Numerical analysis of start-up planar and axisymmetric contraction flows using multi-mode differential constitutive models

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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 where possible. The Phan-Thien/Tanner, Giesekus and 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. These are solved by application of a time-discontinuous/Galerkin least-squares method. Satisfactory agreement with previous work and experimental results is obtained.

Keywords: axisymmetric contraction flow; constitutive models; multi-mode differential model fluids; planar contraction flow

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 Ml 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. [1]. Finally, careful characterization of the fluid's rheology, for instance by Quinzani et al. [2], 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 flow of multi-mode non-linear viscoelastic fluids.

A multitude of numerical schemes to solve viscoelastic flows have been proposed in the past two decades. One of the most successful algorithms, in terms of reaching high values of $De$, is the mixed SU (Streamline Upwind) formulation introduced by Marchal and Crochet [3], and applied in, for instance, Debbaut et al. [4]. This method uses a biquadratic approximation of the velocity field and a four-by-four bilinear subdivision of each velocity element for the stress interpolation. This subdivision was introduced to satisfy the inf–sup compatibility condition between stress and velocity field. This subdivision entails the use of a very high number of degrees of freedom for the stresses, particularly in the case of multi-mode models. Furthermore, the method is inconsistent: upwinding is only applied to the convective terms of the constitutive equation. This possibly leads to enormous consistency errors, as was demonstrated by Tanner and Jin [5] and renders the method of order $h$ (see Crochet and Legat [6]).

Based on the ideas of Renardy [7], King et al. [8] introduced the so-called EEME (Explicitly Elliptic Momentum Equation) formulation. By means of a change of variables, this method maintains the elliptic character of the momentum equation even if $De$ is increased. Yet for non-smooth problems this method cannot reach the same level of elasticity as the SU method described above. It was demonstrated, though, by King et al. [8], Rajagopalan et al. [9, 10] and Coates et al. [11] that the use of non-linear viscoelastic models with bounded elongational viscosity leads to smoother results and convergence at higher values of the $De$ number. Furthermore, Coates et al. [11] conjectured that the order of the singularity as exposed by the particular constitutive model near singular points in the computational domain (for instance the corner in a four-to-one contraction or the transition point in the stick-slip problem) causes a violation of the basic requirements for convergence of the SUPG (Streamline Upwind Petrov–Galerkin) method that is applied to handle the advective term, and hence may cause a breakdown of the convergence of the iterative scheme. A possible remedy for this problem may be the introduction of a discontinuity-capturing operator, as introduced in the context of viscoelastic flows by Baaijens [12]. One aspect that is not handled explicitly by the EEME formulation in its
current setting is the compatibility condition between stress and velocity field.

According to the theoretical results of Baranger and Sandri [13], the presence of a viscous solvent contribution implies satisfaction of the inf-sup compatibility condition with respect to the stresses and velocities. This property is employed in the so-called EVS (Elastic Viscous Split) methods used by Mendelson et al. [14], Beris et al. [15], van Schaftingen and Crochet [16] and Luo and Tanner [17]. Luo and Tanner [17], Rajagopalan et al. [10] and Baaijens [12] have applied the same methodology, but rather than integrating the first-order derivative of the rate of strain tensor by parts, they used a continuous approximation of the rate of strain tensor, allowing a direct computation of the upper convected (Truesdell) derivative of this tensor. This improved results significantly. However, for non-smooth problems as studied by Luo and Tanner [17] and Baaijens [12], the algorithm failed to converge at moderate values of De.

All the methods described heretofore use continuous interpolations of the stress variables. This means that upon using multiple relaxation modes the number of unknowns increases substantially. For instance, for axisymmetric torsionless problems, each node has four stress unknowns per mode and two velocity unknowns, and possibly one pressure unknown. Hence, a four-mode model would lead to eighteen velocity-stress unknowns per node. This count is even more disastrous for the SU method proposed by Marchal and Crochet [3].

A class of methods that can easily handle multiple modes is based on particle tracking, see Dupont and Crochet [18], Luo and Mitsoulis [19], Hulsen and van der Zanden [20]. However, in conjunction with an Oldroyd-B fluid, this method produced highly oscillatory results as demonstrated by Park and Mitsoulis [21]. Furthermore, the iterative method is invariably of the Picard type, giving notoriously slow convergence, as reported by Hulsen and van der Zanden [20] and Rosenberg and Keunings [22]. 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 and Fortin [23]. For equal order velocity discontinuous-stress interpolation, this technique satisfies the inf-sup condition as shown by Ying [24]. The use of discontinuous interpolation of the stress field requires a special procedure to handle the advective terms. Fortin and Fortin [23] applied the Discontinuous Galerkin (DG) method, (see Johnson [25]), also named after Lesaint and Raviart [26]. 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 computa-
tionally 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 inter-
polation and allows a static condensation of the stress variables at the
element level, thereby allowing an efficient handling of multiple 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 [25] and Shakib [27]) 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 De. Furthermore, comparison with
experimental results is sought when appropriate.

