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I. Zúñiga[a,b]; F. M. Leslie[a]
[a] Mathematics Department, Strathclyde University, Glasgow, Scotland [b] Departamento de Fisica Fundamental, U. N. E. D., Madrid, Spain

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Shear-flow instabilities in non-flow-aligning nematic liquid crystals

by I. ZÚÑIGA† and F. M. LESLIE
Mathematics Department, Strathclyde University, Glasgow, Scotland

This paper investigates theoretically the stability of non-flow-aligning nematics in simple shear flow by analyzing the relevant continuum equations. With the aid of numerical techniques, it proves possible to predict thresholds for instability to perturbations both within and out of the shear plane, based on the full equations without approximations. The results obtained are consistent with corresponding experimental studies.

1. Introduction

The behaviour of a nematic liquid crystal in simple shear flow between parallel plates depends crucially upon the orientation of the initial alignment with respect to the plane defined by the imposed velocity vector and the normal to the plates, which is referred to as the shear plane. For example, if the alignment is orthogonal to the shear plane, there is a critical value of the rate of shear beyond which the alignment changes to a new configuration [1]. On the other hand, if the alignment lies initially in the shear plane, the flow can be stable, and for sufficiently large shear rates the alignment is uniform at a small angle to the streamlines [2]. However, there are some nematics that do not exhibit this uniform flow alignment for a range of temperature close to the smectic–nematic transition temperature. This was first reported by Gähwiller [3], who observed that for temperatures lower than a critical value, instead of flow alignment a turbulent state develops. In simple shear-flow experiments Pieranski and Guyon [4] found that the non-alignment is due to the change in sign of the viscosity coefficient α_3 from negative to positive. When α_3 is positive, they observed a critical shear rate at which the alignment comes out of the shear plane. Similar experiments were carried out by Cladis and Torza [5] in Couette flow between concentric cylinders for a nematic with α_3 positive, and they found a first instability threshold at which the alignment changes abruptly to a new configuration, but after this instability, called tumbling, the alignment remains in the shear plane. These somewhat conflicting observations have remained unexplained.

In a recent paper Zúñiga and Leslie [6] investigate the stability of plane shear flow, and employed numerical methods to solve the relevant equations, although they adopted some approximations that may not always be reasonable. A review of earlier theoretical work is given in §3. In the present paper we consider the full equations without approximations and find new instability effects. However, our conclusions are essentially similar to those in the simplified case, and are consistent with the experiments of Pieranski and Guyon [4]. Our results therefore help to clarify the somewhat conflicting experimental evidence, since they tend to confirm that the Cladis and Torza instabilities [5] are possibily peculiar to Couette flow, and so should not be compared with those in plane shear flow.

† Permanent address: Departamento de Física Fundamental, U.N.E.D., Apdo. Correos 50487, 28080 Madrid, Spain.

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2. Basic equations

Consider a layer of nematic confined between two infinite parallel plates a distance $2h$ apart, which are sheared with constant velocity $\mathscr{V}$ in opposite directions along a straight line in their plane. We choose a system of cartesian axes such that the y axis is normal to the bounding plates, with the x axis along the direction of shear and the origin in the centre of the layer. With this choice, it is reasonable to consider the velocity $\mathbf{v}$ and the director $\mathbf{n}$ to be of the following forms:

$$\left.\begin{array}{llll} v_x = u(y,t), & v_y = 0, & v_z = v(y,t), \\ n_x = \cos\theta\cos\phi, & n_y = \sin\theta\cos\phi, & n_z = \sin\phi, \end{array}\right\} \tag{2.1}$$

where θ and ϕ are also functions of y and t. In these expressions, the velocity components, the spatial coordinate and time have been made dimensionless by using h as the natural length scale and $\gamma_1 h^2/K_1$ as the time scale, where K_1 is a Frank constant and γ_1 is the twist viscosity coefficient (see later). Since we examine small perturbations of steady shear flow, the continuum equations are linearized with respect to the variables v, ϕ and $\dot{\theta}$ about the steady in-plane solution with these variables zero, the dot denoting the time derivative. In this event, the resulting equations with these scalings, reduce to

$$\frac{d}{d\theta}[f(\theta)(\theta')^2] - 2\dot{\theta} - (1 + \lambda\cos 2\theta)u' = 0, \tag{2.2}$$

