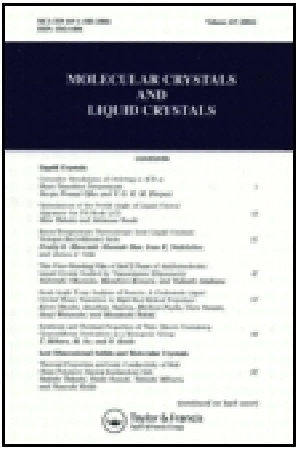

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Steady Flow of a Nematic Liquid Crystal in a Slowly Varying Channel

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We consider steady, two-dimensional flow of a thin film of a nematic liquid crystal between a fixed blade of prescribed shape and a planar substrate moving parallel to itself with a constant velocity. We use a combination of analytical and numerical techniques to analyse the Ericksen–Leslie equations governing the fluid velocity and pressure and the director orientation when both the aspect ratio of the slowly varying channel formed between the blade and the substrate and the distortion of the director field are small. We demonstrate that, in the limit of small orientational elasticity, orientational boundary layers occur close to the substrate and close to the blade, and that, in addition, an orientational internal layer may also occur within which the director orientation changes from $+\theta_0$ *to* $-\theta_0$*, where* θ_0 *is the flow–alignment angle.*

Keywords: Ericksen–Leslie equations; flow alignment; nematic liquid crystal; thin-film flow

INTRODUCTION

The major commercial interest in liquid crystals is a consequence of their optical properties which are exploited in display technologies. These optical properties are directly related to the mean orientation of the molecules in the liquid crystal which can be described by a macroscopic variable, a unit vector called the director. In recent years liquid crystal coating processes have been investigated in

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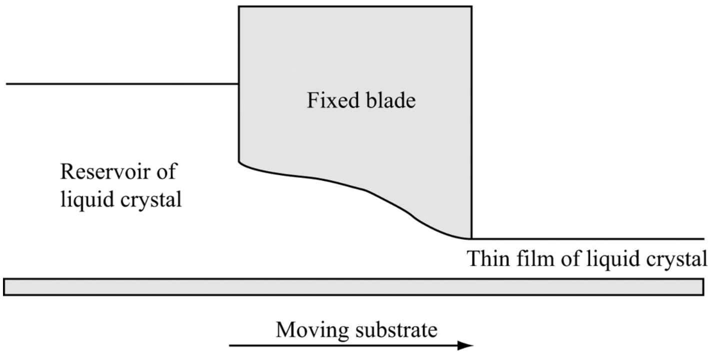

FIGURE 1 Geometry of the coating problem: a substrate is moved to the right under a fixed blade, allowing the liquid crystal to coat the substrate in thin film of (ideally) uniform thickness.

order to facilitate more efficient mass production of liquid crystal displays [1]. These coating techniques typically use a blade, on one side of which there is a reservoir of liquid crystal, and under which the substrate to be coated is pulled. The liquid crystal is then coated onto the substrate in a thin film of (ideally) uniform thickness (see Fig. 1).

The aim of our work is to model the behaviour of a liquid crystal during coating by such a process. Although, in an industrial setting, this process is usually undertaken while the material is in the isotropic phase we will investigate the alignment behaviour in the nematic phase. This will give insight into how flow effects may influence alignment within the coated layer. In particular, an enhanced director alignment within the coated layer, caused by flow effects whilst coating in the nematic phase, would certainly be of interest to device manufacturers since this would lead to contrast enhancement. Specifically we consider steady, two-dimensional flow of a thin film of a nematic liquid crystal between a fixed blade of prescribed shape and a planar substrate moving parallel to itself with a constant velocity.

We use a combination of analytical and numerical techniques to analyse the Ericksen–Leslie equations [2,3] governing the fluid velocity and pressure and the director orientation. The Ericksen–Leslie equations have consistently been successfully applied to many liquid crystal switching and flow problems [4], and we can have confidence that they will accurately model the present system. We will show that, although these equations are rather complicated, analytical solutions can be obtained when some justifiable approximations are made.