2. Problem definition

If \( \Omega \) is the domain of interest in \( \mathbb{R}^2 \) with smooth boundary \( \Gamma \), and
\( I = [0, T] \) the time interval, then the unsteady flow of a Phan-Thien/Tanner
(PTT), a Giesekus and of a Modified Upper Convected Maxwell (MUCM)
fluid is studied in a plane or torsionless axisymmetric flow situation, as
defined by the following problem.

Problem 1 (PVE). Given \( \bar{u}^0: \Gamma_u \times I \mapsto \mathbb{R}^2 \) and \( \bar{t}^0: \Gamma_r \times I \mapsto \mathbb{R}^2 \), find the
plane or axisymmetric stress field \( \tau(\bar{x}, t): \Omega \times I \mapsto \mathbb{R}^{2 \times 2} \), the velocity field
\( \bar{u}(\bar{x}, t): \Omega \times I \mapsto \mathbb{R}^2 \) and the pressure field \( \bar{p}(\bar{x}, t): \Omega \times I \mapsto \mathbb{R} \)
for all \( (\bar{x}, t) \in \Omega \times I \), such that

\[
\bar{V} \cdot (-p I + 2\eta_0 D + \sum_{i=1}^N \tau_i) = \bar{0}, \tag{1}
\]

\[
\bar{V} \cdot \bar{v} = 0, \tag{2}
\]

with for the PTT model

\[
\bar{v} \tau_i + \left[ \frac{1}{\lambda_i} + \frac{\epsilon_i}{\eta_i} \text{tr}(\tau_i) \right] \tau_i = \frac{2\eta_i}{\lambda_i} D \quad i = 1, \ldots, N, \tag{3}
\]

or, for the Giesekus model

\[
\bar{v} \tau_i + \frac{1}{\lambda_i} \tau_i + \frac{\epsilon_i}{\eta_i} \tau_i \cdot \tau_i = \frac{2\eta_i}{\lambda_i} D \quad i = 1, \ldots, N, \tag{4}
\]
or, for the MUCM model
\[ \tau_i + A[\text{tr}(\tau_i)] \tau_i = 2\eta_i A[\text{tr}(\tau_i)] D \quad i = 1, \ldots, N, \] (5)

with
\[ A[\text{tr}(\tau_i)] = \frac{1}{\lambda_i} \left\{ 1 + [F_i \text{tr}(\tau_i)]^{\alpha - 1} \right\} \quad i = 1, \ldots, N, \] (6)

where \( \tau_i = \partial \tau_i / \partial t + \dot{u} \cdot \nabla \tau_i - L \cdot \tau_i - \tau_i \cdot L^T \), with \( L = (\nabla \dot{u})^T \) and \( 2D = L + L^T \), while the following boundary conditions are specified on \( \Gamma \)
\[ \dot{u}(x, t) = \dot{u}^0(x, t) \quad \text{on} \quad \Gamma_u \times I, \] (7)
\[ \left[ -pI + 2\eta_0 D + \sum_{i=1}^{N} \tau_i(x, t) \right] \cdot \hat{n} = \hat{t}^0(x, t) \quad \text{on} \quad \Gamma_i \times I, \] (8)

with \( \Gamma = \Gamma_u \cup \Gamma_i \), and \( \hat{n} \) the unit outward normal at \( \Gamma_i \). Finally, the initial conditions are
\[ \dot{u}(x, 0) = \ddot{0} \quad \text{on} \quad \Omega, \] (9)
\[ \tau_i(x, 0) = \theta \quad \text{on} \quad \Omega \quad i = 1, \ldots, N. \] (10)

Usually, the boundary load \( \hat{t}^0 \) is used to specify the stress state at the inflow boundaries, while the individual components of the extra stress tensors are prescribed along the inflow boundary as well. However, a slightly different procedure is used in this work; it is discussed in Section 4.

