Numerical simulation of three-dimensional free surface flows of Giesekus fluids

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Abstract: *A numerical method for simulating three-dimensional viscoelastic free surface flows governed by the Giesekus constitutive equation has been developed. The momentum equations are solved by the implicit Euler method on a staggered grid while the solution of the Giesekus model is obtained by a second order Runge-Kutta scheme. The free surface is modelled by a front tracking technique based on the Marker-and-Cell method. The numerical method is verified by solving the flow in a tube employing several meshes. Numerical results obtained from the simulation of the jet buckling include the measurements of the frequency of buckling for several values of the Weissenberg number. Furthermore, the effect of the mobility parameter on the jet buckling phenomenon is also investigated.*
Keywords: *Finite difference, Viscoelastic flow, Three-dimensional free surface flow, Giesekus model, Jet buckling*

1. INTRODUCTION

Industrial problems involving fluid flow with free surfaces are present in many manufacturing processes. Applications include, for example, casting, container filling, extrusion and fluid jetting devices. The accurate determination of the free surface is important precisely if the flow strongly depends on the position and curvature of the free surface. In many cases, the flow is non-Newtonian and involves viscoelastic fluids flowing into complex shaped containers. Therefore, there is an industrial interest in developing numerical tools that are capable of dealing with these problems in both two and three-dimensions. Indeed, numerical simulation of viscoelastic free surface flows has been the subject of intense research (e.g. Tomé *et al.* (2012); Mompean *et al.* (2011)). In the literature, a considerable amount of numerical solution of viscoelastic models can be found. For instance, differential models such as, Upper Convected Maxwell (UCM), Oldroyd-B, Phan-Thien-Tanner (PTT), Giesekus, have been the subject of study of many researchers. In particular, the Giesekus model has been investigated by several researchers, e.g. Schleiniger and Weinacht (1991); Ferrás *et al.* (2012); Mu *et al.* (2013) but with regard to free surface flows this model has received litte attention. In this study, we are interested in developing a numerical methodology for solving three-dimensional viscoelastic free surface flows modelled by the Giesekus constitutive equation and apply it to simulate the jet buckling phenomenon. This work is organized as follows: Section 2 presents the governing equations together with the mathematical and numerical formulations while in Section 3 the results obtained from the simulations of a tube filling problem are used to verify the accuracy and convergence of the numerical method. Section 4 provides results obtained with the jet buckling phenomenon and conclusions.

2. MATHEMATICAL FORMULATION

The governing equations for incompressible isothermal flows modelled by the Giesekus model (Schleiniger and Weinacht, 1991) are the mass and momentum equations together with the the Giesekus constitutive equation, that in dimensionless form, can be written in the form as:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla\left(\mathbf{u}\mathbf{u}^T\right) = -\nabla p + \frac{1}{Re}\nabla^2\mathbf{u} + \nabla\cdot\mathbf{S} + \frac{1}{Fr^2}\mathbf{g}, \tag{1a}$$

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

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla\cdot(\mathbf{u}\boldsymbol{\tau}) - (\nabla\mathbf{u})\cdot\boldsymbol{\tau} - \boldsymbol{\tau}\cdot(\nabla\mathbf{u})^T + \boldsymbol{\tau} + \alpha\frac{ReWi}{1-\beta}\left(\boldsymbol{\tau}\cdot\boldsymbol{\tau}\right) = 2\frac{1-\beta}{Re}\mathbf{D}. \tag{2}$$

To obtain the transformed momentum equations (1a) and (1b), the Elastic-Viscous-Splitting-Stress (EVSS) transformation (Rajagopalan *et al.*, 1990) was employed. This transformation permits to write the extra-stress tensor as a linear combination of a Newtonian tensor and a non-Newtonian stress tensor that models the elastic effects in the flow. This transformation is given by

$$\boldsymbol{\tau} = \frac{2}{Re}\mathbf{D} + \mathbf{S}, \tag{3}$$

which was already employed in the formulation of the momentum equations (1a) and (1b). In the equations above, t is the time, $\mathbf{u}$ is the velocity field, p is the pressure, $\mathbf{g}$ is the gravitational field, $\mathbf{S}$ is a non-Newtonian tensor, $\boldsymbol{D} =$

