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Numerical simulation of flow and structure in nematic liquid crystalline materials between eccentric cylinders

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ABSTRACT

In this paper the time transient isothermal flow of lyotropic nematic liquid crystals (LC) between two eccentric cylinders was studied numerically by applying the Landau-de Gennes (LdG) theory. The start-up flow induced by the steady rotation of the inner cylinder was used to model the lubrication problem inside a journal bearing. The ability of liquid crystalline materials to form ordered boundary layers with good load-carrying capacity, outstanding lubricating properties, has been widely demonstrated. The LdG theory for the microstructure of the molecules along with continuity and momentum equations were solved simultaneously using General PDE and Laminar Flow packages of the COMSOL Multiphysics. Flow properties and structure were investigated as a function of simulation time, the Reynolds number and the Energy ratio, *R*. Interconnection and impact of the texture and defects formation/evolution on velocity profile and pressure distribution was observed; nucleation and evolution of disclination line and defect points were detected and pursued over the simulation time. For high Reynolds numbers, the flow reached quasi-stationary condition while the microstructure evolution was at unsteady state. The influence of the Energy ratio and the Reynolds number on the formation and evolution of polydomains was studied. Indeed, it was found that coupling the evolution of liquid crystalline microstructure with the hydrodynamics has a quantitative and qualitative impact on the macro-scale attributes of the flow and on the structure. The standard procedure to classify defects has been applied, oblate and isotropic defects have been identified.

1. Introduction

Nematic liquid crystals are orientationally ordered, textured, anisotropic and viscoelastic materials. They are used as structural or functional materials. An example of functionalities is their application as lubricants, which is related to the anisotropy of the viscosity coefficient, with respect to different flow directions, which is a unique property of the liquid crystalline phase. The remarkable rheological properties of these materials are due to the flow-induced evolution of molecular configurations. Independent studies indicates that LCs change their orientation state in the vicinity of a solid surface. The ability of liquid crystalline materials to form ordered boundary layers with good load-carrying capacity, and to lower the friction coefficients, wear rates and contact temperatures of sliding surfaces, thus contributing to increase the components service life and save energy has been widely demonstrated [1–12].

The present study aims at simulating the transient flow of lyotropic nematic liquid crystalline materials (NLCs) between two eccentric cylinders with small gap size, as a model for the lubrication problem inside a journal bearing.

Since 1888 when liquid crystals were examined for the first time by Friedrich Reinitzer, several continuum theories had been developed to capture different aspects of the rheology and structure formation in liquid crystals. The flow of liquid crystals has been investigated through numerical simulations, in several studies, using Landau-de Gennes theory, Doi–Marrucci–Greco theory and extensions of Doi theory for nematic polymers.

In Doi theory, at any given point in space, the dynamics of rod-like molecules of nematic liquid crystalline polymers (NLCPs) can be found using a diffusion equation of their orientational distribution function by implementing the Maier-Saupe nematic potential function [13]. Start-up flow of lyotropic LCs between two eccentric cylinders has been studied using Doi theory by [14]; defects generation and the coupling between the flow and the molecular structure has been investigated using quadratic closure approximation to estimate the evolution of molecules [15]. Six closure models considered for Doi theory have been compared with each other

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to predict three regimes of director motion: steady alignment, wagging and tumbling. All the closure models foresaw the same distinct attributes of the liquid crystals behaviour. Complex flow simulation of NLCPs has been performed along with the comparison between different closure approximations of Doi theory for rigid rod-like molecules by [16].

The general Poisson-bracket formulation was used by [17] to acquire stochastic dynamical governing equations of nematic LCs for rod-like molecules in nematic/isotropic states. Furthermore, the equations for slow dynamic process of NLCs and nematic suspensions derived by [18], which determined the non-hydrodynamic responses from Leslie–Ericksen equations.

Essential elements in pattern formation of the LCP were solved using the Doi–Marrucci–Greco and moment-averaged theory by [19]. Slow Couette flow of NLCPs was modelled using the Doi–Marrucci–Greco tensorial theory by [20], extending the structural scaling laws developed based on the Leslie–Ericksen theory to incorporate the flow of NLCPs and molecular elasticity. The unsteady shear flow of NLCPs was studied by [21] to determine the range of anisotropic fluctuations in mechanical properties, which depend on orientational distribution functions. They considered that the film processing of nematic polymers is mostly dominated by the shear flow and the orientational order and it is highly sensitive to the rate of shear strain and the ratio of volume of nematic constituent to the total suspension volume.

Moreover, the mesoscopic Doi–Marrucci–Greco theory and the transient Stokes flow of NLCPs were simulated by [22] to study the structural and orientational transition in unsteady shear flow. Moreover, classification of defects and the shape of ellipsoids at each mesoscopic time and space were investigated by [23,24]. Moreover, they predicted the dynamics of oblate defects domains in two space dimensions of shear flow. The texture formation of discotic nematic carbon fibers during the thermal relaxation after the termination of extensional flow was studied by Hong and Chan [25]. The Landau-de Gennes free energy of molecules was used to predict the difference between molecular reorientation time scale and thermal relaxation [26].