3. Remarks on constitutive equations

Each of the models investigated belongs to the category of non-linear models. They all contain the Upper Convected Maxwell (UCM) model as a special case; selecting \( \epsilon_i = 0 \) for the PTT and Giesekus models, and \( A[\text{tr}(\tau_i)] = -1/\lambda_i \) for the MUCM model yields UCM. It has, however, been argued by van der Zanden and Hulsen [28] that the UCM model cannot be integrated stably in a finite element context. The non-linear terms in each of the models investigated give a bounded elongational viscosity (\( \eta_E \)), while UCM gives an unbounded elongational viscosity. Perhaps, at least from a numerical point of view, this is the most important difference of the non-linear models compared to UCM. In addition, the PTT and Giesekus models show a shear-thinning viscosity (\( \eta \)) and also a shear-thinning first normal stress coefficient (\( \Psi_1 \)). This is shown in Fig. 1. Most polymeric liquids share this feature, even model fluids like the PIB and PIB/PB Boger fluids investigated by Quinzani et al. [2]. It has long been assumed, though, that these fluids would be representative for the UCM or Oldroyd-B fluid. Notice that only the shear viscosity curves of the PTT and the Giesekus
Fig. 1. (a), (b)
Fig. 1. (a) Shear viscosity ($\eta$); (b) first normal stress coefficient ($\Psi_1 = \tau_{11} - \tau_{22}/\dot{\gamma}^2$, where $\dot{\gamma}$ denotes the shear rate); (c) elongational viscosity ($\eta_E$). The solid line denotes the MUCM model, the dashed line the PTT model and the dashed-dotted line the Giesekus model. The parameters are $F = 0.064$, $\alpha = 5$, $\epsilon = 0.1$, $\lambda = 1$ and $\eta_0 = 1$.

model differ significantly. The elongational viscosity and the first normal stress coefficient of these two models are quite close.

4. Operator splitting and weak form

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.

Such an approach has been applied before by Fortin and Fortin [23] in conjunction with the method of characteristics to cope with the hyperbolic parts of the constitutive equation. Furthermore, the constitutive equation was transformed into the Lagrangian form, thereby necessitating the need for an additional assumption with respect to the evolution of the deformation tensor. Such an approach could have the advantage of preserving incremental objectivity, as discussed in Baaijens [29].

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

$$\mathcal{L}_t \tau = \frac{\partial \tau}{\partial t} + \bar{u} \cdot \nabla \tau$$  (11)
and define the operators $\mathcal{L}_p$, $\mathcal{L}_G$ and $\mathcal{L}_M$ as

$$\mathcal{L}_p \tau_i = -L \cdot \tau_i - \tau_i \cdot L^T + \left[ \frac{1}{\lambda_i} + \frac{\epsilon_i}{\eta_i} \text{tr}(\tau_i) \right] \tau_i,$$

$$\mathcal{L}_G \tau_i = -L \cdot \tau_i - \tau_i \cdot L^T + \frac{1}{\lambda_i} \tau_i + \frac{\epsilon_i}{\eta_i} \tau_i \cdot \tau_i,$$

$$\mathcal{L}_M \tau_i = -L \cdot \tau_i - \tau_i \cdot L^T + A[\text{tr}(\tau_i)] \tau_i.$$  

The material rate of $\tau$ is formally defined as

$$\frac{D\tau}{Dt} = \mathcal{L}_m \tau = \lim_{\delta \to 0} \frac{\tau(\hat{x}, t + \delta \Delta t) - \tau(\hat{p}, t)}{\delta \Delta t},$$

where $\hat{p}$ denotes the position at time $t$ of the particle that is located at position $\hat{x}$ at time $t + \delta \Delta t$. After splitting the time interval $I$ into $N_t$ time steps,

$$I = \bigcup_{n=1}^{N_t} I_n, \quad I_n = [t_n^+, t_{n+1}^-],$$

with

$$t_n^+ = \lim_{\epsilon \to 0^+} t_n + \epsilon,$$

eqn. (15) suggests the following approximation of the material rate during $I_n$

$$\mathcal{L}_m^n \tau = \frac{\tau(\hat{x}, t_{n+1}) - \tau(\hat{p}, t_n)}{\Delta t}.$$

Suppose, for the time being, that $\tau_i(\hat{p}, t_n)$ is known, then for each time interval $I_n$, the mixed weak formulation of problem PVE is given as follows.

**Problem 2 (MPVE).** Given $\tau_i(\hat{p}, t_n)$, find $(\hat{\tau}_i, \hat{\psi}, \hat{q}) \in H \times H \times X$ at $t = t_{n+1}$, such that for all $(s_i, \tilde{\psi}, q) \in H \times X \times X$, $\xi = P, G$ or $M$

$$\left( s_i, \mathcal{L}_i \hat{\tau}_i + \mathcal{L}_i \tilde{\psi}_i - 2 \frac{\eta_i}{\lambda_i} D_u \right) = 0 \quad i = 1, N,$$

$$-(D_v, 2\eta_0 D_u + \sum_{i=1}^N \tau_i) + (\tilde{\psi} \cdot \hat{\psi}, p) = 0,$$

$$\left( q, \tilde{\psi} \cdot \hat{\psi} \right) = 0,$$

with $\lambda_i = \lambda$, if $\xi = P$ or $G$ and $\lambda_i = A[\text{tr}(\tau_i)]^{-1}$ if $\xi = M$.

