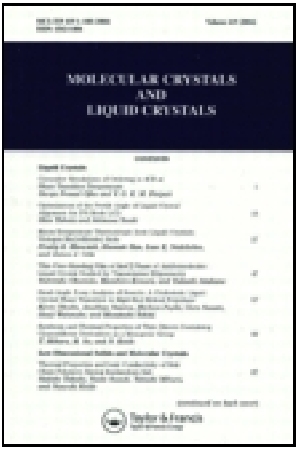

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ANALYSIS OF CONVERGING AND DIVERGING FLOW OF NEMATIC LIQUID CRYSTAL POLYMERS

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Abstract A similarity solution of the Leslie-Ericksen equations for nematic liquid crystals is obtained for converging and diverging flow. The director distribution for parameters characteristic of lyotropic liquid crystal polymer solutions shows a boundary layer resulting from interactions between wall- and flow-induced orientations; the boundary layer scaling with Ericksen number differs, depending on whether the interaction is with the shear flow near the wall or the extensional flow near the channel midplane. Imposition of an azimuthal magnetic field causes a first-order Freedericksz-like transition in director orientation at a critical field strength.

INTRODUCTION

Studies of orientation development in liquid crystalline polymers have generally been restricted to viscometric (i.e., simple shearing) geometries. Shear is an ineffective means of molecular orientation, and in fact most processing flows involve changes in geometry, where the deformation process includes extension and compression; extensional flows typically orient rigid inclusions within one strain unit, and therefore have very different characteristics from shear flows. The simplest model flow that includes extension or compression as well as shear is the *Jeffrey-Hamel flow*, which is a two-dimensional radial flow between infinite planes. This flow field approximates the converging or diverging sections in more complex geometries.

A similarity solution has long been known to exist for

Jeffrey-Hamel flow of Newtonian fluids[1]; the similarity transformation reduces the nonlinear partial differential equations to a set of ordinary differential equations. Leslie[2] extended this result to Ericksen's *Transversely Isotropic Fluid*[3,4], which is the simplest continuum model of a liquid with rod-like structure. We have recently shown[5] that a similarity solution exists for the Leslie-Ericksen fluid[6,7], which is generally believed to be an adequate representation of the rheological properties of low molecular weight nematic liquid crystals. This solution exhibits several characteristics that are of potential practical importance, as follows:

1. There is an orientation boundary layer near the wall, which represents the region of transition from wall-induced orientation to the orientation that is induced by the flow. The boundary layer thickness depends on a dimensionless group known as the Ericksen number (see below), with two different regions of scaling; the boundary layer thickness varies with the reciprocal one-third power of the Ericksen number when the boundary layer extends suffciently far from the wall that it intersects the region of extensional flow, while the boundary layer varies with the reciprocal one-half power of the Ericksen number when the flow is of sufficiently high intensity that the boundary layer is restricted to the shear-dominated region near the wall. This result is obtained analytically in closed form.

2. When an azimuthally-oriented magnetic field is imposed on the converging flow, there is a critical field strength at which a first-order transition from radial to transverse orientation occurs at the centerline. This is a dynamical analog of a Freedericksz transition, and the critical field can be expressed explicitly in terms of a grouping of the Leslie viscosity coefficients. A comparable transition might be expected with a radially-oriented field in diverging flow, but in fact no such transition occurs. There is rather a development of a wall-like orientation transition from radial to azimuthal near the center line.

The rheology of nematic liquid crystalline polymers is not well-understood. Doi's[8] theory is incomplete, and contains no analog of the Oseen-Frank elastic stresses. The Doi theory does reduce in the limit of small deformation rates to the viscous terms in the Leslie-Ericksen theory, giving explicit values of the viscosity coefficients in terms of two scalar parameters, a rotational diffusion coefficient and the scalar order parameter. The Leslie-Ericksen theory may approximate the

TABLE I Parameters Used in the Simulations.

