hydrodynamic and elastic functions, respectively; \( \sigma_{\tau z} = \frac{\delta \mathcal{G}}{\delta \sigma_z} \) is the ST component; the set of the LC parameters \( \delta_j (i = 6, 7, 8, 9) \) is the same as in Section 3; \( \tau = \frac{k_i}{T \beta} t \) is the dimensionless time; and \( \bar{z} = z/d \) is the dimensionless distance away from the lower boundary of the HAN channel. Note that the overbars in the space variable \( z \) in the last three Equations (21)–(23) have been eliminated.

Now, consider that the HAN system confined between two solid surfaces when the director \( \hat{n} \) is strongly anchored to these boundaries, homeotropically to the lower and homogeneously to the upper boundaries,

\[
\theta(z)_{z=0} = 0, \quad \theta(z)_{z=1} = \frac{\pi}{2}, \tag{24}
\]

whereas the velocity on these boundaries must satisfy the no-slip boundary condition,

\[
u(z)_{z=0} = 0, \quad u(z)_{z=1} = 0. \tag{25} \]

Now, the temperature field \( \chi(z, \tau) \) in the HAN channel confined between two solid boundaries when the temperature at the lower boundary is kept constant but where, at the upper boundary, it was assumed that the heat flux vanished must satisfy the boundary conditions [22]

\[
\chi(z)_{z=0} = \chi_1, \; (\chi, \theta)_{z=1} = 0. \tag{26}
\]

The set of parameters that are involved in Equations (21)–(23) are equal to \( \delta_6 \sim 24, \delta_7 \sim 2 \times 10^{-6}, \delta_8 \sim 6 \times 10^{-4} \), and \( \delta_9 \sim 2 \times 10^{-9} \). Using the fact that \( \delta_7, \delta_8, \) and \( \delta_9 \ll 1 \), the linear moment balance (22) and the entropy balance (23) equations can be considerably
simplified. Thus, the whole left-hand side of Equations (22) and (23) can be neglected, and these equations take the following form:

\begin{equation}
\sigma_{xz} = h(\theta)u_{xz} - A(\theta)\theta_{z} - \delta_{b}\chi_{z}\theta_{z}\sin^{2}\theta \left(1 + \frac{1}{2}\sin^{2}\theta\right) = C(\tau),
\end{equation}

where \( \gamma_{1}h(\theta) = a_{1}\sin^{2}\theta \cos^{2}\theta - A(\theta)\theta_{z}u_{xz} + \frac{1}{2}a_{4} + g(\theta), \frac{g(\theta)}{\chi_{z}} = \frac{1}{2}(a_{6}\sin^{2}\theta + a_{5}\cos^{2}\theta) \), \( C(\tau) \) is the function that does not depend on \( z \) and is fixed by the boundary conditions and where

\begin{equation}
\left[\chi_{z}\left(\lambda\cos^{2}\theta + \sin^{2}\theta\right)\right]_{z} = 0.
\end{equation}

To be able to observe the formation of the temperature difference across the HAN channel under the influence of the stationary hydrodynamic flow, the stationary analog of the Equation (21) was considered when \( \theta_{z} = 0 \). In this case, the dimensionless temperature across the hybrid aligned nematic channel is given by [23]

\begin{equation}
\chi(z) = \int_{0}^{\tau} [\mathcal{H}(\theta, u_{xz}) - (\mathcal{H}(\theta, u_{xz}))_{z=1}] / I(\theta, z) dz + \chi_{1},
\end{equation}

where \( \mathcal{H}(\theta, u_{xz}) = h(\theta)u_{xz} - A(\theta)\theta_{z}, I(\theta, z) = \delta_{b}\theta_{z}\sin^{2}\theta \left(1 + \frac{1}{2}\sin^{2}\theta\right) \), and \( \chi_{1} = T_{1}/T_{NI} \).

The formation of the temperature difference across the HAN channel under the influence of the stationary flow with a triangular sharp profile

\begin{equation}
u(z, \zeta) = \begin{cases} \frac{az}{\zeta}, & (0 \leq \zeta < 1), \\ \frac{1}{1 - \zeta}, & (\zeta \leq z < 1), \end{cases}
\end{equation}

was investigated by the standard numerical relaxation method [23], and the results are shown in Figure 12a,b. The relaxation criterion \( \epsilon = |[\theta(T_{R}) - \theta_{eq}] / \theta_{eq}| \) for calculating procedure was chosen to be equal to \( 10^{-4} \) and then, the numerical procedure was carried out until a prescribed accuracy was achieved.

