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A two-phase solver for complex fluids: Studies of the Weissenberg effect

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ABSTRACT

In this work a new two-phase solver is presented and described, with a particular interest in the solution of highly elastic flows of viscoelastic fluids. The proposed code is based on a combination of classical Volume-of-Fluid and Continuum Surface Force methods, along with a generic kernel-conformation tensor transformation to represent the rheological characteristics of the (multi)-fluid phases. Benchmark test problems are solved in order to assess the numerical accuracy of distinct levels of physical complexities, such as the interface representation, the influence of advection schemes, the influence of surface tension and the role of fluid rheology. In order to demonstrate the new features and capabilities of the solver in simulating of complex fluids in transient regime, we have performed a set of simulations for the problem of a rotating rod inserted into a container with a viscoelastic fluid, known as the Weissenberg or Rod-Climbing effect. Firstly, our results are compared with numerical and experimental data from the literature for low angular velocities. Secondly, we have presented results obtained for high angular velocities (high elasticity) using the Oldroyd-B model which displayed very elevated climbing heights. Furthermore, above a critical value for the angular velocity, it was observed the onset of elastic instabilities driven by the combination of elastic stresses, interfacial curvature and secondary flows, that to the authors best knowledge, were not yet reported in the literature.

1. Introduction

Direct numerical simulations of multiphase flows, in which the full continuum equations are solved on a sufficiently refined computational mesh to resolve all continuum scales, date back to the origin of computational fluid dynamics. During the last decades, however, major progresses have been made, by employing a variety of numerical techniques for modeling two-phase flows, either using Lagrangian, Eulerian or Arbitrary Lagrangian–Eulerian (ALE) methodologies. Lagrangian and ALE methods usually represent interfaces accurately, but are rather complex to implement using mesh-dependent discretizations, due to the large mesh distortions involved in fluid flows (Quan, 2011; Montefuscolo et al., 2014). In the ALE method, the mesh follows the interface between the fluid and the solid boundary and the governing equations are discretized on a moving mesh. ALE algorithms require a mesh deformation strategy as the boundaries of the computational domain translate, rotate and deform in order to maintain mesh quality and validity. On the other hand, Eulerian methods are faster and easily parallelizable, but suffer from inherent difficulties for the accuracy of the interface representation, that has to be immersed on the fixed grid. One of the issues of these Eulerian techniques is the increased importance of surface effects (surface tension, Marangoni effects, etc.), quantified by very low capillary (Ca) or Weber (We) numbers. In such cases, the inaccuracies in representing the exact position of the immersed interface generate approximations that are unbalanced, usually between surface, inertial and viscous forces, resulting in the so-called "parasitic currents", a phenomenon that is well documented in the literature Raessi et al. (2009). Additionally, time-step restrictions are a major concern. Since most of interface representations in Eulerian formulations are explicit in time, these restrictions prevent the simulation of real material properties, to the point that recent multiphase codes cannot simulate flows with Reynolds number (Re) and Ca much lower than $O(10^{-2})$ (Hoang et al., 2013; Denner and van Wachem, 2015). Existing

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Eulerian approaches to multiphase flows involve either marker particles, like in Front-tracking techniques (Tryggvason et al., 2001; Pivello et al., 2014), or marker functions as in the Level-set (LS) (Sussman et al., 1994; Scardovelli and Zaleski, 1999; Osher and Fedkiw, 2001; Sussman et al., 1998; Van der Pijl et al., 2005) and Volume-of-Fluid (VOF) (Hirt and Nichols, 1981; Pilliod and Puckett, 2004) approaches. In order to obtain improved interface position and geometric properties such as curvature and normal vector (needed to compute surface tension), hybrid techniques are also available in the literature (Sussman and Puckett, 2000; Sussman et al., 2007), benefiting from the accurate mass conservation of the VOF method and the smooth interface description provided by the LS method.

In recent years, Eulerian mesh-based methodologies have been used for solving interfacial complex fluid flows. Complexity does not arise only from the interaction of different fluid, but also from the physics that governs important phenomena. In some cases, more complex behaviors arise via rheological effects introduced by non-Newtonian and viscoelastic fluids. Many attempts for solving two-phase viscoelastic fluid flows have been presented in the literature see for instance (Pillapakkam and Singh, 2001; Yue et al., 2005; Khismatullin et al., 2006; Stewart et al., 2008; Lind and Phillips, 2010; Habla et al., 2011; Izbassarov and Muradoglu, 2015). Despite of this increase in the development of numerical methods to deal with two-phase viscoelastic fluid flows, there is still unsolved numerical issues and challenges. In non-Newtonian fluids, elastic instabilities can occur even in the absence of inertia, associated with large normal stresses and curvature of streamlines. From a computational perspective, these instabilities present a demanding challenge, such as the High Weissenberg Number Problem (HWNP), leading to the loss of convergence at very low level of elasticity, quantified by the Weissenberg number (Wi). Such numerical failure is usually attained at moderately low Weissenberg numbers ($Wi \sim 1$). This is particularly significant for multi-phase flows, where representing and tracking an interface with complex shape and dynamics are quite challenging. Therefore, the combination of classical numerical methods to represent the interface, surface tension and curvature, along with stabilization techniques to handle the HWNP, can be considered as an useful and innovative framework in current computational rheology.