The spaces $H$, $V \cdot$, $\mathcal{O}$ and $H$ are defined as follows: the velocity trial space $H$

$$H = \{ \tilde{\psi} \mid \tilde{\psi} \in [H^1(\Omega)]^2, \tilde{\psi} = \tilde{\psi}^0 \text{ on } \Gamma_u \},$$
the velocity test space $\mathcal{V}$

$$\mathcal{V} = \{ \hat{\mathbf{v}} \mid \hat{\mathbf{v}} \in [H^1(\Omega)]^2, \hat{\mathbf{v}} = \mathbf{0} \text{ on } \Gamma_u \},$$  

(23)

the pressure (trial) space $\mathcal{Q}$

$$\mathcal{Q} = \{ q \mid q \in L_2(\Omega) \} ,$$  

(24)

and, finally, the stress trial space $\mathcal{S}$

$$\mathcal{S} = \{ s \mid s \in [L_2(\Omega)^2]^2 \} .$$  

(25)

The remaining problem is to determine $\tau(\hat{\mathbf{p}}, t_n)$ for each mode. Equation (19) requires knowledge of $\tau_p(\hat{\mathbf{p}}(\hat{x}, t_{n+1}), t_n)$ for all $\hat{x} \in \Omega$, that is, the value of $\tau$ of the particle that is currently (at $t = t_{n+1}$) located at $\hat{x}$, at its previous location $\hat{\mathbf{p}}(\hat{x}, t_{n+1})$ at the previous time level ($t = t_n$).

One possibility to find this value is to track the particle path back in time and to pick up the previous values by interpolation. However, here it is intended to use a discontinuous approximation for the extra stress tensors. This precludes the use of this particle tracking methodology in combination with numerical Gauss integration, because if neither of the particles initially located at the Gauss points leaves the element during a time step, which is very likely to occur, no information is passed from one element to the other, giving zero advection. Therefore another approach is adopted in this work.

The ‘old’ stress field can be obtained by advecting the stress field at $t = t_n$, $\tau_n \overset{\text{def}}{=} \tau(\hat{x}, t_n)$, by the known velocity field computed from the preceding problem, say $\hat{\mathbf{u}}(\hat{x}, t)$, hence by solving

$$\frac{\partial \tau_p}{\partial t} + \hat{\mathbf{u}} \cdot \nabla \tau_p = 0, \quad \tau_p(t_n) = \tau_n, \quad t \in I_n .$$  

(26)

This advection problem is solved with a so-called space–time Galerkin least-squares finite element method. This means that not only space is discretized in a finite element manner, but also time, rather than invoking a finite difference discretization in time. Also, the time discretization is typically chosen to be piecewise continuous, but discontinuous across so-called time slabs. That is, the domain $\Omega \times I$ is divided into $N_t$ space–time slabs, such that

$$\Omega \times I = \bigcup_{n=1}^{N_t} Q_n, \quad Q_n = \Omega \times I_n, \quad I_n = ]t_n^+, t_{n+1}[ .$$  

(27)

Hence, the solution is allowed to vary discontinuously from one time slab to the other, thereby allowing each time slab to be analysed subsequently.

Material that enters the domain is assumed to have a stress state equal to the value at the inflow boundary at $t = t_n$. So, advection is assumed to vanish at the inflow boundary. In this way, stresses at the inflow boundary
evolve in time as if the upstream flow domain has the same velocity profile as the inflow boundary. This gives a natural specification of the extra stress boundary conditions at the inflow boundary.

**Problem 3 (ADV).** Given \( \dot{u}(\tilde{x}, t), t \in I_n \), find \( \tau_p \in \mathcal{T} \) such that for all \( T \in \mathcal{T} \)

\[
[T + \beta \mathcal{L}_i T, \mathcal{L}_i \tau_p] + (T(t_n^+), \tau_p(t_n^+) - \tau_n(t_n)) = 0. \tag{28}
\]

Let \( \square \) denote a tri-unit cube with local coordinates \( \xi_1, \xi_2 \) and \( \xi_3 \), such that \( \mathcal{X}(\xi) : \square \mapsto Q^r_n = \Omega^r \times I_n \). Then, following Shakib [27]

\[
\beta = \left\{ \frac{\Delta t}{2} + \left[ \frac{\partial^2 T_{ij} \partial^2 T_{jk}}{\partial x_i \partial x_k} v_j v_k \right] \right\}^{1/2} \quad i, j, k = 1, 2. \tag{29}
\]

The notation \([, , ]\) implies

\[
[T, \tau] = \int_{Q_n} T : \tau \, dQ \tag{30}
\]

and the space \( \mathcal{T} \) is given by

\[
\mathcal{T} = \{ T \mid T \in [H^1(\Omega)]^{2 \times 2} \times I_n \}. \tag{31}
\]

Transport of information from one time slab to the next is accomplished with the jump condition on \( t = t_n : (T(t_n^+), \tau_p(t_n^+) - \tau_n(t_n)) \). This term originates from the discontinuous Galerkin method applied in time.

Clearly, the mixed problem MPVE and the advection problem ADV 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 \( \tau_p \) as required to solve problem MPVE. This iterative procedure is continued until convergence.

