A new micro-macro algorithm for simulation of polymer flows

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Abstract

We present a new micro-macro algorithm for the numerical calculation of polymer flows. The system being solved consists of the momentum and mass conservation equations from the continuum mechanics coupled with a microscopic-based rheological model for polymer stress. The integration of the macroscopic part is carried out by combining a new semi-Lagrangian Galerkin projection algorithm for the total derivative operator with a mixed finite element formulation of the linear Stokes problems that have to be solved at each time step of the integration process. The solution of the Stokes problems are calculated by Taylor-Hood $P_2 - P_1$ element. The microscopic part represents the polymer contribution to the stress tensor and is determined from a stochastic simulation of an ensemble of model polymer molecules from whose configurations the polymer stress can be computed as an ensemble average. We shall give details of the stochastic simulation technique and the the procedure to calculate the ensamble average. The model is applied to study the flow in a complex geometry represented by an abrupt 10:1 axisymmetric contraction, assuming incompressibility and isothermal conditions, and the finite extendible nonlinear elasticity (FENE) kinetic model of polymeric fluids.