Chapter 14

The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

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Chapter 14
The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

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1 Introduction 481
2 Mathematical Formulation 481
3 Steady Flow: Variational Formulations 482
4 Time Dependent Flows 488
5 Integral and Stochastic Constitutive Models 490
6 Governing Equations 491
7 The Deformation Fields Method 492
8 Brownian Configuration Fields 493
9 Numerical Methods 494
10 Results 494
11 Conclusions and Discussion 495
12 Related Chapters 496
References 496

1 INTRODUCTION

The development of accurate, stable, efficient, and robust numerical methods for the analysis of viscoelastic flows has proven a challenging task. Nevertheless, significant progress has been made in the finite element formulations for the analysis of viscoelastic flows. The difficulties concern the two major aspects: first, the development of suitable methods to deal with the hyperbolic nature of the constitutive equation (CE); second, the development of appropriate mixed formations for the set of governing equations. Even for seemingly ‘simple’ CEs like the upper-convected Maxwell (UCM) model severe limits appear on the level of elasticity (measured by the dimensionless Weissenberg number) that can be obtained, in particular when geometrical singularities are present.

For a few representative benchmark problems for steady flows, agreement between a number of different formulations has been demonstrated at ever increasing values of the Weissenberg number see for example, Brown and McKinley (1994), Caswell (1996), and more recently Alves, Oliveira and Pinho (2003). And, more importantly, mesh convergent results are achieved here without lowering the maximum achievable Weissenberg number. However, limits in the maximum attainable Weissenberg number still exist for these relative simple flows. The review paper of Baaijens, 1998 discusses various mixed finite element schemes and their applicability for different types of viscoelastic flow problems. A review of the field of computational rheology that covers also other techniques, such as spectral methods, is given in the recent book by Owens and Phillips, 2002. A review focusing particular on integral methods can be found in Keunings (2003).

Similar to the review paper of Baaijens (1998), this work will be restricted to mixed finite element methods, however the emphasis will be on recent developments, such as application to polymer processing, time-dependent simulations, and the application to methods for integral and stochastic models.

2 MATHEMATICAL FORMULATION

The analysis of viscoelastic flows involves the solution of a coupled set of partial differential equations: equations
representing the conservation of mass, momentum, and energy, and CE s for a number of physical quantities present in the conservation equations such as density, internal energy, heat flux, stress and so on. For incompressible, isothermal flow in absence of volume forces, the balance equations of momentum, mass, and the CE for the stress read

\[
\frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \mathbf{p} + \nabla \cdot \left(2\eta \mathbf{D} + \tau\right) \tag{1}
\]

\[
\nabla \cdot \mathbf{u} = 0 \tag{2}
\]

\[
\lambda \nabla \cdot \tau + 2\eta \mathbf{D} + g(\tau) = 0 \tag{3}
\]

where the \( \nabla \mathbf{r} \) denotes the upper-convected time derivative of the stress tensor \( \tau \) defined as

\[
\nabla \mathbf{r} = \frac{\partial \tau}{\partial t} + \mathbf{u} \cdot \nabla \tau - (\nabla \mathbf{u})^T \cdot \tau - \tau \cdot \nabla \mathbf{u} \tag{4}
\]

The velocity is depicted by \( \mathbf{u} \), \( \tau \) denotes the viscoelastic contribution to the extra-stress tensor, \( \rho \) the pressure, and \( \rho \) denotes the density, while \( \mathbf{D} \) denotes the rate of deformation tensor defined as

\[
\mathbf{D} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \tag{5}
\]

Frequently, the extra-stress tensor is defined in terms of a viscous and a viscoelastic contribution, in which \( \eta_0 \) denotes an effective viscosity as appearing in equation (1). The effective viscosity can represent the viscosity of the solvent (for a polymer solution) or an apparent viscosity modeling part of stress by a Newtonian viscosity.