$$[2u'g(\theta) + (1 + \lambda\cos 2\theta)\dot{\theta}]' = 2A\dot{u}, \tag{2.3}$$

$$[f_1(\theta)\phi']' + [f_2(\theta) + \lambda u'\sin\theta\cos\theta]\phi - \dot{\phi} - \alpha v'\sin\theta = 0, \tag{2.4}$$

$$[v'g_1(\theta) + u'g_2(\theta)\phi + \alpha\dot{\phi}\sin\theta]' = A\dot{v}, \tag{2.5}$$

where

$$\left.\begin{array}{rcl} A &=& \dfrac{\varrho K_1}{\gamma_1^2}, \quad \lambda = \dfrac{\gamma_2}{\gamma_1}, \quad \alpha = \dfrac{\alpha_2}{\gamma_1}, \\ K_1 f(\theta) &=& K_1 + (K_3 - K_1)\sin^2\theta, \\ K_1 f_1(\theta) &=& K_2 + (K_3 - K_2)\sin^2\theta, \\ K_1 f_2(\theta) &=& \theta''(K_2 - K_1)\sin\theta\cos\theta \\ && - (\theta')^2\{(3K_2 - K_1 - 2K_3)\sin^2\theta - K_2\}, \\ 2\gamma_1 g(\theta) &=& \alpha_4 + (\alpha_3 + \alpha_6)\cos^2\theta + (\alpha_5 - \alpha_2)\sin^2\theta \\ && + 2\alpha_1\sin^2\theta\cos^2\theta, \\ 2\gamma_1 g_1(\theta) &=& \alpha_4 + (\alpha_5 - \alpha_2)\sin^2\theta, \\ 2\gamma_1 g_2(\theta) &=& (\alpha_3 + \alpha_6 + 2\alpha_1\sin^2\theta)\cos\theta, \\ \gamma_1 &=& \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5 = \alpha_3 + \alpha_2, \end{array}\right\} \tag{2.6}$$

and $\alpha_1 \cdots \alpha_6$ are viscous coefficients, K_1, K_2 and K_3 are elastic constants, ϱ is the density, and the prime denotes the dimensionless spatial derivative.

Assuming that there is strong anchoring at the plates and that the initial alignment is uniform and in the shear plane, the boundary conditions are

$$\left.\begin{array}{l} u(1) = -u(-1) = V, \quad v(1) = v(-1) = 0, \quad V = \gamma_1 h\mathscr{V}/K_1 \\ \theta(1) = \theta_w, \quad \theta(-1) = \theta_w + n\pi, \quad \phi(1) = \phi(-1) = 0, \end{array}\right\} \tag{2.7}$$

where n is an integer. The angle θ_w can take any value, but here we consider only the values zero and $\frac{1}{2}\pi$ that correspond to the two principal configurations of experimental interest.

For small shear rates we expect a steady state in which the director lies in the shear plane with no transverse velocity, i.e. ϕ and v are both zero. In this event, (2.2)–(2.5) reduce to

$$\left.\begin{aligned} \frac{d}{d\theta}[f(\theta)\theta'^2] - \frac{a(1+\lambda\cos 2\theta)}{g(\theta)} &= 0, \\ u'g(\theta) &= a, \end{aligned}\right\} \qquad (2.8)$$

where a is a positive constant equal to the non-dimensional stress exerted on the moving plates.

To study the stability of the steady solution of (2.8), we consider both perturbations $\tilde{v}$, $\tilde{\phi}$ out of the shear plane and perturbations $\tilde{u}$, $\tilde{\theta}$ in the shear plane of the form

$$(\tilde{u}, \tilde{v}, \tilde{\theta}, \tilde{\phi}) = [U(y), V(y), \Theta(y), \Phi(y)]e^{-\omega t}, \qquad (2.9)$$

with ω real. The equations governing these perturbations follow by substitution of the perturbed solution $(u+\tilde{u}, \tilde{v}, \theta+\tilde{\theta}, \tilde{\phi})$ into (2.2)–(2.5), neglecting second-order terms in the perturbations. The inertial terms $A\dot{u}$ and $A\dot{v}$ may be neglected since they are very small ($A \approx 10^{-6}$) compared with $\dot{\theta}$ and $\dot{\phi}$. The quantity A can be interpreted as the ratio of the characteristic time for damping of velocity fluctuations and that for director fluctuations. Thus, by neglecting inertial terms, we are assuming that velocity fluctuations can be regarded as being independent of time compared with director fluctuations. Using (2.3) and (2.5) to eliminate u and v in (2.2) and (2.4), Currie [7] derived the following two Sturm–Liouville equations for the perturbation Φ and Θ:

$$[f_1(\theta)\Phi']' + \left\{f_2(\theta) + \frac{a\sin\theta}{g(\theta)}\left[\lambda\cos\theta + \frac{\alpha g_2(\theta)}{g_1(\theta)}\right]\right\}\Phi + \omega_0\left[1 - \frac{(\alpha\sin\theta)^2}{g_1(\theta)}\right]\Phi = 0, \qquad (2.10)$$

$$2f(\theta)\Theta'' + 2\frac{df(\theta)}{d\theta}\theta'\Theta' + \left\{\frac{d}{d\theta}\left[\frac{df(\theta)}{d\theta}(\theta')^2\right] + \frac{a}{g(\theta)}\left[2\lambda\sin 2\theta + \frac{1+\lambda\cos 2\theta}{g(\theta)}\frac{dg(\theta)}{d\theta}\right]\right\}\Theta + \omega_i\left[2 - \frac{(1+\lambda\cos 2\theta)^2}{2g(\theta)}\right]\Theta = 0. \qquad (2.11)$$

Owing to the non-linearity of (2.8), the steady solution $\theta(y)$ is not readily obtainable in explicit form, and consequently the coefficients in the equations are not expressible in convenient analytic forms.

With strong anchoring of the director at the plates, the boundary conditions for the perturbations are

$$\Phi(\pm 1) = \Theta(\pm 1) = 0. \qquad (2.12)$$

Given that (2.10) and (2.11) are uncoupled, they lead to two independent neutral-stability curves. The steady solution is unstable to perturbations out of the shear plane if there is a shear rate a for which ω_0 is negative, and similarly it is unstable to perturbations in the shear plane if ω_i is less than zero.

3. Simplified models

In order to make progress with the in-plane equations (2.8), previous authors have adopted the two simplifications

$$\text{(i) } \alpha_1 = 0, \quad \text{(ii) } K_1 = K_2 = K_3 = K. \tag{3.1}$$

For nematics with α_3 negative, Currie and MacSithigh [8] have used these approximations and have discussed the stability and dissipation of a number of possible solutions of (2.8) subject to the conditions (2.7). In this way, they show that the system adopts a solution that is symmetric in y and has a single maximum. Thus this solution satisfies

$$\theta(y) = \theta(-y), \quad \theta'(0) = 0, \quad \theta(0) = \theta_m, \tag{3.2}$$

where θ_m is the maximum tilt angle across the gap. With the approximations (3.1), the equations (2.8) integrate to yield

$$\left.\begin{aligned} (\theta')^2 &= 2a[F(\theta) - F(\theta_m)], \\ F(\theta) &= \theta - \frac{\mu}{(\eta_b\eta_c)^{1/2}} \tan^{-1}\left[\left(\frac{\eta_c}{\eta_b}\right)^{1/2} \tan\theta\right], \\ 2\mu &= \alpha_4 + \alpha_5 + \alpha_2, \quad 2\eta_b = \alpha_4 + \alpha_3 + \alpha_6, \quad 2\eta_c = \alpha_4 + \alpha_5 - \alpha_2. \end{aligned}\right\} \tag{3.3}$$

In an earlier paper Pikin [9] studied the stability of an approximate solution of (2.8), valid only for small values of the angle θ such that $\theta^2 \ll 1$. Considering only perturbations in the shear plane, he showed analytically that, when the ratio α_3/α_2 is positive, the flow is stable to infinitesimal perturbations at all values of the velocity V, but that there is a critical value V_c above which his approximate solution becomes unstable when α_3/α_2 is negative.

