Numerical simulation of viscoelastic contraction flows

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Abstract

In this work we present numerical results obtained with a finite volume method for the creeping flow of viscoelastic fluids in both axisymmetric and planar 4 : 1 contractions. Two rheological equations are considered, namely the constant-viscosity Oldroyd-B and the shear-thinning Phan-Thien/Tanner (PTT) models. Accurate solutions are presented over a wide range of the Deborah number (a measure of the elasticity of the flow) extending the attainable values of previous studies [1]. Vortex enhancement was observed for the axisymmetric contraction, with both rheological models, while for the planar contraction vortex enhancement is only observed for the shear-thinning PTT model. In the latter geometry, vortex reduction and the appearance of a small lip vortex is predicted for the constant-viscosity Oldroyd-B fluid.

Keywords: Numerical simulations; Finite-volume method; Viscoelastic fluid; 4 : 1 Contraction; Oldroyd-B; PTT model; Lip vortex; Vortex enhancement; Computational rheology

1. Introduction

The increasing use of computational tools to design industrial equipment for polymer processing requires the ability of existing numerical methods to predict accurately the flow of viscoelastic fluids. This is an area of active research, but there is still a lack of accurate solutions even for some simple benchmark flows. Several benchmark test cases have emerged in the last decade, such as the viscoelastic flow through contractions (both axisymmetric and planar configurations), the flow through corrugated channels, around cylinders or spheres, stick–slip flows, just to cite a few [2,3]. While for most of these test cases accurate solutions are now established through the independent validation of the results by different research groups (although over a limited range of Deborah numbers), there is still a lack of accurate numerical results for the difficult benchmark flow through contractions [1,4]. Nowadays, another emergent challenge is to establish quantitative agreement between numerical results and experimental observations [5]. Matching the numerical solution with experimental results, for different flow conditions, serves not only to judge the accuracy of the numerical method, but also to assess the adequacy of the rheological model used in the simulation. In this respect, there are still some unanswered questions regarding peculiar behaviour shown by some fluids in simple geometries such as contractions [5].

In this work the finite volume method (FVM) developed by the authors [6–8] is applied to the simulation of the flow of viscoelastic fluids in 4 : 1 planar and axisymmetric contraction flows. We start with an outline of the FV procedure for viscoelastic fluid motion, then we present the new numerical results and end up with the main conclusions.

2. Governing equations and numerical method

The equations governing the creeping flow of a viscoelastic fluid are those expressing mass conservation,

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

and momentum conservation in the absence of body forces,

$$\rho \frac{\partial \mathbf{u}}{\partial t} = -\nabla p + \eta_S \nabla \cdot \nabla \mathbf{u} + \nabla \cdot \boldsymbol{\tau} \tag{2}$$

coupled with an adequate constitutive equation for the extra stress tensor $\boldsymbol{\tau}$:

$$\left[1 + \frac{\lambda \varepsilon}{\eta_P} \mathrm{tr}(\boldsymbol{\tau})\right] \boldsymbol{\tau} + \lambda \left[\frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla \cdot \mathbf{u} \boldsymbol{\tau}\right] = \eta_P \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathbf{T}}\right) + \lambda \left(\boldsymbol{\tau} \cdot \nabla \mathbf{u} + \nabla \mathbf{u}^{\mathbf{T}} \cdot \boldsymbol{\tau}\right) \tag{3}$$

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In Eqs. (1) to (3) the constant model parameters are the relaxation time λ, the zero shear-rate polymer viscosity η_P, the solvent viscosity η_S, and the extensibility parameter ε. Eq. (3) represents a simplified form of the PTT model [9] where only the upper convected part of the full Gordon–Schowalter derivative is retained. If ε is set to zero, this constitutive equation becomes identical to the Oldroyd-B model. The ratio between the solvent viscosity and the total viscosity is $\beta = \eta_S/\eta_0$, where $\eta_0 = \eta_S + \eta_P$. Throughout this work $\beta = 1/9$ is used, in accordance with many previous studies.

Eqs. (1) to (3) are transformed into a general nonorthogonal coordinate system for application of the FVM in a collocated mesh arrangement, as explained in detail in Ref. [6]. The governing equations are then integrated in space over the set of control volumes (CV) and in time over a small time step, δt. The resulting set of linearised algebraic equations has the general form

$$a_\mathrm{P}\mathbf{u}_\mathrm{P} = \sum_\mathrm{F}^{6} a_\mathrm{F}\mathbf{u}_\mathrm{F} + \mathbf{S_u} \tag{4}$$

where index P denotes any CV, index F denotes the corresponding surrounding CVs, a_P and a_F are coefficients composed by convective and diffusive contributions, and $\mathbf{S_u}$ is a source term. Eq. (4) is implicitly solved for $\mathbf{u}$ by means of a bi-conjugate gradient method. The resulting velocity field may not satisfy continuity, which must then be enforced by application of velocity and pressure corrections as described in Ref. [6].