A large variety of approaches exists to define a model for the extra-stress tensor \( \tau \) (Bird, Armstrong and Hassager, 1987a; Bird et al., 1987b). Most recent models are derived from kinetic theory. However, from an implementation point of view, a distinction can be made between closed-form constitutive models of the integral and differential type and models that cannot be written as a closed-form constitutive model. First, constitutive models of the differential type will be discussed. Integral and stochastic (nonclosed) models will be the subject of Sections 5 and further. The discussion here will be limited to differential models having the structure as in equation (3), where \( \lambda \) represents a characteristic relaxation time for the polymer system and \( \eta \) represents the polymer viscosity. The function \( g(\tau) \) in equation (3) represents a nonlinear function of the stress, that goes to zero at least as fast as quadratically as \( \tau \) approaches zero. A number of well-known constitutive models are represented by equation (3), including the upper-convected Maxwell, FENE-P (finitely extensible nonlinear elastic (Peterlin)), Phan Thien-Tanner (PTT), Giesekus, and the eXtended pom-pom model. In general both \( \lambda \) and \( \eta \) can be considered as functions of the stress or other state variables, but since this does not seem to drastically influence the behavior of the various numerical schemes to be discussed below, they will be assumed constants here for simplicity.

Clearly, equation (3) may not describe the actual mechanical behavior of many viscoelastic fluids with sufficient accuracy since even in the limit of small deformations a spectrum of relaxation times is necessary to accurately describe the rheology of most viscoelastic fluids. Such a spectrum frequently may be represented by a finite set of relaxation times. For each relaxation time, a CE of the form of equation (3) may be used for a substress \( \tau_i \), such that \( \tau = \sum \tau_i \). However, to discuss the algorithmic developments, a single relaxation time with a CE that obeys equation (3) is sufficient.

### 3 STEADY FLOW: VARIATIONAL FORMULATIONS

Consider the steady, incompressible, inertial-free flow of an Oldroyd-B fluid, that is, equations (1)–(3) with \( \rho = 0 \) and \( \mathbf{g}(\tau) = 0 \). As a natural extension of the common velocity-pressure formulation for Stokes type problems, the classical three field mixed formulation is chosen, in which, besides the momentum and continuity equation, also the CE is cast in a weighted residuals form.

**Problem 1 (MIX)** Find \( \mathbf{u} \), \( \rho \), and \( \tau \) such that for all admissible weighting functions \( \mathbf{v} \), \( q \), and \( S \)

\[
((\nabla \mathbf{v})^T, 2\eta_0 \mathbf{D} + \tau) - (\nabla \cdot \mathbf{v}, \rho) = 0 \tag{6}
\]

\[
(q, \nabla \cdot \mathbf{u}) = 0 \tag{7}
\]

\[
(S, \lambda \nabla \cdot \tau + 2\eta \mathbf{D}) = 0 \tag{8}
\]

where \( (., .) \) denotes the appropriate inner product. Most of the early work on viscoelastic flow analysis is based on this formulation, see for example (Kawahara and Takeuchi, 1977; Crochet and Keunings, 1982).

Assuming that suitable approximation spaces have been selected for the triple stress-velocity-pressure in Problem 1 (MIX), computational difficulties exist with increasing levels of elasticity. The importance of the convective term \( \mathbf{u} \cdot \nabla \tau \) grows and a Galerkin discretization as applied in equation (8) is not optimal (King et al., 1988).

The most widespread method to account for the convective term in the constitutive equation is the so-called streamline-upwind/Petrov Galerkin (SUPG) method of Brooks and Hughes (1982), first applied to viscoelastic flows by Marchal and Crochet (1987):

\[
(S + \alpha \mathbf{u} \cdot \nabla S, \lambda \nabla \cdot \tau + 2\eta \mathbf{D}) = 0 \tag{9}
\]
Several choices for the SUPG parameter $\alpha$ have been proposed in the literature, but are all of the form

$$\alpha = \frac{h}{U}$$  \hspace{1cm} (10)