In the absence of other effects, shearing a flow-aligning liquid crystal induces a director alignment at a well-determined angle θ_0 to the streamlines (the *flow-alignment angle*). Of crucial importance is the *Ericksen number*, a non-dimensional parameter measuring the relative strength of orientational elasticity and viscosity effects. We demonstrate that, in the limit of small orientational elasticity (i.e., large Ericksen number), orientational boundary layers occur close to the substrate and close to the blade, and that, in addition, an orientational internal layer may also occur within which the director orientation changes from $+\theta_0$ to $-\theta_0$.

MATHEMATICAL MODEL

Consider steady, two-dimensional flow of a thin-film of a nematic liquid crystal between a fixed blade of prescribed shape and a moving planar substrate. The substrate is taken to lie in the plane $z = 0$ whilst the blade is taken to lie at $z = h(x)$, a known function of x, the coordinate in the direction of shear (see Fig. 2). The substrate is moved to the right at a constant speed U, and we assume that all dependent variables are functions of x and z only. The nematic director $\mathbf{n}$ is assumed to lie within the plane of shear (a good assumption for realistic values of the shear) and the fluid velocity $\mathbf{v}$ is assumed to have components only in the x and z directions, which is also a good assumption if $\mathbf{n}$ remains in the x–z plane. The director, fluid velocity and pressure

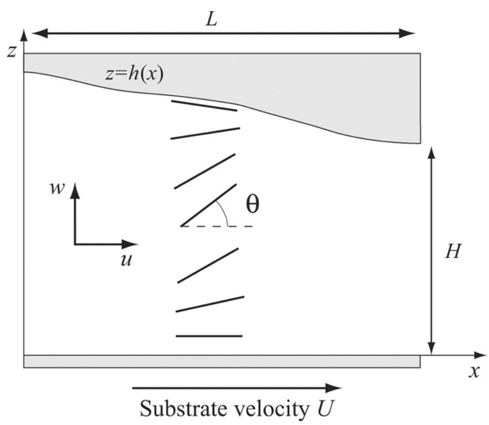

FIGURE 2 The mathematical model of a nematic liquid crystal in a slowly varying channel under a fixed blade.

may therefore be written as

$$\begin{aligned}\mathbf{n} &= (\cos\theta(x,z), 0, \sin\theta(x,z)),\\ \mathbf{v} &= (u(x,z), 0, w(x,z)),\\ p &= p(x,z),\end{aligned} \tag{1}$$

where the director angle θ is the angle that the director makes with the positive x-axis. We use the following non-dimensionalisation of the independent and dependent variables and parameters:

$$x = Lx^*, \quad z = Hz^*, \tag{2}$$

$$h = Hh^*, \quad \alpha_i = \mu_0\alpha_i^*, \quad K_i = K_0K_i^*, \tag{3}$$

$$u = Uu^*, \quad w = \frac{HU}{L}w^*, \quad \tilde{p} = \frac{\mu_0 UL}{H^2}\tilde{p}^*, \tag{4}$$

where μ_0 is some measure of the Leslie viscosities α_i, K_0 is some measure of the elastic constants K_i, H is a typical value of h, and L is the length of the blade in the x direction. The length and velocity in the x and z directions have been non-dimensionalised differently to reflect the slenderness of the slowly varying channel formed between the blade and the substrate, and the standard "lubrication" scaling of the pressure has been employed [5, Chap. 4]. In addition, the standard redefinition of pressure used when studying the Ericksen–Leslie equations [3,4] has been employed so that the modified pressure $\tilde{p}$ includes a term dependent on orientational elasticity.

There are a two important points to make at this stage. In this paper we will assume that α_3 is negative, as is the case in calamitic liquid crystals [6]. In discotic liquid crystals this is not usually the case [7]. However, the analysis below follows through directly, with minor differences, for $\alpha_3 > 0$. When presenting results, we will assume a specific blade shape, namely $h(x) = 1 - \alpha(1 - x)$ with $\alpha < 0$, corresponding to a linearly converging channel. The analogous blade shape corresponding to a linearly diverging channel, namely $h(x) = 1 + \alpha x$ with $\alpha > 0$, can be obtained by using the transformation $(\alpha, x) \to (-\alpha, 1-x)$. However, in the general analysis below, no assumption about the blade shape is made, and the linear blade shape is chosen only in order to plot examples of the velocity profiles and director-orientation patterns.

