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Three-dimensional transient complex free surface flows: Numerical simulation of XPP fluid

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ABSTRACT

In this paper we present a finite difference MAC-type approach for solving three-dimensional viscoelastic incompressible free surface flows governed by the eXtended Pom–Pom (XPP) model, considering a wide range of parameters. The numerical formulation presented in this work is an extension to three-dimensions of our implicit technique [Journal of Non-Newtonian Fluid Mechanics 166 (2011) 165–179] for solving two-dimensional viscoelastic free surface flows. To enhance the stability of the numerical method, we employ a combination of the projection method with an implicit technique for treating the pressure on the free surfaces. The differential constitutive equation of the fluid is solved using a second-order Runge–Kutta scheme. The numerical technique is validated by performing a mesh refinement study on a pipe flow, and the numerical results presented include the simulation of two complex viscoelastic free surface flows: extrudate-swell problem and jet buckling phenomenon.

1. Introduction

Viscoelastic fluid flows are common in many important industrial applications. The need to understand how these flows are processed is of economic and technological interest.

Over the last decades, differential and integral constitutive equations have been widely used to predict complex flows of polymer solutions and melts (e.g. [1–6]). A good overview of different types of constitutive equations describing viscoelastic fluids can be found in several books, as in [7,8] for example.

An important step in the development of a physically realistic and accurate constitutive equation to describe the flow of polymer melts was made recently with the development of the Pom–Pom model [9]. We note, however, that the Pom–Pom model shares many features with the Phan-Thien–Tanner (PTT) model, as shown in [10]. A similar feature is shared by other constitutive models, as shown by Oliveira [11].

An improvement of the original Pom–Pom model is the eXtended Pom–Pom (XPP) formulation, proposed by Verbeeten et al. [12] and Clemeur et al. [13]. Other variants have also been proposed such as the SIPP (Single Improved Pom–Pom), the DIPP (Double Improved Pom–Pom), the SXPP (Single eXtended Pom–Pom), the DXPP (Double eXtended Pom–Pom), the λ^2XPP, the mXPP (modified eXtended Pom–Pom), and the Semi-Linear SXPP. Numerical solution for this type of constitutive equations has taken much effort by several research groups (e.g. [14–20]), and more recently in [21,22].

All the works described above deal with two-dimensional (2-D) flows. One of the first works reported on the literature concerning the numerical simulation of XPP model for three dimensional (3-D) flows was presented by Sirakov et al. [23]. Using a finite element method, the authors investigated the polymer flow in a contraction geometry, and compared the numerical predictions with experimental results. Dressler and Edwards [24] analysed the flow of a Pom–Pom fluid in a tube while Khorsand et al. [25] developed a finite volume method to investigate the single-equation XPP fluid flow in a pipe. More recently, Tenchev et al. [26] investigated the 3-D flow of a XPP fluid past a cylinder and in a contraction geometry using the finite element method.

An additional difficulty appears when the viscoelastic fluid flow involves free surfaces, since an efficient technique to represent the interface with an accurate method for solving the constitutive equations needs to be combined in the numerical simulation. For simulations involving the K-BKZ integral model, one interesting work that deals with free surface flow was presented by Román Marín and Rasmussen [27] who solved the filament stretching between two plates (see also [28]) with third order accuracy in space and time, and analysed the growth of non-axisymmetric disturbances on the free surface. For the extended Pom–Pom constitutive

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equation, Baltussen et al. [29] and Bogaerds et al. [30] examined numerically the stability of the fountain flow, a typical free surface simulation with relevance on injection molding.