At first sight, this algorithm does not have many advantages over other mixed methods. However, if the extra stress tensors are interpolated discontinuously, the stress unknowns can be eliminated at the element level, thereby reducing the number of unknowns significantly, in particular when multiple modes are used. Furthermore, the advection problem can be solved for each component of each extra stress tensor separately (at least for plane flow, torsionless axisymmetric flow and three-dimensional flow conditions, axisymmetric swirling flows are excepted when posed in a polar coordinate system), while, due to the linearity of the problem, the Hessian matrix only needs to be assembled and decomposed once every iteration. This ensures a computationally effective algorithm. Computational cost of the formation of the Jacobian matrix of problem MPVE scales with the number of modes.
involved, and is proportional to the effort of eliminating the stress unknowns on the element level, while the solution of the resulting linearized problem is no more expensive than the solution of a normal Stokes problem in a regular velocity-pressure setting.

5. Numerical experiments

5.1 Discretization

Discretization is accomplished as follows. The domain $\Omega$ is divided into $N_{el}$ elements such that

$$\Omega = \bigcup_{e=1}^{N_{el}} \Omega^e.$$  \hfill (32)

Denote with $P_k(\Omega^e)$ and $Q_k(\Omega^e)$ the $k$th-order interpolation polynomial on a triangular or quadrilateral, respectively, element $e$. Define $R_k$ by

$$R_k(\Omega^e) = \begin{cases} P_k(\Omega^e) & \text{on triangles} \\ Q_k(\Omega^e) & \text{on quadrilaterals.} \end{cases}$$ \hfill (33)

In a more generalized sense, $P_k$ represents linear, quadratic, etc. discretization, while a $Q_k$ discretization contains higher-order terms than strictly implied by the order $k$. The finite dimensional approximations of $\mathcal{U}$, $\mathcal{V}$, $\mathcal{S}$ and $\mathcal{Q}$ are given by

$$\mathcal{U}^h = \{ \hat{u}^h \mid \hat{u}^h \in [R_k]^2, k \geq 1, \hat{u}^h = \tilde{u}^0 \text{ on } \Gamma_u \},$$ \hfill (34)

$$\mathcal{V}^h = \{ \hat{v}^h \mid \hat{v}^h \in [R_k]^2, k \geq 1, \hat{v}^h = \tilde{v}^0 \text{ on } \Gamma_v \},$$ \hfill (35)

$$\mathcal{S}^h = \{ s^h \mid s^h \in [R_k]^{2 \times 2}, k \geq 0 \},$$ \hfill (36)

$$\mathcal{T}^h = \{ T^h \mid T^h \in [R_k]^{2 \times 2} \times P_l, k \geq 0, l \geq 0 \},$$ \hfill (37)

$$\mathcal{Q}^h = \{ q^h \mid q^h \in R_k, k \geq 0 \}.$$ \hfill (38)

The variable $T$ needs to be discretized in both space ($[R_k]^{2 \times 2}$) and time ($P_l$). The spaces $\mathcal{S}$ and $\mathcal{Q}$ may be approximated with either continuous or discontinuous polynomials. The discretization of the triple $(s, \hat{u}, p)$ is identified by $R,R,R_k$. For instance, $Q_2Q_2Q_1$ is a quadrilateral element with quadratic interpolation of both the stress and velocity field, and a bilinear interpolation of the pressure. If a discontinuous interpolation is used, this is signified by the suffix $d$. Hence if a discontinuous stress interpolation is used this might give the $Q_2^dQ_2Q_1$ element.

In this paper only the $(s, \hat{u}, p) \rightarrow Q_2^dQ_2P_1^d$ and $T \rightarrow Q_2 \times P_0^d$ discretization is employed. Experiments have shown that the $(s, \hat{u}, p) \rightarrow P_1^dQ_1P_0^d$ and $T \rightarrow Q_1 \times P_0^d$ discretization gives nearly the same results, but the quadratic approximation gives a better description of the incompressibility constraint.
Clearly, the linear interpolation choice does not satisfy the inf-sup condition on the velocity–pressure interpolation, and occasionally this element may suffer from checkerboarding. Spurious pressure modes can be filtered though, if desired.

The first choice is usually preferred; in that case the extra stress tensor is approximated with a piecewise biquadratic field, that is taken to be discontinuous across element boundaries. In the advection step a continuous biquadratic interpolation in space and a constant in time interpolation is used. It is admitted, as in the advection problem, eqn. (28), that the stress field \( \tau_n(t_n) \) may very well be discontinuous. The result of the advection problem is a continuous biquadratic approximation of \( \tau_p \). This approximation is first projected onto a discontinuous \( Q^d \) field on each element by a least-squares projection. This field is used in the solution of problem MPVE.

5.2 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. 2. 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.

