Continuum Mech. Thermodyn. 4 (1992) 167–175

Continuum Mechanics and Thermodynamics

Continuum theory for nematic liquid crystals

F. M. Leslie

This paper presents a formulation of continuum theory for nematic liquid crystals based upon the balance laws for linear and angular momentum, that derives directly expressions for stress and couple stress in these transversely isotropic liquids. This approach therefore avoids the introduction of generalised forces or torques associated with the director describing the axis of transverse isotropy.

1 Introduction

Continuum theory for nematic liquid crystals has its origins in the work early this century by Oseen [1] and Zocher [2] who laid the basis of the static version, later reformulated more directly by Frank [3] and within a mechanical framework by Ericksen [4]. Ericksen [5] extended his work to propose general balance laws, for which Leslie [6] derived constitutive relations to complete dynamic theory. This theory in both its static and dynamic forms models many phenomena in nematic liquid crystals very well, as described for example in the books by de Gennes [7], Chandrasekhar [8] and Blinov [9], or in the reviews by Stephen and Straley [10], Ericksen [11], Jenkins [12] and Leslie [13].

Our aim here is to present a derivation of continuum theory for nematics based upon the more familiar balance laws for linear and angular momentum, without appeal to generalised forces and moments associated with the director that describes the local axis of transverse isotropy. To do so, we consider the rate of work of body and surface forces and moments, and equate this to the rate of increase of the Frank-Oseen stored energy and kinetic energy, as well as the rate of viscous dissipation. In this way we recover the static theory in a manner not so dissimilar to the approach adopted by Ericksen, and thereafter employ the residual form of this relationship in the form of a viscous dissipation inequality to derive dynamic theory in a way rather analogous to that employed by Leslie [13].

Given that continuum theory is now well-established, one might be tempted to question the need for yet another derivation of these equations, but several reasons can be advanced for our doing so. Firstly our present derivation is in many respects more direct being based simply upon conservation of linear and angular momentum and conventional forces and moments. Also such an alternative formulation provides some insights into the theory and its interpretation, or into proposed generalisations for that matter. At the end of this paper we give an example of the latter. More generally, however, further motivation for this paper at this particular time stems from current interest in formulating similar mathematical models for other classes of liquid crystals, and in this respect the present more compact derivation does have advantages.

Throughout the paper we employ Cartesian tensor notation, so that a comma preceding a suffix denotes partial differentiation with respect to the corresponding spatial coordinate and the summation convention applies.

2 Balance laws

For most purposes it suffices to assume that the nematic is incompressible, and in this event conservation of mass reduces simply to a statement that density is conserved, being constant in a homogeneous liquid. Consequently, if we ignore thermal effects, our conservation laws reduce essentially to two, expressions for the balance of linear and angular momentum. Here, for a volume V bounded by a surface S the former takes the familiar form

$$\frac{d}{dt}\int_V \rho v_i \, dv = \int_V \rho F_i \, dv + \int_S t_i \, ds, \tag{2.1}$$

wherein ρ denotes density, $\mathbf{v}$ velocity, $\mathbf{F}$ body force per unit mass, and $\mathbf{t}$ surface force per unit area, the time derivative being the material time derivative. However, the balance law for angular momentum includes additional terms generally omitted (cf. [14]), and is

$$\frac{d}{dt}\int_V \rho e_{ijk} x_j v_k \, dv = \int_V \rho (e_{ijk} x_j F_k + K_i) \, dv + \int_S (e_{ijk} x_j t_k + l_i) \, ds, \tag{2.2}$$

where $\mathbf{x}$ represents the position vector, $\mathbf{K}$ external body moment per unit mass, $\mathbf{l}$ surface moment per unit area, and e_{ijk} the alternator. The inertial term associated with local rotation of the material element is omitted because in general it is negligible.

If $\mathbf{v}$ is the unit normal at points of the surface S, one may show by the usual tetrahedron argument that the surface force and moment are expressible in terms of stress and couple stress tensors, respectively,

$$t_i = t_{ij} v_j, \qquad l_i = l_{ij} v_j, \tag{2.3}$$

and consequently the above balance laws become in point form

$$\rho \dot{v}_i = \rho F_i + t_{ij,j}, \qquad \rho K_i + e_{ijk} t_{kj} + l_{ij,j} = 0, \tag{2.4}$$

the superposed dot denoting the material time derivative.

