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On the Theory of Extensible Nematic Liquid Crystals

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The theory of heat conducting nematic liquid crystals with stretchable director is considered. The theory of micropolar media with stretch is reviewed and the appropriate field equations are presented. The thermodynamics of the nematic liquid crystals is studied and a set of constitutive equations are derived. The explicit equations of nematodynamics are obtained and some of their features are discussed. The equilibrium state and the rectilinear plane flows are also considered and some simple solutions are presented.

1 INTRODUCTION

The development of a continuum theory of liquid crystals was initiated by Oseen[1] and Zocher.[2] More recent studies have been carried out by Frank.[3] A mathematically complete theory of nematic liquid crystal was developed by Ericksen[4,5] and Leslie.[6,7] Ericksen-Leslie theory of liquid crystals is based on the Ericksen's[4,5] theory of anisotropic fluids.

Recently Lee and Eringen[8–12] developed a theory of liquid crystals which is based on micropolar continuum theories.[13–17] Constitutive equations for heat conducting Nematic liquid crystals were obtained by Narasimhan and Eringen[18] and the explicit equations of motion were derived by Ahmadi and Eringen[19] and Ahmadi.[20] Several simple flows including the flow past a sphere were considered in Ref. 19. It has been shown by Lee and Eringen[21] that as far as the basic laws of motion are concerned the Lee–Eringen and Leslie–Ericksen theories become identical. However, several questions have been raised by Shahinpoor[22,23] about the constitutive equations of the former theory. (See also Lee and Eringen[24]).

An excellent review of the physics of liquid crystal was provided in a recent book by de Gennes.[25]

In both Ericksen–Leslie and Eringen–Lee theories of nematic liquid crystals, it is assumed that the molecules of the liquid crystals behave like rigid rods which can only rotate with no axial deformation.

In the present study, a theory of heat conducting Nematic liquid crystals with deformable molecules is developed. The theory is based on the micropolar continuum theory with stretch as developed by Eringen.[17,26] A set of quasi-linear constitutive equations appropriate for Nematic liquid crystals is presented. The basic equations of motion and heat transfer are derived and discussed. The theory may also find applications to the DNA suspensions and other polymer solutions.

In the section that follows, the fundamental equations of balance and entropy inequality for a micropolar continuum with stretch are presented. In Section 3 the entropy inequality is considered and a set of linear constitutive relations are developed which are appropriate for Nematic liquid crystal with stretch. Section 4 is devoted to the derivation of basic equations of motion and heat transfer. The equilibrium of nematic liquid crystals was considered in Section 5 and their rectilinear plane flows are discussed in Section 6. The paper is concluded by a few remarks in Section 7.

2 LAWS OF MOTION

The basic laws of motion of a micropolar continuum with stretch as derived by Eringen[17–26] are:

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + (\rho v_k)_{,k} = 0 \tag{2.1}$$

Conservation of Microinertia

$$\frac{Di_{kl}}{Dt} + \varepsilon_{lmr} \nu_r i_{km} + \varepsilon_{kmr} \nu_r i_{ml} - 2 i_{kl} \nu = 0, \tag{2.2}$$

Balance of Linear Momentum

$$t_{kl,k} + \rho(f_l - \dot{v}_l) = 0, \tag{2.3}$$

Balance of Angular Momentum

$$m_{kl,k} + \varepsilon_{lmn} t_{mn} + \rho(l_l - \dot{\sigma}_l) = 0, \tag{2.4}$$

Balance of symmetric part of first stress moment

$$\lambda_{k,k} - S + \rho(l - \dot{\sigma}) = 0, \tag{2.5}$$

Conservation of Energy

$$\rho\dot{\varepsilon} = t_{kl}(v_{l,k} - \varepsilon_{klm}v_m) + m_{kl}v_{l,k} + S\nu + \lambda_k \nu_{,k} + q_{k,k} + \rho h, \tag{2.6}$$

Entropy Inequality

$$\rho\dot{\eta} - (q_k/T)_{,k} - \rho h/T \geq 0. \tag{2.7}$$

In these equations ρ is the mass density, $i_{kl} = i_{lk}$ is the microinertia tensor, t_{kl} is the stress tensor, m_{kl} is the couple stress tensor, λ_k is the symmetric part of first stress moment, S is the difference of the trace of microstresses, ε is the internal energy density per unit mass, q_k is the heat flux vector pointing outward, η is the entropy density per unit mass, v_k is the velocity vector, ν_k is the microgyration vector, ν is the microstretch rate, f_k is the body force per unit mass, l_k is the body couple per unit mass, l is the symmetric part of body moment per unit mass, h is the heat source per unit mass, T is the absolute temperature, and $\dot{\sigma}_l$ and $\dot{\sigma}$ are the inertia spins defined by

$$\dot{\sigma}_l \equiv \frac{D}{Dt}[(i_{mm}\delta_{kl} - i_{kl})\nu_k], \tag{2.8}$$

and

$$\dot{\sigma} \equiv (\tfrac{1}{3})[i_{nn}(\dot{\nu} + \nu^2 - \nu_m\nu_m) + i_{nm}\nu_n\nu_m], \tag{2.9}$$

respectively. Throughout this paper the regular Cartesian tensor notation is employed with superposed dot indicating the material time derivative and indices following a comma representing partial differentiations. Equations (2.1–2.9) are the basic laws of motion for a micro-polar continuum with stretch. Equations (2.8) and (2.9) are a generalization of those developed by Eringen[17,22] in the sense that they are applicable to nonmicro-isotropic media such as Nematic liquid crystals.