5.2.1 Example 1: plane 4:1 contraction

Recently, Armstrong et al. [30] 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. [2]. In their study, Armstrong et al. [30] 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

![Fig. 2. Geometry of the four-to-one contraction problem.](image-url)
TABLE 1
Parameters for setting multi-mode PTT model to fit 5.0 wt.% PIB/C14 solution [30]

<table>
<thead>
<tr>
<th>Mode</th>
<th>$\lambda_i$</th>
<th>$\eta_i$</th>
<th>$\epsilon_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.6855</td>
<td>0.0400</td>
<td>0.25</td>
</tr>
<tr>
<td>2</td>
<td>0.1396</td>
<td>0.2324</td>
<td>0.25</td>
</tr>
<tr>
<td>3</td>
<td>0.0389</td>
<td>0.5664</td>
<td>0.25</td>
</tr>
<tr>
<td>4</td>
<td>0.0059</td>
<td>0.5850</td>
<td>0.25</td>
</tr>
<tr>
<td>(0) Solvent</td>
<td>0.0020</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The linear viscoelastic spectrum employed is listed in Table 1.

Based on shear data, $\epsilon_i$ was selected as 0.13. However, normal stress measurements along the centreline of the contraction suggested the use of $\epsilon_i = 0.25$. This value is used in all multi-mode computations of this PIB solution. A one-mode fit is also experimented with: $\lambda_1 = 0.06$ and $\eta_1 = 1.424$, while $\epsilon_1 = 0.1$ and $\eta_0 = 0$.

Figure 3(a) shows the predicted viscosity of the 4-mode and 1-mode models. Likewise, Fig. 3(b) shows the computed first normal stress coefficient, defined as

$$\Psi_1 = N_1 / \dot{\gamma}^2,$$

where the first normal stress difference $N_1 = \tau_{xx} - \tau_{yy}$ and $\dot{\gamma}$ denotes the shear rate. In this case, the Deborah number ($De$) is defined as

$$De = \frac{\Psi_1(\dot{\gamma})\dot{\gamma}}{2\eta(\dot{\gamma})}.$$  (40)

In all computations the shear rate is specified by

$$\dot{\gamma} = \frac{\langle v \rangle}{H_2},$$  (41)

where $\langle v \rangle$ is the average velocity in the downstream channel, and $H_2$ is half the gapwidth of the downstream strip. Figure 4 shows $De$ as a function of the shear rate. Hence, given a certain $De$ the average downstream velocity can be computed directly.

The channel dimensions are given in Table 2.

Two situations have been analysed in detail: $De = 0.55$ and $De = 0.77$. Both at the exit and inlet a parabolic velocity profile is prescribed. The maximum velocity at the exit is $0.1277 \text{ m s}^{-1}$ for $De = 0.55$ and $0.2554 \text{ m s}^{-1}$ for $De = 0.77$. Clearly, as the 5.0 wt.% PIB/C14 solution is shear thinning,
Fig. 3. (a) Viscosity ($\eta$) vs. shear rate; (b) first normal stress coefficient ($\Psi_1$) vs. shear rate ($\dot{\gamma}$); solid line; 4-mode model; dashed line; 1-mode model.
Fig. 4. $De$ vs. shear rate ($\dot{\gamma}$); solid line, 4-mode model; dashed line, 1-mode model.

**TABLE 2**

Dimensions (m) of the channel

<table>
<thead>
<tr>
<th>$L_1$</th>
<th>$L_2$</th>
<th>$H_1$</th>
<th>$H_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.01</td>
<td>0.0127</td>
<td>0.0032</td>
</tr>
</tbody>
</table>

This does not correspond to a fully developed velocity profile at steady state. Yet, no apparent difficulty has been encountered in using these profiles. Sufficiently far away from the inlet and outlet fully developed profiles will emerge as time proceeds.

Four meshes have been used, called Mesh1, Mesh2, Mesh3 and Mesh4, as depicted in Fig. 5. Some characteristic mesh parameters are given in Table 3. The minimum element length occurs at the corner.

Figure 6 compares the computed first normal stress difference along the centreline for Mesh1 (solid line) and Mesh2 (dashed line) with the measurements of Armstrong et al. [30]. For $De = 0.77$ this is done in Fig. 7, but now the results for Mesh3 and Mesh4 have also been included (dotted line). The local parameter $s$ is defined as $s = (x - L_1)/H_2$. Computed and measured results are in reasonable agreement. Clearly, the algorithm does not break
down with mesh refinement near the re-entrant corner, while little difference is found in the computed results on Mesh2, Mesh3, and Mesh4. This also holds for the results presented in the sequel when approaching the corner.
singularity from the upstream direction along $y = H_2$. Hence, convergence upon mesh refinement is suggested. Yet, a more thorough investigation of this aspect may be necessary.
TABLE 3
Characteristic mesh parameters

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$h_{\text{min}}$</th>
<th>No. of elements</th>
<th>No. of nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.15e-4</td>
<td>270</td>
<td>1167</td>
</tr>
<tr>
<td>2</td>
<td>1.06e-4</td>
<td>520</td>
<td>2197</td>
</tr>
<tr>
<td>3</td>
<td>2.07e-4</td>
<td>540</td>
<td>2291</td>
</tr>
<tr>
<td>4</td>
<td>1.04e-4</td>
<td>720</td>
<td>3033</td>
</tr>
</tbody>
</table>

Fig. 6. $N_1$ vs. $s = (x - L_1)/H_2$ along the centreline $y = 0(m)$ at $De = 0.55$; solid line, Mesh2; dashed line, Mesh1; ○, experiment [30].