where $h$ is a characteristic element size, that is, the element size along the local flow direction and $U$ is a characteristic velocity. A possible choice for $U$ is to use the velocity in the direction of the local coordinates at the midpoint of a biquadratic element (Marchal and Crochet, 1987), or at each integration point (Baaijens, 1992). Other choices are the norm of the velocity $u$ (King et al., 1988), or a characteristic velocity of the flow (Lunsmann et al., 1993). Owens, Chauvière and Philips (2002) introduced a locally upwinded spectral technique (LUST) for viscoelastic flows, in which locally within each member of the partition of a spectral element is formed by the quadrature grid. Marchal and Crochet (1987) demonstrated the limitations of the MIX/SUPG formulation for problems with a geometrical singularity, such as the stick-slip problem or contraction flows. On the basis of these findings, they suggested to apply the upwind term to the convective part of the CE only, yielding the so-called streamline-upwind (SU) formulation:

$$\left(S, \lambda \nabla \cdot \mathbf{v} + \tau - 2\eta \mathbf{D}\right) + \left(\alpha u \cdot \nabla S, \lambda u \cdot \nabla \mathbf{v}\right) = 0$$  \hspace{1cm} (11)

The obvious limitation of this formulation is its inconsistency, in the sense that if the exact solution is inserted into equation (11), that is, $\lambda \nabla \cdot \mathbf{v} + \tau - 2\eta \mathbf{D} = 0$, a residual $(\alpha u \cdot \nabla S, \lambda u \cdot \nabla \mathbf{v})$ remains. Moreover, the method is reported to be first-order accurate only such that achieving mesh converged results is extremely difficult.

An alternative to the SUPG method is the discontinuous Galerkin (DG) or Lesaint–Raviart method. Here, the extra-stress tensor is approximated discontinuously from one element to the next, and upwind stabilization is obtained as follows:

$$\left(S, \lambda \nabla \cdot \mathbf{v} + \tau - 2\eta \mathbf{D}\right) - \sum_{e=1}^{N} \int_{\Gamma_e^p} S : \lambda u \cdot n (\tau - \tau^{\text{ext}}) \, d\Gamma = 0$$  \hspace{1cm} (12)

with $n$ the unit outward normal on the boundary of element $e$, $\Gamma_e^p$ the part of the boundary of element $e$, where $u \cdot n < 0$, and $\tau^{\text{ext}}$ the extra-stress tensor in the neighboring upwind element. In the context of viscoelastic flows, this method was first introduced by Fortin and Fortin (1989) on the basis of ideas of Lesaint and Raviart (1974), who proposed the method to solve the neutron transport equation. Compared to the SUPG formulation, the implementation of the DG method in a standard finite element code is more involved. This is due to the boundary integral along the inflow boundary of each element in which stress information of the neighboring, upwind, element is needed. This drawback is circumvented for unsteady flows by Baaijens (1994b) by using an implicit/explicit implementation.

Several methods have been proposed in the literature to retain an elliptic contribution of the form $((\nabla \mathbf{v})^T, \mathbf{D})$ in the weak form of the momentum equation, equation (6), which is particularly important if a purely viscous contribution is absent or small compared to the viscoelastic contribution. One way to achieve this is the application of a change of variables, known as the elastic-viscous stress splitting (EVSS) formulation, first introduced by Perera and Walters (1977) and Mendelson et al. (1982) for the flow of a second-order fluid and later extended to viscoelastic flows by Beris, Armstrong and Brown (1984, 1986):

$$\Sigma = \tau - 2\eta \mathbf{D}$$  \hspace{1cm} (13)

Substitution of this into equations (8) and (6), respectively, yields

**Problem 2 (EVSS/SUPG)** Find $\mathbf{u}$, $p$, $\tau$, and $\mathbf{H}$ such that for all admissible weighting functions $v$, $q$, $S$, and $H$

$$(\nabla \mathbf{v})^T, \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \mathbf{H} = 0$$  \hspace{1cm} (17)