3 CONSTITUTIVE EQUATIONS

In order to complete the theory a set of constitutive equations must be derived. Introducing the Helmholtz free energy

$$\psi = \varepsilon - T\eta, \tag{3.1}$$

and eliminating ρh between (2.6) and (2.7) we find an alternative form of Clausius–Duhem inequality,

$$-\rho(\dot{\psi} + \eta\dot{T}) + t_{kl}(v_{l,k} - \varepsilon_{klm}\nu_m) + m_{kl}\nu_{l,k} + S\nu + \lambda_k\nu_{,k} + q_k(\ln T)_{,k} \geq 0. \tag{3.2}$$

We now consider the following set of general constitutive equations:

$$\psi = \psi(\rho^{-1}, T, T_{,k}, v_{l,k} - \varepsilon_{klm}\nu_m, \phi_{k,l}, \phi_{,k}, \nu_{,k}, \phi, \nu), \tag{3.3}$$

$$\begin{aligned} t_{kl} &= t_{kl}(\cdots), m_{kl} = m_{kl}(\cdots), \lambda_k = \lambda_k(\cdots), \\ S &= S(\cdots), q_k = q_k(\cdots), \eta = \eta(\cdots), \end{aligned} \tag{3.4}$$

where t_{kl}, m_{kl}, λ_k, S, q_k and η are functions of the same constitutive variables as ψ. In (3.3) and (3.4) we have introduced the displacement vector u_k, microrotation ϕ_k and microstretch ϕ.

Taking the total time derivative of (3.3) and employing the resulting equation in inequality (3.2) we find

$$\begin{aligned} &\left(t_{(kl)} + \rho\frac{\partial\psi}{\partial\phi_{m,k}}\phi_{m,l} + \rho\frac{\partial\psi}{\partial\phi_{,k}}\right)v_{l,k} + t_{[kl]}(v_{l,k} - \varepsilon_{klm}\nu_m) \\ &- \rho\left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T} - \rho\frac{\partial\psi}{\partial T_{,k}}\dot{\overline{T_{,k}}} + \frac{\partial\psi}{\partial\rho^{-1}}v_{k,k} \\ &+ \left(\rho\frac{\partial\psi}{\partial(v_{l,k} - \varepsilon_{klm}\nu_m)}\right)(\dot{\overline{v_{l,k}}} - \varepsilon_{klm}\dot{\nu}_m) \\ &+ \left(m_{kl} - \rho\frac{\partial\psi}{\partial\phi_{l,k}}\right)\nu_{l,k} - \rho\frac{\partial\psi}{\partial\nu_{l,k}}\dot{\overline{\nu_{l,k}}} \\ &+ \left(\lambda_k - \rho\frac{\partial\psi}{\partial\phi_{,k}}\right)\nu_{,k} - \rho\frac{\partial\psi}{\partial\nu_{,k}}\dot{\overline{\nu_{,k}}} \\ &+ \left(S - \rho\frac{\partial\psi}{\partial\phi}\right)\nu - \rho\frac{\partial\psi}{\partial\nu}\dot{\nu} + q_k T_{,k}/T \geq 0, \end{aligned} \tag{3.5}$$

where $t_{(kl)}$ and $t_{[kl]}$ are the symmetric and antisymmetric parts of the stress tensor. In the derivation of (3.5) we employed the continuity equation (2.1) and the relations

$$\begin{aligned} v_k = \dot{u}_k, \qquad \nu_k = \dot{\phi}_k, \qquad \nu = \dot{\phi}, \\ \frac{d}{dt}\phi_{,k} = \dot{\phi}_{,k} - \phi_{,j}v_{j,k}. \end{aligned} \tag{3.6}$$

The inequality (3.5) must hold for arbitrary variation of $\dot{T}$, $\dot{\overline{T_{,k}}}$, $v_{(l,k)}$ $\dot{v}_{[l,k]}$, ν_m, $\dot{v}_{l,k}$, $\dot{\nu}_m$, ν and $\dot{\nu}$. It is then concluded that

$$\eta = -\frac{\partial\psi}{\partial T}, \tag{3.7}$$

$$\frac{\partial\psi}{\partial T_{,k}} = \frac{\partial\psi}{\partial(v_{l,k} - \varepsilon_{klm}\nu_m)} = \frac{\partial\psi}{\partial\nu_{l,k}} = \frac{\partial\psi}{\partial\nu_{,k}} = \frac{\partial\psi}{\partial\nu} = 0, \tag{3.8}$$

$${}_Dt_{kl}(v_{l,k} - \varepsilon_{klm}\nu_m) + {}_Dm_{kl}\nu_{l,k} + 3_D\lambda_k\nu_{,k} + 3_DS\nu + q_kT_{,k}/T \geq 0, \tag{3.9}$$

where we have introduced the decomposition of the stress, couple stress and stress moments into nondissipative and dissipative parts. These are

$$t_{kl} = {}_Et_{kl} + {}_Dt_{kl} - p\delta_{kl}, \; m_{kl} = {}_Em_{kl} + {}_Dm_{kl},$$
$$\lambda_k = {}_E\lambda_k + {}_D\lambda_k, \qquad S = {}_ES + {}_DS, \tag{3.10}$$