Figures 8 and 9 show the computed $\tau_{11}$ and $\tau_{12}$ profiles along the line $y = H_2$ for $De = 0.55$ and $De = 0.77$, respectively. For $De = 0.55$ the results are shown on Mesh1 and Mesh2, while for $De = 0.77$ only the results for Mesh2 are shown. The results of Mesh3 and Mesh4 show little difference.

Only to give an impression of the distribution of $\tau_{11}$, $\tau_{22}$ and $\tau_{12}$, a contour plot is shown in Fig. 10 at $De = 0.77$, all on Mesh3. In all cases 10 contour levels are drawn, that are equally spaced between the minimum and maximum values. Actual stress values can much better be obtained from the previous figures, i.e. Fig. 9.
Fig. 7. $N_1$ along the centreline at $De = 0.77$; solid line, Mesh2; dashed line; Mesh1; dotted line, Mesh3; dashed-dotted line; Mesh4; ○, experiment [30].

Fig. 8. $\tau_{11}$ and $\tau_{12}$ profiles along $y = H_2$ at $De = 0.55$. 
Fig. 9. $\tau_{11}$ and $\tau_{12}$ profiles along $y = H_2$ at $De = 0.77$.

Fig. 10. (a)
Fig. 10. (a) Distribution of $\tau_{11}$; (b) distribution of $\tau_{22}$; (c) distribution of $\tau_{12}$, all at $De = 0.77$. 
To access some of the quality of the solution, a particle tracking solution based upon a 4th- and 5th-order Runge–Kutta integration is compared with the finite element method solution in Fig. 11 at $De = 0.77$. Figure 11(a)
Fig. 11. (a) Particle path of point injected at $x_0 = 0$, $y_0 = 0.012$; (b) $\tau_{11}$ profile along particle path; (c) $\tau_{22}$ profile along particle path; (d) $\tau_{12}$ profile along particle path, all at $De = 0.77$. Solid line; FEM results; dashed line, 4th/5th-order Runge–Kutta integration.
shows the path of the particle that is injected at \((x_0, y_0) = (0, 0.012)\) (m). This particle passes the singularity very closely. Except for a small region near the singularity, the two solutions compare well, see Figs. 11(b–11(d). At this point it is not known what causes the discrepancy, but it is not nearly as large as the results reported by Rosenberg and Keunings [22].

Armstrong et al. [30] also investigated the first normal stress difference along \(y = H_2\) for \(x \in [0, L_1]\), thus approaching the corner singularity from the upstream channel. Taking \(s = (x - L_1)/H_2\) in accordance with the definition of Armstrong et al. [30], Figs. 12 and 13, show the computed first normal stress difference upstream of the singularity. For \(De = 0.55\), \(N_1\) approaches the corner singularity with a logarithmic slope of approximately \(-0.5\). This value is also obtained by Armstrong et al. [30]. However, at \(De = 0.77\), the computed slope is positive, which is in contradiction to experimental results.

Figures 14 and 15 show the computed \(|\tau_{12}|\) upon approaching the corner singularity along the line \(x \in ]0, L_1[\), \(y = H_2\). In both cases the slope is about \(-0.4\). The computed values at \(De = 0.77\) match the experimental values remarkably well. This is in contradiction to the results for \(N_1\).

Finally, it is of interest to compare the behaviour of a one-mode PTT model and a one-mode Giesekus model with the predictions of the four-mode PTT model. All computations are run on Mesh1, with the flow

\[|N_1| \ (Pa)\]

Fig. 12. \(N_1\) along the line \(y = H_2\) for \(x \in [0, L_1]\) at \(De = 0.55\).
Fig. 13. $N_1$ along the line $y = H_1$ for $x \in [0, L_1]$ at $De = 0.77$, ○, experiment [30].