3 Static theory

A common starting point for continuum theory of nematic liquid crystals is the assumption of a local stored energy associated with distortions of the uniform equilibrium alignment of these transversely isotropic liquids. Thus, employing a unit vector field or director **n** to describe their axis of anisotropy, Oseen [1], Zocher [2], Frank [3] and Ericksen [4] all assume the existence of a stored energy density W such that at any point

$$W = W(n_i,\, n_{i,j}), \tag{3.1}$$

this function being subject to the invariance and symmetry requirements

$$W(n_i,\, n_{i,j}) = W(Q_{ip}n_p,\, Q_{ip}Q_{jq}n_{p,q}) = W(-n_i,\, -n_{i,j}), \tag{3.2}$$

where Q is any orthogonal tensor. If one assumes a quadratic dependence upon the gradients, the function takes the form proposed by Oseen [1] and Frank [3]

$$\begin{aligned} 2W &= K_1(n_{i,i})^2 + K_2(n_i e_{ijk} n_{k,j})^2 + K_3 n_{i,p} n_p n_{i,q} n_q \\ &+ (K_2 + K_4)\left(n_{i,j} n_{j,i} - (n_{i,i})^2\right), \end{aligned} \tag{3.3}$$

the K's being constant coefficients. As Ericksen [4, 5] shows, whatever the choice of the function (3.1), it must satisfy

$$e_{ipq}\left(n_p \frac{\partial W}{\partial n_q} + n_{p,k} \frac{\partial W}{\partial n_{q,k}} + n_{k,p} \frac{\partial W}{\partial n_{k,q}}\right) = 0 \tag{3.4}$$

this being a consequence of the invariance requirement in (3.2).

Ericksen [4, 5] was the first to give a mechanical interpretation to equilibrium theory for nematics by employing a virtual work formulation. Here we present a somewhat similar derivation that considers the rate at which forces and moments do work on a volume of nematic, and assumes that this work goes into changes in either the above stored energy or the kinetic energy, or is lost in viscous dissipation. Our basic postulate is therefore

$$\int_V \rho(F_i v_i + K_i w_i)\, dv + \int_S (t_i v_i + l_i w_i)\, ds = \frac{d}{dt}\int_V \left(\frac{1}{2}\rho v_i v_i + W\right) dv + \int_V D\, dv, \tag{3.5}$$

where **w** denotes the local angular velocity of the material element, and D the rate of viscous dissipation per unit volume. In point form the above reduces to

$$t_{ij} v_{i,j} + l_{ij} w_{i,j} - w_i e_{ijk} t_{kj} = \dot{W} + D, \tag{3.6}$$

a result that we exploit below to obtain the equilibrium forms for the stress and couple stress.

Given that the vector **w** represents the angular velocity of the material element, one has

$$\dot{n}_i = e_{ipq} w_p n_q, \tag{3.7}$$

and noting that

$$\overline{n_{i,j}}^{\cdot} = (\dot{n}_i)_{,j} - n_{i,k}v_{k,j}, \tag{3.8}$$

it follows in turn that

$$\begin{aligned}\dot{W} &= \frac{\partial W}{\partial n_p}\dot{n}_p + \frac{\partial W}{\partial n_{p,k}}\overline{n_{p,k}}^{\cdot} \\ &= e_{iqp}\left[\left(n_q\frac{\partial W}{\partial n_p} + n_{q,k}\frac{\partial W}{\partial n_{p,k}}\right)w_i + n_q\frac{\partial W}{\partial n_{p,k}}w_{i,k}\right] - \frac{\partial W}{\partial n_{p,k}}n_{p,q}v_{q,k} \\ &= e_{iqp}\left(n_q\frac{\partial W}{\partial n_{p,j}}w_{i,j} - n_{k,q}\frac{\partial W}{\partial n_{k,p}}w_i\right) - \frac{\partial W}{\partial n_{p,j}}n_{p,i}v_{i,j},\end{aligned} \tag{3.9}$$

the latter manipulation using the identity (3.4). Combining the above with (3.6) yields

$$\begin{aligned}&\left(t_{ij} + \frac{\partial W}{\partial n_{p,j}}n_{p,i}\right)v_{i,j} + \left(l_{ij} - e_{iqp}n_q\frac{\partial W}{\partial n_{p,j}}\right)w_{i,j} \\ &- w_ie_{iqp}\left(t_{pq} - \frac{\partial W}{\partial n_{k,p}}n_{k,q}\right) = D.\end{aligned} \tag{3.10}$$

Clearly the terms in the above linear in the angular velocity and the gradients of the velocity and angular velocity must be zero, given that the rate of dissipation is necessarily positive. One therefore concludes that

$$t_{ij} = -p\delta_{ij} - \frac{\partial W}{\partial n_{p,j}}n_{p,i} + \tilde{t}_{ij}, \quad l_{ij} = e_{ipq}n_p\frac{\partial W}{\partial n_{q,j}} + \tilde{l}_{ij}, \tag{3.11}$$

where p is an arbitrary pressure arising from the assumed incompressibility, and $\tilde{\mathbf{t}}$ and $\tilde{\mathbf{l}}$ denote dynamic contributions. The relationship (3.10) thus reduces to

$$\tilde{t}_{ij}v_{i,j} + \tilde{l}_{ij}w_{i,j} - w_ie_{ijk}\tilde{t}_{kj} \geqq 0, \tag{3.12}$$

given that the rate of viscous dissipation is positive. This inequality is exploited below to impose restrictions upon the dynamic terms.