with

$$p = -\frac{\partial\psi}{\partial\rho^{-1}}, \tag{3.11}$$

is the thermodynamic pressure and

$${}_Et_{(kl)} = -\rho\frac{\partial\psi}{\partial\phi_{m,k}}\phi_{m,l} - \rho\frac{\partial\psi}{\partial\phi_{,l}}\phi_{,k} \tag{3.12}$$

$${}_Em_{kl} = \rho\frac{\partial\psi}{\partial\phi_{l,k}}, \tag{3.13}$$

$${}_E\lambda_k = \rho\frac{\partial\psi}{\partial\phi_{,k}}, \tag{3.14}$$

$${}_ES = \rho\frac{\partial\psi}{\partial\phi}. \tag{3.15}$$

It is now possible to derive general constitutive equations for the stress, couple stress and the stress moments. In the present analysis we restrict ourselves to linear theory. The quasi-linear constitutive equations appropriate for nematic liquid crystals are

$$t_{kl} = -p\delta_{kl} + a_{klmn}(v_{n,m} - \varepsilon_{mnp}v_p) + c_{kl}v - \tfrac{1}{2}(B_{jkmn}\phi_{m,n}\phi_{j,l}$$
$$+ B_{jlmn}\phi_{m,n}\phi_{j,k} + F_{km}\phi_{,m}\phi_{,l} + F_{lm}\phi_{,m}\phi_{,k}) \tag{3.16}$$

$$m_{kl} = B_{lkmn}\phi_{m,n} + b_{lkmn}v_{m,n} + e_{lkmn}\varepsilon_{mnr}v_{,r}$$
$$+ E_{lkmn}\varepsilon_{mnr}\phi_{,r} + \gamma_{lkmn}\tau_{mn}, \tag{3.17}$$

$$\lambda_k = f_{kl}v_{,l} + F_{kl}\phi_{,l} + g_{kl}\varepsilon_{lmn}v_{n,m}$$
$$+ G_{kl}\varepsilon_{lmn}\phi_{n,m} + \alpha_{kl}\varepsilon_{lmn}\tau_{mn}, \tag{3.18}$$

$$S = \eta v + \zeta_0\phi, \tag{3.19}$$

$$q_p = \tfrac{1}{2}(d_{lkmn}v_{m,n} + k_{lkmn}\varepsilon_{mnq}v_{,q} + \delta_{lkmn}\tau_{mn})\varepsilon_{lkp}, \tag{3.20}$$

where η, ζ are material constants and

$$\tau_{mn} = \tfrac{1}{2}\varepsilon_{mnp}T_{,p}/T. \tag{3.21}$$

The coefficients a_{klmn}, B_{lkmn}, b_{lkmn}, c_{kl}, e_{lkmn}, E_{lkmn}, k_{lkmn}, f_{kl}, F_{kl}, g_{kl}, G_{kl}, α_{kl}, γ_{lkmn}, d_{lkmn} and δ_{lkmn} are related to coefficients of viscosity, heat conductivity, etc.

These coefficients must satisfy the condition of transverse isotropy along the local average direction of the Nematic liquid crystals molecules. This restriction reduces the number of material constants present in those coefficients. Employing the most general forms of the transversly isotropic tensors of fourth and second order together with symmetry properties, it is found that

$$\begin{aligned} a_{ijkl} = {} & \lambda\delta_{ij}\delta_{kl} + (\mu + \kappa)\delta_{ki}\varepsilon_{lj} + \mu\delta_{kj}\delta_{il} \\ & + a_l h_m \varepsilon_{mij} h_n \varepsilon_{nkl} + a_2 \delta_{ij} h_k h_l + a_3 \delta_{kl} h_i h_j \\ & + a_4 \delta_{ki} h_l h_j + a_5 \delta_{lj} h_k h_i + a_6 \delta_{kj} h_l h_i \\ & + a_7 \delta_{li} h_k h_j + a_8 h_i h_j h_k h_l, \end{aligned} \tag{3.22}$$

$$\begin{aligned} B_{ijkl} = {} & \alpha_B \delta_{kl}\delta_{ij} + \beta_B \delta_{ki}\delta_{lj} + \gamma_B \delta_{kj}\delta_{il} \\ & + B_l h_m \varepsilon_{mij} h_n \varepsilon_{nkl} + B_2(\delta_{ij} h_k h_l + \delta_{kl} h_i h_j) \\ & + B_3 \delta_{ki} h_l h_j + B_4 \delta_{lj}\, h_k h_i \\ & + B_5(\delta_{kj} h_l h_i + \delta_{li} h_k h_j) + B_6 h_i h_j h_k h_l, \end{aligned} \tag{3.23}$$

$$g_{kl} = g_l \delta_{kl} + g_2 h_k h_l, \tag{3.24}$$

where the director h_k is the local average direction of the Nematic liquid crystals molecules.

The coefficients E_{lkmn}, e_{lkmn}, b_{lkmn}, γ_{lkmn}, d_{lkmn}, k_{lkmn} and δ_{lkmn} have expression similar to (3.23) with the material constants α_B, β_B, γ_B, ... , etc. being replaced by their corresponding values. The expression for c_{kl}, f_{kl}, F_{kl}, G_{kl} and α_{kl} are similar to (3.24). It must be pointed out that in the derivation of the constitutive equations (3.16–3.24) the difficulty of consideration of a "reference configuration" which was proposed in Refs. 8–12 and questioned by Shahinpoor[22,23] is completely eliminated and the macrodeformation was assumed not to be a constitutive variable.

