Coating of a substrate with a nematic liquid crystal

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The Ericksen–Leslie equations for anisotropic materials are used to model a blade-coating process in which a nematic liquid crystal is coated onto a planar substrate. Such a process has recently been used to deposit liquid crystal and polariser layers in the construction of display devices. The direction and uniformity of the mean molecular alignment (described by a unit vector called the director) are important factors for the performance of the devices, particularly when this alignment is "frozen in" within a polariser layer. We restrict our attention to thin films and small director distortions, and we study the two particular cases in which either orientational elasticity effects or flow effects dominate the orientation of the liquid crystal. In both cases we obtain analytical solutions for the fluid velocity and pressure. When orientational elasticity effects dominate we obtain an analytical solution for the director. When flow effects dominate we find that the director is uniform in the bulk of the liquid crystal and exhibits thin orientational boundary layers.

1 Introduction

The aim of this paper is to study a blade-coating process in which a nematic liquid crystal is coated onto a planar substrate moving parallel to itself. In previous work [1] we described the flow and alignment behaviour of the liquid crystal in the region under the blade; here we describe the flow and alignment patterns within the liquid crystal layer after emerging from the region under the blade (drag out) or before entering the region under the blade (drag

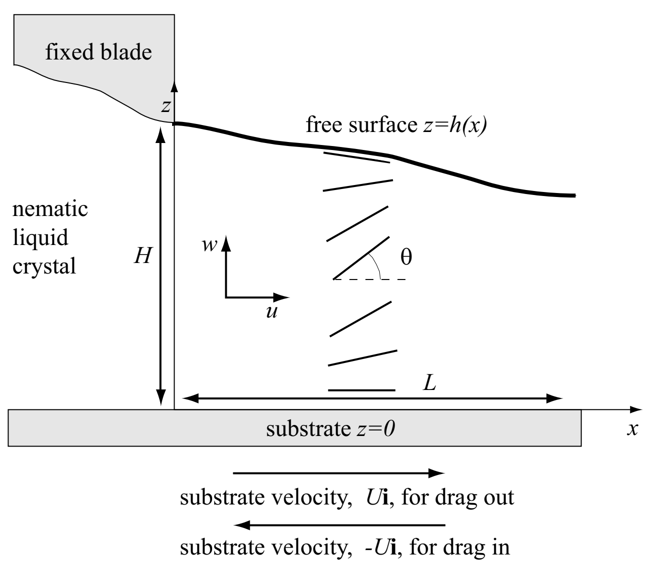

Figure 1: Geometry of the mathematical model of blade coating of a nematic liquid crystal.

in), as shown in Fig. 1. Such a process has been used to deposit liquid crystal and polariser layers in the construction of display devices [2]. The direction and uniformity of alignment are important factors for the performance of the device, particularly when this alignment is "frozen in" within a polariser layer. We are therefore particularly interested in the mean molecular orientation of the liquid crystal, described by a unit vector $\mathbf{n}$, called the director. We use both analytical and numerical techniques to analyse the Ericksen–Leslie equations [3, 4] governing the fluid velocity, pressure and director orientation, in cases when both the aspect ratio of the film of liquid crystal and the distortion of the director field are small.

2 Governing equations

We consider a thin film of liquid crystal of constant density ρ and surface-tension coefficient γ, lying on a planar substrate $z = 0$ which moves away from (or towards) a fixed blade with constant velocity $U\mathbf{i}$ (or $-U\mathbf{i}$), with $U > 0$. We will assume that a steady state has been reached, that the dependent variables (velocity, pressure and director) have no y dependence, and that the director remains in the xz-plane. These assumptions have been shown to be valid for many common liquid crystals and for moderate flow rates [5]. The velocity $\mathbf{v}$, modified pressure $\tilde{p}$ and director $\mathbf{n}$ can therefore be written as $\mathbf{v} = (u(x, z), 0, w(x, z))$, $\tilde{p} = \tilde{p}(x, z)$ and $\mathbf{n} = (\cos\theta(x, z), 0, \sin\theta(x, z))$. The standard continuum equations for the fluid dynamics of anisotropic materials are the Ericksen–Leslie equations [3, 4, 5] which have frequently been shown to model such systems accurately. These equations are nonlinear partial differential equations, and we will employ certain simplifying assumptions in order to obtain analytical solutions.