The tensor $\mathbf{H}$ is introduced as an additional variable obtained by an $L_2$-projection of $\mathbf{D}$ in equation (17), where $\mathbf{E}$ denotes a suitable weighting function. The purpose of this projection is to facilitate evaluation of the upper-convected derivative of $\mathbf{H}$ as appearing in equation (16). This derivative contains the gradient of $\mathbf{H}$, and use of $\mathbf{D}$ in this expression instead of the projection $\mathbf{H}$ would require second-order derivatives of the velocity field, and therefore continuity of the gradient of the velocity field $\mathbf{u}$. This extension is due to Rajagopalan, Armstrong and Brown (1990) and is used by many others.

One may proceed one step further by performing a projection of $(\mathbf{E}, G - (\nabla \mathbf{u})^T) = 0$, and using $G$ as an additional unknown rather than $\mathbf{D}$, and subsequently use the projection of $G$ in the CEs as well. The latter leads to the so-called EVSS-G method, introduced by Brown et al. (1993) and Szady et al. (1995).

A major disadvantage of EVSS is that the change of variables (see, equation (13)) is not possible for all constitutive relations, in particular it cannot be applied to integral models and models that cannot be written in a closed-form closed expression. Guénette and Fortin (1995a) introduced a modification of the EVSS formulation, known as the discrete EVSS method (DEVSS). Here, a stabilizing elliptic
operator is introduced in the discrete version of momentum equation, which is similar to the EVSS method, but the objective derivative of the rate of strain tensor is avoided. Moreover, the method is not restricted to a particular class of CEs and has the same computational costs as EVSS. Using the Oldroyd-B model and SUPG, we introduce the so-called DEVSS-G/SUPG form.

**Problem 3 (DEVSS-G/SUPG)** Find \( u, p, G, \) and \( \tau \) such that for all admissible weighting functions \( v, q, E, \) and \( S \)

\[
\begin{align*}
((\nabla v)^T, \alpha \eta (2D - (G + G^T)) + \tau) - (\nabla \cdot v, p) &= 0 \\
(q, \nabla \cdot u) &= 0 \\
(S + au \cdot \nabla S, \lambda \left( \frac{\partial \tau}{\partial t} + u \cdot \nabla \tau - G - \tau \cdot G^T \right) - \eta (G + G^T) &= 0 \\
(E, \nabla u - G^T) &= 0
\end{align*}
\]

In the discrete momentum equation (18), an elliptic operator \( \alpha \eta (2D - (G + G^T)) \) is introduced, where \( G \) is a discrete approximation of the velocity gradient tensor \((\nabla u)^T\) obtained from equation (21). The auxiliary parameter \( \alpha \) is generally set to 1. Notice that if the exact solution is recovered, the elliptic operator \( \alpha \eta (2D - (G + G^T)) \) vanishes. However, in a finite element calculation, this is generally not the case because \( D \) is derived from the velocity field, and \( G \) results from the projection equation (21), and therefore generally belong to a different approximation space. The first application of discrete elastic-viscous split stress (DEVSS) to the DG method is reported by Baaijens et al. (1997).

The acronym DEVSS is not really an appropriate name for the method because the stress splitting is not present in either the momentum or CE. As has been observed by Fan, Tanner and Phan-Thien (1999b), Bogaers, Verbeeten and Baaijens (2000), and Bogaers (2002), most of the above-mentioned formulations can be interpreted as being a member of the family of the Galerkin/Least-square concept. It is well known that, for the Navier–Stokes equations, various stabilizing algorithms can be derived by introducing perturbation terms to the potential functional of the variational problem. For viscoelastic flows, a thorough analysis of the addition of such terms is still lacking.