4 EQUATIONS OF NEMATODYNAMICS

Employing the constitutive equations (3.16–3.19) into the equations of balance (2.3–2.5) we find the basic equations of motion of Nematic liquid crystals. These are

$$\begin{aligned} \rho\dot{v}_l = {} & \rho f_l - p_{,l} + [a_{klmn}(v_{n,m} - \varepsilon_{mnp} v_p)]_{,k} + (c_{kl} v)_{,k} \\ & - \tfrac{1}{2}[B_{jkmn}\phi_{m,n}\phi_{j,l} + B_{jlmn}\phi_{m,n}\phi_{j,k} + F_{km}\phi_{,m}\phi_{,l} + F_{lm}\phi_{,m}\phi_{,k}]_{,k}, \end{aligned} \tag{4.1}$$

$$\begin{aligned} \rho\dot{\sigma}_l = {} & \rho l_l + (B_{lkmn}\phi_{m,n})_{,k} + (b_{lkmn} v_{m,n})_{,k} \\ & + \varepsilon_{mnr}[e_{lkmn} v_{,r} + E_{lkmn}\phi_{,r}]_{,k} + (\gamma_{lkmn}\tau_{mn})_{,k} \\ & + \varepsilon_{lmn} a_{mnpq}(v_{q,p} - \varepsilon_{pqr} v_r), \end{aligned} \tag{4.2}$$

$$\begin{aligned}\rho\dot{\sigma} = \rho l &+ (f_{kl} v_{,l})_{,k} + (F_{kl}\phi_{,l})_{,k} \\ &+ \varepsilon_{lmn}(g_{kl} v_{n,m} + G_{kl}\phi_{n,m})_{,k} \\ &+ (\alpha_{kl}\varepsilon_{lmn}\tau_{mn})_{,k} - \zeta v - \zeta_o \phi.\end{aligned} \tag{4.3}$$

Introducing (3.1) into (2.6) we find the equation for the transfer of heat in Nematic liquid crystals, i.e.

$$\rho C\dot{T} = \nabla \cdot \mathbf{q} + \Phi, \tag{4.4}$$

where C is the heat capacity defined as

$$C = -T\frac{\partial^2 \psi}{\partial T^2}, \tag{4.5}$$

$$\begin{aligned}\Phi = (t_{kl} + p\delta_{kl})(v_{l,k} - \varepsilon_{klm} v_m) &+ (m_{kl} - B_{lkmn}\phi_{m,n} \\ + E_{lkmn}\varepsilon_{mnr}\phi_{,r})v_{l,k} &+ (\lambda_k - F_{kl}\phi_{,l} \\ - G_{kl}\varepsilon_{lmn}\phi_{n,m})v_{,k} &+ \zeta v^2,\end{aligned} \tag{4.6}$$

and $\mathbf{q}$ is given by equation (3.20).

Equations (4.1–4.4) together with equations (2.1) and (2.2) are the complete set of equations for the dynamics and heat transfer of Nematic liquid crystals.

We now consider further simplifications which are direct consequence of the nature of Nematic liquid crystals. It is well known[24] that the molecules of Nematic liquid crystals have the shape of relatively long cylinders. It has been shown previously[20,21] that the microinteria is related to the director field, i.e.

$$\rho i_{kl} = \rho_1 h_k h_l, \tag{4.7}$$

with ρ_1 given by

$$\rho_1 = \frac{\rho' \xi^2}{12}, \tag{4.8}$$

where ξ is the length and ρ' is the local mass density of the director field. Assuming that ρ' is constant and

$$\xi \approx \xi_0, \tag{4.9}$$

with

$$\dot{\xi} = \xi_0 v. \tag{4.10}$$

Employing (4.7) into (2.2) we find that

$$\dot{h}_k = \varepsilon_{klm} v_l h_m. \tag{4.11}$$

In the derivation of (4.11) we have used the following properties of the directors;

$$h_k h_k = 1, \qquad \dot{h}_k h_k = 0, \tag{4.12}$$

and (4.10).

The expression for the inertia spins become

$$\rho\dot{\sigma}_r = \frac{D}{Dt}[\rho_1(\delta_{rm} - h_r h_m)v_m], \tag{4.13}$$

$$\rho\dot{\sigma} = \tfrac{1}{3}\rho_1[\dot{v} + v^2 - (\delta_{nm} - h_n h_m)v_n v_m], \tag{4.14}$$

with

$$\dot{\rho}_1 = \rho_1 v. \tag{4.15}$$

We now summarize the basic linearized equations of motion in vectorial form. These are

