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Numerical Investigation of a New Two-Fluid Model for Semi-Dilute Polymer Solutions

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Abstract : Many soft materials such as polymer solutions can develop localized bands with different shear rates, which are known as shear bands. Using the generalized bracket approach of nonequilibrium thermodynamics, we recently developed a new two-fluid model to study shear banding for semi-dilute polymer solutions. The two-fluid approach is an appropriate means for describing diffusion processes such as Fickian diffusion and stress-induced migration. In this approach, it is assumed that the local gradients in concentration and, if accounted for, also stress generate a nontrivial velocity difference between the components. Since the differential velocity is treated as a state variable in our model, the implementation of the boundary conditions arising from the derivative diffusive terms is straightforward. Our model is a good candidate for benchmark simulations because of its simplicity. We analyzed its behavior in cylindrical Couette flow, a rectilinear channel flow, and a 4:1 planar contraction flow. The latter problem was solved using the OpenFOAM finite volume package and the impact of shear banding on the lip and salient vortices was investigated. For the other smooth geometries, we employed a standard Chebyshev pseudospectral collocation method. The results showed that the steady-state solution is unique with respect to initial conditions, deformation history, and the value of the diffusivity constant. However, smaller the value of the diffusivity constant is, the more time it takes to reach the steady state.

Keywords : nonequilibrium thermodynamics, planar contraction, polymer solutions, shear banding, two-fluid approach
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