![Figure 12](image)

\textbf{Figure 12.} (a) The distance \( z \) dependence of the temperature \( \chi(z) \) over the HAN channel under the effect of the stationary flow \( \nu = u(z, \zeta)\hat{\imath} \), with a triangular profile, for a number of values of \( a \) [23]: 0.0009 (curve 1), 0.0007 (curve 2), and 0.0005 (curve 3). In this case, the vector \( \nu \) is in the positive direction. (b) The same as in (a), but \( \nu = -u(z, \zeta)\hat{\imath} \) is in the negative direction.

When the stationary hydrodynamic flow \( \nu = u(z, \zeta)\hat{\imath} \) is directed in the positive direction (see Figure 12a), and the temperature at the lower boundary of the HAN channel keeps a constant value \( \chi_{z=0} = \chi_{1} = 0.97 \ (\sim 298 \, \text{K}) \), across the nematic sample, a vertical temperature gradient \( \nabla \chi \) directed to warmer upper boundary forms. The highest tempera-
ture difference \( \chi_{\text{max}}(\zeta) \equiv \Delta \chi = \chi_{\text{up}} - \chi_{\text{lw}} = 0.03 \) (\( \sim 9 \) K), which was initially equal to zero, is built in the HAN channel under the influence of the hydrodynamic flow \( u(z, \zeta) \), where the magnitude of the factor \( a \) is equal to 0.0009 (\( \sim 12 \) nm/s) (see Figure 12a, curve (1)). The rest curves (2) and (3) correspond to \( a = 0.0007 \) (\( \sim 1 \) nm/s) and 0.0005 (\( \sim 0.7 \) nm/s), respectively. In the case of the reverse direction \( v = -u(z, \zeta) \mathbf{i} \) (see Figure 12b), the temperature on the upper bounded surface remains constant \( \chi_{z=1} = \chi_1 = 0.99 \) (\( \sim 304 \) K), while the lower surface cools to 0.96 (\( \sim 295 \) K), which is close to the nematic-solid phase transition temperature at \( a = 0.0009 \) (curve (1)). In all of these cases, \( \zeta \) (\( \sim 0.98 \)) is close to the upper boundary of the HAN channel. The value of \( \chi_{\text{max}}(\zeta) \) has a huge influence on the location of the maximum of \( u(z, \zeta) \). In the case where \( \zeta \) is placed in the middle part of the nematic channel, \( \zeta = 0.5 \) (see Figure 13a), the temperature difference, which was initially equal to zero, increases to \( \Delta \chi \sim 0.0008 \) (\( \sim 0.3 \) K) at the value of \( a = 0.0009 \) and only with the increase in \( a \) by up to a two order of magnitude, from 0.0009 up to 0.09 (\( \sim 0.1 \mu m/s \)); that difference in temperature increases to a few degrees \( \Delta \chi \sim 0.02 \) (\( \sim 6 \) K). The effect of the \( \zeta \) position on the value of the maximum temperature difference \( \chi_{\text{max}}(\zeta) \) when a constant temperature is kept at \( \chi_{z=0} = \chi_1 = 0.97 \) (\( \sim 298 \) K) at the lower boundary for a number of values of the hydrodynamic velocities \( u(z, \zeta) \) is shown in Figure 13b. Notes that the velocity \( u(z, \zeta) \) and the temperature \( \chi(z) \) at the boundaries must satisfy the boundary conditions Equations (24) and (25), respectively. We found that the value of \( \chi_{\text{max}}(\zeta) \) is sensitive to the position of \( \zeta \) and shows an increase in the magnitude of the highest temperature difference when \( \zeta \) is close to both boundaries of the HAN channel. This behavior of \( \chi_{\text{max}}(\zeta) \) is dictated by Equation (29). Indeed, in the case of the stationary flow, the value of the shear rate shift \( \Delta u_z = u_z^\alpha - u_z^\beta \sim \frac{1}{(1-\alpha)} \) increases to infinity in the vicinity of the bounding surfaces, when the position of \( \zeta \to 0 \) or 1. Physically, this means that only the stationary flow with a triangular sharp profile and a maximum position near boundaries can create the highest temperature difference in the hybrid aligned nematic channel of several degrees. With another hydrodynamic flow with profiles that cannot demonstrate the sharp growth of \( u_z(z) \), the same result can be achieved only by using the “high-speed” hydrodynamic flow \( \sim 0.1 \mu m/s \).