The constitutive equation is discretised in a way similar to that of the momentum equation, resulting in:

$$a_\mathrm{P}^{\tau}\boldsymbol{\tau}_\mathrm{P} = \sum_\mathrm{F}^{6} a_\mathrm{F}^{\tau}\boldsymbol{\tau}_\mathrm{F} + \mathbf{S}_{\boldsymbol{\tau}}. \tag{5}$$

Due to the hyperbolic nature of Eq. (3), a key point in the algorithm is the calculation of the convective terms in the constitutive equation. A new convection scheme, especially designed to be used with differential viscoelastic constitutive relations, was proposed recently by the authors [8] and is here adopted throughout. The CUBISTA scheme (Convergent and Universally Bounded Interpolation Scheme for the Treatment of Advection) has the advantage over more classical schemes, like the SMART scheme of Gaskell and Lau [10], of promoting iterative convergence when used with implicit methods. It has been found that this high-resolution scheme is accurate and very stable, thus being very adequate for the simulation of viscoelastic flows [4,8].

3. Problem description

A schematic representation of the geometry is presented in Fig. 1, where some of the relevant nomenclature is defined. The half-width of the downstream channel, H_2, is taken as the characteristic length scale and its average velocity, U_2, is the characteristic velocity scale. Therefore, comparison between plane and axisymmetric flows is based on the characteristic velocity U_2, and not on the flow rate, Q.

A zoomed view near the contraction plane of the coarse computational grid is shown in Fig. 1 to illustrate the local refinement of the mesh near the re-entrant corner, where the highest stress gradients are expected to occur. Extensive mesh refinement studies were done in previous works [4,7] to assess the accuracy of the numerical solutions. Good mesh convergence was established, and based on that information two meshes are retained for this work, with 10,587 and 42,348 cells and a minimum normalised cell size near the re-entrant corner of 0.014 and 0.0071, respectively.

Concerning fluid rheology, similar parameters are chosen as in previous studies [1,4]. Creeping flow is assumed (Re = 0), with solvent viscosity fraction $\eta_S/\eta_0 = 1/9$. The extensibility parameter in the PTT model is taken as $\varepsilon = 0.25$, a typical value for polymer melts [11]. A number of simulations are performed at different elasticity levels, measured by the Deborah number, here defined as $\mathrm{De} = \lambda U_2/H_2$.

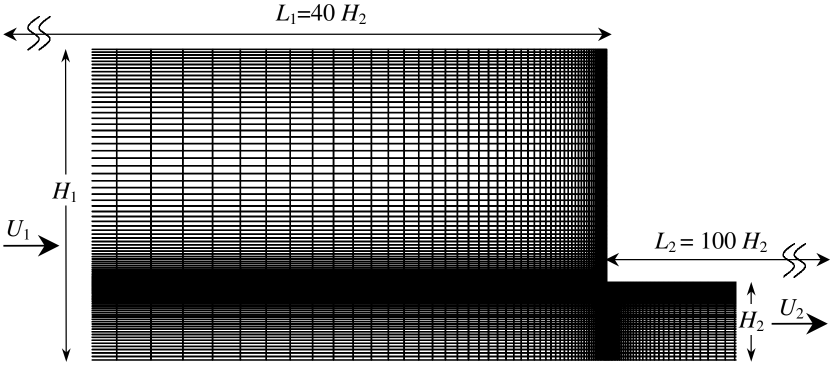

Fig. 1. Zoomed view of the coarse mesh near the contraction plane, and definition of some of the relevant variables.

