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A front-tracking method for computational modeling of viscoelastic two-phase flow systems

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ABSTRACT

A front-tracking method is developed for direct numerical simulations of viscoelastic two-phase systems in which one or both phases could be viscoelastic. One set of governing equations is written for the whole computational domain and different phases are treated as a single fluid with variable material and rheological properties. The interface is tracked explicitly using a Lagrangian grid while the flow equations are solved on a fixed Eulerian grid. The surface tension is computed at the interface using the Lagrangian grid and included into the momentum equations as a body force. The Oldroyd-B, FENE-CR and FENE-MCR models are employed to model the viscoelasticity. The viscoelastic model equations are solved fully coupled with the flow equations within the front-tracking framework. A fifth-order WENO scheme is used to approximate the convective terms in the viscoelastic model equations and second-order central differences are used for all other spatial derivatives. A log-conformation method is employed to alleviate the high Weissenberg number problem (HWNP) and found to be stable and very robust for a wide range of Weissenberg numbers. The method has been first validated for various benchmark single-phase and two-phase viscoelastic flow problems. Then it has been applied to study motion and deformation of viscoelastic two-phase systems in a pressure-driven flow through a capillary tube with a sudden contraction and expansion. The method has been demonstrated to be grid convergent with second-order spatial accuracy for all the cases considered in this paper.

1. Introduction

Viscoelastic emulsions are ubiquitous in a wide range of engineering applications such as materials and food processing, pharmaceuticals, polymer blends and droplet-based microfluidics [51,49]. In particular, almost all the particle-laden biological fluids in nature exhibit viscoelastic behavior. Therefore it is of crucial importance to understand the dynamics of an individual viscoelastic droplet in a viscoelastic or Newtonian medium [51].

Computational modeling of viscoelastic fluid flow is a difficult task mainly due to the large disparity in time scales especially at high Weissenberg numbers known as the high Weissenberg number problem (HWNP). The existence of a moving and deforming interface in two-phase systems makes the problem even more complicated and challenging. Viscoelasticity has been usually modeled based on the microstructure of dilute polymer solutions and expressed by various constitutive differential equations such as upper convected Maxwell (UCM)/Oldroyd-B [40], Giesekus [22] and finitely extensible nonlinear elastic (FENE-P [5], FENE-CR [13]) models for single and multiphase flow systems [51,42]. Various numerical approaches have been proposed to solve these models coupled with the flow equations. However the conventional numerical algorithms usually failed to converge above a certain Weissenberg number limit [42]. This stability problem is primarily caused by the exponential growth of viscoelastic stresses in regions of high shear rates or near stagnation points [42]. The failure of the numerical methods to properly approximate this exponential growth results in a numerical instability. Moreover this instability is pronounced if the positive definiteness of the conformation tensor is not preserved at the numerical solution level. The conformation tensor has a definite physical origin and interpretation stemming from the internal microstructure of polymer molecules in a continuum level [4] dictating the conformation tensor to be positive definite. Hulsen [26] proved that the conformation tensor must be initialized and remain positive definite for numerical stability. However, this condition can be violated in numerical approximations due to accumulation of numerical errors [42].

In a pioneering study, Keunings [28] observed failure of existing numerical methods at high Weissenberg numbers and attributed this failure to the inappropriate numerical methodologies. Since

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then, a number of stabilization approaches have been proposed to overcome the HWNP in viscoelastic flow simulations as recently discussed in details by Chen et al. [12]. Marchal and Crochet [31] developed one of the first successful numerical methods for simulations of viscoelastic flows at high Weissenberg numbers using upwind discretization of the convective terms in a mixed finite-element framework. Mompean and Deville [32] developed a finite-volume method and successfully performed simulations of Oldroyd-B fluid flow in a 3D planar contraction at high Weissenberg numbers. More recently, Fattal and Kupferman [20] developed the log-conformation method (LCM) based on reformulation of the constitutive equations using a logarithmic transformation of conformation tensor. The LCM has been shown to be stable and accurate at high Weissenberg numbers, i.e., as high as $Wi = 100$ [27]. This representation makes the problem more stable at numerical solution level since it preserves the positive definiteness of the conformation tensor and successfully captures sharp elastic stress layers. Sarkar and Schowalter [48] proposed a semi-analytical method (SAM) in which the exponential time variation is retained explicitly. In contrast with the LCM, the SAM does not require any eigen-decomposition so it has an advantage of having lower computation cost and implementation simplicity. However the positive definiteness of the conformation tensor is not preserved automatically in the SAM. Thus it may diverge at high Weissenberg numbers unless special treatments are done to guarantee the positive definiteness at numerical solution level. The SAM has been successfully used for two-phase viscoelastic flow simulations including shear [1,33] and buoyancy-driven [34] flows. However we found that, although the SAM is efficient at low or moderate Weissenberg numbers, it diverges when Weissenberg number exceeds a certain limit, i.e., $Wi > 2$, in simulating a viscoelastic droplet in a pressure-driven constricted channel. Therefore the SAM is used for low or moderate Weissenberg numbers while the LCM is employed at high Weissenberg numbers in the present study.