![Figure 13](image_url)

**Figure 13.** (a) The distance \( z \) dependence of the temperature \( \chi(z) \) for the stationary flow \( v = -u(z, \zeta = 0.5) \mathbf{i} \) in the negative direction and calculated for a number of \( a \) [23]: 0.0009 (curve 1), 0.009 (curve 2), and 0.09 (curve 3). (b) Dependence of \( \chi_{\text{max}}(\zeta) \) vs. position of \( \zeta \) for a number of \( a \): 0.0011 (curve 1), 0.0009 (curve 2), and 0.0007 (curve 3).

It was shown by the Brewster angular spectroscopy (BAS) method that the hydrodynamic flow of arachidic (eicosanoic) acid through the narrow channel with the width of \( \sim 0.1 \mu m \) and with the triangular velocity profile at a shear rate of more than 0.2 s\(^{-1} \) at different values of surface pressure can be achieved [22]. It has also been shown that, as the flow rate increases, the velocity profile gradually becomes sharper, eventually becoming triangular. In a typical fluid, such a profile would indicate shear thickening. If this is the
case, we do not exclude the possibility of extending the BAS method to the case of the abovementioned nematic system.

4. Conclusions

This section discusses some recent numerical advances in predicting the structural and hydrodynamic behavior of thermally excited flow in microfluidic hybrid aligned nematic (HAN) channels. Despite the fact that certain quantitative and qualitative advances have been made in the hydrodynamic description of relaxation processes in microsized nematic channels under the effect of a temperature field, there are still a number of questions concerning the temperature gradient formation across these channels. It is shown that, under the influence of the temperature gradient, the horizontal nematic layer, initially at rest, starts moving in the horizontal direction when heated both from below and from above. In the case of strong homeotropic and planar anchorings at the boundaries, the equilibrium distribution of the velocity field $u_{st}(z)$ over the HAN channel is characterized by a sharp increase in the absolute value of $u_{st}(z)$ in the vicinity of the boundary with the planar anchoring [7]. This result, in turn, leads to a number of questions. Is it possible for a temperature difference $\Delta T$ to occur between two boundaries of the HAN microfluidic channel as a result of the stationary hydrodynamic flow distribution of the flow $u_{st}(z)$ across the channel or by applying the SS $\sigma_{zx}$ to the boundaries of this channel? Alternatively, in more general terms, how does $\Delta T$ depend on $u_{st}(z)$ or $\sigma_{zx}$?

The second set of questions is related to the study of the influence of the microscopic width of the LC channel (confining) on the nature of the orientation dynamics of such an LC system. First, it should be noted that, in our case, the shear flow is formed under conditions of strong anchoring of the director field to the boundaries of the LC channel despite the fact that we deal with a microsized channel. Thus, confining also plays a crucial role in the formation of orientation dynamics in such an LC system. Apparently, with an increase in the width of the LC channel, the nature of the orientation dynamics of the director field changes in the direction of continuous rotation of the director, as we described in the article [19].

The absence of continuous rotation of the director field in the tumbling regime is actually due to the combined effect of both anchoring and the size of the HAN channel. Undoubtedly, further investigation of changes in the orientation dynamics in a microscopic LC channel under the influence of a shear stress applied to one of the boundaries of the LC channel as the channel width increases will be continued.

The above numerical results show that both the stationary flow with a triangular velocity profile $u_{st}(z)$ and SS $\sigma_{zx}$ applied to the boundaries of the HAN channel can, under certain conditions, overcome the viscous, elastic, thermomechanical, and anchoring forces and cause a temperature gradient across this channel, with the maximum absolute temperature difference being up to several degrees.

This once again shows that the macroscopic description of the nature of the hydrodynamic flow of an anisotropic liquid subtly senses the microscopic structure of an LC material.

We believe that the present investigation can shed some light on the problem of precise handling of microvolume LC drops, which requires self-contained micropumps.

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