Viscosity coefficients (poise)					
α_1	α_2	α_3	α_4	α_5	α_6
-5052	-2636	-439	1889	2725	-350
Elastic constants (dynes x 10^6)					
K_{11}	K_{33}				
1.817	0.8395				
Magnetic susceptibility (cgs emu g^{-1} x 10^7)					
$\chi_\perp$	$\Delta\chi$				
-5.0	1.0				

properties of lyotropic liquid crystalline polymer solutions, and there have been some attempts to estimate the material parameters. It is unlikely that the theory is directly applicable to thermotropic systems; Moore and Denn[9] have shown, for example, that the analog of the Oseen-Frank elasticity in a thermotropic liquid crystal polymer must allow for creep.

We have applied the similarity solution for Jeffrey-Hamel flow of a Leslie-Ericksen fluid to two cases that might be characteristic of lyotropic liquid crystalline polymer solutions; we have used a set of parameters for poly (1,4-phenylene-2,6-benzobisthiazole) estimated by Se and Berry[10], as well as the viscosity coefficients that follow from the limiting case of the Doi theory. The parameters estimated by Se and Berry, which are shown in Table 1, are not consistent with the Doi theory, but the flow behavior for both sets of parameters is essentially the same and we show only the former here. The general conclusion is that, except for scaling because of the different orders of magnitude of viscosities, the predictions for the polymeric liquid crystals in Jeffrey-Hamel flow do not differ from those for the low molecular weight nematics.

FLOW FIELD

The geometry is shown schematically in Figure 1. The major assumption leading to the similarity solution is that the velocity vector contains only a radial component, v_r, which is a function of r and ψ. Conservation of mass requires

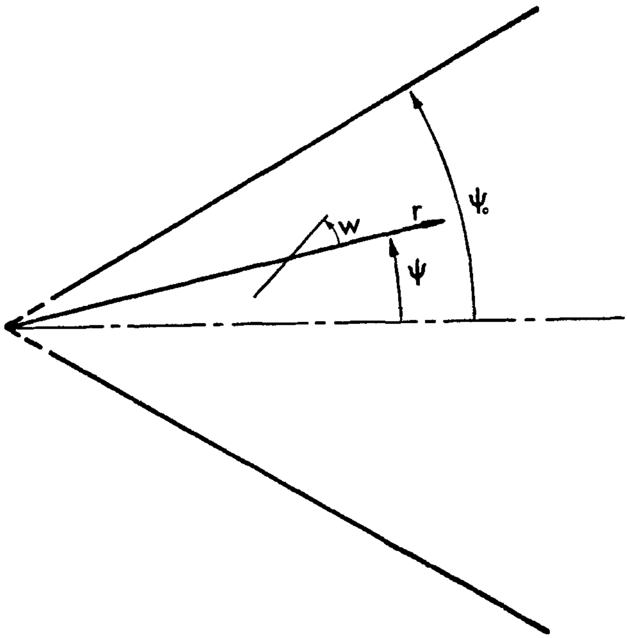

FIGURE 1. Schematic of the flow.

that the velocity be of the form $u(\psi)/r$. The director is assumed to lie in the ψ-r plane, in which case it is represented by a function $W(\psi)$, as follows:

$$n_r = \cos W(\psi), \qquad n_\psi = \sin W(\psi)$$

W defines the director angle relative to a ray passing through the origin, so $W = 0$ represents radial alignment at *any azimuthal position. The flow is characterized by a* single dimensionless group, the *Ericksen number*, E, defined as follows:

$$E = (\alpha_2 - \alpha_3)q/K_{11}$$

K_{11} is the elasticity coefficient for splay deformations. The flow rate per unit width, q, is defined

$$q = \int_{-\psi_o}^{\psi_o} u(\psi)\, d\psi$$

E is positive for converging flow and negative for diverging flow. In the absence of an imposed electromagnetic field it can be established through a stability analysis that the center line orientation must be radial (W = 0) for converging flow and transverse (W = $\pm \pi/2$) for diverging flow.

