

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Polydomain Simulation of Liquid Crystalline Polymer Orientation in Channel Flows JUN FANG, WESLEY BURGHARDT, Northwestern University — The properties of liquid crystalline polymers are strongly affected by the molecular orientation state induced by processing flows. LCP structure development under flow is quite complex, due to the propensity towards 'director tumbling' dynamics in rodlike nematics, and the resulting complicated 'polydomain' distributions of orientation. Many models of LCP structure & rheology begin with a detailed description of the molecular orientation state, possibly including a molecular description of distortional elasticity. While well suited for simulations of fundamental phenomena in simple flows, application of these models to processing flows is far out of reach. Conversely, the phenomenological polydomain model of Larson & Doi is sufficiently simple to allow for its application to process simulations. This is further facilitated by a nearly exact analogy between the Larson-Doi model and the Folger-Tucker model for predicting orientation in fiber dispersions, which is incorporated in commercial process simulation software. We use this available modeling infrastructure to test the ability of the Larson-Doi model to predict orientation distributions in kinematically complex but isothermal channel flows of liquid crystalline polymers, comparing simulation results orientation distribution data previously obtained using in situ x-ray scattering methods.

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Date submitted: 27 Nov 2007

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