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Numerical Analysis of Unsteady Viscoelastic Contraction Flows of Multi-Mode Fluids

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Abstract. The flow of multi-mode differential model fluids through planar and axisymmetric 4:1 contractions is studied numerically, and comparison with experimental results is made when appropriate. The Phan-Thien/Tanner and the Modified Upper Convected Maxwell constitutive models are investigated. An efficient algorithm is constructed by employing discontinuous interpolants for the extra stress components and the pressure field. An operator splitting methodology is adopted to extract the advective parts of the constitutive equation. The advective parts of the constitutive equations are solved by application of a Time-Discontinuous/Galerkin Least-Squares method. Satisfactory agreement with previous work and experimental results is obtained.

1 Introduction

Accurately solving general viscoelastic flow problems for high values of elasticity is still a major research challenge. A particularly difficult task is the resolution of flow problems involving multiple relaxation modes in a computationally effective way. This is necessary because most existing polymeric fluids (even carefully constructed test fluids like the so-called Boger fluids or the M1-fluid) require the use of multiple relaxation modes. Furthermore, there is an experimentally driven thrust towards unsteady computations, as upon increasing the so-called Deborah number (De), and thereby the relative importance of elastic effects over viscous phenomena, polymer flows may pass through a number of dynamic flow transitions, as is for instance elegantly demonstrated by McKinley et al. [12]. Finally, careful characterization of the fluids rheology, for instance by Quinzani et al. [14], has revealed that non-linear viscoelastic models are required to model the fluid.

The above observations form the basis of the objectives of the current study: to construct an efficient numerical algorithm to analyse unsteady viscoelastic flows of multi-mode non-linear viscoelastic fluids.

The use of continuous interpolations of the extra stress components, see e.g. Marchal and Crochet [11], yields an inefficient algorithm as it entails the use of a very high number of degrees of freedoms for the stresses, particularly in the case of multi-mode models. Furthermore, a special interpolation of the extra stress tensor is needed to satisfy the so-called inf-sup condition on the velocity-stress interpolation.

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A class of methods that can easily handle multiple modes is based on particle tracking, see Dupont et al. [5], Luo and Mitsoulis [10], Hulsen et al. [7]. However, in conjunction with an Oldroyd-B fluid, this method produced highly oscillatory results as is demonstrated by Park et al. [13]. Furthermore, the iterative method is invariably of the Picard type, giving notoriously slow convergence, as reported by Hulsen et al. [7] and Rosenberg et al. [15]. As yet, no unsteady version of this method appears to be available.

Mixed methods using a discontinuous interpolation of the extra stress tensor(s) bypass the computational restrictions of the aforementioned class of mixed methods. This methodology was first introduced for viscoelastic flows by Fortin et al. [6]. For equal order velocity discontinuous-stress interpolation, this technique satisfies the inf-sup condition as shown by Ying [17]. The use of discontinuous interpolation of the stress field requires a special procedure to handle the advective terms. Fortin et al. [6] applied the Discontinuous Galerkin (DG) method, see Johnson [8], also named after Lesaint and Raviart [9]. Although this technique is very effective and is one of the best-known linear advection algorithms, its implementation is cumbersome and non-standard. In order to be computationally effective for multiple mode models, the stress variables need to be eliminated by static condensation at the element level. To be able to do this, the elements need to be sequenced in a special ordering. Such an ordering is only possible for flows without recirculation, otherwise a block relaxation process needs to be applied, giving a slowdown in convergence of the iterative method.

In this study a discontinuous stress interpolation is applied because it results in satisfaction of the inf-sup condition of the stress velocity interpolation and allows a static condensation of the stress variables at the element level, thereby allowing an efficient handling of muliple modes. However, the advection algorithm will be different. Rather than using a DG method, the so-called Time-Discontinuous / Galerkin Least-Squares method (TD/GLS), see Johnson [8] and Shakib et al. [16] is applied, in conjunction with a discretization of the total (or material) derivative. The method is shown to be convergent upon mesh refinement for a number of flow problems using a number of non-linear material models with single or multiple modes up to moderate values of the *De* number. Furthermore, comparison with experimental results is sought when appropriate.