The main objectives of this work are two-folded: (i) present to the scientific community, a validated new two-phase solver that can deal with multi-phase flows and fluids of complex rheology, and (ii) report interesting results obtained for the Weissenberg effect, related to the dynamical aspects of the onset of elastic instabilities and unsteady flow patterns formed at high rod angular velocities. As far as we are aware, such flow features have not been reported in previous studies based on numerical simulations and it is the ability of this new solver that makes these predictions possible. This numerical framework combines the classic VOF and Continuum surface force (VOF-CSF) and the Height Function (HF) method, along with the generic kernel-conformation tensor transformations. To the authors knowledge, in the context of viscoelastic two-phase flows, it is the first work that describes the implementation of the VOF method, using a piecewise linear interface construction method (PLIC) to reconstruct the interface and a least squares VOF interface reconstruction algorithm (ELVIRA), for solving the HWNP. The code is verified with several benchmark tests, as the viscoelastic laminar lid-driven cavity flow, the axisymmetric concentric annulus with inner cylinder rotation and the droplet spreading of a viscoelastic fluid. Finally, we performed a set of simulations for the application problem of a rotating rod inserted into a container with viscoelastic fluid, named the Weissenberg or Rod-Climbing effect.

The paper is organized as follows. The governing equations used to define the dynamics of an isothermal and incompressible flow of complex multi-fluids are discussed in Section 2. Section 3 describes the numerical algorithms used in the finite difference code. The validation of the numerical formulations are presented in Section 4. The obtained results and corresponding discussions of the numerical simulations for the Weissenberg effect are presented in Section 5. Finally, the conclusions from this study are presented in Section 6.

2. Governing equations

The flow is assumed to be isothermal, laminar, and the fluids incompressible. The governing equations are those expressing conservation of mass

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

and conservation of momentum

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = \nabla\cdot(-p\mathbf{I} + \boldsymbol{\tau} + 2\mu_s\mathbf{D}) + \mathbf{g} + \mathbf{F}, \tag{2}$$

where $\mathbf{u}$ is the velocity field, t is time, ρ is the density, μ_s is the Newtonian solvent viscosity, p is the pressure, $\mathbf{g}$ is the gravity force and $\mathbf{F}$ is the surface tension force. The symbol $\mathbf{D} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ is the rate of deformation tensor, $\boldsymbol{\tau}$ is the elastic stress and $\mathbf{I}$ is the identity tensor.

Several polymeric constitutive equations are implemented in the current version of the solver: the Oldroyd-B model (Bird et al., 1987), the linear form of the Phan-Thien–Tanner (LPTT) model (Phan-Thien and Tanner, 1977) and the Giesekus model (Giesekus, 1982). For an isothermal flow, these rheological equations of state can be written in a compact form as:

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + (\mathbf{u}\cdot\nabla)\boldsymbol{\tau} - \left[(\nabla\mathbf{u})^T\cdot\boldsymbol{\tau} + \boldsymbol{\tau}\cdot\nabla\mathbf{u}\right] = \frac{1}{\lambda}\mathbf{M}(\boldsymbol{\tau}), \tag{3}$$

where $\mathbf{M}(\boldsymbol{\tau})$ is defined by the viscoelastic model

$$\mathbf{M}(\boldsymbol{\tau}) = \begin{cases} 2\mu_p\mathbf{D} - \boldsymbol{\tau} & \text{Oldroyd-B,} \\ 2\mu_p\mathbf{D} - \boldsymbol{\tau} - \dfrac{\alpha\lambda}{\mu_p}\boldsymbol{\tau}\cdot\boldsymbol{\tau} & \text{Giesekus,} \\ 2\mu_p\mathbf{D} - \left(1 + \dfrac{\epsilon\lambda}{\mu_p}\mathrm{tr}(\boldsymbol{\tau})\right)\boldsymbol{\tau} & \text{LPTT,} \\ \quad -\lambda\xi(\boldsymbol{\tau}\cdot\mathbf{D} + \mathbf{D}\cdot\boldsymbol{\tau}) & \end{cases} \tag{4}$$

where λ is a relaxation time and μ_p is the polymer viscosity coefficient. The stress coefficient function of the LPTT model, depends on the trace of $\boldsymbol{\tau}$, $\mathrm{tr}(\boldsymbol{\tau})$, and introduces the dimensionless parameter ϵ which is closely related to the steady-state elongational viscosity in extensional flows. The slip parameter, ξ, takes into account the non-affine motion between the polymer molecules and the continuum. The polymer strands embedded in the medium may slip with respect to the deformation of the macroscopic medium, thus each strand may transmit only a fraction of its tension to the surrounding continuum. When $\xi = 0$ there is no slip and the motion becomes affine. The parameter ξ is responsible for a non-zero second normal-stress difference in shear, leading to secondary flows in ducts having non-circular cross-sections, which is superimposed on the streamwise flow. In the nonlinear term of the Giesekus model, α represents a dimensionless "mobility factor". The amount of Newtonian solvent is controlled by the dimensionless solvent viscosity coefficient, $\beta = \frac{\mu_S}{\mu_0}$, where $\mu_0 = \mu_S + \mu_P$ denotes the total shear viscosity.

An alternative form of describing viscoelastic models is by using the conformation tensor, $\mathbf{A}$, as proposed by Fattal and Kupferman (2005). In this formulation the velocity gradient is defined as

$$\nabla\mathbf{u}^{\mathbf{T}} = \boldsymbol{\Omega} + \mathbf{B} + \mathbf{N}\mathbf{A}^{-1}, \tag{5}$$

where $\boldsymbol{\Omega}$ and $\mathbf{N}$ are anti-symmetric tensors, $\mathbf{B}$ is symmetric and commutes with $\mathbf{A}$. Thus the constitutive equation based on the