Using a finite-difference scheme and these approximations (3.1), Manneville [10] integrates the two-dimensional equations (2.8) numerically, and found that for a certain range of velocities V of the plates two different solutions coexist when α_3 is positive. Each solution corresponds to different values of θ_m, which are $\frac{1}{2}\pi$ apart. The tumbling observed by Cladis and Torza [5] is then explained as a discontinuous jump from one solution to the other. Carlsson [11] integrated (3.3) and the second of (2.8) by quadrature, and showed that the function $\theta_m(V)$ is multivalued for small negative values of the ratio α_3/α_2. In that event the tumbling should disappear as the temperature decreases and approaches the smectic–nematic transition. However, this is in apparent conflict with the experimental observations of Cladis and Torza (see figure 2 (*a*) in [5]).

All of these papers seem to give some support to the tumbling instability found by Cladis and Torza [5], in conflict with the findings of Pieranski and Guyon [4]. However, an initial assumption that the director remains in the shear plane can hardly explain an instability with the director departing from the shear plane. The need to consider perturbations out of the shear plane was first appreciated by Pieranski, Guyon and Pikin [12], and, making further approximations over and above those in (3.1), they found an instability threshold at which the director comes out of the plane. The value of this threshold is about twice as large as that corresponding to instability to perturbations in the plane, the latter calculated numerically using Pikin's analysis [9]. However, as the authors acknowledged, the analysis is valid only for shear rates smaller than that corresponding to the first threshold.

In a recent paper Zúñiga and Leslie [6] have obtained a numerical solution of (3.3) and the second of (2.8), and have examined its stability with respect to perturbations both out of and in the shear plane by solving (2.10) and (2.11) with the simplifications (3.1). The calculations employ three different sets of values for the viscosities, but the same value for the elastic constant. It is possible to characterize the sets of viscosities by the value of the ratio

$$\varepsilon = \alpha_3/|\alpha_2|. \tag{3.4}$$

The critical maximum tilt angle calculated for the instability out of the plane in the planar configuration is quite large, varying between 180° and 130° for the different viscosity values used (see table I in [6]). For the homeotropic configuration the same angle is found to be slightly greater than 90° for all three sets of viscosity values. On the other hand, the instability to perturbations in the plane depends strongly upon ε (see figures 1 and 2), the solution becoming stable as ε increases. The critical maximum tilt angle is again close to 90° in the homeotropic configuration for the three sets of constants, but in the planar configuration this value tends to zero with ε. In fact, when ε is equal to 10^{-3}, two tumblings occur before the solution becomes unstable to perturbations out of the plane. The first tumbling corresponds to a jump from θ_m with value $-2.2°$ to $-170°$, and this new state is stable until θ_m becomes larger than a second threshold at $-181°$, but now this instability will take the director out of the plane since the new configuration is unstable to out-of-plane perturbations. Although this is similar to the observations of Cladis and Torza [5], they used a different geometry (cylindrical) and configuration (homeotropic).

Except in extreme cases when ε is small compared with unity, Zúñiga and Leslie have found that the director comes out of the plane following the instability. For their second set of viscosity values, ε is relatively small and close to the value relevant to the experiments by Pieranski and Guyon [4]. In this case tumbling occurs first, but the new configuration is soon unstable to out of plane perturbations. For larger values of ε, there is no tumbling, and the instability taking the director out of the plane occurs first.

4. Numerical studies of the full equations

Near the smectic–nematic transition the viscous coefficients α_1, α_3 and α_6 and the elastic constants K_2 and K_3 diverge, while K_1, α_2, α_4 and α_5 remain finite. Therefore in (3.1) neither the one-elastic–constant approximation nor the assumption that α_1 is zero can be justified. Near the temperature at which α_3 becomes positive, the term α_1 does not seem to be important in the viscosity function $g(\theta)$. On the other hand, the twist elastic constant K_2 is always smaller than K_3 and K_1 ($2K_2 \approx K_3$), and so should play a role in the instability out of the plane. In order to study the effects of the two approximations in (3.1), we consider the full equations without the approximations.

