A Tale of Two Micelles: The Analysis and Simulation of a Two-Species Scission/Reforming Model for Wormlike Micellar Solutions
Michael Earl Cromer, Jr.
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Wormlike micellar mixtures consist of self-assembled micellar aggregates, which, due to their length, can entangle in solution thus exhibiting viscoelastic properties. Additionally these aggregates, or wormlike micelles, continuously break and reform in equilibrium due to, for example, thermal fluctuations, and do break in flow due to stress. In wall-driven shearing flows such as circular Taylor-Couette flow, many wormlike micellar solutions exhibit a shear-banding transition resulting in a high shear-rate region near the inner, rotating cylinder and a low shear-rate region located towards the outer, fixed wall. A model developed to capture the physics of concentrated solutions of wormlike micelles, which does predict this spatially inhomogeneous shear-banding phenomenon, is the VCM model (Vasquez, McKinley and Cook, J. Non-Newtonian Fluid Mech. 2007). This model, a microstructural network model with linear elastic network elements, is a two species model describing the coupled evolution of two wormlike chain species, long chains ‘A’ which can break in half to form shorter chains ‘B’ which can themselves recombine to form a long ‘A’ chain. The VCM governing constitutive equations comprise a coupled, nonlinear partial differential equation system which allows for reptative and Rouse-like stress-relaxation mechanisms, in addition to breakage. In this dissertation, steady and transient predictions of the VCM model are examined in both shear and extensional flows using computational, asymptotic and analytic methods.

The one-dimensional pressure-driven flow in a rectilinear channel is investigated first. The rectilinear pressure-driven flow velocity profile deviates from the parabolic profile expected for a Newtonian fluid, exhibiting a complex spatial structure including a wall boundary layer as well as, above a critical pressure drop, an interior layer connecting shear bands. At a critical pressure drop the flow transitions to a shear banded flow, and volumetric spurt is observed. In the time-dependent simulations, the interior layer, which connects the shear bands, forms near the walls and evolves in time towards the center of the channel. An adaptive spectral method is developed to track and resolve the spatial and temporal evolution of the thin interior layer. Linear stability analysis of the steady pressure-driven flow shows that at banding an interfacial instability can arise resulting in a 2D sinuous (snake-like) perturbation flow in the flow/gradient plane, with local fluctuations along the interface between bands. Further analysis shows that decreasing the channel height, for other parameters fixed, leads to a critical height at which the flow stabilizes.

In homogeneous uniaxial extensional flow, the VCM model exhibits a non-montonic elastic tensile stress versus extension rate curve reminiscent of the non-monotonic flow curve in homogeneous shear flow. As such, linear stability analysis was carried out on this steady curve showing that within the multi-valued region of the stress versus extension rate curve the VCM model is extremely unstable to axial perturbations along the filament. To this end a 1+1D Lagrangian formulation is used to simulate the inhomogeneous filament stretching of the VCM model. The stretching simulations show that elongating filaments described by the VCM model exhibit a dramatic and sudden rupture event similar to that observed in filament stretching experiments of wormlike micelles. This rupturing event is accompanied by a mass breakage of the long species.