Mass

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0, \tag{4.16}$$

Microinertia

$$\dot{\mathbf{h}} = \mathbf{v}\times\mathbf{h}, \tag{4.17}$$

Microstretch

$$\dot{\rho}_l = \rho_l v, \tag{4.18}$$

Linear Momentum

$$\begin{aligned}\rho\dot{\mathbf{v}} = \rho\mathbf{f} &- \nabla p + (\lambda+\mu)\nabla\nabla\cdot\mathbf{v} + (\mu+\kappa)\nabla^2\mathbf{v} \\ &+ \kappa\nabla\times\mathbf{v} - a_1[\nabla\times(\mathbf{hh}\cdot\nabla\times\mathbf{v}) - 2\nabla\times(\mathbf{hh}\cdot\mathbf{v})] \\ &+ a_2\nabla(\mathbf{h}\cdot\nabla\mathbf{v}\cdot\mathbf{h}) + a_3\nabla\cdot(\mathbf{hh}\nabla\cdot\mathbf{v}) + a_4[\nabla\cdot(\nabla\mathbf{v}\cdot\mathbf{hh}) \\ &- \nabla\cdot(\mathbf{h}\times\mathbf{vh})] + a_5\nabla\cdot[\mathbf{h}(\mathbf{h}\cdot\nabla\mathbf{v} + \mathbf{h}\times\mathbf{v})] \\ &+ a_6\nabla\cdot[\mathbf{h}(\nabla\mathbf{v}\cdot\mathbf{h} - \mathbf{h}\times\mathbf{v})] + a_7\nabla\cdot[(\mathbf{h}\cdot\nabla\mathbf{v} + \mathbf{h}\times\mathbf{v})\mathbf{h}] \\ &+ a_8\nabla\cdot[\mathbf{h}(\mathbf{h}\cdot\nabla\mathbf{v}\cdot\mathbf{h})\mathbf{h}] + c_1\nabla v + c_2\nabla\cdot(\mathbf{hh}v) \\ &+ \nabla\cdot{}_E\boldsymbol{t},\end{aligned} \tag{4.19}$$

Angular Momentum

$$
\begin{aligned}
\frac{D}{Dt}[\rho_1(\mathbf{v} - \mathbf{hh}\cdot\mathbf{v})] = {} & \rho\mathbf{l} + \kappa(\nabla\times\mathbf{v} - 2\mathbf{v}) + a_1\mathbf{hh}\cdot(\nabla\times\mathbf{v} - 2\mathbf{v}) \\
& + (a_6 - a_4)[\mathbf{h}\times\nabla\mathbf{v}\cdot\mathbf{h} + \mathbf{v} - \mathbf{h}(\mathbf{h}\cdot\mathbf{v})] \\
& + (a_7 - a_5)[\mathbf{h}\cdot\nabla\mathbf{v}\times\mathbf{h} \\
& + \mathbf{v} - \mathbf{h}(\mathbf{h}\cdot\mathbf{v})] + (\alpha_B + \beta_B)\nabla\nabla\cdot\boldsymbol{\phi} + \gamma_B\nabla^2\boldsymbol{\phi} \\
& - B_1\nabla\times(\mathbf{hh}\cdot\nabla\times\boldsymbol{\phi}) + B_2[\nabla(\mathbf{h}\cdot\nabla\boldsymbol{\phi}\cdot\mathbf{h}) \\
& + \nabla\cdot(\mathbf{hh}\nabla\cdot\boldsymbol{\phi})] \\
& + B_3\nabla\cdot(\mathbf{hh}\cdot\nabla\boldsymbol{\phi}) + B_4\nabla\cdot(\nabla\boldsymbol{\phi}\cdot\mathbf{hh}) \\
& + B_5[\nabla\cdot(\mathbf{h}\cdot\nabla\boldsymbol{\phi}\mathbf{h}) \\
& + \nabla\cdot(\mathbf{h}\nabla\boldsymbol{\phi}\cdot\mathbf{h}) + B_6\nabla\cdot(\mathbf{hhh}\cdot\nabla\boldsymbol{\phi}\cdot\mathbf{h}) \\
& + (\alpha_b + \beta_b)\nabla\nabla\cdot\mathbf{v} + \gamma_b\nabla^2\mathbf{v} - b_1\nabla\times(\mathbf{hh}\cdot\nabla\times\mathbf{v}) \\
& + b_2[\nabla(\mathbf{h}\cdot\nabla\mathbf{v}\cdot\mathbf{h}) + \nabla\cdot(\mathbf{hh}\nabla\cdot\mathbf{v})] + b_3\nabla\cdot(\mathbf{hh}\cdot\nabla\mathbf{v}) \\
& + b_4\nabla\cdot(\nabla\mathbf{v}\cdot\mathbf{hh}) + b_5[\nabla\cdot(\mathbf{h}\cdot\nabla\mathbf{v}\mathbf{h} + \nabla\cdot(\mathbf{h}\nabla\mathbf{v}\cdot\mathbf{h})] \\
& + b_6\nabla\cdot(\mathbf{hhh}\cdot\nabla\mathbf{v}\cdot\mathbf{h}) + 2\gamma_1\nabla\times(\mathbf{hh}\cdot\boldsymbol{\theta}) \\
& + (\gamma_3 - \gamma_5)\nabla\cdot(\mathbf{hh}\times\boldsymbol{\theta}) + (\gamma_4 - \gamma_5)\nabla\cdot(\boldsymbol{\theta}\times\mathbf{hh}) \\
& + 2e_1\nabla\times(\mathbf{hh}\cdot\nabla v) + (e_3 - e_5)\nabla\cdot(\mathbf{hh}\times\nabla v) \\
& + (e_4 - e_5)\nabla\cdot(\nabla v\times\mathbf{hh}) + 2E_1\nabla\times(\mathbf{hh}\cdot\nabla\phi) \\
& + (E_3 - E_5)\nabla\cdot(\mathbf{hh}\times\nabla\phi) + (E_4 - E_5)\nabla\cdot(\nabla\phi\times\mathbf{hh}),
\end{aligned} \tag{4.20}
$$

Symmetric part of first stress moment

$$
\begin{aligned}
\tfrac{1}{3}\rho_1[\dot{v} + v^2 - \mathbf{v}\cdot\mathbf{v} + (\mathbf{h}\cdot\mathbf{v})^2] = {} & \rho l + f_1\nabla^2 v \\
& + f_2\nabla\cdot(\mathbf{hh}\cdot\nabla v) + F_1\nabla^2\phi + F_2\nabla\cdot(\mathbf{hh}\cdot\nabla\phi) \\
& + g_2\nabla\cdot(\mathbf{hh}\cdot\nabla\times\mathbf{v}) + G_2\nabla\cdot(\mathbf{hh}\cdot\nabla\times\boldsymbol{\phi}) \\
& + 2\alpha_1\nabla\cdot\boldsymbol{\theta} + 2\alpha_2\nabla\cdot(\mathbf{hh}\cdot\boldsymbol{\theta}) - \zeta v - \zeta_o\phi,
\end{aligned} \tag{4.21}
$$

Energy

$$
\begin{aligned}
\rho C\dot{T} = {} & [\beta_\delta + (\delta_3 + \delta_4)/2 - \gamma_\delta - \delta_5]\nabla\cdot\boldsymbol{\theta} \\
& + [\delta_1 + \delta_5 - (\delta_3 + \delta_4)/2]\nabla\cdot(\mathbf{hh}\cdot\boldsymbol{\theta}) \\
& + \tfrac{1}{2}\{(d_3 - d_5)\nabla\cdot(\mathbf{h}\cdot\nabla\mathbf{v}\times\mathbf{h}) \\
& + (d_4 - d_5)\nabla\cdot(\mathbf{h}\times\nabla\mathbf{v}\cdot\mathbf{h}) - 2d_1\nabla\cdot(\mathbf{hh}\cdot\nabla\times\mathbf{v})\} \\
& + [\beta_k + (k_3 + k_4)/2 - \gamma_k - k_5]\nabla^2 v \\
& + [k_1 + k_5 - (k_3 + k_5)/2]\nabla\cdot(\mathbf{hh}\cdot\nabla v) + \Phi,
\end{aligned} \tag{4.22}
$$

where

$$\boldsymbol{\theta} = \nabla T/2T. \tag{4.23}$$

In equation (4.19) the elastic part of the stress tensor is given by

$$\begin{aligned}
2_E t_{jm} = {} & \alpha_B \phi_{k,k}(\phi_{j,m} + \phi_{m,j}) + 2\beta_B \phi_{i,j}\phi_{i,m} \\
& + \gamma_B(\phi_{j,i}\phi_{i,m} + \phi_{m,i}\phi_{i,j}) \\
& + B_1 h_n \varepsilon_{nkl} \phi_{k,l} h_r(\varepsilon_{rij}\phi_{i,m} + \varepsilon_{rim}\phi_{i,j}) \\
& + B_2[h_k \phi_{k,l} h_l(\phi_{j,m} + \phi_{m,j}) + \phi_{k,k} h_i(\phi_{i,m} h_j + \phi_{i,j} h_m)] \\
& + B_3 \phi_{i,l} h_l(h_j \phi_{i,m} + h_m \phi_{i,j}) \\
& + 2B_4 h_k \phi_{k,j} h_i \phi_{i,m} \\
& + B_5 h_i h_l(\phi_{j,l}\phi_{i,m} + \phi_{m,l}\phi_{i,j}) \\
& + B_6 \phi_{k,l} h_k h_l h_i(\phi_{i,m} h_j + \phi_{i,j} h_m) \\
& + 2F_1 \phi_{,j}\phi_{,m} + F_2 h_k \phi_{,k}(h_j \phi_{,m} + h_m \phi_{,j}).
\end{aligned} \tag{4.24}$$

This completes our summary of the basic equations for dynamics of extensible nematic liquid crystals. Note that by taking ρ_1 as constant,

$$\phi = \nu \equiv 0, \tag{4.25}$$

and discarding equations (4.18) and (4.21) the equations for regular nematic liquid crystals would be obtained. In other words equations (4.16), 4.20) and (4.22) are the basic equation for the regular nematodynamics.

5 EQUILIBRIUM STATE

The equilibrium state of Nematic liquid crystal is considered in this section. The constitutive equation (3.16)–(3.19) in the absence of thermal effects and in the equilibrium state reduce to

$$\begin{aligned}
t_{kl} = {} & -p\delta_{kl} + c_{kl}\phi - \tfrac{1}{2}(B_{jkmn}\phi_{m,n}\phi_{j,l} \\
& + B_{jlmn}\phi_{m,n}\phi_{j,k} + F_{kl}\phi_{,m}\phi_{,l} + F_{lm}\phi_{,m}\phi_{,k}),
\end{aligned} \tag{5.1}$$

$$m_{kl} = B_{lkmn}\phi_{m,n} + E_{lkmn}\varepsilon_{mn,r}\phi_{,r}, \tag{5.2}$$

$$\lambda_k = F_{kl}\phi_{,l} + G_{kl}\varepsilon_{lmn}\phi_{n,m}, \tag{5.3}$$

$$S = -\zeta_o \phi. \tag{5.4}$$

From (5.1) it is clearly observed that shear stress is supported by the liquid crystal gives rise to the gradient of microroration and the gradient of microstretch fields. It should be mentioned here that even when microstretch ϕ is identically zero, the equilibrium stress tensor do have nonzero shear terms. (This question has been raised by Shahinpoor[23]).