$\frac{1}{2}\left((\nabla u)+(\nabla u)^T\right)$ is the Newtonian contribution to the extra-stress tensor and α is the parameter that models the mobility of the fluid. The nondimensional numbers, $Fr = \dfrac{U}{\sqrt{gL}}$, $Re = \dfrac{\rho U L}{\eta_0}$, $Wi = \dfrac{\lambda U}{L}$ are, respectively, the Froude, Reynolds and Weissenberg numbers. The constants, L, U and ρ denote typical scalings for length, velocity and density, respectively. Furthermore, the amount of Newtonian solvent present in the fluid is controlled by the constant $\beta = \dfrac{\eta_s}{\eta_0}$, where $\eta_0 = \eta_s + \eta_p$ represents the total viscosity at zero shear, while η_s and η_p represent the Newtonian and polymeric viscosities, respectively. When $\alpha = 0$, the Giesekus model reduces to the Oldroyd-B model and making $\alpha = \beta = 0$, the UCM model is obtained.

To solve the equations (1a)-(3), it is necessary to specify appropriate initial and boundary conditions. At the inlet, the velocity is specified by $\mathbf{u} = \mathbf{U}_{inf}$ and the extra-stress tensor is set as $\boldsymbol{\tau} = \boldsymbol{\tau}_{inf}$. At fluid exits (outflows), homogeneous Neumann conditions both for velocity and extra-stress tensor, $\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}} = \dfrac{\partial \boldsymbol{\tau}}{\partial \mathbf{x}} = \mathbf{0}$, are set and the no-slip condition, $\mathbf{u} = \mathbf{0}$, on rigid boundaries is assumed. allows

We are interested in three-dimensional flows with free surfaces in which the fluid flows into a passive atmosphere. Assuming that surface tension forces can be neglected at the interface between the fluids (viscous fluid and air) the extra-stress tensor components should be continuous so that the proper boundary condition is described by (for details see (Batchelor, 1967), page. 157):

$$\mathbf{n}^T \cdot (\boldsymbol{\sigma} \cdot \mathbf{n}) = 0, \qquad \mathbf{m_1}^T \cdot (\boldsymbol{\sigma} \cdot \mathbf{n}) = 0, \qquad \mathbf{m_2}^T \cdot (\boldsymbol{\sigma} \cdot \mathbf{n}) = 0,$$

where $\mathbf{n}, \mathbf{m_1}$ and $\mathbf{m_2}$ denote unit normal and tangential vectors to the free surface and $\boldsymbol{\sigma} = -p\mathbf{I} + \dfrac{2}{Re}\boldsymbol{D} + \mathbf{S}$ is the total stress tensor. These conditions are applied making local approximations to the unit vectors $\mathbf{n}, \mathbf{m_1}$ and $\mathbf{m_2}$. Details of the approximations employed can be found in Tomé *et al.* (2012).

The method of solution is based on the projection method introduced by Chorin and Marsden (2000). The GENSMAC (GENeralized Simplified Marker-And-Cell) methodology, which has been in constant improvement by Tomé and McKee (1994) and co-workers (Tomé *et al.*, 2012), is the base to the present methodology. The momentum equations are solved on a 3D-staggered grid while the Giesekus constitutive equation is solved by a finite difference method that approximates the time derivative by a second order Runge-Kutta method. The spatial derivatives are approximated by second-order differences. More details about the classification of cells and the discretization of the equations at the free surface can be found in McKee *et al.* (2008).

3. VERIFICATION RESULTS

To verify the capability of the numerical methodology presented in Section 2, the filling of a three-dimensional tube was simulated. To analyse the convergence of the numerical results, this problem was solved on four computational meshes: Mesh 1: $16 \times 16 \times 80$ cells ($dx = dy = dz = 0.125$), Mesh 2: $20 \times 20 \times 100$ cells ($dx = dy = dz = 0.1$), Mesh 3: $32 \times 32 \times 160$ cells ($dx = dy = dz = 0.0625$) and Mesh 4: $40 \times 40 \times 200$ cells ($dx = dy = dz = 0.05$). The process of filling consisted in considering a totally empty tube at time $t = 0s$ and then, the fluid is injected in through the tube entrance until it became completely full and steady state flow was established. The following data were considered: tube radius $L = 1m$, tube length $10L$, $U = 1m/s$, $Re = 1.0$, $Wi = 1.0$, $\beta = 0.5$ and $\alpha = 0.1$. Figure 1(a) shows the frontal visualization of the viscoelastic flow at the time $t = 5s$ while Figs. 1(b)-1(e) display the numerical profiles obtained for velocity w and extra-stress tensor components τ^{xx}, τ^{xz} and τ^{zz} at the middle section of the tube ($z = 5, y = 1$ and $0 < x < 2$). We can observe in Fig. 1 that the numerical solutions displayed good agreement with the solution obtained on the finer mesh M4 and convergence of the results can be observed.