Using the standard thin-film approximation [6] based on the assumption that the liquid crystal film deposited onto the substrate is "thin", that is, the length scale of the film in the z direction H is much smaller than the length scale in the x direction L, so that the aspect ratio ϵ of the film, defined as $\epsilon = H/L$, is small, the governing equations can be greatly simplified. The appropriate thin-film Ericksen–Leslie equations, which consist of a mass-conservation equation and balance laws of linear and angular momentum, are

$$\begin{aligned} 0 &= u_x + w_z, && (1)\\ 0 &= \tilde{p}_x - (g(\theta)u_z)_z + O(\epsilon), && (2)\\ 0 &= \tilde{p}_z + G + O(\epsilon), && (3)\\ 0 &= E\, m(\theta)u_z - \left[f(\theta)\,\theta_{zz} + \frac{1}{2}\frac{df(\theta)}{d\theta}\,\theta_z^2\right] + O(\epsilon), && (4) \end{aligned}$$

where

$$\begin{aligned} g(\theta) &= \cos^2\theta + \frac{\eta_2}{\eta_1}\sin^2\theta + \frac{\alpha_1}{\eta_1}\cos^2\theta\sin^2\theta, && (5)\\ f(\theta) &= \cos^2\theta + \frac{K_3}{K_1}\sin^2\theta, && (6)\\ m(\theta) &= \frac{\alpha_3}{\eta_1}\cos^2\theta - \frac{\alpha_2}{\eta_1}\sin^2\theta, && (7) \end{aligned}$$

in which the α_i are the *Leslie viscosities* [4], $\eta_1 = (\alpha_4 + \alpha_3 + \alpha_6)/2$ and $\eta_2 = (\alpha_4 + \alpha_5 - \alpha_2)/2$ are two of the *Miesowicz viscosities* [7], and K_1 and K_3 are elastic constants. In formulating these equations standard non-dimensionalisations and rescalings of the variables have been used (more details of which may be found in [1]). The non-dimensional gravity term in eq. (3) is

$$G = \frac{\rho g H^3}{\eta_1 U L}, \tag{8}$$

and the non-dimensional parameter $E = \eta_1 U H / K_1$ in eq. (4) is the *Ericksen number*, a measure of the ratio of viscous to elastic effects.
We will assume that the director lies parallel to the substrate at $z = 0$ and the fluid velocity is equal to the velocity of the substrate. At the free surface $h(x)$ we assume that the usual normal and tangential stress balances hold and that the director lies parallel to the free surface. With appropriate non-dimensionalisation the boundary conditions are therefore

$$u = 1, \ w = 0, \ \theta = 0 \quad \text{on} \quad z = 0, \tag{9}$$

$$u_z = 0, \ \tilde{p} = -S h_{xx}, \ \theta = \epsilon h_x \quad \text{on} \quad z = h, \tag{10}$$

where

$$S = \frac{\gamma H^3}{\eta_1 U L^3} \tag{11}$$

denotes the non-dimensional surface-tension coefficient. Note that the constant volume flux of fluid along the channel per unit width, Q, given by

$$Q = \int_0^h u \, \mathrm{d}z, \tag{12}$$

will be assumed to be prescribed a priori.
To make analytical progress we restrict our attention to small director-angle distortions; in other words, scaling θ as $\theta = \delta \theta^*$ with $\theta^* = O(1)$ we assume that $\delta \ll 1$. Furthermore, for a "flow-aligning" material (that is, one with $\alpha_2 \alpha_3 > 0$ [5]) the flow-aligning angle θ_0, which is defined by $\theta_0 = \tan^{-1} \sqrt{\alpha_3/\alpha_3}$ and is the angle at which the director would orient in the absence of any elastic terms, is usually small. Hence, at this point we have three small parameters to consider, namely ϵ, δ and θ_0; the possible orderings in these parameters result in different sets of equations and boundary conditions. In this paper we will discuss the following two orderings.
Case 1: $\epsilon \sim \delta \ll \theta_0 \ll 1$. In this case orientational elasticity effects dominate flow effects which are insufficient to increase θ significantly from its value at the boundary. The governing equations (1)–(4) simplify to