The free energy function corresponding to equation (5.1)–(5.4) is given by

$$\rho\psi = \tfrac{1}{2}B_{lkmn}\phi_{m,n}\phi_{l,k} + E_{lkmn}\varepsilon_{mnr}\phi_{,r}\phi_{l,k} + \tfrac{1}{2}F_{kl}\phi_{,k}\phi_{,l} + \tfrac{1}{2}\zeta_o\phi^2. \tag{5.5}$$

When the molecules of the nematic liquid crystal behave like rigid rods with no axial deformation the free energy reduces to the following simple equation, i.e.

$$\rho\psi = \tfrac{1}{2}B_{lkmn}\phi_{m,n}\phi_{l,k}. \tag{5.6}$$

Employing (3.24) the explicit form of the free energy (5.6) becomes

$$\begin{aligned} 2\rho\psi = {} & \alpha_B(\nabla\cdot\boldsymbol{\phi})^2 + \beta_B(\nabla\boldsymbol{\phi})^2 + \gamma_B\nabla\boldsymbol{\phi}:\nabla\boldsymbol{\phi} \\ & + B_1(\mathbf{h}\cdot\nabla\times\boldsymbol{\phi})^2 + 2B_1(\nabla\cdot\boldsymbol{\phi})(\mathbf{h}\cdot\nabla\boldsymbol{\phi}\cdot\mathbf{h}) \\ & + B_3(\mathbf{h}\cdot\nabla\boldsymbol{\phi})^2 + B_4(\nabla\boldsymbol{\phi}\cdot\mathbf{h}) \\ & + 2B_5(\mathbf{h}\cdot\nabla\boldsymbol{\phi})\cdot(\nabla\boldsymbol{\phi}\cdot\mathbf{h}) + B_6(\mathbf{h}\cdot\nabla\boldsymbol{\phi}\cdot\mathbf{h})^2. \end{aligned} \tag{5.7}$$

The corresponding free energy according to the Ericksen–Leslie theory in our notation is

$$\begin{aligned} 2\rho\psi = {} & k_{22}\cdot(\nabla\mathbf{h})^2 + (k_{11} - k_{22} - k_{24})(\nabla\cdot\mathbf{h})^2 \\ & + (k_{33} - k_{22})(\mathbf{h}\cdot\nabla\mathbf{h})^2 + k_{24}\nabla\mathbf{h}:\nabla\mathbf{h}, \end{aligned} \tag{5.8}$$

where k_{11}, k_{22}, etc. are material constant. A similar expression with different constants have been considered in the book by de Gennes.[25]

It is interesting to note that if $\boldsymbol{\phi}$ is replaced by $\mathbf{h}$ in (5.7) the expression for the free energy of Ericksen–Leslie theory of nematic liquid crystal is recovered with a few extra terms. It is therefore concluded that the main difference between the present theory and that of Ericksen–Leslie is the consideration of the gradient of the rotation of director field as an independent constitutive variable in the present theory (which is a generalization of Eringen–Lee theory) in contrast to the consideration of the gradient of the director field itself as an independent constitutive variable in the Ericksen–Leslie theory.

6 RECTILINEAR PLANE FLOWS

Let us consider a flow which is in x direction and the flow variables are functions of only y and t, i.e.

$$\begin{aligned} & v = (v_x(y,t), o, o), \qquad \mathbf{v} = (o, o, v_z(y,t)), \\ & h = (\cos\theta, \sin\theta, o), \qquad \boldsymbol{\phi} = (o, o, \phi_z(y,t)), \\ & \theta = \theta(y,t). \end{aligned} \tag{6.1}$$

From equation (4.17) it follows that

$$v_z = \dot{\theta} = \frac{\partial \theta}{\partial t}, \tag{6.2}$$

and hence

$$\phi_z = \theta(y, t). \tag{6.3}$$

Equation (4.16) for ρ constant is identically satisfied. Equation (4.18) becomes

$$\frac{\partial \rho_1}{\partial t} = \rho_1 v. \tag{6.4}$$

The nonzero component of the linear momentum equation is

$$\begin{aligned}\rho \frac{\partial v_x}{\partial t} = \rho f_x - \frac{\partial p}{\partial x} + (\mu + \kappa)\frac{\partial^2 v_x}{\partial y^2} + \kappa \frac{\partial \dot{\theta}}{\partial y} + a_4 \frac{\partial}{\partial y}\left[\cos^2\theta\left(\theta + \frac{\partial v_x}{\partial y}\right)\right] \\ + a_5 \frac{\partial}{\partial y}\left[\sin^2\theta\left(\dot{\theta} + \frac{\partial v_x}{\partial y}\right)\right] - a_6 \frac{\partial}{\partial y}(\sin^2\theta\dot{\theta}) \\ - a_7 \frac{\partial}{\partial y}(\cos^2\theta\dot{\theta}) + a_8 \frac{\partial}{\partial y}\left(\sin^2\theta\cos^2\theta\frac{\partial v_x}{\partial y}\right) \\ + c_2 \frac{\partial}{\partial y}(\sin\theta\cos\theta v) - \tfrac{1}{2}B_1 \frac{\partial}{\partial y}\left[\sin\theta\cos\theta\left(\frac{\partial \theta}{\partial y}\right)^2\right] \\ + \tfrac{1}{2}B_3 \frac{\partial}{\partial y}\left[\sin\theta\cos\theta\left(\frac{\partial \theta}{\partial y}\right)^2\right] + \tfrac{1}{2}F_2 \frac{\partial}{\partial y}\left[\sin\theta\cos\theta\left(\frac{\partial \phi}{\partial y}\right)^2\right].\end{aligned} \tag{6.5}$$

