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NEMATIC LIQUIDS IN WEAK CAPILLARY POISEUILLE FLOW: STRUCTURE SCALING LAWS AND EFFECTIVE CONDUCTIVITY IMPLICATIONS

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Abstract. We study the scaling properties of heterogeneities in nematic (liquid crystal) polymers that are generated by pressure-driven, capillary Poiseuille flow. These studies complement our earlier drag-driven structure simulations and analyses. We use the mesoscopic Doi-Marrucci-Greco model, which incorporates excluded-volume interactions of the rod-like particle ensemble, distortional elasticity of the dispersion, and hydrodynamic feedback through orientation dependent viscoelastic stresses. The geometry likewise introduces anchoring conditions on the nano-rods which touch the solid boundaries. We first derive flow-orientation steady-state structures for three different anchoring conditions, by asymptotic analysis in the limit of weak pressure gradient. These closed-form expressions yield scaling laws, which predict how lengthscales of distortions in the flow and orientational distribution vary with strength of the excluded volume potential, molecule geometry, and distortional elasticity constants. Next, the asymptotic structures are verified by direct numerical simulations, which provide a high level benchmark on the numerical code and algorithm. Finally, we calculate the effective (thermal or electrical) conductivity tensor of the composite films, and determine scaling behavior of the effective property enhancements generated by capillary Poiseuille flow.

Key Words. Liquid crystal (nematic) polymers, asymptotic expansions, partial differential equations, capillary Poiseuille flow, conductivity

1. Introduction

The rheological behavior of Poiseuille flow of liquid crystal polymers is of interest for technology applications in processing of high performance fibers and films. Rey and co-workers have studied capillary Poiseuille flows using the Leslie-Ericksen theory for discotic nematic liquid crystals ([4, 5, 6]). Denniston *et al.* have used lattice Boltzmann simulations of Landau-deGennes orientation tensor models to explore the behavior of liquid crystal polymers subject to Poiseuille flow ([9]). In this work we study capillary Poiseuille flow using the Doi-Marrucci-Greco model, which also employs an orientation (second-moment) tensor description of the rod distribution.

We extend our early work ([3], [17]) in the following ways: 1) asymptotic results for tilted anchoring condition are derived; 2) the rotary diffusivity is explicitly coupled in the asymptotic results; 3) direct numerical simulations are carried out to validate asymptotic results; and 4) effective conductivity properties of Poiseuille flow-generated composite films are calculated.

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The paper is organized as follows. First, we describe the model of liquid crystal polymer hydrodynamics proposed by Doi, Marrucci and Greco ([10, 25, 26, 27]). Second, we present the structure scaling properties of the orientation tensor for different anchoring conditions; this is achieved by asymptotic analysis that yields exact orientation modes with spatial variations controlled by material and boundary conditions in the limit of weak pressure gradient. We perform direct numerical simulations to verify the asymptotic results, and then observe new properties as the asymptotic conditions are violated. Finally, we calculate the effective (thermal or electrical) conductivity tensor of the composite films, and determine scaling behavior of the effective property enhancements generated by capillary Poiseuille flow.

2. Model Formulation

We consider capillary Poiseuille flow of nematic liquid crystal polymers (LCPs). Capillary Poiseuille flow is the flow between two non-slip boundaries at $y = -h$ and $y = h$ driven by a pressure gradient in this context. The flow is described by a velocity field $\mathbf{v} = (v_x(y,t), 0, 0)$ with the centerline of the pipe located at $y = 0$. Figure 1 depicts the cross-section of the Poiseuille flow on the (x, y) plane. For simplicity here we suppress variations in the direction of flow (x) and primary vorticity direction (z), and transport in the vertical (y) direction.

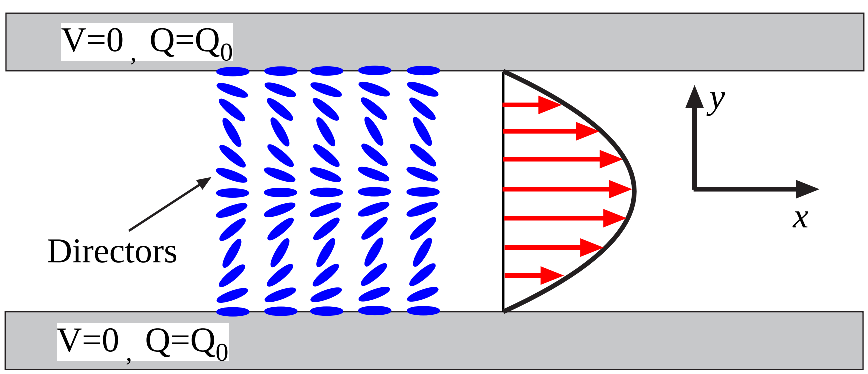

FIGURE 1. Plane Poiseuille flow geometry. Non-slip boundary conditions for the velocity and boundary anchoring for the orientation tensor given by the stable nematic rest state are prescribed, with major director angle $\psi_0 = 0$ shown here.

The dimensionless governing equations consist of the balance of linear momentum, stress constitutive equation, continuity equation, and the equation for the