The integration of the steady solution of the system of non-linear ordinary differential equations (2.8) subject to the boundary conditions (2.7) was achieved by means of a finite-difference technique with deferred correction and Newton inter-action. We have used a NAG routine based on the technique described in [13]. For a given value of the shear rate a, the NAG routine, supplied with an initial guess for the profiles, iterates until the difference between two successive solutions is within a small prescribed tolerance; in this way, the steady solutions $\theta(y)$ and $u(y)$ could be obtained to any desired accuracy. For the range of values of a in which there are two solutions, both are found by choosing an appropriate initial guess. Starting with

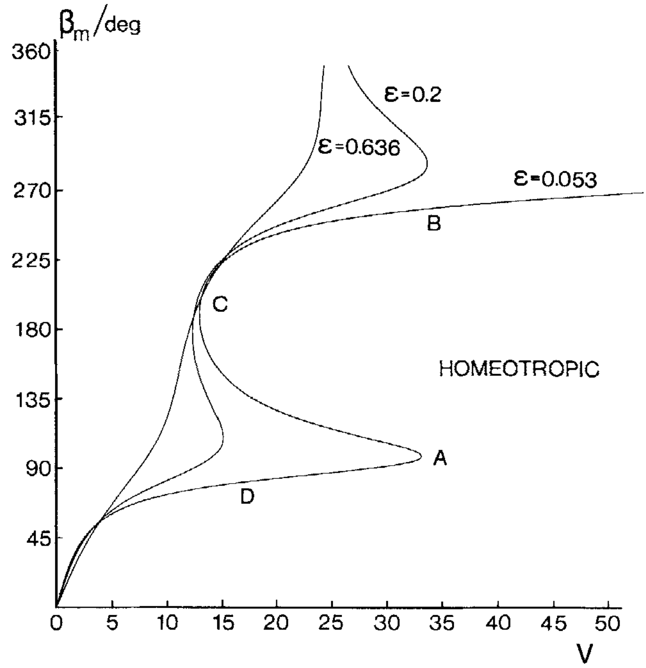

Figure 1. The orientation at the plates is homeotropic. $\beta_m = |\theta_m - \frac{1}{2}\pi|$ is the maximum tilt angle and V is the non-dimensional velocity. In this figure and in figure 2 we have used set 3 of the material constants, but with $\alpha_1 = 0$ and $K_1 = K_2 = K_3 = 10^{-11}$ N in order to use (2.8) and (3.3).

a small value of a and incrementing to higher values, at each stage using as the initial guess the previous solution, we eventually encounter the tumbling (point A, figure 1), which is a jump to the second solution at point B. However, using this second solution as initial guess and decreasing the value of a, the upper branch to the point C at which one jumps back to the first solution at D is followed. This hysteresis was avoided in the simplified model [11, 6] because by quadrature of (3.3) it is possible to obtain a as a function of θ_m, which is a single-valued relation (whereas θ_m is a multivalued function of V; see figures 1 and 2). Figures 3 and 4 give typical director and velocity profiles.

For each solution $\theta(y)$ we have computed the eigenvalue of both Sturm–Liouville equations (2.10) and (2.11) subject to the boundary conditions (2.12). Instead of the Galerkin method used in the previous paper [6], we obtained the eigenvalues by means of a shooting method with a Runge–Kutta–Merson integration. A comparison of the results from the Galerkin method with those from the shooting method gives a useful check on the accuracy of the results.

We have used several sets of material constants taken from data for 4-n-octyl-4′-cyanobiphenyl (8CB) some of which are shown in table 1. The results of the calculations are presented in table 2. They show that the approximate steady solution is close to the exact one, but for the exact solution there is a slight additional stabilizing effect due to the extra viscosity α_1. The approximate analysis is very good for describing the instability to perturbations in the plane because it essentially reflects the coexistence of two solutions for certain ranges of values of the shear rate. This is why the stability analysis developed by Pikin [9] gives accurate results. On the other hand, a dramatic reduction of the threshold for instability out of the plane is obtained. It