The above equilibrium forms of the relationships (3.11) for stress and couple stress are of course identical to the expressions obtained by Ericksen [4, 5]. Also, we show below that the balance of moments $(2.4)_2$ reduces to the familiar Euler-Lagrange equation of static theory.

4 Dynamic theory

To continue our derivation of nematic theory it is now necessary to derive constitutive relations for the dynamic contributions to stress and couple stress. Here we assume that any material point at any instant

$$\tilde{t}_{ij} \text{ and } \tilde{l}_{ij} \text{ are functions of } n_i,\ v_{i,j},\ w_i, \tag{4.1}$$

evaluated at that point at that instant. However, since no dependence upon gradients of the local angular velocity is included, it follows at once from the inequality (3.12) on account of this gradient occurring linearly that

$$\tilde{l}_{ij} = 0. \tag{4.2}$$

This result is analogous to that obtained by Leslie [6].

The above and invariance to superposed rigid body motions lead to our assumption (4.1) being reformulated as

$$\tilde{t}_{ij} \text{ is a hemitropic function of } n_i,\, D_{ij},\, \omega_i, \tag{4.3}$$

where the rate of strain $\mathbf{D}$ and the relative angular velocity $\mathbf{w}$ are defined by

$$2D_{ij} = v_{i,j} + v_{j,i}, \qquad \omega_i = w_i - \frac{1}{2}\, e_{ijk} v_{k,j}, \tag{4.4}$$

For nematic liquid crystals, material symmetry further requires that the above functional dependence be isotropic, and also even in the director. With the assumption that the viscous stress is linear in the velocity gradients and the angular velocity, and noting that the latter is an axial vector and also the identity

$$e_{ijk}\omega_k = n_i e_{jkq}\omega_k n_q + n_j e_{iqk}\omega_k n_q + e_{ijq} n_q n_p \omega_p, \tag{4.5}$$

one ultimately obtains from (4.3)

$$\begin{aligned} \tilde{t}_{ij} &= \alpha_1 n_p n_k D_{pk} n_i n_j + \alpha_2 N_i n_j + \alpha_3 N_j n_i + \alpha_4 D_{ij} \\ &+ \alpha_5 D_{ip} n_p n_j + \alpha_6 D_{jp} n_p n_i + \alpha_7 e_{ijp} n_p \omega, \end{aligned} \tag{4.6}$$

where

$$N_i = e_{ipq}\omega_p n_q, \qquad \omega = \omega_p n_p .$$

In the present context the α's are simply constants. This dissipative stress differs from that given by Leslie [6] only through the presence of the final term.

Straightforwardly, the axial vector associated with the asymmetric viscous stress can be written as

$$e_{ijk}\tilde{t}_{kj} = e_{ijk} n_j \tilde{g}_k + \tilde{g} n_i, \tag{4.7}$$

where the vector $\tilde{\mathbf{g}}$ and the scalar $\tilde{g}$ take the forms

$$\begin{aligned} &\tilde{g}_i = -\gamma_1 N_i - \gamma_2 D_{ip} n_p, \qquad \gamma_1 = \alpha_3 - \alpha_2, \qquad \gamma_2 = \alpha_6 - \alpha_5, \\ &\tilde{g} = -\gamma_3 \omega, \qquad \gamma_3 = 2\alpha_7 . \end{aligned} \tag{4.8}$$

Also it follows from the latter equations (4.6) that

$$\omega_i = e_{ijk} n_j N_k + \omega n_i, \tag{4.9}$$

this and (4.7) simply decomposing the respective vectors into components perpendicular and parallel to the director.

In view of the result (4.2) the inequality (3.12) reduces to

$$\tilde{t}_{ij}v_{i,j} - w_i e_{ijk}\tilde{t}_{kj} \geqq 0, \tag{4.10}$$

which noting (4.4) may be written as

$$\tilde{t}_{ij}D_{ij} - \omega_i e_{ijk}\tilde{t}_{kj} \geqq 0. \tag{4.11}$$

Given (4.7) and (4.9), however, this is equivalent to

$$\tilde{t}_{ij}D_{ij} - \tilde{g}_i N_i - \tilde{g}\omega \geqq 0, \tag{4.12}$$

which differs from the corresponding form derived by Leslie [6] solely through the final term.