4. JET BUCKLING PHENOMENON

When a viscous jet flows onto a rigid plate several phenomena can occur as for example jet buckling. This event is associated with very viscous jets and in the past decades, has attracted the attention of many researchers (e.g. Paulo *et al.* (2007), Ville *et al.* (2011), Tomé *et al.* (2012), Cruickshank and Munson (1981); Cruickshank (1988)). This problem was studied by Cruickshank and Munson (1981) who performed a series of experiments showing an asixymmetric Newtonian jet falling onto a flat surface and varied the jet diameter (D), height of the jet to the flat surface (H) and fluid viscosity (η). From the results obtained they derived sufficient conditions under which a Newtonian viscous jet would present buckling after reaching a rigid plate. They found that an axisymmetric jet should undergo buckling if the following conditions

$$Re < 1.2 \qquad \text{and} \qquad \frac{H}{D} > 7.2, \text{ are satisfied.}$$

To verify these conditions we simulated a jet containing Newtonian fluid flowing onto a plate with $Re = 0.5$ and $Re = 1.5$. Figure 2 displays the fluid flow configuration at time $t = 0.8$s, where it can be observed that the jet with $Re = 0.5$ did undergo buckling whereas the jet with $Re = 1.5$ did not. These results confirm Cruickshank and Munson (1981) predictions.