In general, very little analytical progress can be made since the governing equations are partial differential equations that involve nonlinear functions of θ. For instance, in the momentum equations the effective viscosity is a nonlinear function of θ,

$$\alpha_{\text{eff}} = \frac{1}{2}(\alpha_4 + \alpha_3 + \alpha_6)\cos^2\theta + \frac{1}{2}(\alpha_4 + \alpha_5 - \alpha_2)\sin^2\theta + \alpha_1\cos^2\theta\sin^2\theta. \tag{5}$$

In order to make analytical progress, we will make some justifiable approximations, as described in the next two sections.

THIN-FILM APPROXIMATION

The first approximation we make is a thin-film approximation [5, Chap. 4] based on the assumption that the aspect ratio ϵ of the channel (defined by $\epsilon = H/L$) is small, that is, $\epsilon \ll 1$. In the limit $\epsilon \to 0$ the Ericksen–Leslie equations give (dropping the superscript star from the non-dimensional variables)

$$0 = \tilde{p}_x - (g(\theta)u_z)_z + O(\epsilon), \tag{6}$$

$$0 = \tilde{p}_z + O(\epsilon), \tag{7}$$

$$0 = Em(\theta)u_z - \left[f(\theta)\theta_{zz} + \frac{1}{2}f'(\theta)\theta_z^2\right] + O(\epsilon), \tag{8}$$

where

$$g(\theta) = \eta_1\cos^2\theta + \eta_2\sin^2\theta + \alpha_1\cos^2\theta\sin^2\theta, \tag{9}$$

$$f(\theta) = K_1\cos^2\theta + K_3\sin^2\theta, \tag{10}$$

$$m(\theta) = \alpha_3\cos^2\theta - \alpha_2\sin^2\theta, \tag{11}$$

in which $\eta_1 = 1/2(\alpha_4 + \alpha_3 + \alpha_6)$ and $\eta_2 = 1/2(\alpha_4 + \alpha_5 - \alpha_2)$ are two of the so-called *Miesowicz viscosities* [8]. The non-dimensional parameter $E = \mu_0 UH/K_0$ is the *Ericksen number* and represents the ratio of orientational elasticity and viscosity effects. Appropriate choices of μ_0 and K_0 are η_1 and K_1, respectively.

The non-dimensional boundary conditions on u, θ and $\tilde{p}$ are

$$u = 1,\ \theta = 0 \quad \text{on} \quad z = 0, \tag{12}$$

$$u = 0,\ \theta = \epsilon h_x \quad \text{on} \quad z = h, \tag{13}$$

$$\tilde{p} = 0 \quad \text{at} \quad x = 0,\, 1. \tag{14}$$

The boundary conditions on u and θ correspond, respectively, to no slip and strong homogeneous orientation (i.e., the director is parallel to the boundary) at both boundaries. The boundary conditions on $\tilde{p}$ follow from (7), which requires that the pressure at either end of the blade is constant, and the assumption that the pressure is the same at these points. Since the pressure enters the Ericksen–Leslie equations through derivative terms, and is therefore degenerate up to an additive constant, we can then take the rescaled pressure to be equal to zero at $x = 0$ and $x = 1$.

Because of the nonlinear dependence of $g(\theta)$, $f(\theta)$ and $m(\theta)$ on θ it still seems that, in general, no significant analytical progress can be made. In order to make progress we will consider a second approximation concerning the size of θ.