To complete our derivation of nematic theory it is necessary to examine to what extent if any our conservation of angular momentum differs from the generalised director balance law commonly employed. This we do in the following section.

5 Angular momentum

The present formulation of nematic theory differs from earlier derivations primarily through a direct appeal to conservation of angular momentum rather than indirectly through generalised forces or torques. Consequently, it is natural to turn first to this balance law.

Recalling the constitutive relations (3.11) and the result (4.2) the balance law $(2.4)_2$ becomes

$$e_{ipq}\left(n_p \frac{\partial W}{\partial n_{q,j}}\right)_{,j} - e_{ipq}\frac{\partial W}{\partial n_{k,p}} n_{k,q} + e_{ipq}\tilde{t}_{qp} + \rho K_i = 0, \tag{5.1}$$

or after some re-arrangement employing the identity (3.4) and the definition (4.7)

$$e_{ipq}n_p\left[\left(\frac{\partial W}{\partial n_{q,j}}\right)_{,j} - \frac{\partial W}{\partial n_q} + \tilde{g}_q\right] + \tilde{g}n_i + \rho K_i = 0. \tag{5.2}$$

However, for a nematic liquid crystal the body moment due to an external magnetic or electric fields is generally assumed to take the form [4]

$$\rho K_i = e_{ipq}n_p G_q, \tag{5.3}$$

where for a magnetic field **H**

$$G_i = \Delta\chi n_p H_p H_i \tag{5.4}$$

with $\Delta\chi$ the diamagnetic susceptibility anisotropy, and for an electric field **E**

$$G_i = \Delta\varepsilon n_p E_p E_i, \tag{5.5}$$

$\Delta\varepsilon$ denoting the dielectric permittivity anisotropy. As a consequence the equation (5.2) can be written as the sum of two parts, one perpendicular and the other parallel to the director,

$$e_{ipq}n_p\left[\left(\frac{\partial W}{\partial n_{q,j}}\right)_{,j} - \frac{\partial W}{\partial n_q} + \tilde{g}_q + G_q\right] + \tilde{g}n_i = 0, \tag{5.6}$$

from which one immediately concludes that

$$\tilde{g} = 0, \tag{5.7}$$

and

$$\left(\frac{\partial W}{\partial n_{i,j}}\right)_{,j} - \frac{\partial W}{\partial n_i} + \tilde{g}_i + G_i = \gamma n_i, \tag{5.8}$$

γ being an arbitrary scalar. Recalling (4.8), the former requires that

$$\omega = 0 \text{ or } w_p n_p = \frac{1}{2} n_p e_{pjk} v_{k,j}, \tag{5.9}$$

so that in this theory the local spin about the director must always be equal to the local component of vorticity in that direction.

Given the result (5.9), the viscous stress tensor reduces to its familiar form. Also, equation (5.8) is simply the director balance law of nematic theory, in its static form being equivalent to the Euler-Lagrange equations of a variational formulation. It is therefore evident that our present approach simply reproduces the theory proposed earlier by Ericksen and Leslie [5, 6].

6 Second order elasticity

In this final section we consider a slight modification of the above theory proposed by Nehring and Saupe [15] that has within the last few years led to some controversy [16, 17], and show that within the context of the present formulation the various problems encountered are not unexpected.

By rather plausible reasoning Nehring and Saupe [15] argue that one should replace the assumption (3.1) by

$$W = W(n_i, n_{i,j}, n_{i,jk}), \tag{6.1}$$

this function as before quadratic in the first gradients, but linear in the second partial derivatives. For our purposes there is no need to restrict the energy in this way, and we therefore proceed more generally. A repetition of Ericksen's argument leads to

$$e_{ipq}\left(n_p \frac{\partial W}{\partial n_q} + n_{p,k}\frac{\partial W}{\partial n_{q,k}} + n_{k,p}\frac{\partial W}{\partial n_{k,q}} + n_{p,jk}\frac{\partial W}{\partial n_{q,jk}} + 2n_{j,kp}\frac{\partial W}{\partial n_{j,kq}}\right) = 0, \tag{6.2}$$

as consequence of the usual invariance assumption. Also, as for the result (3.8) one finds

$$\dot{\overline{n_{i,jk}}} = (\dot{n}_i)_{,jk} - v_{p,j}n_{i,pk} - v_{p,k}n_{i,pj} - n_{i,p}v_{p,jk}. \tag{6.3}$$