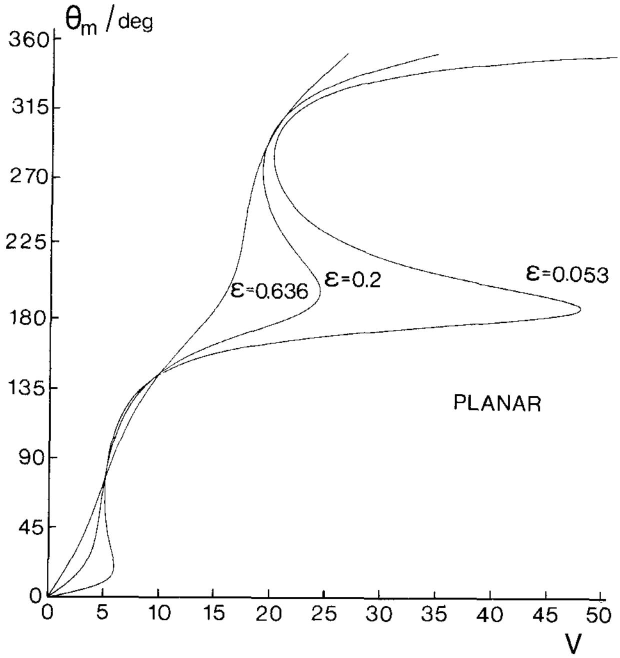

Figure 2. The orientation at the plates is planar. θ_m is the maximum tilt angle and V the non-dimensional velocity. We have used the same values of the material constants as in figure 1.

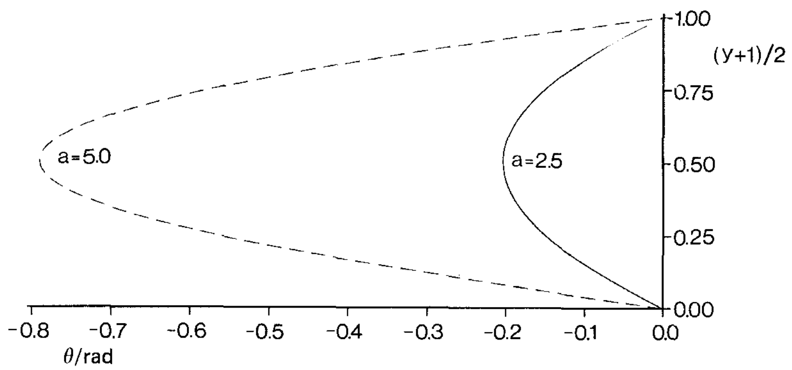

Figure 3. The tilt angle across the layer for two values of the shear rate, using set 3 of the material constants.

is rather surprising that this reduction takes place even if only one of the approximations (3.1) is removed. This can be understood by inspection of (2.10), which gives the total torque in the x direction. The first term is a stabilizing elastic torque, whereas the second term is a destabilizing torque, which has a contribution $f_2(\theta)$ from the deformation of the director and a viscous torque proportional to a. When these stabilizing and destabilizing torques cancel each other, the solution will be marginally stable. The important contribution to the destabilizing torque when $K_2 \neq K_1$ is through $f_2(\theta)$, and the corresponding contribution from α_1 is through $g_2(\theta)$. This latter contribution is significant when $\alpha_3 + \alpha_6$ is small compared with $2\alpha_1 \sin^2 \theta$; since α_6 is generally negative, this is likely to occur when α_3 is positive and approximately equal to $|\alpha_6|$.

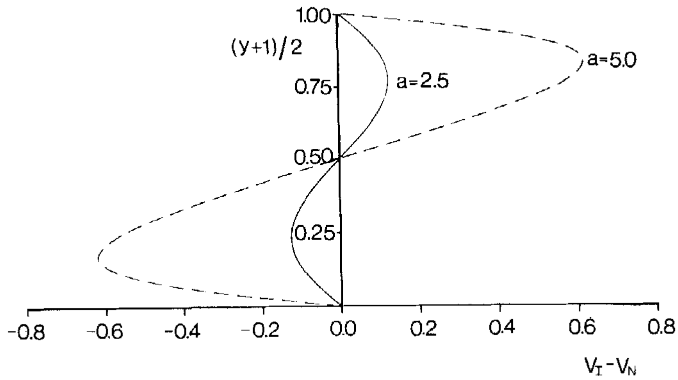

Figure 4. The difference between the non-dimensional velocity profile for the nematic V_N and the corresponding velocity profile for an istropic liquid V_I, again using set 3 of the material constants.

Table 1. Material constants.