$$0 = u_x + w_z, \quad 0 = \tilde{p}_x - u_{zz}, \quad 0 = \tilde{p}_z + G, \quad \theta_{zz} = -E_\epsilon u_z, \tag{13}$$

where we have introduced the appropriate Ericksen number $E_\epsilon = -(\alpha_3 E)/(\eta_1 \epsilon)$. Note that, since $\epsilon \sim \delta$, the leading order boundary condition on θ at $z = h$ is $\theta = h_x$.
Case 2: $\epsilon \ll \delta \sim \theta_0 \ll 1$. In this case flow effects dominate orientational elasticity effects and θ achieves flow alignment. The governing equations (1)–(4) simplify to

$$0 = u_x + w_z, \quad 0 = \tilde{p}_x - u_{zz}, \quad 0 = \tilde{p}_z + G, \quad \theta_{zz} = -E_{\theta_0}(1 - \theta^2) u_z, \tag{14}$$

where we have introduced the appropriate Ericksen number $E_{\theta_0} = -(\alpha_3 E)/(\eta_1 \theta_0)$. Note that, since $\epsilon \ll \delta$, the leading order boundary condition on θ at $z = h$ is $\theta = 0$.

The other possible orderings of the small parameters ϵ, δ and θ_0 are either not considered because they are not tractable analytically, or are rejected because they are not physically realisable.

3 Drag out

First we consider the situation in which the substrate $z = 0$ is moving away from the fixed blade. The leading order equations for the fluid pressure and velocity in Case 1 and Case 2 are the same, and furthermore they are decoupled from θ; hence the solution can be calculated directly from either eqs (13 a–c) or eqs (14 a–c) with boundary conditions (9) and (10) to be, in both cases,

$$\tilde{p}(x, z) = G(h - z) - Sh_{xx}, \tag{15}$$

$$u(x, z) = -\frac{\tilde{p}_x}{2}(2h - z)\, z + 1, \tag{16}$$

$$w(x, z) = \frac{\tilde{p}_{xx}}{2}\left(h - \frac{z}{3}\right) z^2 + \frac{\tilde{p}_x}{2} h_x z^2. \tag{17}$$

Substituting the solution (16) for u into eq. (12) and using (15) leads to the governing equation for the free surface h, namely

$$Sh_{xxx} - Gh_x = \frac{3(Q - h)}{h^3}. \tag{18}$$

The free surface profile can be computed numerically from (18). Furthermore, by linearising about the uniform solution $h = h_\infty = Q$ $(Q > 0)$ of (18) one may show that the decay of h towards the uniform solution as $x \to +\infty$ is always monotonic.
From eqs (15), (16) and (18) we find that the solution for u may be written as

$$u(x, z) = \frac{3(Q - h)(2h - z)z}{2h^3} + 1, \tag{19}$$

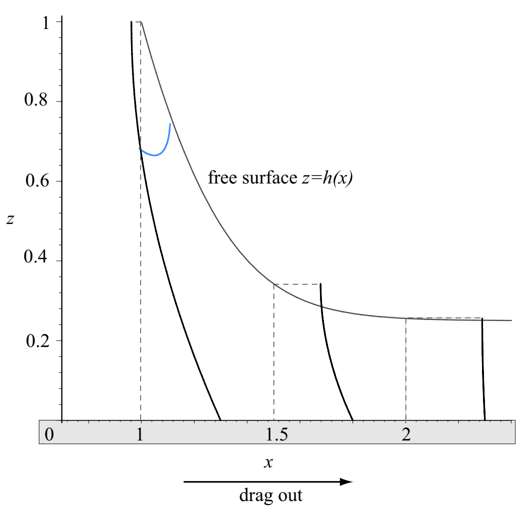

Figure 2: Velocity (in the x direction) profiles at $x = 1, 1.5, 2$ in the drag-out problem, when $Q = 0.25$, $G = 1$ and $S = 1$. Reverse flow occurs above the curve $z = z_0$ on which $u = 0$ (indicated with a blue line) when $h > 3Q = 0.75$.

so that the curve $z = z_0$ on which $u = 0$ is given by

$$\frac{z_0}{h} = 1 - \left[\frac{3Q - h}{3(Q - h)}\right]^{1/2}. \tag{20}$$

Hence, if $h > 3Q$ then there are regions of reverse flow (that is, regions in which $u < 0$) (see Fig. 2). We also see from eq. (19) that $u_z = 0$ not only at the free surface $z = h$, but also when $h = Q$, when there would be a change in the sign of the shear. However, in this situation, numerical solutions of (18) suggest that the free surface h is monotonic for all x, so there is no change in the sign of the shear.

3.1 Case 1: $\epsilon \sim \delta \ll \theta_0 \ll 1$

Substituting the solution (19) for u into the angular momentum balance (13d), integrating twice and applying boundary conditions (9) and (10) leads to the solution for θ, namely

$$\theta = \frac{h_x}{h} z + E_\epsilon \frac{(Q - h)(h - z)(2h - z)z}{2h^3}. \tag{21}$$

In this case orientational elasticity effects dominate flow effects and we expect the flow to have only a weak effect on the director angle. The solution in eq. (21) shows that the flow changes the θ profile from a linear profile when $E_\epsilon = 0$ to a cubic function of z when $E_\epsilon \neq 0$ (see Fig. 3). As flow effects become more important, corresponding to increasing the Ericksen number, the tendency of the flow to try to align the director, and thus distort it from the linear profile, is seen.

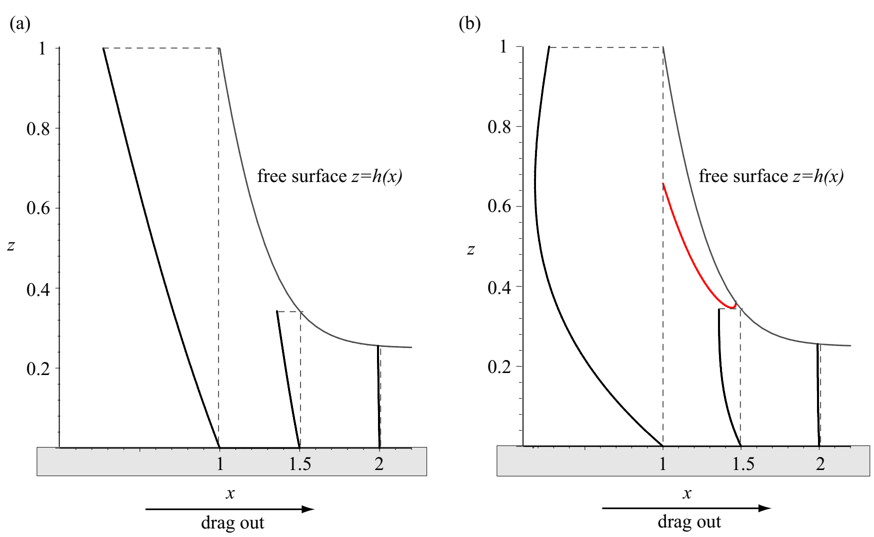

Figure 3: The director angle θ at $x = 1, 1.5, 2$ in the drag-out problem for Case 1, when $Q = 0.25$, $G = S = 1$ and (a) $E_\epsilon = 1$ and (b) $E_\epsilon = 10$. The curve on which $\theta_z = 0$ is indicated by a red line.

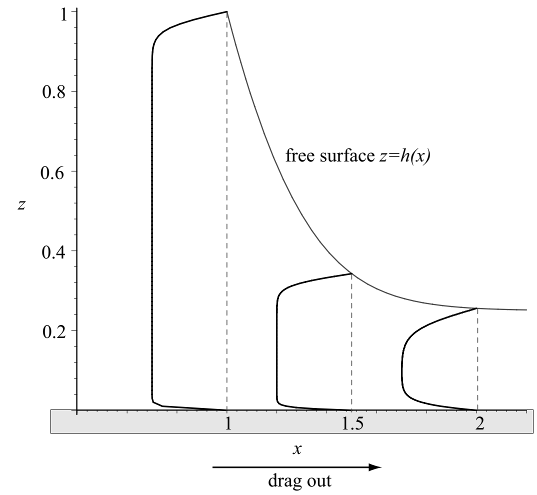

Figure 4: The director angle θ at $x = 1, 1.5, 2$ in the drag-out problem for Case 2, when $Q = 0.25$, $G = S = 1$ and $E_{\theta_0} = 10^4$.

3.2 Case 2: $\epsilon \ll \delta \sim \theta_0 \ll 1$

In general, equation (14d) for the director angle θ must be solved numerically. However, when $E_{\theta_0} \gg 1$ flow effects dominate orientational elasticity effects and the solution for θ in the bulk is $\theta = 1$ (equivalent to the unscaled value θ_0) if $u_z > 0$ and $\theta = -1$ (equivalent to the unscaled value $-\theta_0$) if $u_z < 0$, with thin boundary layers where θ changes rapidly to its prescribed boundary values, one near the substrate $z = 0$ of thickness $E_{\theta_0}^{-1/2}$ and another near the free surface $z = h(x)$ of thickness $E_{\theta_0}^{-1/3}$. Thus, when $E_{\theta_0} \gg 1$, applying boundary-layer analysis [8] we find an appropriate composite, uniformly valid leading-order asymptotic solution for θ, namely

$$\theta \sim -\mathrm{sgn}(Q-h)\left\{2 - 3\tanh^2\left(\left(\frac{3|Q-h|E_{\theta_0}}{2}\right)^{1/2}\frac{z}{h} + \beta\right)\right.$$
$$\left. + \phi\left(\left(\frac{|Q-h|E_{\theta_0}}{2}\right)^{1/3}\frac{h-z}{h}\right) + 1\right\}, \tag{22}$$

where $\beta = \tanh^{-1}\sqrt{2/3}$, and $\phi(\zeta)$ is obtained numerically by solving

$$\phi_{\zeta\zeta} = \zeta(1-\phi^2), \quad \phi(0) = 0, \quad \phi \to -1 \quad \text{as} \quad \zeta \to +\infty. \tag{23}$$

Figure 4 shows the director profile given by eq. (22) and it clearly shows the boundary-layer structures. Note that in this case the shear never changes sign, and thus neither does the director orientation in the bulk.

4 Drag in

So far we have considered the situation when the substrate $z = 0$ is moving away from the fixed blade; we now study the situation when the substrate is moving towards the blade. In

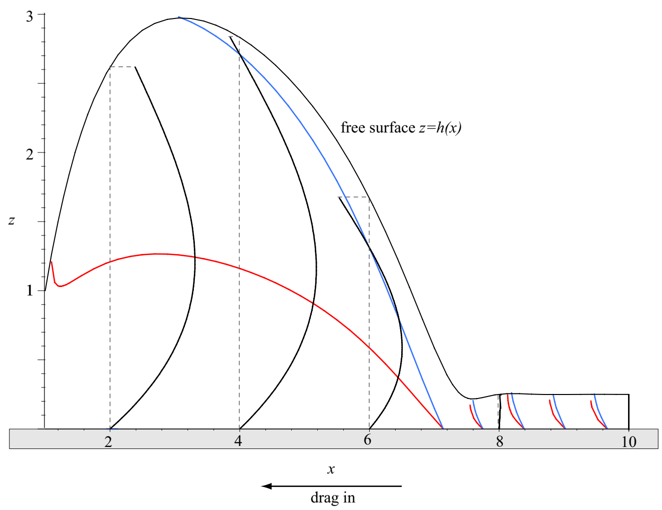

Figure 5: The director angle θ at $x = 2, 4, 6, 8, 10$ in the drag-in problem for Case 1, when $Q = -0.25$, $G = S = 1$ and $E_\epsilon = 5$. The curve on with $\theta = 0$ is indicated by a blue line, and the curve on which $\theta_z = 0$ is indicated by a red line.

this case, the boundary conditions (9) should be replaced by

$$u = -1, \; w = 0, \; \theta = 0 \quad \text{on} \quad z = 0, \tag{24}$$

and the analysis above follows with minor differences. In particular, the free surface now satisfies

$$Sh_{xxx} - Gh_x = \frac{3(Q+h)}{h^3}. \tag{25}$$

Linearising this equation about the uniform solution $h = h_\infty = -Q$ ($Q < 0$) we can show that the decay of h towards the uniform solution as $x \to +\infty$ is monotonic when S and G satisfy

$$0 < \frac{S}{Q^6 G^3} < \left(\frac{2}{9\sqrt{3}}\right)^2 \simeq 0.01646, \tag{26}$$

but is oscillatory otherwise.