2 Viscous flow

Problem definition: To access and illustrate some of the difficulties encountered in a mixed stress-velocity-pressure formulation in the presence of singularities, Newtonian flow is studied first.

Problem 1 (MV) *Find* $(\boldsymbol{\tau}, \vec{u}, p)$ *, such that for all* $(\boldsymbol{s}, \vec{v}, q)$

$$(\boldsymbol{s}, \boldsymbol{\tau} - 2\eta \boldsymbol{D}_u) = 0 \tag{1}$$

$$-(\boldsymbol{D}_v, \boldsymbol{\tau}) + (\vec{\nabla} \cdot \vec{v}, p) = 0 \tag{2}$$

$$(q, \vec{\nabla} \cdot \vec{u}) = 0 \tag{3}$$

The notation (.,.) implies: $(\boldsymbol{A},\boldsymbol{B}) = \int_\Omega \boldsymbol{A} : \boldsymbol{B}\, d\Omega$ if $\boldsymbol{A}$ and $\boldsymbol{B}$ are two tensors, while $(a,b) = \int_\Omega ab\, d\Omega$ if a and b are two scalars.

Discretization: Let Q_i, P_i denote a discretization of order i on quadrilaterals and triangles respectively. The suffix $()^d$ denotes the use of a *dis*continuous interpolation, i.e. continuous within an element, but discontinuous at element interfaces. Three discretization are investigated. First, in the case of a regular velocity-pressure formulation a $(\vec{u},p) \rightarrow Q_2P_1^d$ element is used. Secondly, a continuous interpolation for the extra stress tensor is employed: $(\boldsymbol{\tau},\vec{u},p) \rightarrow Q_2Q_2P_1^d$. Thirdly, a discontinuous interpolation of $\boldsymbol{\tau}$ is incorporated: $(\boldsymbol{\tau},\vec{u},p) \rightarrow Q_2^dQ_2P_1^d$.

Test problem: As a test problem the four-to-one contraction problem is used. The geometry is depicted in fig. 1. The dimensions are chosen as: $H_1 = 4$, $H_2 = 1$, $L_1 = L_2 = 8$. The flow is from left to right. Along the entry, a parabolic velocity profile is prescribed with a maximum velocity of 0.1.

The predicted extra stress τ_{12} is depicted in fig. 2. The continuous interpolation of $\boldsymbol{\tau}$ clearly causes significant oscillations that are not present in the other two interpolations. Hence, upon using a mixed formulation it is advantageous to apply a discontinuous interpolation of the extra stress field.

3 Viscoelastic flow

Problem definition: The unsteady flow of a Phan-Thien Tanner (PTT) and of a Modified Upper Convected Maxwell (MUCM) fluid is studied in a plane or torsionless axisymmetric flow situation.

The method proposed in this manuscript is based on an operator splitting methodology. The material rate in the constitutive equation represents the advective part. During each time step this stress advection is dealt with separately from the remaining part of the constitutive equation.

Introduce the operator $\mathcal{L}_t$ that represents the material rate as

$$\mathcal{L}_t\boldsymbol{\tau} = \frac{\partial\boldsymbol{\tau}}{\partial t} + \vec{u}\cdot\vec{\nabla}\boldsymbol{\tau} \tag{4}$$

and define the operators $\mathcal{L}_P$ (for PTT) and $\mathcal{L}_M$ (for MUCM) as

$$\mathcal{L}_P\boldsymbol{\tau}_i = -\boldsymbol{L}\cdot\boldsymbol{\tau}_i - \boldsymbol{\tau}_i\cdot\boldsymbol{L}^T + (\frac{1}{\theta_i} + \frac{\epsilon_i}{\eta_i}\mathrm{tr}(\boldsymbol{\tau}_i))\boldsymbol{\tau}_i \tag{5}$$

and

$$\mathcal{L}_M\boldsymbol{\tau}_i = -\boldsymbol{L}\cdot\boldsymbol{\tau}_i - \boldsymbol{\tau}_i\cdot\boldsymbol{L}^T + A(\mathrm{tr}(\boldsymbol{\tau}_i))\boldsymbol{\tau}_i,\ \ A(\mathrm{tr}(\boldsymbol{\tau}_i)) = \frac{1}{\theta_i}(1+(F_i\mathrm{tr}(\boldsymbol{\tau}_i))^{\alpha-1}) \tag{6}$$