In spite of significant progress made for viscoelastic single-phase flow simulations, numerical methods have not yet reached maturity for simulating multiphase viscoelastic flows especially at high Weissenberg numbers. Tanner [50] performed a pioneering numerical study of die-swell problem using a Maxwell fluid model. Later Crochet and Keunings [19] simulated a circular and slit die-swell problem using the Oldroyd-B fluid model. Keunings and co-worker have also performed numerical simulations of various free-surface viscoelastic flows [9,10,28]. Kolte et al. [29] used a Lagrangian method to simulate the transient filament stretching rheometer. More recently various one-field formulations have been employed to perform direct numerical simulations of interfacial viscoelastic flows. Examples include the level-set [3,45], the volume of fluid (VOF) [14,23,25], marker and cell [43,53,54], phase-field [8,62,67], the conservative semi-Lagrangian advection scheme of constrained interpolation profile method with rational function (CIP-CSLR) [21] and the front-tracking methods [17,18,48]. In addition, versions of the arbitrary Lagrangian–Eulerian (ALE) [15,28,59,63,64] and the Lagrangian [47,61] methods have been also employed. Lind and Phillips [30] recently studied the effect of viscoelasticity on a rising gas bubble using a boundary element method. These methods have been used to investigate a wide range of interfacial viscoelastic flow problems including the jet buckling [6,39,54], extrudate swell [15,53,54], viscoelastic drop dynamics [17,18,33,43] and the cross-slot flow [43], among others.

The front-tracking method developed by Unverdi and Tryggvason [57] has been widely used to examine many aspects of Newtonian interfacial flows [55,36,52,37,41,38]. The method was extended to treat viscoelastic interfacial flows first by Sarkar and Schowalter [48] and has been successfully used to study viscoelastic drop dynamics in shear and buoyancy-driven flows [1,33–35]. Sarkar and Schowalter [48] used the semi-analytical method that is limited to low or moderate Weissenberg numbers as mentioned earlier. Chung et al. [17,18] developed a finite-element/front-tracking method for simulation of viscoelastic interfacial flows in two-dimensional planar geometries using the log-conformation approach but the method is restricted to low Reynolds number (creeping) flows. This method has been successfully applied to study viscoelastic two-phase systems in a planar channel with a sudden constriction.

In the present study, a finite-difference/front-tracking method is developed for direct numerical simulation of viscoelastic two-phase flow systems including a Newtonian droplet in a viscoelastic medium (NV), a viscoelastic droplet in a Newtonian medium (VN) and a viscoelastic droplet in another viscoelastic medium (VV). Although the method is general and applicable to virtually any interfacial flow involving viscoelastic fluids, our main goal is to simulate the drop dynamics encountered or inspired by micro/bio-fluidic applications [52,58,65,66]. The method is designed to accommodate the generic family of viscoelastic model equations including the Oldroyd-B, FENE-CR of Chilcott Rallison [13] and FENE-MCR of Coates et al. [11]. The convective terms in viscoelastic constitutive equations are approximated using a second-order ENO [24] and fifth-order upwinded WENO-Z [7] schemes. It is found that the WENO-Z scheme outperforms the ENO scheme in resolving thin high viscoelastic stress layers near the interface. All the other spatial derivatives are approximated using central differences on a staggered grid. Both the semi-analytical and log-conformation methods are employed to overcome high Weissenberg number problem. It is found that the SAM is computationally more efficient than the LCM but fails to achieve convergence at high Weissenberg numbers especially for the pressure-driven viscoelastic two-phase flows in constricted capillary tubes. On the other hand, the LCM successfully achieves convergence for much higher Weissenberg numbers, e.g., as high as $Wi = 100$ without any difficulty but with a higher computational cost and increased implementation complexity. The method has been first validated for two benchmark single-phase problems. The first problem deals with the start-up Poiseuille flow of an Oldroyd-B fluid in a circular capillary tube. For this case, the numerical results are found to be in excellent agreement with the analytical solution obtained by Waters and King [60] both for the transient and steady state cases. The second benchmark problem concerns with a pressure-driven single-phase FENE-MCR fluid flow through an abrupt 4:1 constricted pipe. The results are compared and found to be in good agreement with the computational results of Coates et al. [11]. Then the method is applied to simulate the motion and deformation of a buoyancy-driven droplet in viscoelastic two-phase systems moving through a capillary tube studied computationally by You et al. [64]. The results are found to be in good agreement with You et al. [64] especially when the WENO-Z scheme is used to discretize the convective terms in the viscoelastic model equations. Finally the method has been successfully applied to a more challenging case involving motion and deformation of a droplet in pressure-driven viscoelastic two-phase systems flowing through a capillary tube with a sudden contraction and expansion. This test case holds a great promise to be a benchmark problem for testing performance of numerical methods developed to simulate viscoelastic two-phase systems of practical interest. The present numerical algorithm has been found to be very robust and grid convergent with second-order spatial accuracy for all the cases considered in this paper.

The main contributions of the present work can be summarized as follows: