On a 3D isothermal model for nematic liquid crystals accounting for stretching terms

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Abstract. In the present contribution, we study a PDE system describing the evolution of a nematic liquid crystals flow under kinematic transports for molecules of different shapes. More in particular, the evolution of the velocity field $u$ is ruled by the Navier–Stokes incompressible system with a stress tensor exhibiting a special coupling between the transport and the induced terms. The dynamics of the director field $d$ is described by a variation of a parabolic Ginzburg–Landau equation with a suitable penalization of the physical constraint $|d| = 1$. Such equation accounts for both the kinematic transport by the flow field and the internal relaxation due to the elastic energy. The main aim of this contribution is to overcome the lack of a maximum principle for the director equation and prove (without any restriction on the data and on the physical constants of the problem) the existence of global in time weak solutions under physically meaningful boundary conditions on $d$ and $u$.

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1. Introduction

In this paper, we consider a hydrodynamical system modeling the flow of nematic liquid crystals. Assuming that the material occupies a bounded spatial domain $\Omega \subset \mathbb{R}^3$ with a smooth boundary $\Gamma$, the system couples the 3D incompressible Navier–Stokes equations governing the motion of the velocities with a modified Allen–Cahn equation for the director field, that is

\[
\begin{align*}
\text{div } u &= 0, \quad \text{in } (0, T) \times \Omega, \\
\partial_t u + \text{div}(u \otimes u) + \nabla p &= \text{div } T + f, \quad \text{in } (0, T) \times \Omega, \\
\partial_t d + u \cdot \nabla d - \alpha d \cdot \nabla u + (1 - \alpha) d \cdot \nabla^T u &= \gamma (\Delta d - \nabla d W(d)), \quad \text{in } (0, T) \times \Omega,
\end{align*}
\]

where

\[
\begin{align*}
T &= S - \lambda (\nabla d \otimes \nabla d) - \alpha \lambda (\Delta d - \nabla d W(d)) \otimes d + (1 - \alpha) \lambda d \otimes (\Delta d - \nabla d W(d)), \\
S &= \mu (\nabla u + \nabla^T u),
\end{align*}
\]

$T$ and $S$ being the Cauchy stress and the Newtonian viscous stress tensors, respectively. Here, $u$ denotes the velocity field of the flow, $d$ is the director field and stands for the averaged macroscopic/continuum molecular orientation in $\mathbb{R}^3$, $p$ is a scalar function representing the hydrodynamic pressure (including the hydrostatic part and the induced elastic part from the orientation field) and $f$ is a given external force. The positive constants $\mu, \lambda$ and $\gamma$ stand for the viscosity, the competition between kinetic energy and potential energy, and the microscopic elastic relaxation time (Deborah number) for the molecular

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orientation field, respectively. The function $W$ penalizes the deviation of the length $|\mathbf{d}|$ from the value 1, which is due to liquid crystal molecules being of similar size (cf. [11]). A typical example is a double-well potential as, for example, $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$. In general, $W$ may be written as a sum of a convex part and a smooth, but possibly non-convex one. Finally, the constant $\alpha \in [0, 1]$ is a parameter related to the shape of the liquid crystal molecules. For instance, the spherical, rod-like and disk-like liquid crystal molecules correspond to the cases $\alpha = \frac{1}{2}$, 1 and 0, respectively (cf., e.g., [3, 7] and [20]).

Concerning the notation, $\nabla \mathbf{d}$ represents the gradient with respect to the variable $\mathbf{d}$. $\nabla \mathbf{d} \otimes \nabla \mathbf{d}$ denotes the $3 \times 3$ matrix whose $(i, j)$th entry is given by $\nabla_i \mathbf{d} \cdot \nabla_j \mathbf{d}$, for $i \leq j \leq 3$, and $\otimes$ stands for the usual Kronecker product, that is, $(\mathbf{u} \otimes \mathbf{u})_{ij} := u_i u_j$, for $i, j = 1, 2, 3$. Finally, $\nabla^T$ indicates the transpose of the gradient.

We notice that this system was very successful in describing the coupling between the velocity field $\mathbf{u}$ and the director field $\mathbf{d}$, especially in the liquid crystals of nematic type.

The hydrodynamics theory of liquid crystals was due to Ericksen and Leslie (cf. [3] and [10]). However, the general Ericksen–Leslie system was so complicated that only some special cases of it have been investigated theoretically or numerically in the literature.

In this context, Lin and Liu (cf. [11] and [12]) formulated a simplified version of the original model, which has been analyzed also by several other authors, see, for example, [18, 19, 22]. In the simplified model, some meaningful physical terms, such as the stretching and rotation effects of the director field induced by the straining of the fluid, are not taken into account.

In a following paper by Coutand and Shkoller [2], the authors considered a model in which the stretching term is present and proved a local well-posedness result. Here, due to the presence of the stretching term, the total energy balance does not hold. To overcome such an inconvenience, Sun and Liu [20] proposed a variant of the Lin and Liu model [11] in which not only the stretching term is included in the system, but also a suitable new component to the stress tensor is added.

In our paper, we refer to a slightly more general model derived by Wu et al. in [22].

The main interests in the topic come essentially from two directions. First, the previous results in the literature were only obtained in 2D or in 3D, under the assumption that the viscosity coefficient $\mu$ in the stress $\mathbf{S}$ (cf. (1.5)) is sufficiently big with respect to proper norms of the initial data and with respect to other coefficients like $\lambda$. In the previous contributions [20] and [22], it was claimed that, due to the impossibility of proving the boundedness in $L^\infty$ for $\mathbf{d}$ (because the maximum principle cannot be applied to the director field equation), the existence of solution was out of reach without assuming to have a big viscosity coefficient in the velocity equation. Our main result shows that, even if the existence of classical solutions cannot be proved without any restriction on the size of the coefficients and the data (as it is for the uncoupled 3D Navier–Stokes system), however, it is possible to obtain the existence of weak solutions. This is in agreement with the previous contributions in the field of incompressible 3D Navier–Stokes equations.

The main point here is an appropriate choice of the test functions leading to a rigorous weak formulation of the system (cf. the following formulas (3.8–3.10)). Let us notice that in the recent paper [1], formal computations are performed in order to show the existence of weak solutions for such a problem, but no rigorous definition of the weak formulation as well as no proof of existence of such solutions is given. In particular, in our manuscript, choosing properly the space of the test functions in the weak momentum equation (cf. (3.9)), we obtain well-defined weak solutions. This is necessary in order to deal with the stretching term in the Cauchy stress $\mathbf{T}$ (cf. (1.4)). More comments on this point are given in Remark 3.2.

The second novelty of our analysis consists in the fact that, to our knowledge, all the previous contributions in the literature (except for [1] where formal results are stated in case of Dirichlet, Neumann and periodic boundary conditions) were obtained assuming periodic boundary conditions on the director field $\mathbf{d}$. However, from the applications point of view, the cases of non-homogeneous Dirichlet or Neumann boundary conditions look more appropriate (cf., e.g., [15] where it is pointed out that the Neumann