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A finite difference technique for solving a time strain separable K-BKZ constitutive equation for two-dimensional moving free surface flows

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ABSTRACT

This work is concerned with the numerical solution of the K-BKZ integral constitutive equation for two-dimensional time-dependent free surface flows. The numerical method proposed herein is a finite difference technique for simulating flows possessing moving surfaces that can interact with solid walls. The main characteristics of the methodology employed are: the momentum and mass conservation equations are solved by an implicit method; the pressure boundary condition on the free surface is implicitly coupled with the Poisson equation for obtaining the pressure field from mass conservation; a novel scheme for defining the past times t' is employed; the Finger tensor is calculated by the deformation fields method and is advanced in time by a second-order Runge–Kutta method. This new technique is verified by solving shear and uniaxial elongational flows. Furthermore, an analytic solution for fully developed channel flow is obtained that is employed in the verification and assessment of convergence with mesh refinement of the numerical solution. For free surface flows, the assessment of convergence with mesh refinement relies on a jet impinging on a rigid surface and a comparison of the simulation of a extrudate swell problem studied by Mitsoulis (2010) [44] was performed. Finally, the new code is used to investigate in detail the jet buckling phenomenon of K-BKZ fluids.

1. Introduction

Viscoelastic free surface flows are important in many industrial processes as for example in injection molding and profile extrusion. These problems are challenging as the flow may possess several moving free surfaces and although many

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researchers have been working on the development of numerical methods for simulating viscoelastic free surface flows, the accurate application of the free surface stress conditions is a problem that has not yet been fully resolved. Most of the works and methods to deal with free surface flows of viscoelastic fluids concern constitutive equations of the differential type such as the models known as UCM [1–3], Oldroyd-B [4–7], Phan–Thien–Tanner [8–10], FENE-CR (also FENE-P) [11], eXtended Pom–Pom [12,13], among others. Notwithstanding, the advances in computational resources have motivated researchers to consider more sophisticated rheological models that employ integral equations instead of partial differential equations. One reason is that integral constitutive models are known to provide a good fitting to the rheology of polymer melts, as for example high density polyethylene (HDPE) [14,15] and low density polyethylene (LDPE) [16], that are usually employed by many industries. Among the most successful integral models stands the K-BKZ equation [17,18] which has also been employed by many researchers that have developed numerical methods for this class of fluids (e.g. [19,20]). However, most of the problems investigated with integral models involve confined flows as for example entry flows [21,22] and flows through abrupt contractions [16,23–25].

The K-BKZ model was originally developed using ideas of rubber elasticity theory in a general framework accounting for the strain free energy associated with the elastic strain imposed on the material [17,18]. In its original form, this model consists of a class of constitutive equations because it admits a large variety of functions for the free energy and it considers a viscoelastic liquid as a relaxing rubber in which both the elastic energy and stress are allowed to relax. One of the methods to arrive at a specific K-BKZ model is to fit it to single or double step strain data. The response of the model is often poor if the two sudden strains are of opposite sign [26] and this is observed not only in shear, as documented in [26], but also in extension as well shown by Rasmussen and co-workers [27,28]. These authors measured stress relaxation of some polymer melts in well-controlled extensional flow experiments, including reversed flow due to imposition of normal strain rate steps, and showed that multimode versions of models akin to the K-BKZ constitutive equation, such as the Doi–Edwards with or without interchain alignment, could not capture adequately the observed stress evolution of the melt, especially when a uniaxial extensional flow was followed by a biaxial extensional flow. In the absence of such severe strains, which is often the case, the performance of the model is significantly better and its parameters can still be determined using data from measurements of the viscosity and first normal stress difference in steady shear flow, in addition to the basic shear stress growth and shear stress relaxation experiments. If more than one mode is needed to fit the relaxation spectrum, data from small amplitude oscillatory shear provides the coefficients of the memory function.

For some polymer melts, such as LDPE, polydimethylsiloxane or polystyrene, the stress dependence of the K-BKZ equation is factorable on time and strain dependencies and the nonlinear behavior can be accommodated through a damping function, for which many forms have been proposed [29], including the Papanastasiou–Scriven–Macosko (PSM) form used here [30]. Fittings of the K-BKZ/PSM model to experimental data in steady and transient shear and extension of LDPE and HDPE are also shown in [31].

It should also be said that, as the complexity of flow kinematics increases, simple models are not able to quantitatively describe experimental data. More capable and adequate constitutive models are of integrodifferential type and are based on molecular theories for linear, branched and star polymers. These mathematically more complex models are outside the scope of the present work, but some contributions to such developments have been presented by Mead et al. [32], Ianniruberto and Marrucci [33] and Wagner et al. [34], among others.

Dealing numerically with flows of fluids described by integrodifferential models relies most commonly on extensions of Lagrangian approaches, such as the Lagrangian integral method of Hassager and Bisgaard [35], subsequently extended to 3D flows by Rasmussen and Hassager [36], or with extensions of the method of deformation fields of Peters et al. [37] used here also. One example of an extension of Lagrangian methods is by Peters el al. [38], whereas an early extension of the Eulerian method is by Wapperom et al. [39] who performed simulations in a sudden contraction–expansion.

Flow problems possessing free surface(s) have also been considered by some investigators. For example, one work involving transient free surface flows and integral models is the filament stretching presented by McKinley and Sridhar [40] and was also studied in [36,41,42]. Another free surface flow problem which has been numerically investigated is the extrudate swell phenomenon [14,43–52]. However, these investigations employ the finite element method and their application to flows possessing time-dependent folding free surfaces has yet to be demonstrated. A detailed discussion on the importance of the K-BKZ integral constitutive model and current developments on numerical techniques for solving integral models are provided in the review papers of Tanner [53] and Mitsoulis [31]. For this reason, a more general introduction on numerical methods for solving integral constitutive equations is not given here.

Free surface flows in which there is a moving free surface interacting with solid walls are common in practical applications such as container filling. Even though the K-BKZ model has been applied to solve a variety of viscoelastic flows, to the best of our knowledge, integral constitutive models have not been applied to simulate the buckling effect that can occur when a jet interacts with a solid wall. It is true that such interaction results in a combination of uniaxial and biaxial extensional flows for which the K-BKZ, and several other simple integral constitutive equations [27,28], cannot provide an accurate quantitative solution, but as indicated above and below, there is sufficient novelty in the set of characteristics of this work to justify this numerical experience. Although there are various versions of the K-BKZ integral model, this work deals with the so-called K-BKZ/PSM model (Papanastasiou–Scriven–Macosko [30]).

We present a numerical method for solving two-dimensional flows governed by the K-BKZ/PSM integral constitutive equation that is capable of resolving multiple moving free surface flows and their interaction with rigid walls. We formulate