### 3.1 Spatial discretization; finite elements

In the well-known velocity-pressure formulation of the Stokes problem, recovered by omitting \( \tau \) from equations (6) to (7), the so-called inf–sup or Ladyshenskaja-Babuška-Brezzi (LBB) compatibility condition between the velocity and pressure interpolation needs to be satisfied (Brezzi and Fortin, 1991). Likewise, the addition of the weak form of the CE, equation (8), imposes compatibility constraints on the interpolation of the triple stress-velocity-pressure. Fortin and Pierre (1987) have shown that in the absence of a purely viscous contribution, for example, \( \eta_v = 0 \) and using a regular Lagrangian interpolation, the following conditions must hold:

1. The velocity-pressure pressure interpolation must satisfy the usual LBB condition to prevent for locking and spurious oscillation phenomena.
2. If a discontinuous interpolation of the extra-stress tensor \( \tau \) is used, the space of the strain rate tensor \( D \) as obtained after differentiation of the velocity field \( u \) must be a member of the interpolation space of the extra-stress tensor \( \tau \), that is, \( D \subset \tau \).
3. If a continuous interpolation of \( \tau \) is used, the number of internal nodes must be larger than the number of nodes on the side of an element used for the velocity interpolation.

Condition (2) is relatively easily satisfied using a DG method; see, for example, Fortin and Fortin (1989) and Baaijens (1994a). Condition (3) is confirmed by the earlier work of Marchal and Crochet (1987), who introduced a four-by-four bilinear subdivision of the extra stresses on a biquadratic velocity element. Baranger and Sandri (1992) have shown that the third condition need not be imposed if a purely viscous contribution is present (\( \eta_v \neq 0 \)), which allows a much larger class of discretization schemes.

Prior to the introduction of (D)EVSS, it was customary to use an equal-order interpolation of the velocity and stress field. Exceptions to this are the so-called 4 × 4 element of Marchal and Crochet (1987), and discontinuous interpolations of the extra stresses by Fortin and Fortin (1989). Because of the introduction of (D)EVSS, a larger selection is possible, yet the most common scheme is to use a stress and strain rate discretization that is one order lower than the velocity interpolation.

If (D)EVSS(-G) and a continuous interpolation of the extra-stress tensor are used, the strain rate tensor (or the velocity gradient tensor) is interpolated in the same way as the extra-stress tensor. The most commonly applied element for the (D)EVSS(-G) method has a biquadratic velocity, bilinear pressure, stress and strain rate (or velocity gradient) interpolation; see Debae, Legat and Crochet (1994).

In case of the DG method, hence with a discontinuous interpolation of the extra-stress tensor, a variety of choices have been experimented with by Fortin and Fortin (1989). Baaijens et al. (1997) shows that with a biquadratic velocity...
interpolation and a bilinear discontinuous interpolation of the stresses, the most stable results are obtained with a bilinear continuous interpolation of the strain rate tensor. This differs from the DEVSS/SUPG formulation, in which the rate of strain tensor is interpolated equal to the extra-stress tensor.

A special class of methods is formed by so-called (pseudo-) spectral collocation formulations; see Plitisis and Beris (1989), Xu, Davies and Phillips (1993), and Phillips (1994). These may generally be viewed as a special form of MIX and EVSS in the sense that the discretization is not of the Galerkin type since the weighting function are chosen unity at the collocation points. A different class of discretization models are the higher-order finite volume methods, which recently have been used to obtain second-order accuracy for a number of benchmark problems (Alves, Oliveira and Pinho, 2003). Earlier models based on finite volumes were not able to provide accurate results. Fan (2003) and others have applied $h-p$ type of finite elements, which provide stable discretizations to viscoelastic flow problems in smooth geometries with an exponential convergence rate. A drawback of these higher-order discretizations is that they are limited for problems with singularities.

An illustration of the effect of the formulation and associated discretization is obtained by examining the planar stick-slip problem assuming Newtonian flow, but in a mixed setting. Hence, in equations (1) and (3), the viscosity $\eta = 0$ and the relaxation time $\lambda = 0$. The stick-slip problem is schematically represented in Figure 1. Along $\Gamma_{st}$ the velocity is set to zero, while along $\Gamma_{sl}$ only the normal component of the velocity is zero. Along the inflow boundary, $\Gamma_{i}$ a parabolic inflow velocity profile is prescribed, and along the symmetry line $\Gamma_{s}$, the velocity in the vertical direction is also suppressed.

