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Numerical Solution of the Upper-Convected Maxwell Model for Three-Dimensional Free Surface Flows

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Abstract. This work presents a finite difference technique for simulating three-dimensional free surface flows governed by the Upper-Convected Maxwell (UCM) constitutive equation. A Marker-and-Cell approach is employed to represent the fluid free surface and formulations for calculating the non-Newtonian stress tensor on solid boundaries are developed. The complete free surface stress conditions are employed. The momentum equation is solved by an implicit technique while the UCM constitutive equation is integrated by the explicit Euler method. The resulting equations are solved by the finite difference method on a 3D-staggered grid. By using an exact solution for fully developed flow inside a pipe, validation and convergence results are provided. Numerical results include the simulation of the transient extrudate swell and the comparison between jet buckling of UCM and Newtonian fluids.

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Key words: Viscoelastic flow, Upper-Convected Maxwell, finite difference, free surface, implicit techniques, Marker-and-Cell.

1 Introduction

A common industrial process is extrusion whereby a complex fluid is passed through a die under pressure. The extrudate, the polymer that exits the die, may be the final product or may be an intermediate stage in the industrial process. Other industrial applications involving complex fluids include container filling and polymer injection. These problems are often time-dependent, non-isothermal, and viscoelastic: they also often

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have multiple free surfaces and the geometries can be complex. Computational rheology, and in particular viscoelastic free surface flows, has been an active area (see, for example, [1–4, 16, 24, 27, 41, 43] to mention a few). However, much of the work has dealt with two-dimensional, steady state, creeping flows. Notwithstanding, 3D confined flows employing the Upper-Convected Maxwell (UCM), Oldroyd-B, Phan-Thien-Tanner (PTT) models can be found in the literature (eg. [5–10]). More recently, there have been several attempts to model three-dimensional viscoelastic free surface flow: for example, Rassmussen and Hassager [11] used a 3D-Lagrangian integral model to simulate the elastic end-plate instability of polymeric filaments employing the UCM model. Kim et al. [12] developed a finite element code using the Volume-of-Fluid (VOF) technique to simulate 2D/3D free surface flows of Newtonian and Generalized Newtonian (GNF) fluids. Kim's code is in principle capable of dealing with three-dimensional moving free surfaces, but is yet to be tested on real problems. More recently, Bonito et al. [13] presented a finite element/finite volume technique that was capable of solving three-dimensional viscoelastic flows with moving free surfaces. In particular, Bonito et al. [13] presented jet buckling results for both Newtonian and Oldroyd-B fluids.

On the millennium, Castelo et al. [18] developed a fully three-dimensional code called Freeflow3D. In this code the governing equations were solved by the finite difference method on a staggered grid and the free surface(s) modeled by a Marker-and-Cell method [14]. Freeflow3D can deal with time-dependent free surface flows and can cope with multiple moving free surfaces. It can simulate container filling and jet buckling of Newtonian fluids (e.g. Tomé et al. [17]), deal similarly with Generalized Newtonian flows [22], and more recently it has been extended to viscoelastic free surface flows of Oldroyd-B fluids (see Tomé et al. [25]).

In this work we develop a numerical method for simulating three-dimensional viscoelastic free surface flows governed by the Upper-Convected Maxwell constitutive equation. The momentum equations are solved by the implicit Euler method combined with an implicit technique for calculating the pressure on the free surface. The UCM constitutive equation is solved by the explicit Euler scheme. The method is validated by simulating fully developed flow in a 3D-pipe and convergence results are obtained through mesh refinement. Results of fully three-dimensional viscoelastic flows with moving free surfaces are given.

2 Governing equations

Incompressible and isothermal flows are governed by the mass conservation equation and the equation of motion which can be written as

$$\nabla\cdot\mathbf{u}=0, \tag{2.1}$$

$$\frac{\partial\mathbf{u}}{\partial t}+\nabla\cdot(\mathbf{u}\mathbf{u})=\frac{1}{\rho}\left[-\nabla p+\nabla\cdot\mathbf{T}\right]+\mathbf{g}, \tag{2.2}$$