Fig. 14. $|\tau_{12}|$ (Pa) along the line $y = H_1$ for $x \in [0, L_1]$ at $De = 0.55$. The slope is -0.4.
Fig. 15. $|\tau_{12}|$ along the line $y = H_1$ for $x \in [0, L_1]$ at $De = 0.77$; solid line, computed results; $\odot$, experiment [30].

conditions corresponding to $De = 0.55$ for the four-mode PTT model. The first normal stress difference along the centreline is compared in Fig. 16. The single mode PTT model gives smaller values than the four-mode model, while the Giesekus model produces markedly lower values of $N_1$. The behaviour of $N_1$ along the line $x \in ]0, L_1[$, $y = H_2$, i.e. upon approaching the singularity from the upstream direction, is depicted in Fig. 17. In this case the single mode PTT model produces a different qualitative behaviour than the four-mode PTT model, while, surprisingly, the one-mode PTT model compares well with the one-mode Giesekus model.

5.2.2 Example 2: axisymmetric 4:1 contraction

Coates et al. [11] 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. [11] for the four-to-one contraction problem. The channel dimensions are given in Table 4; $L_1$ and $L_2$ are the lengths and $R_1$ and $R_2$ the radii of the entrance and exit sections, respectively.

At both the entrance and exit a parabolic velocity profile is prescribed; in all cases the maximum velocity at the exit $v_{\text{max}}/R_2 = 2 \text{ s}^{-1}$. A sequence of $De$
Fig. 16. $N_1$ along centreline at $De = 0.55$ for the 4-mode PTT model (solid line), 1-mode PTT model (dashed line) and the 1-mode Giesekus model (dotted line).

is computed by increasing the relaxation time $\lambda$; Table 5 shows the $De$ sequence and the related choice of $\lambda$. $De$ is computed by specifying the shear rate as in eqn. (41). The parameters $F$ and $\alpha$, eqn. (5), are fixed at 0.064 and 5, respectively.

A detail of the mesh near the singularity is depicted in Fig. 18.

The stress solution at $De = 2.29$ is depicted in Fig. 19. This can be compared with Fig. 13 of Coates et al. [11]; results compare well.

Figure 20 shows the computed vortex at $De = 2.29$ and at $De = 6.11$, respectively. Both vortices have a concave shape, confirming the results of Coates et al. [11].

Figure 21 compares the computed vortex size of this work as a function of $De$ with experimental results of Boger et al. [31] and the numerical results

|TABLE 4|

Dimensions of axisymmetric contraction

<table>
<thead>
<tr>
<th>$L_1/R_2$</th>
<th>$L_2/R_2$</th>
<th>$R_1/R_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>32</td>
<td>4</td>
</tr>
</tbody>
</table>
Fig. 17. $N_1$ along $y = H_2$ for $x \in [0, L_1]$ at $De = 0.55$, upon approaching the corner singularity from the upstream direction, for the 4-mode PTT model (solid line), 1-mode PTT model (dashed line) and the 1-mode Giesekus model (dotted line).

Fig. 18. Partial view of mesh used to analyse the axisymmetric 4:1 contraction flow.
of Coates et al. [11]. The dimensionless vortex size ($\chi$) is defined as the vortex length ($L_v$) divided by the upstream tube diameter ($2R_1$). As reported by Coates et al. [11], the computed results match the experimental results.

Fig. 19. (a), (b)
unexpectedly well. Coates et al. [11] 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 $De$. 
6. 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. [11], shows that upon using the MUCM model the computed stress fields at $De = 2.29$ compare well, while the vortex growth matched the experimental results of Boger et al. [31]. Also, much higher $De$ could be obtained with the current method than with the EEME method employed by Coates et al. [11]. The good correspondence between the computed vortex size and the experimentally observed values may very well be misleading. The MUCM model as such does not predict the material functions of the PAC solution employed by Boger et al. [31] well enough. 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. [30] are therefore extremely valuable. A detailed comparison of the predicted stress fields along the symmetry line of the plane 4:1 contraction and upon approaching the corner singularity from the upstream direction with experimental results is made where possible. In particular, the computed first normal stress difference along the symmetry line compares well with experimental observations. The behaviour near the singularity approximates the experimental results reasonably well. The shear stress at $De = 0.77$ matches the experimental results particularly well, sufficiently far away from the singularity. It is, however, disappointing to see that in this case the first normal stress difference is poorly predicted.

It is a great challenge to push the current method towards predicting the unsteady three-dimensional flow patterns in axisymmetric contraction flows.

---

TABLE 5
Deborah number vs. relaxation time

<table>
<thead>
<tr>
<th>$De$</th>
<th>2.29</th>
<th>3.53</th>
<th>4.71</th>
<th>5.41</th>
<th>6.11</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{\gamma}$</td>
<td>1.76</td>
<td>3</td>
<td>5</td>
<td>7</td>
<td>10</td>
</tr>
</tbody>
</table>

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described by McKinley et al. [1]. It is believed that the current method is sufficiently efficient to be extended towards three-dimensional computations. This will be the subject of future work.
Fig. 21. Dimensionless vortex size $\chi = L_c/2R_1$ as a function of the $De$ number. *, Experimental results of Boger et al. [31]; +, computed results from Coates et al. [11]; O, this work.

References