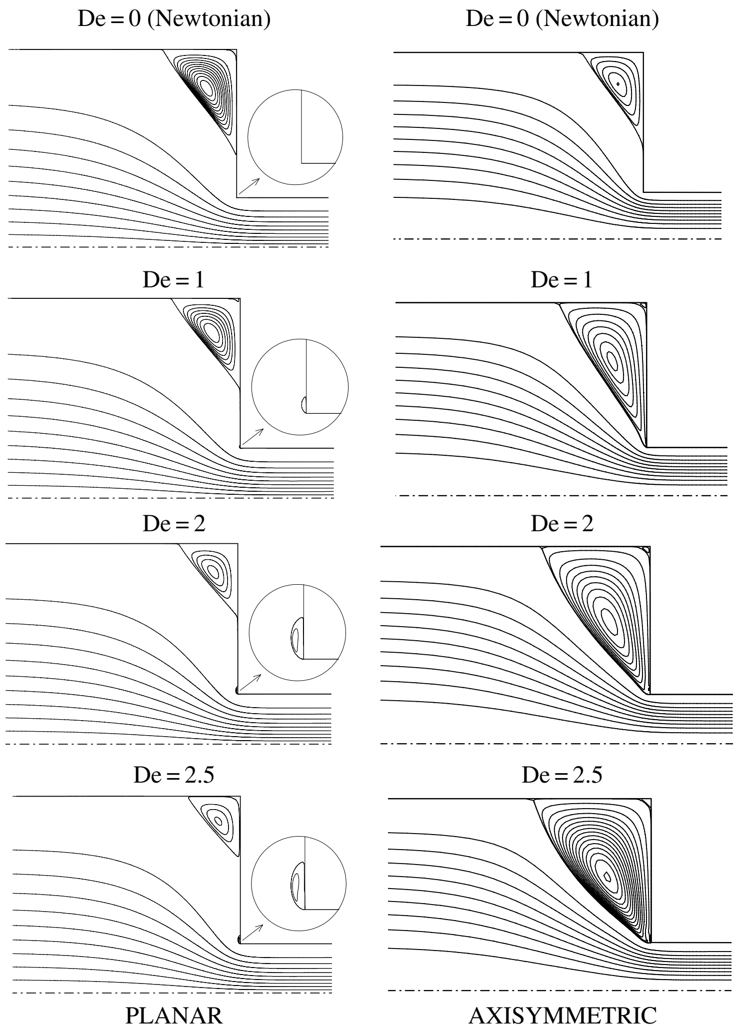

Fig. 2. Flow patterns with the Oldroyd-B fluid in the planar and axisymmetric contractions.

4. Results and conclusions

In Fig. 2, the results obtained for the constant-viscosity Oldroyd-B model are presented in terms of streamline plots, for increasing Deborah numbers. For the planar contraction geometry, vortex intensity is reduced with an increase in the elasticity, whereas for the axisymmetric situation extreme vortex enhancement is observed, in accordance with experimental observations for Boger fluids [5]. Similar trends were obtained by Aboubacar and co-workers [1], although for the axisymmetric case we were able to achieve a significantly higher De number (De = 2.5 compared with De = 0.85 in [1]). For the planar contraction flow, the presence of a small lip vortex near the re-entrant corner (which increases with elasticity) was also observed in the numerical results of Ref. [1].

For the shear-thinning PTT model, vortex enhancement is observed in Fig. 3 for both planar and axisymmetric contractions, in accordance with experimental observations and the numerical results presented in Ref. [1]. For this rheological model we were able to obtain converged solutions at extremely high De numbers (De = 100 for the planar and De > 1000 for the axisymmetric contractions), which demonstrates the robustness of the present approach and in particular of the new high-resolution scheme developed in Ref. [8]. For comparison purposes, in Ref. [1] convergence could be achieved only up to De = 9 and 4 for the planar and axisymmetric contractions, respectively, and on much coarser meshes. It is known that the difficulty in computing non-Newtonian viscoelastic flows raises sharply with the degree of mesh refinement.

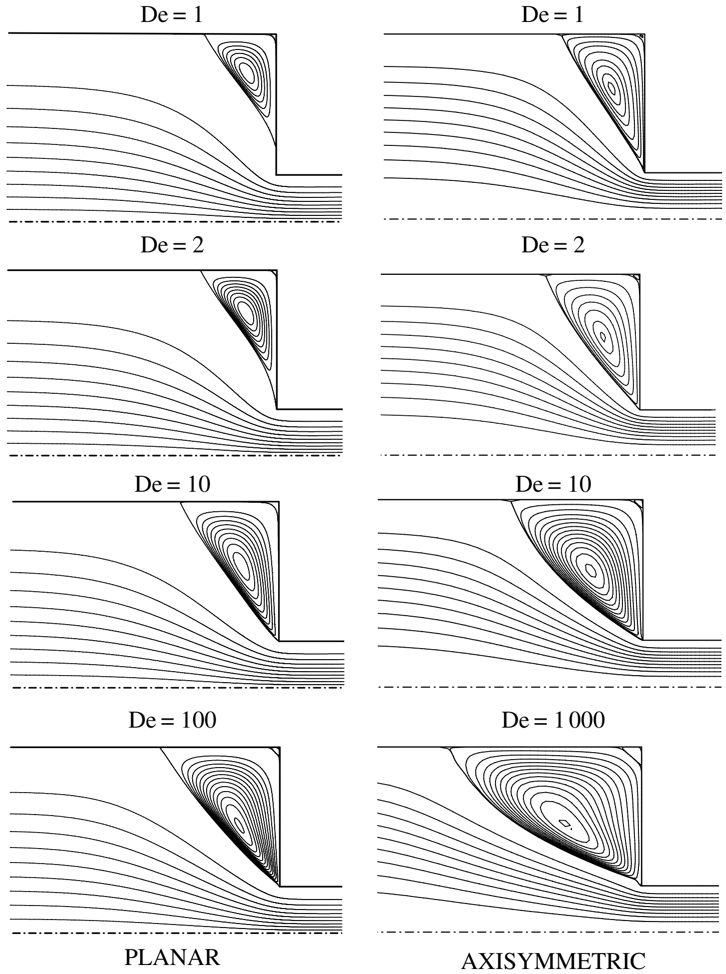

Fig. 3. Flow patterns with the PTT fluid in the planar and axisymmetric contractions.

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