Physica D 351–352 (2017) 1–13

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Solution landscapes in nematic microfluidics

M. Crespo [a,*], A. Majumdar [b], A.M. Ramos [c], I.M. Griffiths [d]

[a] UMR MISTEA - Mathématiques, Informatique et Statistique pour l´ Environnement et l´Agronomie (INRA/SupAgro). 2, Place P.Viala, 34060 Montpellier, France

[b] Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, UK

[c] Departamento de Matemática Aplicada & Instituto de Matemática Interisciplinar, Universidad Complutense de Madrid, Plaza de Ciencias, 3, 28040 Madrid, Spain

[d] Mathematical Institute, Radcliffe Observatory Quarter, University of Oxford, Oxford, OX2 6GG, UK

HIGHLIGHTS

- We explore the equilibria in nematic microfluidics as a function of pa- rameters ($\mathcal{G}$, $\mathcal{B}$).
- We demonstrate multistability for admissible pairs ($\mathcal{G}$, $\mathcal{B}$).
- We perform an asymptotic analysis of the static equilibria in the limits $\mathcal{G} \to 0$ and $\mathcal{G} \to \infty$.
- We study the sensitivity of the dynamic solutions to initial conditions.
- We control the final steady state by manipulating the rate of change of $\mathcal{G}$ and $\mathcal{B}$.

ARTICLE INFO

Article history:
Received 21 July 2016
Received in revised form
21 April 2017
Accepted 25 April 2017
Available online 4 May 2017
Communicated by C. Josserand

Keywords:
Leslie–Ericksen model
Nematic microfluidics
Asymptotic analysis
Anchoring strength

ABSTRACT

We study the static equilibria of a simplified Leslie–Ericksen model for a unidirectional uniaxial nematic flow in a prototype microfluidic channel, as a function of the pressure gradient $\mathcal{G}$ and inverse anchoring strength, $\mathcal{B}$. We numerically find multiple static equilibria for admissible pairs ($\mathcal{G}$, $\mathcal{B}$) and classify them according to their winding numbers and stability. The case $\mathcal{G} = 0$ is analytically tractable and we numerically study how the solution landscape is transformed as $\mathcal{G}$ increases. We study the one-dimensional dynamical model, the sensitivity of the dynamic solutions to initial conditions and the rate of change of $\mathcal{G}$ and $\mathcal{B}$. We provide a physically interesting example of how the time delay between the applications of $\mathcal{G}$ and $\mathcal{B}$ can determine the selection of the final steady state.

1. Introduction

Recent years have seen a tremendous surge in research in complex fluids, of which nematic liquid crystals (NLC) are a prime example [1–3]. Nematic liquid crystals are anisotropic liquids that combine the fluidity of liquids with the orientational order of solids i.e. the constituent rod-like molecules typically align along certain preferred or distinguished directions and this orientational anisotropy can have a profound optical signature [4]. Various researchers have already looked at effects of magnetic, electric or flow fields on pattern formation in confined nematic systems [1,5]. In particular, microfluidics is a thriving area of research; scientists typically manipulate fluid flow, say conventional isotropic fluids, in narrow channels complemented by different boundary treatments, leading to novel transport and mixing phenomena for fluids and potentially new health and pharmaceutical applications [6–8]. A natural question to ask is what happens when we replace a conventional isotropic liquid with an anisotropic liquid, such as a nematic liquid crystal? [3] Nematic microfluidics have recently generated substantial interest by virtue of their optical, rheological and backflow properties along with their defect profiles [9].

In Sengupta et al. [3], the authors investigate, both experimentally and numerically, microfluidic channels filled with nematic solvents. The authors work with a thin microfluidic channel with length much greater than width and width much greater than depth. A crucial consideration is the choice of boundary conditions and the authors work with homeotropic or normal boundary conditions on the top and bottom channel surfaces, which

* Corresponding author.
E-mail addresses: maria.crespo-moya@umontpellier.fr (M. Crespo), a.majumdar@bath.ac.uk (A. Majumdar), angel@mat.ucm.es (A.M. Ramos), ian.griffiths@maths.ox.ac.uk (I.M. Griffiths).

http://dx.doi.org/10.1016/j.physd.2017.04.004
0167-2789/

require the molecules to be oriented in the direction of the surface normal. The anchoring strength is a measure of how strongly the boundary conditions are enforced: strong anchoring roughly corresponds to Dirichlet conditions for the director field and zero anchoring describes free (Neumann homogeneous) boundary conditions. We expect most experiments to have moderate to strong anchoring conditions. The authors impose a flow field transverse to the anchoring conditions so that there are at least two competing effects in the experiment: anchoring normal to the boundaries and flow along the length of the microfluidic channel. They work with weak, medium, and strong flow speeds in qualitative terms and observe complex flow transitions. In the weak-flow regime, the molecules are only weakly affected by the flow and the molecular orientations are largely determined by the anchoring conditions. As the flow strength increases, a complex coupling between the molecular alignments and the flow field emerges and the nematic molecules reorient to align somewhat with the flow field. The medium-flow director field exhibits boundary layers near the center and the boundaries where the director field is strongly influenced by either the flow field or the boundary conditions. In the strong-flow regime, the molecules are almost entirely oriented with the flow field, with the exception of thin boundary layers near the channel surfaces to match the boundary conditions. The authors study these transitions experimentally and their experimental results suggest a largely *uniaxial* profile wherein the molecules exhibit a single distinguished direction of molecular alignment and this direction is referred to as being the *director* in the literature [1]. The authors present experimental measurements for the optical profiles and flow fields and their experimental work is complemented by a numerical analysis of the nematodynamic equations in the Beris–Edwards theory [10]. The Beris–Edwards theory is one of the most general formulations of nematodynamics, that accounts for both uniaxial and biaxial systems (with a primary and secondary direction of molecular alignment) and variations in the degree of orientational order. The authors numerically reproduce the experimentally observed flow transitions, the director and flow-field profiles, all of which are in good qualitative agreement with the experiments.