PROFILES

The computed velocity distribution is shown in Figure 2 for a fluid with the parameters of PBT in Table 1 and a half angle (ψ_o) of 0.5 radians. Curve C is the result for a Newtonian fluid. The velocity profile is relatively insensitive to the Ericksen number, and never deviates significantly from the profile for a Newtonian fluid. This result, which is also observed for the parameters characteristic of low molecular weight nematic, is useful for obtaining approximate analytical solutions, since the Newtonian result is known in closed form. The orientation distribution is shown in Figure 3 for different possible wall anchoring angles. The solution clearly illustrates the presence of a core orientation that is independent of

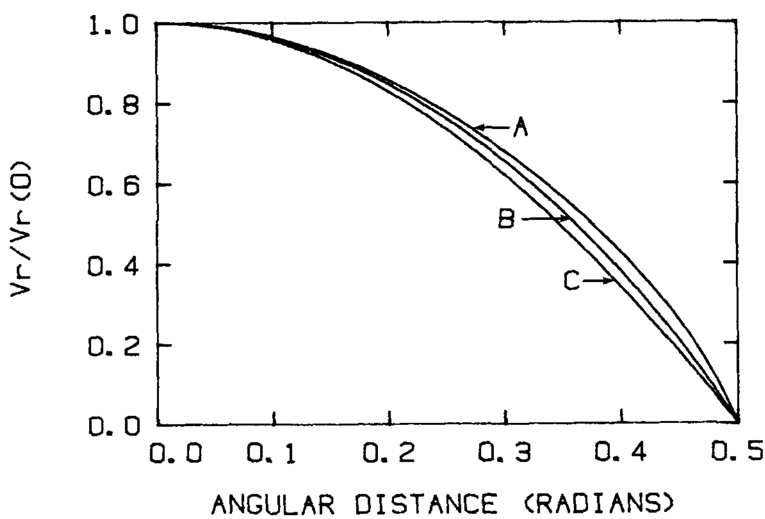

FIGURE 2. Velocity profile for converging flow, normalized relative to the centerline velocity. A: E = 66; B: E = 6; C: Newtonian fluid.

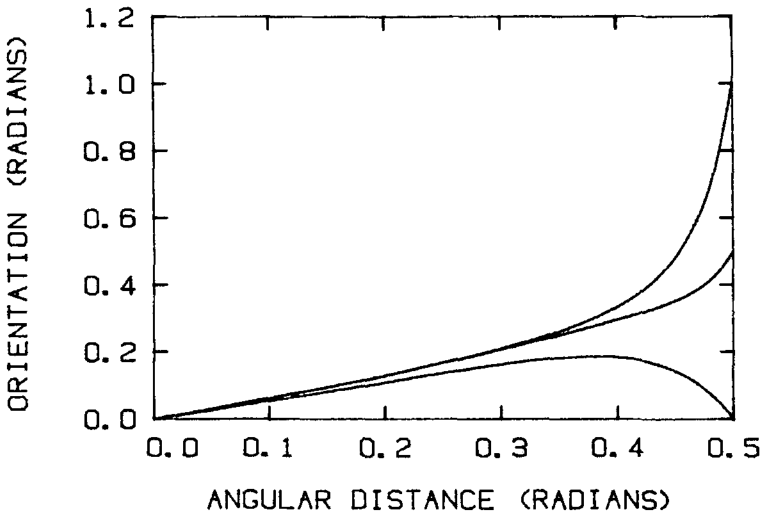

FIGURE 3. Effect of wall-induced orientation on the director orientation profile.

the wall behavior and a boundary layer determined by the competition between the elasticity and flow; the boundary layer thickness is well approximated by the analytical result obtained previously[5] using asymptotic analysis, as follows:

$$E<2000: \ \delta \sim 2 \left[\frac{\tan 2\psi_o - 2\psi_o}{2E} \right]^{1/3} \frac{(\lambda^2 - 1)^{1/2}}{2}$$

$$E>2000: \ \delta \sim 3.5 \left[\frac{\tan 2\psi_o - 2\psi_o}{E} \right]^{1/2} (\lambda^2 - 1)^{-1/4}$$

The result for low Ericksen number represents the competition between wall-induced elasticity and the extensional flow along the center line, while the result for higher values of the Ericksen number reflects the fact that the boundary layer has thinned sufficiently so that the extensional flow has little significance and the competition is between wall anchoring and the shear flow in the neighborhood of the wall. The results using viscosity parameters developed from the Doi theory are essentially the same.