The die-swell (or extrudate-swell) phenomenon is a common benchmark flow problem in computational rheology that involves free surfaces. One of the earliest 3-D free surface viscoelastic computation was presented by Tran-Cong and Phan-Thien [31]. In that pioneer work, the authors employed a boundary element method to design extrusion dies using the Upper-Convected Maxwell (UCM) model. Recently, a number of works analysed the behavior of XPP fluids for this flow problem. In two-dimensions, Russo and Phillips [32] presented a spectral method to simulate the extrudate-swell, while Oishi et al. [33] developed a finite difference scheme to study the influence of the XPP model parameters on the extrudate swell ratio. For the three-dimensional case, there are less works that analyse the extrudate-swell problem. For instance, Debbaut and Marchal [34] numerically modeled this problem using the POLYFLOW commercial software, while Aloku and Yuan [35] simulated the double convected Pom–Pom model on a foaming process in extrusion flow. A recent study of axisymmetric extrudate swell for the XPP model using an Arbitrary Lagrangian Eulerian (ALE) finite element formulation was presented by Ganvir et al. [36], showing good agreement with experimental results.

The development of accurate methods for solving moving free surface flows of viscoelastic fluids is still challenging. This fact has motivated the work of some researchers on computational rheology, and important insights have been obtained over the years. In particular, for the XPP model we highlight the following works: Yang et al. [37] simulated the mold filling process combining a level set method and the finite volume method on a non-staggered grid; Jiang et al. [38] studied the impact of liquid droplets on solid surfaces using an improved Smoothed Particle Hydrodynamics method; Qiang et al. [39] analysed the gas-assisted injection molding process using Level Set/SIMPLEC methods; more recently, Li et al. [40] simulated the full three-dimensional packing process in injection molding.

Despite these important developments, in the context of the Marker-And-Cell (MAC) approach, using finite differences and staggered grids, numerical predictions for 3D moving free surface flows of branched polymers have received relatively little attention and, to our best knowledge, this is the first work to address this problem for the XPP model. Within this context, this paper presents a numerical method to simulate complex 3-D free surface flows. The numerical technique implemented in this work is an original extension to 3-D flows of the implicit method developed for viscoelastic flows, which is described in detail in [33].

2. Mathematical model

Incompressible isothermal viscoelastic flows are governed by a system of partial differential equations consisting of the equations of momentum and mass conservation, coupled with a constitutive equation for the extra-stress tensor. The differential constitutive equation used in this work is based on the single mode XPP model (details presented in [12]). Mass conservation and momentum equations can be expressed in dimensionless form respectively by

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

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \frac{\beta}{Re}\nabla^2 \mathbf{u} + \nabla \cdot \boldsymbol{\tau} + \frac{1}{Fr^2}\mathbf{g}, \tag{2}$$

where $\mathbf{u}$ is the velocity vector field, p is the pressure, $\boldsymbol{\tau}$ is the polymeric contribution to the extra-stress tensor, and $\mathbf{g}$ is the gravitational field.

In this work, we use the XPP model which is given by

$$f(\lambda,\boldsymbol{\tau})\boldsymbol{\tau} + We\,\overset{\nabla}{\boldsymbol{\tau}} + \frac{1-\beta}{Re\ We}(f(\lambda,\boldsymbol{\tau})-1)\mathbf{I} + \alpha\frac{Re\ We}{1-\beta}\boldsymbol{\tau}\cdot\boldsymbol{\tau} = 2\frac{1-\beta}{Re}\boldsymbol{D}, \tag{3}$$

where $f(\lambda,\boldsymbol{\tau})$ and λ are given by

$$f(\lambda,\boldsymbol{\tau}) = \frac{2}{\gamma}\left(1-\frac{1}{\lambda}\right)e^{Q_0(\lambda-1)} + \frac{1}{\lambda^2}\left[1-\frac{\alpha}{3}\left(\frac{Re\ We}{1-\beta}\right)^2 tr(\boldsymbol{\tau}\cdot\boldsymbol{\tau})\right] \tag{4}$$

and

$$\lambda = \sqrt{1+\frac{1}{3}\left(\frac{Re\ We}{1-\beta}\right)|tr(\boldsymbol{\tau})|}. \tag{5}$$