DIRECTOR APPROXIMATION

The boundary conditions on θ are $\theta = 0$ at $z = 0$ and $\theta = \epsilon h_x$ at $z = h$, and it may be possible that θ remains no larger than $O(\epsilon)$ throughout the channel. Since no external torques (such as those induced by an applied electric field) are present, the only internal torque that might cause the director to be larger than $O(\epsilon)$ is the torque due to the fluid flow. In a flow-aligning material the flow effects will tend to align the director so that $\theta = \pm\theta_0$, where $\theta_0 = \tan^{-1}(\sqrt{\alpha_3/\alpha_2})$ is the flow-alignment angle, whereas in a non-flow-aligning material the flow will cause the director to rotate continuously ("tumble"). In flow-aligning materials, α_3 is typically two orders of magnitude smaller than α_2, and so θ_0 is usually small. Therefore, the maximum director angle in the layer is at least as large as ϵ, since it attains this value at the blade, and, if $\theta_0 > \epsilon$, will be no larger than θ_0, since this is the maximum value that flow aligning can achieve. Therefore, since both ϵ and θ_0 are small, we can confidently assert that $\theta << 1$, i.e., that the distortion of the director field is small.

We now have three small parameters to consider: the aspect ratio ϵ, a director-angle scale δ which is defined by $\theta = \delta\theta^*$ with $\theta^* = O(1)$, and the flow-alignment angle θ_0. Since, as explained above, θ cannot be smaller than ϵ everywhere in the channel, there are two main cases to consider: $\delta = O(\epsilon)$ and $\delta >> \epsilon$. Within these two main cases we must consider various sub-cases depending on the size of the parameter θ_0. If $\delta << \theta_0$ then the flow has only a small effect on the director. If, however, $\delta = O(\theta_0)$ then the flow aligns the director. Finally, if $\delta >> \theta_0$ then the blade aligns the director at an angle much greater than the flow-alignment angle.

Case 1: $\epsilon \sim \delta << 1$, i.e., the maximum value of θ is of a similar size to the boundary–dictated value of the director angle. In this case there are three subcases to consider.

Case 1a: $\delta << \theta_0$ or θ_0 does not exist: flow effects are insufficient to increase θ significantly from the boundary–dictated value and flow alignment is not achieved.

Case 1b: $\delta \sim \theta_0$: flow effects are sufficiently strong to achieve flow alignment in part of the channel.

Case 1c: $\delta >> \theta_0$: the flow–alignment angle is much less than the boundary–dictated value. Flow alignment may occur, but the director angle will attain its maximum value at the blade.

Case 2: $\epsilon << \delta << 1$, i.e., the maximum value of θ is much larger than the boundary–dictated value of the director angle. In this case there are again three subcases to consider.

Case 2a: $\delta << \theta_0$ or **θ_0 does not exist:** flow effects increase θ significantly above the boundary–dictated value, but they are not sufficiently strong to achieve flow alignment.

Case 2b: $\delta \sim \theta_0$: flow effects are sufficiently strong to achieve flow alignment in part of the channel.

Case 2c: $\delta >> \theta_0$: this situation (in which the director angle is much greater than both the boundary–dictated value and the flow-alignment angle) is not physically realisable if the liquid crystal is flow aligning and no external torque is present.

Of the physically realistic cases, two possibilities (Cases 1b and 1c) result in partial differential equations that include derivatives in the x direction and fluid velocity in the z direction; these must, in general, be solved numerically. In Cases 1a and 2a the equations simplify significantly and the solutions for u and θ are readily found to be polynomial functions of z (θ being found to be a cubic function of z in both cases). The situation in Case 2b is more interesting and this is the case we will concentrate on in the remainder of the present work.

RESULTS

When $\epsilon << \delta \sim \theta_0 << 1$ flow effects are sufficiently strong to achieve flow alignment in part of the channel. If we set $\delta = \theta_0$ then in the limit $\theta_0 \to 0$ Eqs. (6)–(8) become

$$0 = \tilde{p}_x - u_{zz} + O(\theta_0), \tag{15}$$

$$0 = \tilde{p}_z + O(\theta_0), \tag{16}$$

$$0 = \theta_{zz} + E(1-\theta^2)u_z + O(\theta_0), \tag{17}$$

where the appropriate scaled Ericksen number is $E = -\alpha_3 UH/\theta_0 K_1$. The boundary conditions (12) and (14) again hold, but at leading order (13) is replaced by $u = 0$ and $\theta = 0$ on $z = h$.

