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A method for calculating rheological and morphological properties of constant-volume polymer blend models in inhomogeneous shear fields

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Abstract

We show how to formulate two-point boundary-value problems in order to compute fully-developed laminar channel and tube flow profiles for viscoelastic fluid models. The formulation is applied to Couette and pressure-driven flows separately, or a combination of both. The application of this methodology is illustrated analytically for the Upper-Convected Maxwell Model, and it is applied computationally for the Phan-Thien/Tanner and Giesekus Models. Numerical solutions exist for the last two models [J.Y. Yoo, H.C. Choi, On the steady simple shear flows of the one-mode Giesekus fluid, Rheol. Acta 28 (1989) 13–24; P.J. Oliveira, F.T. Pinho, Analytical solution for fully developed channel and pipe flow of Phan-Thien–Tanner fluids, J. Fluid Mech. 387 (1999) 271–280; M.A. Alves, F.T. Pinho, P.J. Oliveira, Study of steady pipe and channel flows of a single-mode Phan-Thien–Tanner fluid, J. Non-Newtonian Fluid Mech. 101 (2001) 55–76], allowing verification of the computational technique. Subsequently, the computational algorithm is applied to the constant-volume polymer blend models of Maffettone and Minale [P.L. Maffettone, M. Minale, Equation of change for ellipsoidal drops in viscous flow, J. Non-Newtonian Fluid Mech. 84 (1999) 105–106 (Erratum), J. Non-Newtonian Fluid Mech. 78 (1998) 227–241] and Dressler and Edwards [M. Dressler, B.J. Edwards, The influence of matrix viscoelasticity on the rheology of polymer blends, Rheol. Acta 43 (2004) 257–282; M. Dressler, B.J. Edwards, Rheology of polymer blends with matrix-phase viscoelasticity and a narrow droplet size distribution, J. Non-Newtonian Fluid Mech. 120 (2004) 189–205]. Rheological and morphological properties of the model blends are thus obtained as functions of the spatial position within the channel, applied pressure drop, and shear rate at the wall.

Keywords: Viscoelasticity; Laminar channel flow; Constant-volume models; Microstructural constraints; Polymer blend models

1. Introduction

The processing of polymer blends is a critical issue in the plastics industry, since the mechanical properties of the finished product are greatly impacted by the deformational and thermal histories of the specific process. In the past decade, the Doi/Ohta [7] model was developed to describe the rheological and morphological properties of polymer blends under isothermal flow conditions. Very recently, the need for blend models to conserve volume of the dispersed (droplet) phase was recognized, and new models have since been developed which guarantee the satisfaction of this constraint [4–6,8,9].

The models mentioned in the preceding paragraph can be quite complicated, incorporating different physical processes in the governing set of evolution equations. For example, terms appear in the dynamical equations that describe the interaction of matrix-phase viscoelasticity with the morphology of the dispersed phase, and vice-versa. Due to this complexity, to date most examinations of this model behavior have studied only homogeneous shear fields, either under steady-state conditions, or start-up and cessation of homogeneous shear flow behavior. To be useful in real process simulations, techniques must be developed that can deal with the additional complexities of these models in inhomogeneous flow fields.

Of course, computational viscoelastic fluid mechanics is a mature field, wherein many different types of rheological constitutive equations have been tested in inhomogeneous flow fields relevant to the polymer processing industry. Many different techniques have been developed for performing these simulations. However, because of the additional complexity of the constant-volume polymer blend models, applying most of these

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approaches to these new models is extremely demanding heuristically, although conceptually similar in principle.

In this article, we are going to strike down a middle road between the relative ease of use of the homogeneous shear calculations, and the overriding complexity of sophisticated inhomogeneous shear field calculations. In homogeneous calculations, one typically uses Newton's method for steady-state computations, and a Runge–Kutta method for transient calculations. Both methods are fairly simple to implement, even for complicated models such as those that concern us here. We would like very much to keep the complexity of our inhomogeneous calculations on the same level as this. Of course, doing so requires a compromise, and something must be given up to compensate for our requirement concerning ease of use.

Herein, we consider steady-state, fully developed, laminar, Couette and pressure-driven flows of polymer blends down channels or tubes. Thus we give up the ability to study start-up effects, entrance/exit effects, etc., but gain the ability to compute flow, rheological, and morphological profiles for the model blends under these restricted conditions. One should not think, therefore, that the results of the calculations would be uninteresting: as shown below, blend models exhibit much more interesting behavior than the typical results generated by most viscoelastic fluid models, solved under the same conditions.