Let $\vec{p}$ denote the previous (at $t = t_n$) position of the particle currently (at $t = t_{n+1}$) located at $\vec{x}$. Then, for each time interval $t_n \rightarrow t_{n+1}$, the following approximation of the material rate is employed,

$$\mathcal{L}_t{}^n\boldsymbol{\tau} = \frac{\boldsymbol{\tau}(\vec{x},t_{n+1}) - \boldsymbol{\tau}(\vec{p},t_n)}{\Delta t} \tag{7}$$

Suppose, for the time being, that $\boldsymbol{\tau}_i(\vec{p}, t_n)$ is known, then for each time interval I_n, the mixed weak formulation of problem PVE is given by

Problem 2 (MPVE) *Given* $\boldsymbol{\tau}_i(\vec{p}, t_n)$*, find* $(\boldsymbol{\tau}_i, \vec{u}, p)$ *at* $t = t_{n+1}$*, such that for all* $(\boldsymbol{s}_i, \vec{v}, q)$, $\alpha = P$ *or* M

$$(\boldsymbol{s}_i, \mathcal{L}_t{}^n \boldsymbol{\tau}_i + \mathcal{L}_\alpha \boldsymbol{\tau}_i - 2\frac{\eta_i}{\bar{\theta}_i}\boldsymbol{D}_u) = 0, \quad i = 1, \ldots, N \tag{8}$$

$$-(\boldsymbol{D}_v, 2\eta_0 \boldsymbol{D}_u + \sum_{i=1}^{N} \boldsymbol{\tau}_i) + (\vec{\nabla} \cdot \vec{v}, p) = 0 \tag{9}$$

$$(q, \vec{\nabla} \cdot \vec{u}) = 0 \tag{10}$$

with $\bar{\theta}_i = \theta_i$ *if* $\alpha = P$ *and* $\bar{\theta}_i = A(tr(\boldsymbol{\tau}_i))^{-1}$ *if* $\alpha = M$.

The remaining problem is to determine $\boldsymbol{\tau}(\vec{p}, t_n)$ for each mode. Eq. (8) requires knowledge of $\boldsymbol{\tau}_p \doteq \boldsymbol{\tau}(\vec{p}(\vec{x}, t_{n+1}), t_n)$ for all $\vec{x} \in \Omega$. This field can be obtained by advecting the stress field at $t = t_n$, $\boldsymbol{\tau}_n \doteq \boldsymbol{\tau}(\vec{x}, t_n)$, by the known velocity field computed from the preceding problem, say $\vec{u}(\vec{x}, t)$. This advection problem is solved with a so-called space-time Galerkin Least-Squares finite element method, see Shakib [16] and Baaijens [2].

Clearly, the mixed problem MPVE and the advection problem are coupled. To find the actual solution they are solved in a decoupled fashion in association with an iterative procedure. Problem MPVE is non-linear and the Newton iteration scheme is used to find an approximate solution. At the beginning of each Newton iteration, the advection problem is solved first, using the most recently computed approximation of the velocity field. This supplies an estimate for $\boldsymbol{\tau}_p$ as required to solve problem MPVE. This iterative procedure is continued until convergence.

Discretization: Based on the results of the Newtonian flow example, the following discretization is employed:$(\boldsymbol{\tau}_i, \vec{u}, p) \rightarrow Q_2^d Q_2 P_1^d$. In the advection step a continuous bi-quadratic interpolation is used.

Test problems: Two test geometries are experimented with: the plane and axisymmetric four-to-one (4:1) contraction problem. These geometries are selected due to the presence of a corner singularity.

The 4:1 contraction geometry is sketched in fig. 1. In all computations a one-step Newton iteration procedure is adopted and the time step is fixed at $\Delta t = 0.01$ for example 1 and $\Delta t = 0.1$ for example 2.