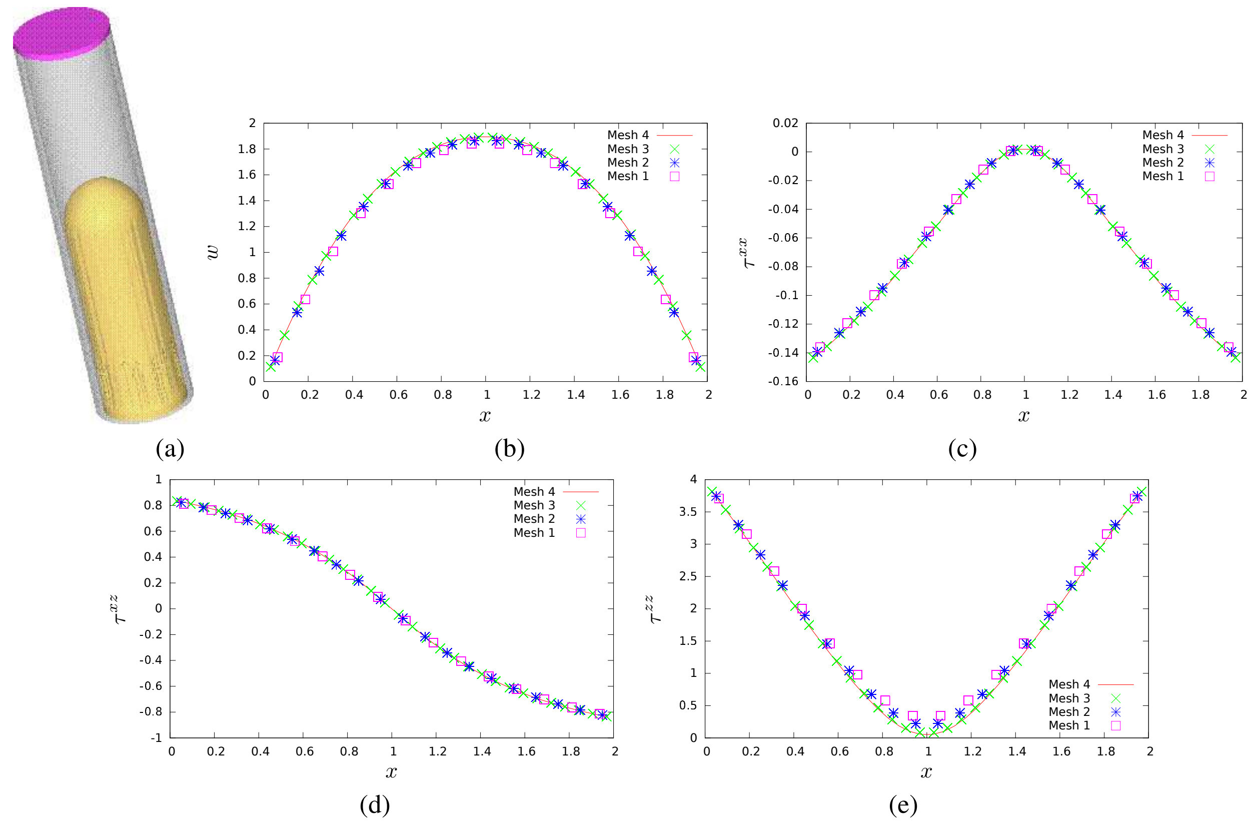

Figure 1: Filling of a tube with a viscoelastic fluid: $Re = 1$, $Wi = 1$, $\beta = 0.5$ and $\alpha = 0.1$. (a) Three-dimensional visualization of the flow at $t = 5s$. Figures (b)-(e) display the solutions at the middle of the tube at $t = 50s$. (b) w, (c) τ^{xx} , (d) τ^{xz} (e)τ^{zz}.

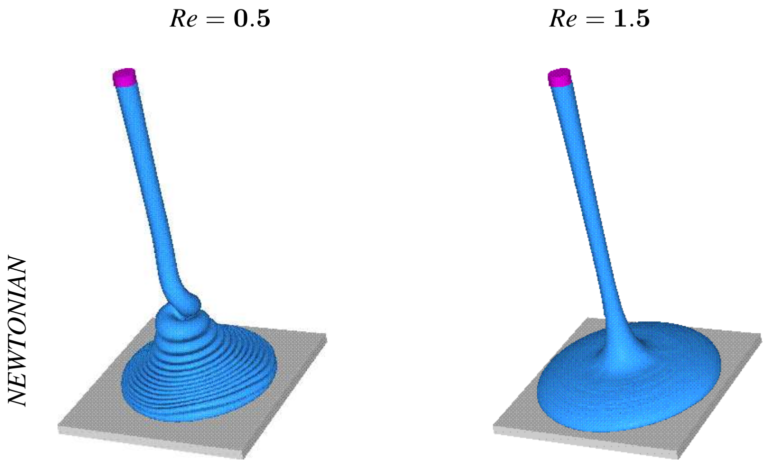

Figure 2: Simulation of a Newtonian jet flowing down to a rigid plate with $H/D = 16$. Fluid flow visualization at time $t = 0.8$s.

As it is shown in Fig. 2, for a Newtonian fluid the Reynolds number is an important parameter that controls the buckling phenomenon. On the contrary, in viscoelastic flows the Weissenberg number models the elastic forces in the flow and also has a strong influence on the buckling phenomenon as it was demonstrated in the works Paulo *et al.* (2007) and Tomé *et al.* (2012). In the case of the Giesekus viscoelastic constitutive model, the parameter α dictates the shear thinning behaviour of the fluid. This makes the “Reynolds number” to change locally according to the local shear rate and may have a strong effect in the jet buckling phenomenon. To demonstrate this fact we performed four simulations showing a jet hitting a rigid plate with $Re = 1.5$ and $Wi = 10$. The input data used in these simulations where the same employed by Tomé et al. (2011) who simulated this problem with the UCM model, while the parameter α was assigned the values 0, 0.1, 0.3 and 0.5. The results obtained in these simulations are summarized in Fig. 3 which shows the fluid flow visualization at times $t = 0.4$s and 0.8s. Indeed, in Fig. 3, the results with $\alpha = 0$ shows that at time $t = 0.4$s the jet already hitted the plate, starting to accumulate upon itself and at time $t = 0.8$s the jet clearly buckled. These results are in good agreement with those of Tomé *et al.* (2012) which obtained similar results employing the UCM model. The results with $\alpha = 0.1$ presented similar results to those with $\alpha = 0$ which shows that the Giesekus model produced similar results obtained with the UCM model. As the value of α increases, the shear thinning behaviour predicted by the Giesekus model makes the fluid to gain more mobility so with $\alpha = 0.3$ the results show that the buckling effect was suppressed and similar results were obtained with $\alpha = 0.5$. This shows that the buckling frequency decreases as the value of α increases. These results indicate that the numerical method employed to solve the Giesekus constitutive equation can cope with three-dimensional free surface flows governed by this constitutive model.