The velocity profile can be calculated directly from (15) and (16) to be

$$u = \frac{h-z}{h^3}\left[h^2 - 3(h-h_{\mathrm{m}})z\right], \tag{18}$$

where $h_{\mathrm{m}} = I_2/I_3$ with

$$I_n = \int_0^1 \frac{1}{h^n(\tilde{x})}\,\mathrm{d}\tilde{x}. \tag{19}$$

Since θ does not enter (15) and (16) at leading order the velocity profile is exactly the same as that for a Newtonian fluid [5, Chap. 4, p. 66]. If $h > 3h_{\mathrm{m}}/2$ there is a region of reverse flow (i.e., a region in which $u < 0$) between the curve on which $u = 0$ and the blade $z = h$, and a region of reverse shear (i.e., a region in which $u_z > 0$) between the curve on which $u_z = 0$, denoted by $z = z_{\mathrm{m}}$ where

$$z_{\mathrm{m}} = \frac{h(4h - 3h_{\mathrm{m}})}{6(h-h_{\mathrm{m}})}, \tag{20}$$

and the blade $z = h$. If $h < 3h_{\mathrm{m}}/4$ there is a region of reverse shear between $z = z_{\mathrm{m}}$ and the substrate $z = 0$. These regions of reverse shear will be important when we consider the director reorientation in response to the fluid flow.

Figure 3 shows the velocity profiles in the linearly converging channel $h = 1 - \alpha(1-x)$ when $\alpha = -2$. In this case

$$h_{\mathrm{m}} = \frac{2(1-\alpha)}{(2-\alpha)} = \frac{3}{2}, \tag{21}$$

and so when $h > 3h_{\mathrm{m}}/2 = 9/4$ (i.e., when $x < 3/8$) there is a region of reverse flow above the curve on which $u = 0$ (marked with a dashed line) and a region of reverse shear above $z = z_{\mathrm{m}}$ (marked with a dotted line), and when $h < 3h_{\mathrm{m}}/4 = 9/8$ (i.e., when $x > 15/16$) there is a region of reverse shear below $z = z_{\mathrm{m}}$ (again marked with a dotted line). Note that if the blade angle is sufficiently small in magnitude (specifically if $\alpha > -1$) then the regions of reverse flow and shear do not occur.

From (17) we see that, if $E \ll 1$ then orientational elasticity effects dominate flow effects and the leading order solution for θ is a linear

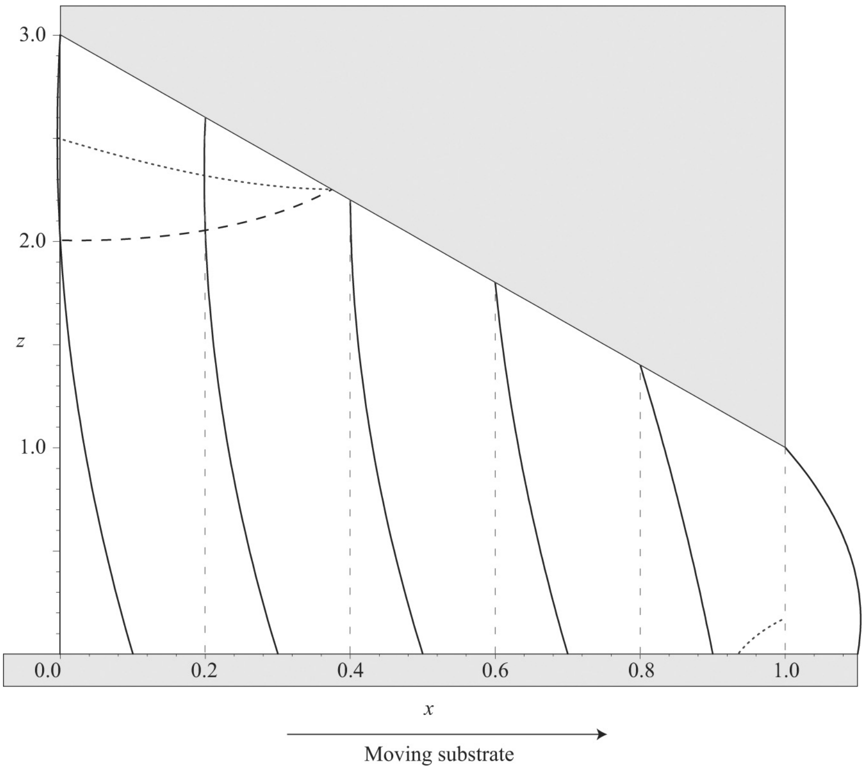

FIGURE 3 Velocity profiles in the case $h(x) = 1 + 2(1 - x)$ at $x = 0, 0.2, 0.4, 0.6, 0.8, 1$. Reverse flow occurs above the curve on which $u = 0$ (indicated with a dashed line), and reverse shear occurs above $z = z_{\mathrm{m}}$ (indicated with a dotted line) when $h > 9/4$ (i.e., when $x < 3/8$) and below $z = z_{\mathrm{m}}$ when $h < 9/8$ (i.e., when $x > 15/16$).

function of z. If $E = O(1)$ then orientational elasticity effects are comparable with flow effects and little analytical progress can be made because of the presence of the θ^2 term in (17). However, if $E >> 1$ then flow effects dominate orientational elasticity effects and $\theta = \pm 1$ (equivalent to the unscaled statement $\theta = \pm\theta_0$) everywhere except for thin regions over which θ changes rapidly from $+1$ to -1.

By substituting the velocity profile (18) into the angular momentum balance (17), and performing a standard boundary–layer analysis [9], we find that there are thin orientational boundary layers of thickness $O(E^{-1/2})$ near $z = 0$ and $z = h$ in which θ changes from its "outer" value of $+1$ or -1 to its "wall" value of $\theta = 0$. If $h < 3h_{\mathrm{m}}/4$ or $h > 3h_{\mathrm{m}}/2$ then there is also a thin orientational internal layer of thickness $O(E^{-1/3})$ near $z = z_{\rm m}$ within which the shear changes sign and θ changes between its outer values of $+1$ and -1. A composite, uniformly valid leading-order asymptotic solution for θ throughout the channel is found to be

$$\begin{aligned}\theta \sim\ & \mathrm{sgn}(q_0)\left[3\tanh^2\left(\left(\frac{|q_0|E}{2}\right)^{1/2} z \pm \beta\right) - 2\right]\\ &+ \mathrm{sgn}(q_h)\left[3\tanh^2\left(\left(\frac{|q_h|E}{2}\right)^{1/2} (h - z) \pm \beta\right) - 2\right]\\ &- \tilde{\phi}\left((|h - h_{\rm m}|E)^{1/3}\frac{z - z_{\rm m}}{h}\right),\end{aligned} \tag{22}$$