Example 1: plane 4:1 contraction. Recently, Armstrong et al. [1] published detailed LDV and birefringence measurements of a 5.0 % wt PIB/C14 solution through a plane contraction. This material has been extensively characterized by Quinzani et al. [14]. In their study, Armstrong et al. used measured velocity profiles along the centreline of the contraction to compute the viscoelastic response of the material using several non-linear constitutive models (Giesekus, Bird-DeAguiar, PTT and Acierno et al.). They concluded that the PTT model gave the best fit on the elongational viscosity. The PTT model is therefore used in this work to compute the viscoelastic flow.

The linear viscoelastic spectrum employed is listed in table 1.

mode #	θ_i	η_i	ε_i
1	0.6855	0.0400	0.25
2	0.1396	0.2324	0.25
3	0.0389	0.5664	0.25
4	0.0059	0.5850	0.25
(0) solvent		0.0020	

Table 1: Parameter setting of multi-mode PTT model to fit 5.0 %wt PIB/C14 solution

Based on shear data, ε_i was selected as 0.13. However, normal stress measurements along the centreline of the contraction suggested the use of $\varepsilon_i = 0.25$. This value is used in all multi-mode computations of this PIB solution.

The shear-rate-dependent Deborah number (De) is defined as

$$De = \frac{\Psi_1(\dot{\gamma})\dot{\gamma}}{2\eta(\dot{\gamma})} \tag{11}$$

with

$$\Psi_1 = \frac{\tau_{xx} - \tau_{yy}}{\dot{\gamma}^2} \tag{12}$$

In all computations the shear rate is specified by $\dot{\gamma} = \frac{<v>}{H_2}$ where $< v >$ is the average velocity in the downstream channel, and H_2 is half the gapwidth of the downstream strip. The channel dimensions are: $L_1 = 0.05$, $L_2 = 0.01$, $H_1 = 0.0032$ and $H_2 = 0.0095$.

Only one analysis is discussed here: $De = 0.77$. The maximum velocity at the exit is 0.2554, while a parabolic velocity profile is assumed.

Three meshes have been used, called Mesh1, Mesh2 and Mesh3. As a representative, Mesh1 is depicted in fig. 3. Some characteristic mesh parameters are given in table 2

Mesh #	h_{min}	# elements	# nodes
1	2.15e-4	270	1167
2	1.06e-4	520	2197
3	2.07e-4	540	2291

Table 2: Characteristic mesh parameters

Fig. 4 compares the computed first normal stress difference along the centreline for Mesh1 (solid line), Mesh2 (dashed line) and Mesh3 (dotted line) with the measurements of Armstrong et al. [1]. Computed and measured results are in reasonable agreement, while convergence upon mesh refinements is also demonstrated.

Example 2: axisymmetric 4:1 contraction. Coates et.al [4] studied the behaviour of the MUCM model in axisymmetric contractions for a single relaxation time. The MUCM model is designed to give Newtonian behaviour near the singularity. In this study a qualitative comparison is made with the results of Coates et al. [4] for the four-to-one contraction problem. The channel dimensions are: $L_1 = 16$, $L_2 = 32$, $H_1 = 4$ and $H_2 = 1$.

At both the entrance and exit a parabolic velocity profile is prescribed; in all cases the maximum velocity at the exit $v_{max} = 2$. A sequence of De numbers is computed by increasing the relaxation time θ.

Fig. 5 compares the computed vortex size of this work as a function of the De number with experimental results of Boger et al. [3] and the numerical results of Coates et al. [4]. The dimensionless vortex size is defined as the vortex length divided by the upstream tube diameter. As reported by Coates et al. [4], the computed results match the experimental results unexpectedly well. Coates et.al [4] could not reach values of De larger than 2.69, while the current method converges at least up to $De = 6.11$. No attempt has been made yet to reach higher values of De.

4 Conclusions

An efficient algorithm to compute the unsteady flow of multi-mode differential model fluids through planar and axisymmetric contractions has been constructed. The algorithm is efficient in the sense that all stress and pressure degrees of freedom can be eliminated on the element level by means of static condensation. Therefore, computation of the Jacobian matrix roughly scales with the number of modes, while solving the resulting system of equations is no more expensive than solving the regular Stokes problem in a velocity-pressure setting.