With the above a somewhat tedious calculation ultimately yields

$$\dot{W} = e_{ipq}\left(n_p \frac{\partial W}{\partial n_{q,j}} + 2n_{p,k}\frac{\partial W}{\partial n_{q,kj}}\right) w_{i,j} + e_{ipq}n_p \frac{\partial W}{\partial n_{q,jk}} w_{i,jk}$$
$$- \left(\frac{\partial W}{\partial n_{k,j}} n_{k,i} + 2\frac{\partial W}{\partial n_{q,kj}} n_{q,ki}\right) v_{i,j} - \frac{\partial W}{\partial n_{q,jk}} n_{q,i} v_{i,jk}$$
$$- e_{ipq}\left(\frac{\partial W}{\partial n_{j,q}} n_{j,p} + 2\frac{\partial W}{\partial n_{j,kq}} n_{j,kp}\right) w_i . \tag{6.4}$$

While the extra terms involving the angular velocity and the first gradients of velocity and angular velocity cause no problems, those involving second gradients present new difficulties. Clearly, in order to accommodate the latter, some modification of our assumption (3.5) is necessary, this requiring the introduction of terms involving higher order forces and moments of the type discussed by Green and Rivlin [18, 19], and associated additional conservation laws.

Thus the modification proposed by Nehring and Saupe proves to be rather more than it first appears, requiring concepts with which we have little experience. Not surprisingly from this viewpoint, it does lead to difficulties with regard to the interpretation of additional boundary conditions required. While Hinov [20] does attempt to address such complications, it may be wiser to await some sound evidence that such complexity is necessary before considering such generalisations.

References

1. Oseen, W. C.: The theory of liquid crystals. Trans. Faraday Soc. 29 (1933) 883–899
2. Zocher, H.: The effect of a magnetic field on the nematic state. Trans. Faraday Soc. 29 (1933) 945–957
3. Frank, F. C.: On the theory of liquid crystals. Discussions Faraday Soc. 25 (1958) 19–28
4. Ericksen, J. L.: Hydrostatic theory of liquid crystals. Arch. Rat. Mech. Anal. 9 (1962) 371–378
5. Ericksen, J. L.: Conservation laws for liquid crystals. Trans. Soc. Rheol. 5 (1961) 23–34
6. Leslie, F. M.: Some constitutive equations for liquid crystals. Arch. Rat. Mech. Anal. 28 (1968) 265–283
7. de Gennes, P. G.: The physics of liquid crystals. Oxford University Press, London and New York, 1974
8. Chandrasekhar, S.: Liquid crystals. Cambridge University Press, 1977
9. Blinov, L. M.: Electro-optical and magneto-optical properties of liquid crystals. John Wiley and Sons, New York, 1983
10. Stephen, M. J. and Straley, J. P.: Physics of liquid crystals. Rev. Mod. Phys. 46 (1974) 617–704
11. Ericksen, J. L.: Equilibrium theory of liquid crystals. Adv. Liq. Cryst. 2 (1976) 233–298
12. Jenkins, J. T.: Flows of nematic liquid crystals. Ann. Rev. Fluid Mech. 10 (1978) 197–219

13. Leslie, F. M.: Theory of flow phenomena in liquid crystals. Adv. Liq. Cryst. 4 (1979) 1–81
14. Truesdell, C. and Toupin, R. A.: The classical field theories. Handbuch der Physik, Bd. III/1, (1960) 225–793
15. Nehring, J. and Saupe, A.: On the elastic theory of uniaxial liquid crystals. J. Chem. Phys. 54 (1971) 337–343
16. Oldano, C. and Barbero, G.: Possible boundary discontinuities of the tilt angle in nematic liquid crystals. J. Physique Lett. 46 (1985) 451–456
17. Hinov, H. P.: Comment on the criticism of the one-dimensional solution of the K_{13} elastic problem in nematics. Mol. Cryst. Liq. Cryst. 168 (1989) 7–12
18. Green, A. E. and Rivlin, R. S.: Simple force and stress multipoles. Arch. Rat. Mech. Anal. 16 (1964) 325–353
19. Green, A. E. and Rivlin, R. S.: Multipolar continuum mechanics. Arch. Rat. Mech. Anal. 17 (1964) 113–147
20. Hinov, H. P.: On the variation of the K_{13} nematic surface-like volume energy and the nematic surface energy of Mada. Mol. Cryst. Liq. Cryst. 148 (1987) 197–224

Prof. F. M. Leslie
Dept. of Mathematics
University of Strathclyde
Livingstone Tower
Glasgow G1 1XH
Scotland

Received January 6, 1992