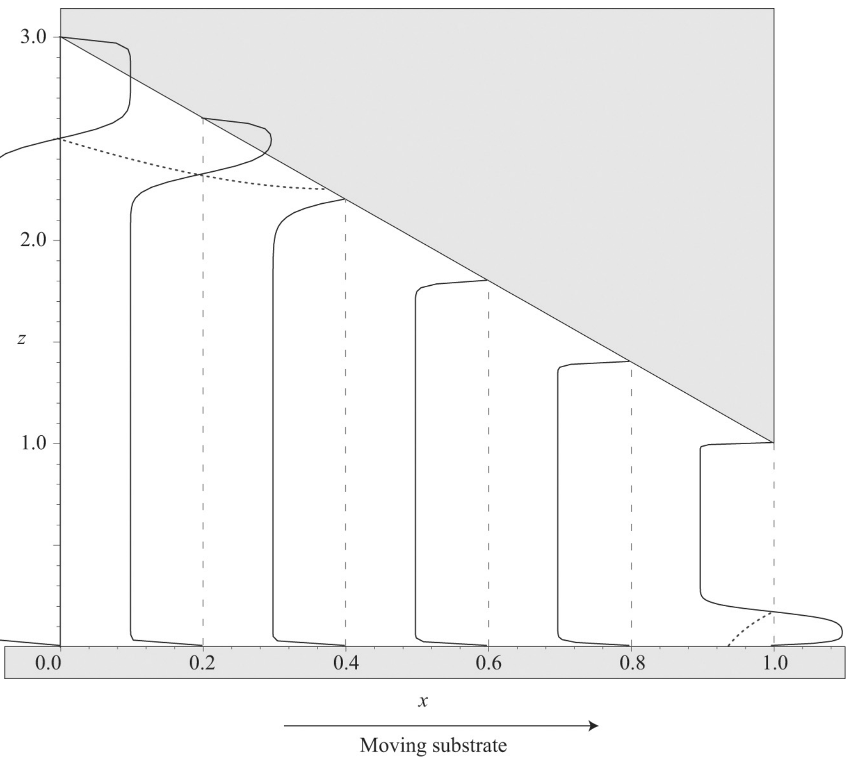

FIGURE 4 The director–orientation profiles in the case $h(x) = 1 + 2(1 - x)$ at $x = 0, 0.2, 0.4, 0.6, 0.8, 1$ when $E = 10^4$. Orientational boundary layers occur near $z = 0$ and $z = h$, and an orientational internal layer occurs near $z = z_{\rm m}$ (indicated with a dotted line).

where

$$q_0 = u_z\big|_{z=0} = \frac{3h_{\mathrm{m}} - 4h}{h^2}, \tag{23}$$

$$q_h = u_z\big|_{z=h} = \frac{2h - 3h_{\mathrm{m}}}{h^2}, \tag{24}$$

$$\beta = \tanh^{-1}\sqrt{\frac{2}{3}} \simeq 1.14622, \tag{25}$$

and

$$\tilde{\phi}(\xi) = \begin{cases} -1 & \text{if} \quad \dfrac{3h_{\mathrm{m}}}{4} < h < \dfrac{3h_{\mathrm{m}}}{2} \\ \mathrm{sgn}(h - h_{\mathrm{m}})\phi(\xi) & \text{if} \quad h < \dfrac{3h_{\mathrm{m}}}{4} \quad \text{or} \quad h > \dfrac{3h_{\mathrm{m}}}{2}, \end{cases} \tag{26}$$

where $\phi = \phi(\xi)$ satisfies

$$\phi_{\xi\xi} = 6\xi(1 - \phi^2) \ \text{ subject to } \ \phi \to \pm 1 \quad \text{as} \quad \xi \to \mp\infty. \tag{27}$$

This system for ϕ, which describes the behaviour within the internal layer, must be solved numerically; however, since it does not contain any parameters, it needs to be solved only once.

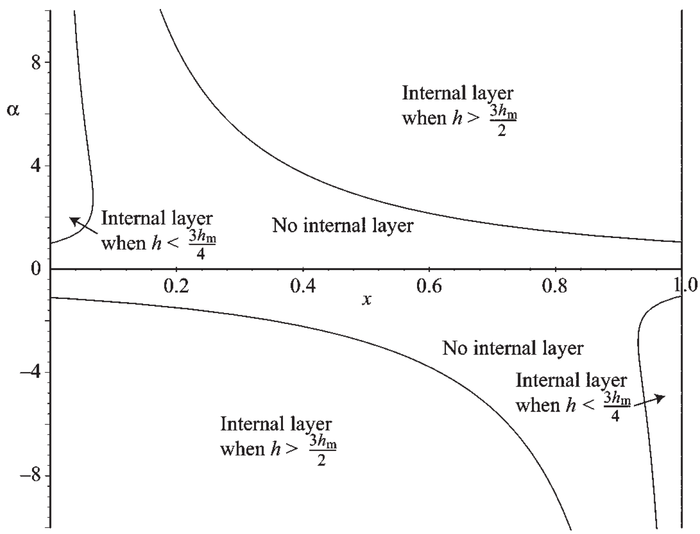

FIGURE 5 The x-α parameter plane showing the regions within which an orientational internal layer occurs for both linearly converging ($\alpha < 0$) and linearly diverging ($\alpha > 0$) channels.