In a similar way to the drag-out problem we find that if $h > -3\,Q$ then there are regions of reverse flow (that is, regions in which $u > 0$), and that there is a change in the sign of the shear when $h = -Q$. The sign of the shear will be important in the next two subsections in which we study the director orientation in response to the fluid flow.

4.1 Case 1: $\epsilon \sim \delta \ll \theta_0 \ll 1$

The director profile has a similar form to that in the drag-out problem:

$$\theta = \frac{h_x}{h} z + E_\epsilon \frac{(Q+h)(h-z)(2h-z)z}{2h^3}. \tag{27}$$

Again, the flow effects change the θ profile from a linear to a cubic function of z (see Fig. 5).

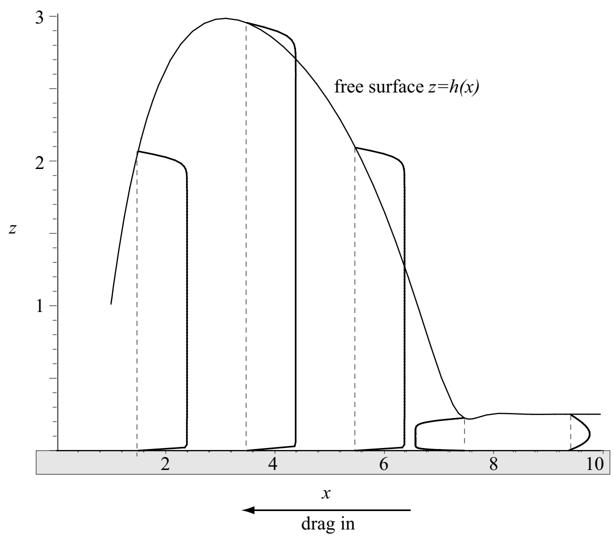

Figure 6: The director angle θ at $x = 1.5, 3.5, 5.5, 7.5, 9.5$ in the drag-in problem for Case 2, when $Q = -0.25$, $G = S = 1$ and $E_{\theta_0} = 10^4$.

4.2 Case 2: $\epsilon \ll \delta \sim \theta_0 \ll 1$

In this case, as in the drag-in problem, boundary-layer analysis leads to the appropriate leading order solution for the director in the form

$$\theta \sim -\mathrm{sgn}(Q+h)\left\{2 - 3\tanh^2\left(\left(\frac{3|Q+h|E_{\theta_0}}{2}\right)^{1/2}\frac{z}{h} + \beta\right) + \phi\left(\left(\frac{|Q+h|E_{\theta_0}}{2}\right)^{1/3}\frac{h-z}{h}\right) + 1\right\}, \tag{28}$$

where ϕ is given again by eq. (23).
Figure 6 shows the director profile given by eq. (28). In this case, the shear changes sign within the film and thus the director orientation in the bulk also changes from $+1$ to -1, accordingly.

5 Conclusions

Using the Ericksen–Leslie equations we have modelled a blade-coating process in which a thin film of a nematic liquid crystal is deposited onto a planar substrate. Analytical results were obtained by assuming that the liquid crystal film is thin and the director distortions are small.
In the drag-out problem the decay of the free surface towards its uniform state far from the blade was found to be always monotonic; furthermore, numerical results suggest that the free surface is monotonic for all x. An analytical solution for the pressure and velocity was found, and also for the director when elasticity effects dominate. In such a case, we showed that the director is monotonic for small values of E_ϵ. When flow effects dominate, the director aligns with $-\theta_0$ in the bulk exhibiting thin boundary layers near the boundaries and, since the shear does not change sign, neither does the alignment of the director in the bulk.

In the drag-in problem it was found that the decay of the free surface towards its uniform state far from the blade can be either monotonic (in which case the behaviour of the director is qualitatively similar to that in the drag-out problem) or oscillatory, depending on the relative strengths of surface tension and gravity. Again, an analytical solution for the pressure and velocity is found, and also for the director when elasticity effects dominate. When the decay of h is oscillatory we found that, when elasticity effects dominate, the film always contains regions where θ is non-monotonic and, when flow effects dominate, θ changes its orientation in the bulk from $-\theta_0$ to θ_0, exhibiting thin boundary layers near the boundaries.

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