In these equations, the Reynolds number Re, the solvent viscosity ratio parameter β, the Weissenberg number We, the γ parameter, the Q parameter and the Froude number Fr are defined by

$$Re = \frac{\rho UL}{\mu},\quad \beta = \frac{\mu_S}{\mu},\quad We = \frac{\lambda_1 U}{L},\quad \gamma = \frac{\lambda_2}{\lambda_1},\quad Q = \frac{2}{Q_0},\quad Fr = \frac{U}{\sqrt{gL}}, \tag{6}$$

where λ_1 and λ_2 are the orientation and backbone stretch relaxation times, ρ is the fluid density, $\mu = \mu_S + \mu_P$ (with μ_S and μ_P representing the solvent viscosity and polymeric viscosity coefficient, respectively) is the zero shear rate viscosity, Q is the number of arms at the extremity of the Pom–Pom molecule and the α parameter controls the anisotropic drag [22]. In addition, L, U and g are length, velocity and gravity characteristic scales, respectively.

The upper-convected derivative of tensor $\boldsymbol{\tau}$ in (3) is defined by

$$\overset{\nabla}{\boldsymbol{\tau}} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla\cdot(\mathbf{u}\boldsymbol{\tau}) - (\nabla\mathbf{u})\cdot\boldsymbol{\tau} - \boldsymbol{\tau}\cdot(\nabla\mathbf{u})^T, \tag{7}$$

while the rate-of-deformation tensor $\boldsymbol{D}$ is given by

$$\boldsymbol{D} = \frac{1}{2}[\nabla\mathbf{u} + (\nabla\mathbf{u})^T]. \tag{8}$$

In order to solve numerically Eqs. (1)–(3) it is necessary to impose boundary conditions for the velocity field and non-Newtonian extra-stress tensor $\boldsymbol{\tau}$. If the velocity at inflows is constant, then the non-Newtonian tensor is set as $\boldsymbol{\tau} = \mathbf{0}$, while for parabolic velocity at inflows the non-Newtonian tensor $\boldsymbol{\tau}$ is defined as in the Oldroyd-B model [18,33]. At outflows the homogeneous Neumann conditions are employed for $\mathbf{u}$ and $\boldsymbol{\tau}$ (see [41]), namely,

$$\frac{\partial \mathbf{u}}{\partial n} = \mathbf{0} \quad \text{and} \quad \frac{\partial \boldsymbol{\tau}}{\partial n} = \mathbf{0} \tag{9}$$

where n represents the normal direction of the outflow boundary. For rigid walls, the no-slip condition $\mathbf{u} = \mathbf{0}$ is used and $\boldsymbol{\tau}$ is computed directly from Eq. (3) (details are given in [33]).

Assuming a passive atmosphere, the correct boundary conditions for the free surface are given by

$$\boldsymbol{n}\cdot(\boldsymbol{\sigma}\cdot\boldsymbol{n}) = 0, \tag{10}$$

$$\boldsymbol{t}_1\cdot(\boldsymbol{\sigma}\cdot\boldsymbol{n}) = 0, \tag{11}$$

$$\boldsymbol{t}_2\cdot(\boldsymbol{\sigma}\cdot\boldsymbol{n}) = 0, \tag{12}$$

where $\boldsymbol{\sigma} = -p\mathbf{I} + 2\frac{\beta}{Re}\boldsymbol{D} + \boldsymbol{\tau}$ is the total stress tensor and $\boldsymbol{n} = (n_x, n_y, n_z)$, $\boldsymbol{t}_1 = (t_{1x}, t_{1y}, t_{1z})$ and $\boldsymbol{t}_2 = (t_{2x}, t_{2y}, t_{2z})$ are, respectively, unit normal and tangential vectors to the free surface.

3. Overview of numerical implementation

The governing and constitutive equations are solved using the strategy of Oishi et al. [33], which combines projection methods with an implicit technique for the treatment of pressure on free