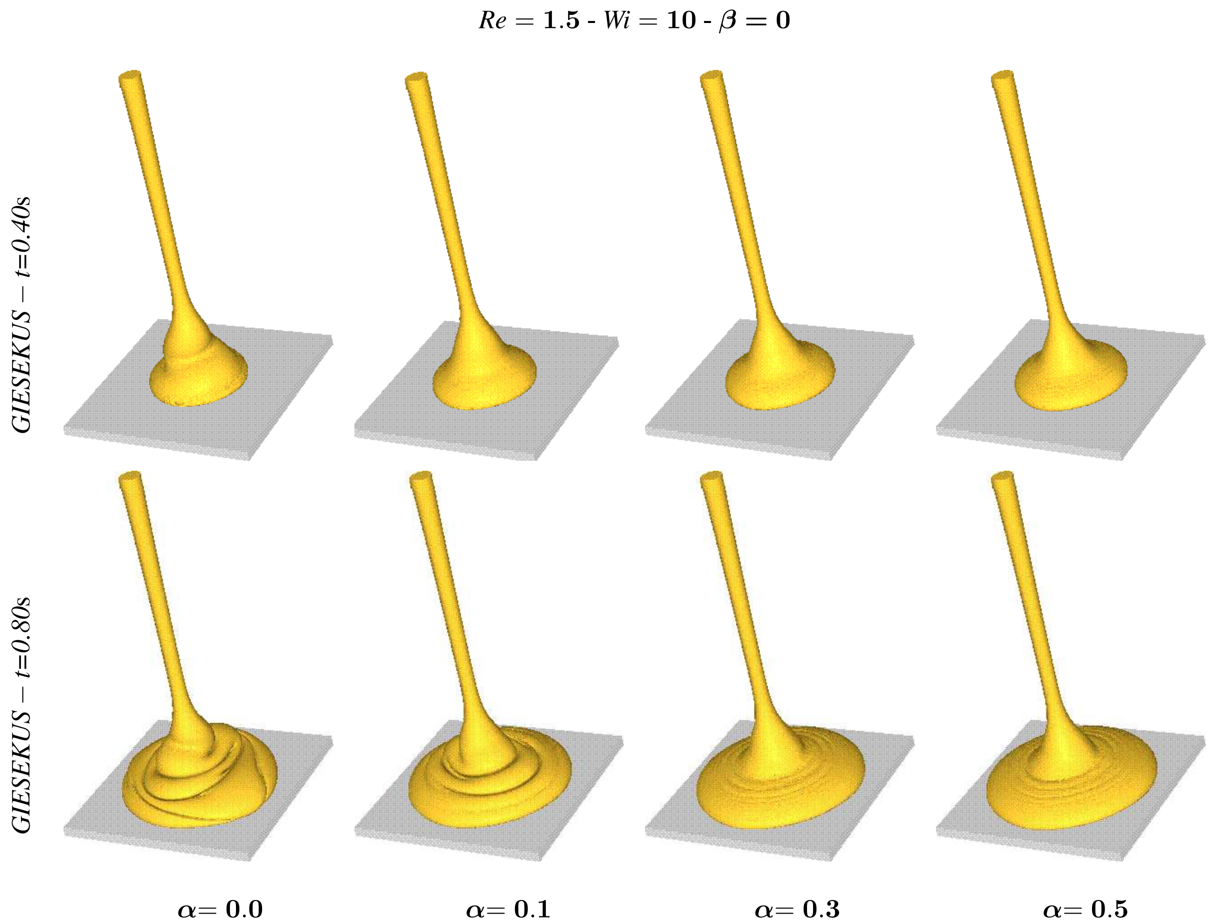

Figure 3: Numerical simulation of a Giesekus fluid jet hitting a rigid plate. Data used: $Re = 1.5$, $H/D = 16$, $Wi = 10$, $\beta = 0$ and several values of the mobility factor α.

5. CONCLUDING REMARKS

This paper presented a finite difference technique to simulate viscoelastic flows governed by the constitutive equation Giesekus. Verification results in the problem of filling a circular tube were provided where mesh refinement showed convergence of the numerical methodology. The technique was applied to simulate the jet buckling phenomenon for various values of the mobility factor α. The numerical results are in agreement with the model which predicts stronger shear thinning effect as the value of α is increased. Indeed, for $\alpha = 0.3$ and 0.5, the effects of shear thinning intensify the fluid mobility that avoided the appearance of the jet buckling phenomenon.

6. ACKNOWLEDGEMENTS

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