The equation of balance of angular momentum reduces to

$$\begin{aligned}\frac{\partial}{\partial t}(\rho_1\theta) = \rho l_x - \kappa\left(\frac{\partial v_x}{\partial y} + 2\dot{\theta}\right) + (a_6 - a_5)\left(\dot{\theta} + \cos^2\theta\frac{\partial v_x}{\partial y}\right) \\ + (a_7 - a_5)\left(\dot{\theta} + \sin^2\theta\frac{\partial v_x}{\partial y}\right) + \frac{\partial^2}{\partial y^2}(\gamma_B\theta + \gamma_b\dot{\theta}) \\ + \frac{\partial}{\partial y}\left[\cos^2\theta\frac{\partial}{\partial y}(B_1\theta + b_1\dot{\theta})\right] + \frac{\partial}{\partial y}\left[\sin^2\theta\frac{\partial}{\partial y}(B_3\theta + b_3\dot{\theta})\right] \\ + \frac{\partial}{\partial y}\left\{\cos\theta\sin\theta\frac{\partial}{\partial y}[E_3 - E_5 - 2E_1)\phi + (e_3 - e_5 - 2e_1)v]\right\}.\end{aligned} \tag{6.6}$$

Equation (4.21) also simplifies to

$$\tfrac{1}{3}\rho_1(\ddot{\phi} + \dot{\phi}^2 - \dot{\theta}^2) = \rho l + f_1 \frac{\partial^2 \dot{\phi}}{\partial y^2} + f_2 \frac{\partial}{\partial y}\left(\sin^2\theta \frac{\partial \dot{\phi}}{\partial y}\right)$$
$$+ F_1 \frac{\partial^2 \phi}{\partial y^2} + F_2 \frac{\partial}{\partial y}\left(\sin^2\theta \frac{\partial \phi}{\partial y}\right) + g_2 \frac{\partial}{\partial y}\left(\sin\theta\cos\theta \frac{\partial \dot{\theta}}{\partial y}\right) \quad (6.7)$$
$$+ G_2 \frac{\partial}{\partial y}\left(\sin\theta\cos\theta \frac{\partial \theta}{\partial y}\right) - \zeta_o \phi - \zeta \dot{\phi}.$$

Equations (6.4)–(6.7) are the basic equations for the unsteady rectilinear shear flow of an extensible nematic liquid crystals. The solution of this set of highly nonlinear couple partial differential equation is quite cumbersome and will not be considered here. However the following limiting case will be treated in more detail.

In the absence of body force, body couple and longitudinal microdeformation discarding equation (6.7) we consider the steady shear flow between two parallel plates. It is observed that for

$$\phi = v = 0, \quad (6.8)$$

equation (6.4) implies that

$$\rho_1 = \text{const.}, \quad (6.9)$$

and equation (6.5) accepts a simple steady shearing flow solution for constant pressure field, i.e.

$$v_x = Ny, \quad (6.10)$$

where N is the shear rate. Assuming now θ is only time dependent equation (6.6) reduces to the following nonlinear differential equation,

$$\rho_1\ddot{\theta} - (a_6 - a_4 + a_7 - a_5 + 2\kappa)\dot{\theta} - N(a_7 - a_5 + a_4 - a_6)\sin^2\theta = (\kappa + a_6 - a_4)N. \quad (6.11)$$

For the special case when

$$\kappa + a_6 - a_4 = 0 \quad (6.12)$$

the steady equilibrium solution of (6.11) is simply $\theta = 0$ independent of the initial condition. In other words the director field would align itself to the direction of shear flow regardless of the initial starting direction. However, if (6.12) is not satisfied, the equilibrium direction will be at some angle to the flow direction, i.e.

$$\theta = \text{Arc}\sin\left(\frac{\kappa + a_6 - a_4}{a_6 - a_4 + a_5 - a_7}\right)^{1/2}. \quad (6.13)$$

Note that the equilibrium angle θ as predicted by (6.13) is independent of shear rate N. This is in agreement with the results of Gahwiller[27] and Wahl and Fischer[28] who have observed steady angle as large as 17.5° with streamlines, independent of the magnitude of the shear rate.

7 FURTHER REMARKS

A theory of nematodynamics with stretch is presented in this study where the effect of axial deformation of the director field is also considered. The aims of this investigation were two-fold. The main objective was to present a direct derivation (without using the concept of "reference configuration") of the quasi-linear version of Eringen–Lee theory of nematic liquid crystals, which is generalized by consideration of the nonlinear microrotational effect in stress tensor which follows from the nonlinear coupling in the entropy inequality (3.5). By doing so, further similarities between the Ericksen–Leslie theory and the present theory is revealed and some of the questions of Shahinpoor[23] is clarified.

Another objective of the present study was the consideration of the effect of the axial stretch of the directors. According to de Gennes[25] liquid crystals could be formed of small organic molecules such as *p*-azoxyanisole (PAA) which are rigid rods with length 20A and width 5A as well as long helical rods with a typical length of the order 300A and widths 20A. Good examples of this latter type are suspensions of the deoxyribonucleic acids (DNA) or plastic fibers with length of the order of 100μ and diameter of the order of 10μ.

The present theory could find applications in analysis of the dynamical properties of liquid crystals made of such long and possibly stretchable elements.

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