Set	1	2	3	4	5	6
α_1/Pa s	0·026	0·014	0.038	0·0078	0·134	0·39
α_2/Pa s	−0·052	−0·049	−0·059	−0·045	−0·070	−0·070
α_3/Pa s	$0{\cdot}825 \times 10^{-3}$	$0{\cdot}15 \times 10^{-2}$	$0{\cdot}305 \times 10^{-2}$	$0{\cdot}42 \times 10^{-2}$	0·014	0·027
α_4/Pa s	0·05	0·049	0·052	0·048	0·056	0·057
α_5/Pa s	0·043	0·036	0·047	0·026	0·053	0·059
α_6/Pa s	$-0{\cdot}82 \times 10^{-2}$	−0·011	$-0{\cdot}84 \times 10^{-2}$	−0·014	$-0{\cdot}29 \times 10^{-2}$	0·016
$10^{11}K_1$/N	1·29	0·90	1·20	0·70	1·40	1·45
$10^{11}K_2$/N	0·60	0·40	0·56	0·35	0·70	0·90
$10^{11}K_3$/N	1·30	0·90	1·20	0·67	2·10	2·80
ε	0·016	0·031	0·052	0·093	0·2	0·39

Viscosity values are taken from [14, 15] and elastic constants from [16, 17].

Table 2. Stability in terms of maximum tilt angle θ_m.

	Planar, $\theta_w = 0°$			Homeotropic, $\theta_w = 90°$		
ε	$\theta_c^{in}/°$	$\theta_c^{out}/°$	V_c	$\theta_c^{in}/°$	$\theta_c^{out}/°$	V_c
0·016	−10·3	−9·2	9·9	−4·0	−4·0	69·4
0·031	−22·3	−13·2	7·4	−7·0	−5·7	46·0
0·053	−18·3	−14·9	6·0	−7·1	−7·4	33·2
0·093	−177·6	−25·8	5·0	−10·9	−10·4	22·9
0·20	−183·3†	−22·3	3·8	−57·3	−11·2	15·8
0·39	−160·4†	−23·5	3·2	22·9	−11·5	11·9

θ_c^{in} and θ_c^{out} are the critical values of θ_m. Thus the solution is stable to perturbations in the shear plane when $\theta_w > \theta_m > \theta_c^{in}$, and is stable to perturbations out of the shear plane when $\theta_w > \theta_m > \theta_c^{out}$.

V_c is the non-dimensional velocity of the top plate corresponding to the first instability. The actual velocity $\mathscr{V}_c$ is equal to $K_1 V_c/\gamma_1 h$. Note that the use of $\mathscr{V}$ and h differs by a factor 2 in the present paper from that in [6], this implying a corresponding factor 4 in the critical value for the scale velocity.

† These values do not correspond to an instability but rather to a very sharp continuous tumbling.

With the full equations, the solution first becomes unstable to perturbations out of the plane for all sets of constants that we have considered, except in single instances for sets 3 and 6 when the initial orientation is homeotropic. However, the tumbling instability produces a tilt configuration that is immediately unstable to perturbations out of the plane. It is also interesting to note that the critical velocity V_c for stability increases (apparently without bound) as ε tends to zero, but tends to a (non-zero) constant value for large ε. This dependence of the critical velocity on ε corresponds to that found in the experiments of Pieranski, Guyon and Pikin [12]. It also corresponds to the dependence found by Cladis and Torza [5] of the critical velocity for the first tumbling on temperature, i.e. on ε. As we have explained, the theoretical explanation for the tumbling, namely that θ_m is a multivalued function of V, is valid only for small ε. Therefore, even if an instability out of the plane did not arise, the nature of tumbling could not be explained in terms of plane flow.

5. Conclusions

A numerical integration of the basic steady solution in simple shear flow has been obtained. Without the usual approximations adopted by previous authors, we have studied the stability of the solution to certain perturbations both in and out of the plane, and find in general that there is a critical value for the shear rate above which the solution becomes unstable out of the plane. This is the case both for homeotropic and for planar configurations, and for a number of sets of material constants. The different sets of material constants from data on 8CB were chosen in order to investigate the dependence of the instability threshold on temperature. All our results are consistent with the experiments of Pieranski and Guyon [4, 12]. This work therefore clarifies the apparently conflicting evidence provided by the experiments of Cladis and Torza [5] and those of Pieranski and Guyon [4]. Our results suggest that the tumbling observed in the former experiments may not be explained by means of an analysis of plane shear flow, and is more likely to be associated with the cylindrical geometry used in the experiments. However, before drawing too firm conclusions, perhaps some consideration should be given to other selections of material parameters, and possibly, also more general perturbations notwithstanding the experimental evidence of apparent homogeneous instabilities.

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