The isothermal, incompressible flow of liquid crystalline polymers was formulated by Farhudi and Rey using a tensorial approach for microstructure characterization; the transient and steady simple shear flow of uniaxial NLCs was studied. Furthermore, the elastic contribution for the molecular field and the elastic stress tensors were neglected to simplify the model and a spatially homogenous director vector for the molecules were assumed. Two types of orientational modes were predicted according to the nematic potential (simple aligning mode and complex modes). Three different subdivision regimes of complex modes were further investigated via the change in shear rates, which resulted in describing two distinct critical shear rates that characterize the transition between tumbling, oscillatory and stationary regime [27,28].

Tsuji and Rey solved constitutive equations for evolution of LCs in rectilinear simple shear flow. Both, short-range elasticity and long-range elasticity were considered in their model. The compatibility of this tensorial theory was tested with the Leslie–Ericksen and Doi theory for asymptotic cases of $De \rightarrow \infty$ and $Er \rightarrow \infty$respectively. A mechanism for compatibility between the Doi's tumbling effect and fixed anchoring angle of the molecules on the boundaries was suggested [29]. A generalized version of tensorial governing equation was proposed by Tsuji; in these governing equations, short-range elasticity, flow contributions and long-range elasticity were included. Shear flow of liquid crystalline materials as a function of the Ericksen and Deborah numbers and for a fixed anchoring angle of the molecules on the boundaries was investigated. In their study, the counter impact of the microstructure on flow characteristics of LC was neglected [30].

Grecov and Rey adapted the Landau-de Gennes theory to describe the flow of flow-aligning thermotropic LCs. Well known thermodynamic restrictions along with ordering of Miesowicz viscosities and flow-aligning angle of the director emerging from the Leslie–Ericksen theory were implemented to characterize shear viscosity coefficients of NLCs [31]. Start-up shear responses for different anchoring angles of the director at the wall boundaries and various Ericksen and Deborah numbers were investigated [32]. Grecov and Rey implemented the Landau-de Gennes equations along with decoupling simplification and constant shear rate, to achieve an insight on defects nucleation in shear-induced flow of flow-aligning liquid crystalline polymers (LCPs). The understanding of defect-defect annihilation and defect-wall interactions resulted from this study was needed to achieve a defect-free monodomain melts of LCPs [33,34].

The LdG theory is well suited to simulate texture formation since defects are non-singular solutions to the governing equations. However, solving LdG model for realistic applications is computationally expensive; thus, numerous simplifications of this theory have been done in the past to make it simpler to solve. For example, neglecting the counter impact of the microstructure on the flow or neglecting the long-range contribution on shear stress tensors for solving the fluid flow have been used as simplifying assumptions.

In order to fully understand the lubrication problem of modified/enhanced lubricants by liquid crystalline materials in journal bearings, transitional and turbulent flow regimes of LCs between two eccentric cylinders with micro-scale gap size have to be investigated. Therefore, characteristic length scales can be classified with respect to the molecular size, defect, gap, and large geometrical length scales. In this case, the multi-scale phenomenon significantly increases the degree of difficulty of solving this set of equations. Furthermore, considering the transient/turbulent flow regime of liquid crystalline materials will remarkably increase the number of degrees of freedom, hence complexity of the system. The combination of the multi-scale phenomenon inherited from liquid crystalline nature and transient/turbulent flow regime of the actual flow of any lubricant in journal bearing make the numerical analysis immensely complicated to be solved in a realistic timeframe. Consequently, the main objective was adjusted to investigate the laminar flow regime of liquid crystalline materials between two eccentric cylinders with larger gap sizes as a preliminary step of the lubrication problem. Although, the gap size used in this numerical analysis is considerably larger than the actual gap size in journal bearings and the laminar flow regime was enforced, the results of this investigation are worthy to discuss since this study is one of the very few attempts on numerical simulation of unabridged Landau-de Gennes nematodynamics governing equations of a nematic liquid crystalline materials under shear, extensional and rotational flows. It is essential to emphasize that the results of this study are intrinsically valuable to shed light on the intertwined interaction of microstructure and flow of liquid crystalline materials and potentially useful for rheological and tribological study of liquid crystalline materials.

In order to approach the objective, a complete set of equations for the evolution of the microstructure coupled with 2-D Navier–Stokes equations was solved. In this study, the evolution of the microstructure modelled using the Landau-de Gennes theory, was linked with the Navier–Stokes equations using a modified total stress tensor established in the momentum equations. The flow characteristics and the orientation of the liquid crystalline molecules for different rotational velocities of the inner cylinder were investigated. Flow and rheological properties, defects nucleation/evolution inside the domain have been studied. The flow-induced structural changes and the orientation-induced flow were analyzed for different Reynolds numbers and Energy ratios.