Comparison with other work, notably Coates et al. [4], shows that upon using the MUCM model the computed stress fields at $De = 2.29$ compare well, while the vortex growth matches the experimental results of Boger et al. [3]. Also, much higher De could be obtained with the current method than with the EEME method employed by Coates et al. [4].

Knowledge of the local stress behaviour in the contraction flow is essential for judging the behaviour of a particular constitutive equation. The results presented by Armstrong et al. [1] are therefore extremely valuable. The agreement of the predicted stress fields along the symmetry line of the plane 4:1 contraction with experimental results is satisfactory.

It is a great challenge to push the current method towards predicting the unsteady three-dimensional flow patterns in axisymmetric contraction flows described by McKinley et al. [12]. It is believed that the current method is sufficiently efficient to be extended towards three-dimensional computations. This will the subject of future work.

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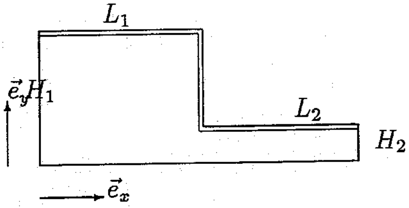

Figure 1: Geometry of the four-to-one contraction problem

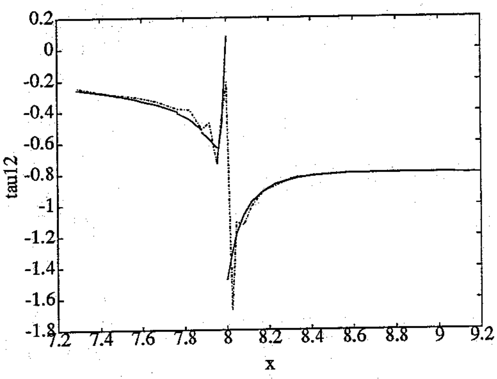

Figure 2: τ_{12} Component along $y = 1$; Dashed-dot: $Q_2Q_2P_1^d$, Solid: $Q_2^dQ_2P_1^d$. The velocity-pressure solution coincides with the solid line

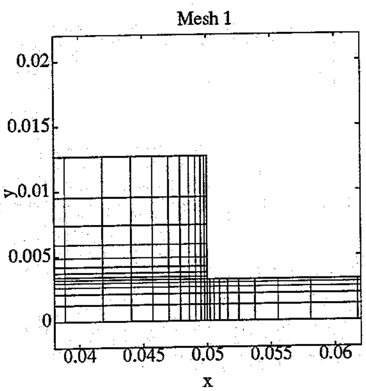

Figure 3: Mesh1

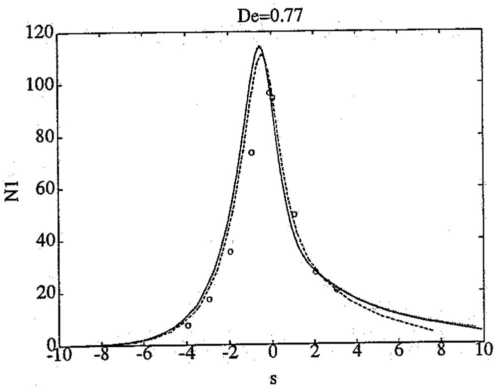

Figure 4: N_1 versus s at $De = 0.77$, Solid line: Mesh2, Dashed line: Mesh1, Dotted line: Mesh3

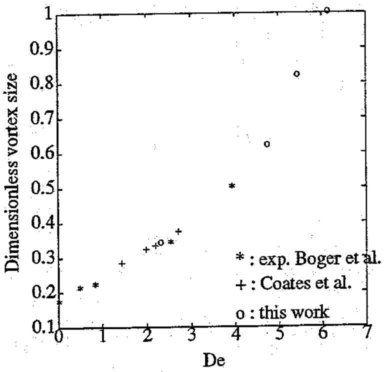

Figure 5: Dimensionless vortex size as a function of the De number. $*$: experimental results of Boger et al. , $+$: computed results from Coates et al. , o: this work