The director profile for diverging flow is shown in Figure 4. The inelastic core/boundary layer behavior is

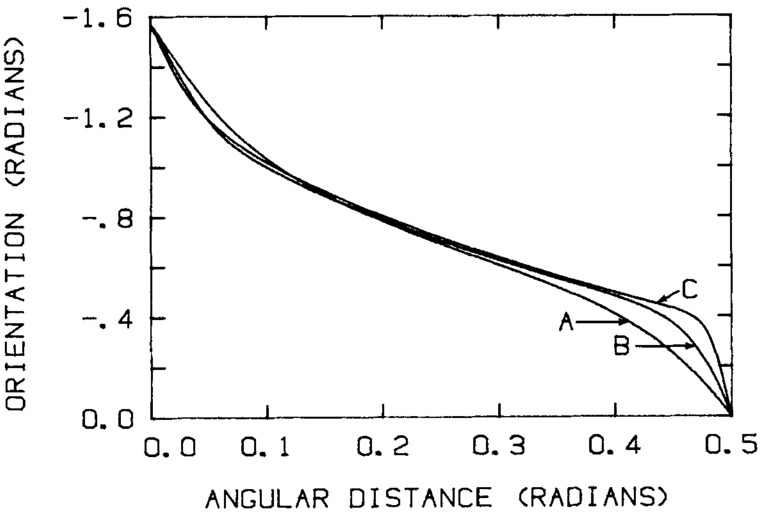

FIGURE 4. Director orientation profile for diverging flow. A: E = −96; B: E = −515; C: E = −1819.

clearly seen here as well; the boundary layer thickness is described by the asymptotic theory. It is perhaps useful to note that the boundary layer is an inevitable feature of flows of nematic liquids and is the probable cause of the thin, highly oriented regions that are commonly observed on parts that have been molded from liquid crystalline polymers. High Ericksen numbers in processing could be undesirable, since a very thin boundary layer like the one that is seen to be developing in Figure 4 might have an enhanced tendency to peel.

MAGNETIC FIELDS

Similarity solutions can be obtained where there is a magnetic field with the form H = [A/r, B/r, 0]. The presence of the magnetic field introduces a new dimensionless group, as follows:

$$\mathcal{D} = (\alpha_2 - \alpha_3)\ q/(A^2 + B^2)\ \Delta\chi$$

$\Delta\chi$ is the anisotropic magnetic susceptibility. The effect of a radial field on converging flow is shown in Figure 5; increasing field strength causes a more uniform radial alignment, while also decreasing the intensity of the flow for a fixed upstream pressure.

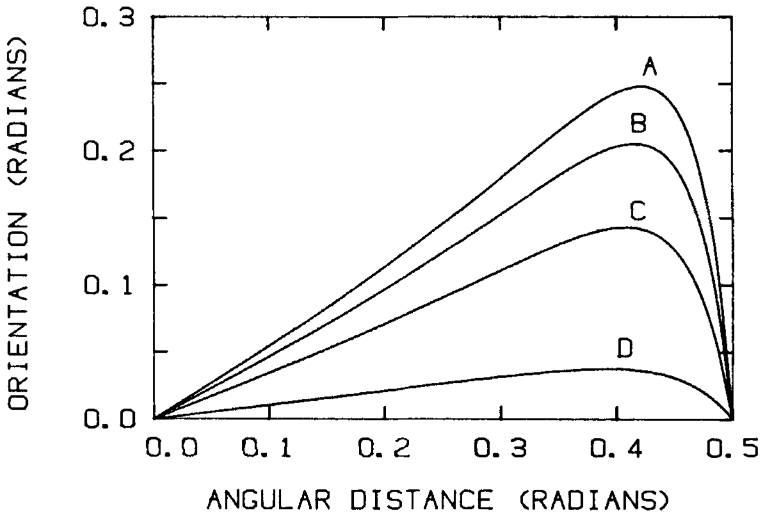

FIGURE 5. Effect of a radial magnetic field on director orientation profile. A: $\mathcal{D} = \infty$ (no field); B: $\mathcal{D} = 1.71$; C: $\mathcal{D} = 0.53$; D: $\mathcal{D} = 0.078$.