The choices of plus or minus signs in (22) lead to four distinct solutions. The choice of either of the minus signs corresponds to a solution with higher energy than the solution where both plus signs are chosen, and is therefore unlikely to be achieved in practice. We will therefore be concerned only with the solution in (22) with both plus signs chosen.

Figure 4 shows the director–orientation profiles in the linearly converging channel $h = 1 - \alpha(1 - x)$ when $\alpha = -2$. Figure 4 clearly shows the boundary and internal layer structure; in particular, it shows how the internal layer merges with the top boundary and reappears again from the bottom boundary as x increases. Note that the corresponding director profiles for a linearly *diverging* channel can easily be constructed by exploiting the transformation $(\alpha, x) \to (-\alpha, 1 - x)$. Figure 5 shows the regions of the x-α parameter plane within which an internal layer occurs for both linearly converging ($\alpha < 0$) and linearly diverging ($\alpha > 0$) channels. In particular, Figure 5 shows that there are no internal layers when $|\alpha| < 1$.

Note that it is also possible to construct the director profiles for a *nonlinear* blade shape. Since the x coordinate enters (8) essentially as a parameter, the director angle $\theta(x, z)$ at any point x along the channel may be found by using the *local* slope of the blade $\alpha = h_x$ in (22).

DISCUSSION

We considered steady, two-dimensional flow of a thin film of a nematic liquid crystal between a fixed blade of prescribed shape and a planar substrate moving parallel to itself with a constant velocity. A simplified version of the Ericksen–Leslie equations was obtained by assuming that both the aspect ratio of the slowly varying channel formed between the blade and the substrate and the distortion of the director field are small. In this paper we considered the situation when flow effects dominate orientational elasticity effects (Case 2b). In this case orientational boundary layers occur close to the substrate and close to the blade, and, in addition, an orientational internal layer also occurs when $h > 3h_{\mathrm{m}}/2$ and when $h > 3h_{\mathrm{m}}/4$ (i.e., when the channel is sufficiently wide and when it is sufficiently narrow).

Although not presented in this paper, in the case when orientational elasticity dominates flow effects (Cases 1a and 2a) we have found that the equations simplify significantly and the solutions for u and θ are readily found to be polynomial functions of z (θ being a cubic function of z in both cases). When orientational elasticity and flow effects are comparable (Cases 1b and 1c) the equations simplify to partial differential equations that include derivatives in the *x* direction and fluid velocity in the *z* direction; these must, in general, be solved numerically.

REFERENCES

[1] Penterman, R., Klink, S. I., de Koning, H., Nisato, G., & Broer, D. J. (2002). *Nature*, *417*, 55.
[2] Ericksen, J. L. (1960). *Arch. Ration. Mech. Anal.*, *4*, 231.
[3] Leslie, F. M. Q. (1966). *J. Mech. Appl. Math.*, *19*, 357.
[4] Stewart, I. W. (2004). *The Static and Dynamic Continuum Theory of Liquid Crystals*, Taylor and Francis.
[5] Ockendon, H. & Ockendon, J. R. (1995). *Viscous Flow*, Cambridge University Press.
[6] Dunmur, D. A., Fukuda, A., & Luckhurst, G. (2000). *Physical Properties of Liquid Crystals*: *Nematics*, INSPEC.
[7] de Andrade Lima, L. R. P. & Rey, A. D. (2003). *J. Non–Newt. Fluid Mech.*, *110*, 103.
[8] Miesowicz, M. (1935). *Nature*, *17*, 261.
[9] Nayfeh, A. H. (1973). *Perturbation Methods*, Wiley.