In Anderson et al. [11], the authors model this experimental set-up within the Leslie–Ericksen model for nematodynamics. Their Leslie–Ericksen model is restricted to uniaxial nematics with constant ordering (a constant degree of orientational order) [5]. They present governing equations for the flow field and the nematic director field along with the constitutive relations that describe the coupling between the director and the flow field (see Appendix A for details) and assume that all dependent variables only vary along the channel depth, with a unidirectional flow along the channel length, consistent with the experiments. These assumptions greatly simplify the mathematical model, yielding a decoupled system of partial differential equations for the director field, which captures the flow dynamics through a single variable: the pressure gradient, $\mathcal{G}$, along the channel length. The authors define two separate boundary-value problems: one for weak-flow solutions and one for strong-flow solutions, described by two different sets of boundary conditions for the director field. They find weak- and strong-flow solutions for all values of the pressure gradient and they relate the resulting flow profile to the mean flow speed by a standard Poiseuille-flow-type relation. The energy of the weak-flow solution is lower than the strong-flow solution for small $\mathcal{G}$ and there is an energy cross-over at some critical value, $\mathcal{G}^*$, that depends on the anchoring strength at the channel surfaces. Recently, Batista et al. [12] undertook a comprehensive study of the interplay between the pressure gradient and anchoring conditions on the transition between the weak-flow and strong-flow solutions, which they related to a discontinuity in the mass flow rate function.

In this paper, we build on the work in Anderson et al. [11] by performing an extensive study of the static solution landscape, complemented by some numerical investigations of the dynamical behavior, as the system evolves to these equilibrium configurations. We adopt the same model with the same underpinning assumptions as in Anderson et al. [11], but we do not define two separate boundary-value problems. We impose weak anchoring conditions for the director field on the top and the bottom surfaces since it includes both the weak and strong anchoring configurations and allows us to capture the competition between the flow field and the anchoring strength. In Bevilacqua et al. [13], the authors adopt a similar approach to study the competition between the magnetic field and the anchoring strength on static equilibrium profiles, described by critical points of a suitably defined energy.

We compute the static equilibrium solutions, using a combination of analytic and numerical methods, as a function of $\mathcal{G}$ and the inverse anchoring strength $\mathcal{B}$. The case $\mathcal{G} = 0$ is analytically tractable and we identify two different classes of solutions and characterize their stability. This is complemented by an asymptotic analysis in the limits $\mathcal{G} \to 0$ and $\mathcal{G} \to \infty$, with the latter regime yielding useful information about the boundary layers near channel surfaces, which are experimentally observed in the strong-flow regimes [3]. We then study the solution landscape for $\mathcal{G} \neq 0$ and track the stable and unstable solution branches as a function of $(\mathcal{G}, \mathcal{B})$. Our work largely focuses on the static equilibria but the last section is devoted to a numerical study of the dynamic Leslie–Ericksen model and its sensitivity to the initial condition. In particular, we present a numerical example for which we can control the final steady state by manipulating the rate of change of the pressure gradient and anchoring conditions.

The paper is organized as follows. In Section 2, we present the Leslie–Ericksen dynamic model, the governing equations and boundary conditions. In Section 3, we explore the static solution landscape as a function of the pressure gradient and anchoring strength. In Section 4, we study the dynamic model, with focus on the effects of initial conditions and the time-dependent forms of the pressure gradient and anchoring strength, and conclude in Section 5 by putting our work in context and discuss future developments.

2. Mathematical model

As in Anderson et al. [11], we model the NLC within the microfluidic channel in the Leslie–Ericksen framework. The channel has dimensions, $L_{\hat{x}} \gg L_{\hat{y}} \gg L_{\hat{z}}$, in the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions respectively, consistent with the experimental set-up in Anderson et al. [11] and Sengupta et al. [3] The NLC is purely uniaxial with constant order parameter, by assumption, and is hence fully described by a director field, $\boldsymbol{n}$, that represents the single preferred direction of nematic alignment. Here, $\boldsymbol{n}$ and $-\boldsymbol{n}$ are physically indistinguishable (in the absence of polarity the sign of $\boldsymbol{n}$ has no physical meaning). We additionally assume that all dependent variables only depend on the $\hat{z}$-coordinate, along the channel depth, as depicted in Fig. 1. Then the director field is of the form $\boldsymbol{n} = (\sin(\theta(\hat{z}, \hat{t})), 0, \cos(\theta(\hat{z}, \hat{t})))$ and the velocity field is unidirectional, of the form $\boldsymbol{v} = (\hat{u}(\hat{z}, \hat{t}), 0, 0)$, with $-h \leq \hat{z} \leq h$. Since $\boldsymbol{n}$ and $-\boldsymbol{n}$ are indistinguishable, θ and $\theta + k\pi$, $k \in \mathbb{Z}$, describe the same director profile. We assume that $\hat{u}(\hat{z}, \hat{t})$ is symmetric around the center-line (i.e. around $\hat{z} = 0$) and no-slip conditions are imposed on the channel walls (i.e. $\hat{u}(\pm h, \hat{t}) = 0$). We assume weak anchoring boundary conditions for θ on $\hat{z} = \pm h$, that can be derived from the well-known Rapini–Papoular weak-anchoring energy [14],

$$E_S = \int_{\hat{z}=\pm h} \frac{A}{2} \sin^2 \theta \, d\hat{x} \, d\hat{y},$$