The effect of an azimuthal field on converging flow is shown in Figure 6. Curve A represents the stable orientation distribution just prior to the imposition of the critical field, after which there is a first-order Freedericksz-like transition; the critical field is given by the equation

$$B_c^{\,2} = 2(\alpha_6 - \alpha_5)\, u(0)/\Delta\chi$$

u(0) can be estimated from the analytical solution for a Newtonian fluid. Curve A in Figure 7 shows the orientation distribution just prior to transition, while curve C shows the stable distribution for a field slightly in excess of the critical field; increasing the field still further will stop the flow completely, with an orientation distribution given by curve B, and the flow will be reversed at still higher field strengths. The time scales associated with this transition will be long because of the high viscosity, and it is possible that meta-stable intermediate structures might be observed (c.f. Meyer[11]).

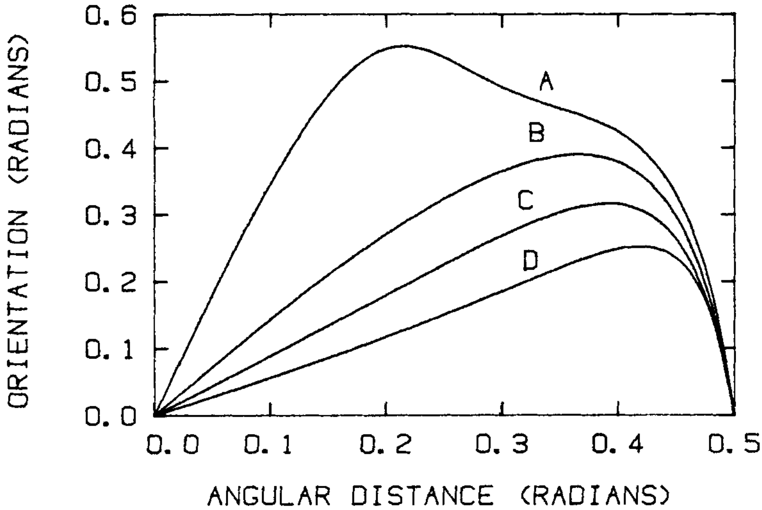

FIGURE 6. Effect of an azimuthal magnetic field on director orientation in converging flow. A: $\mathcal{D}$ = 0.42; B: $\mathcal{D}$ = 0.49; C: $\mathcal{D}$ = 0.76; D: $\mathcal{D}$ = 8.

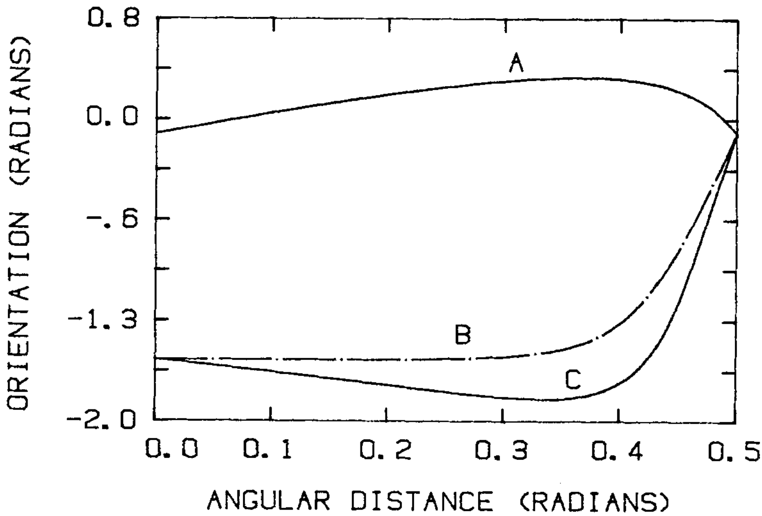

FIGURE 7. Director orientation distribution in converging flow near the critical field. A: $\mathcal{D}$ = 0.45; B: $\mathcal{D}$ = 0 (flow reversal); C: $\mathcal{D}$ = 0.40.

The interaction of the magnetically- and flow-induced orientation in diverging flow is such that no transitions occur.

ACKNOWLEDGMENT

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