The method that we use here is to adapt a Two-Point Boundary-Value (TPBV) Technique [10] to the complexities of constant-volume polymer blend models undergoing the flow processes described in the preceding paragraph. As will be demonstrated below, this is not more difficult than applying Newton's method or a Runge–Kutta method to a homogeneous shear-flow problem; however, some initial methodological issues must be overcome to apply the TPBV Technique to viscoelastic fluids. Nevertheless, the basic idea behind this computational scheme has been used in prior stability analyses of laminar channel flow of viscous fluids heated from below [11].

Fortunately, much work has been done in the past to solve various rheological models for the viscometric flows considered herein: e.g., Schleiniger and Weinacht [12,13] solved the boundary-value problem for the Giesekus Model, and in Refs. [2,3,14,15] analytical solutions for the Phan-Thien/Tanner (PTT) Model can be found. These past efforts allow us the opportunity to test the technique used herein for accuracy using the much simpler (relative to the constant-volume blend models) viscoelastic fluid constitutive equations.

In the remainder of this article, we first work out the theoretical framework for expressing constitutive equations for implementation in the TPBV methodology developed herein. This is not difficult, and merely means that we need to re-express the viscoelastic constitutive equations used as test cases in terms of an internal microstructural variable instead of the extra stress tensor. We do this because the more complicated polymer blend models are expressed in terms of microstructural variables, and cannot easily (or even with great difficulty) be rewritten in terms of the extra stress tensor. After this, we provide an overview of the theoretical concepts involved in using the TPBV technique. These are subsequently illustrated analytically by solving the Upper-Convected Maxwell Model (UCMM) in a channel under simultaneous Couette and pressure-driven flow. Following this, the methodology is applied computationally to generate velocity and stress profiles under the same flow condition for the Phan-Thien/Tanner (PTT) [16] and Giesekus [17,18] Models. These profiles are then compared with solutions for the same models available in the literature. Afterwards, the TPBV methodology is applied to two constant-volume polymer blend models, and the somewhat surprising results are discussed.

2. Theoretical background and problem formulation

For the purpose of the present article, the physical variables that describe the system, x, are the velocity vector field, $\mathbf{v}$ and one or more internal variables, $\mathbf{X}$, which are either contravariant second-rank tensors or scalars: hence $x = [\mathbf{v}, \mathbf{X}]$. At present, the variables $\mathbf{X}$ are left unspecified because they change with the different models to be discussed in the subsequent sections. Furthermore, the variables $\mathbf{X}$ can be unconstrained or obey a scalar constraint that is expressed in terms of the scalar invariants of the microstructural variables [19].

The generic forms of the evolution equations for this variable set are

$$\rho \frac{\partial v_\alpha}{\partial t} = -\rho v_\beta \nabla_\beta v_\alpha - \nabla_\alpha p + \nabla_\beta \sigma_{\alpha\beta}, \tag{1}$$

$$\frac{\partial X_{\alpha\beta}}{\partial t} = \left.\frac{\partial X_{\alpha\beta}}{\partial t}\right|_{\text{cons}} + \left.\frac{\partial X_{\alpha\beta}}{\partial t}\right|_{\text{diss}}, \tag{2}$$

where we have assumed that $\mathbf{X}$ is a second-rank tensorial variable and we have introduced the Einstein summation convention over repeated indices. Eq. (1) is the Cauchy momentum equation, where the pressure, constant mass density, and the extra stress tensor have been denoted with p, ρ, and $\boldsymbol{\sigma}$, respectively. Note that in this formulation, the extra stress tensor is a known function of $\mathbf{X}$, dependent on the particular model under investigation. The first term on the right-hand side of Eq. (1) is the nonlinear convective term, the second one represents the negative pressure gradient, and the last one is the divergence of the extra stress tensor field. Eq. (2) is a general representation of the microstructural dynamics. The first term on the right-hand side of Eq. (2) represents the reversible contribution to the microstructural-dynamics (note that the term $\mathbf{v} \cdot \nabla\mathbf{X}$ is included in this term), whereas the second term is the irreversible contribution. Both of these terms are typically specified explicitly in polymer blends models, but need to be inferred for typical viscoelastic fluid models. This is easily accomplished following methodology described by Beris and Edwards [20].

In the present article, we wish to solve the continuum Eqs. (1) and (2) for a superposition of Couette flow with plane pressure-driven (Poiseuille) flow. Tube flow is considered in the appendix. Therefore, the dynamical equations will be solved numerically to match prescribed boundary conditions on the channel walls. Here, we want to assume no-slip boundary conditions to be imposed on the velocity field at the channel walls. Mathematically, this is a two-point boundary-value problem. The methodology to solve the boundary value problem is straightforward and computer algorithms are available (cf., e.g., [10]). However, it is not immediately obvious how to manipulate the continuum Eqs. (1)