Employing the MIX method, the horizontal velocity component along $\Gamma_{st} \cup \Gamma_{sl}$ is shown in Figure 2. In Figure 2(a), the velocity and stress are discretized with a biquadratic ($Q_{2}^2$) interpolation, while the pressure is discretized with a bilinear $Q_{1}$ polynomial. The use of a continuous bilinear approximation of the stress results in the velocity field of Figure 2(b).

![Figure 1. Geometry of the stick-slip problem.](image)

![Figure 2. Horizontal velocity along $\Gamma_{st} \cup \Gamma_{sl}$. (a) $\mathbf{u}, \mathbf{\tau}, p : Q_{2}Q_{2}Q_{1}$, (b) $\mathbf{u}, \mathbf{\tau}, p : Q_{2}Q_{1}Q_{1}$.](image)

The oscillations in the velocity field along the slip boundary $\Gamma_{sl}$ clearly demonstrate the limitation of this formulation.

Analysis of the same problem, but now with the DEVSS formulation, yields the velocity in Figure 3. Now, both discretizations, $\mathbf{u}, \mathbf{\tau}, p, H : Q_{2}Q_{2}Q_{2}Q_{1}$, and $\mathbf{u}, \mathbf{\tau}, p, H : Q_{2}Q_{1}Q_{1}Q_{1}$, yield smooth and accurate velocity curves. Notice that in the latter case, the stress approximation is discontinuous, while a continuous approximation of $H$ is used. Other discretizations may also be used; for example, Baaijens et al. (1997) and Baaijens (1998).

### 3.2 Solution technology

The resulting set of nonlinear equations is often solved using a Newton–Raphson scheme in combination with a first-order continuation in the Weissenberg number $Wi$. The resulting linear set of equations is generally solved using a direct LU factorization and a frontal solver. This is referred to as a fully coupled approach, in which the full set of equations is solved simultaneously.

Even for two-dimensional problems with modest geometrical complexity and a single relaxation time, memory limitations prohibit the use of direct solvers. The need for fine meshes maintains to resolve the steep stress boundary layers near curved boundary and singularities that occur with many of the existing CEs. Consequently the coupled approach requires a (frequently too) large amount of memory and may lead to excessive CPU time consumption. In particular for three-dimensional computations, the coupled approach with direct solvers is not feasible.
One way to reduce memory requirements is to decouple the viscoelastic extra stresses from the momentum and continuity equation. Coupling between the two sets of equations is then achieved iteratively by means of a Picard iteration. However, convergence of this scheme is slow and the maximum attainable Weissenberg number is usually significantly lower than with a coupled solver.

The use of iterative solvers for the set of equations resulting from methods like DEVSS is not that trivial. Often the matrix is ill conditioned and the number of iterations to reach convergence is too large. The development of appropriate preconditioners for these iterative methods is still an active field of research. Advantages of the decoupled set of equations are that simpler matrix systems need to be inverted where iterative solvers converge much faster. The application of domain decomposition based techniques in combination with parallel iterative solvers appears to be particularly attractive for future developments.

### 3.3 Performance evaluation

The falling-sphere-in-a-tube problem, using the UCM model, is by far the most cited benchmark problem for numerical methods for viscoelastic flow computations. It is well known that the major difficulty for this problem results from the development of stress boundary layers on the sphere wall and the increase of the stress wake after the rear stagnation point as the Weissenberg number increases. Recent analysis of Fan (2003) show that the numerical simulation of the falling-sphere problem for an Oldroyd-B fluid is even more complicated than for the UCM fluid, which is a contradiction with earlier beliefs. For most other problems, the maximum achievable Weissenberg number is minimal for the UCM model.

The falling-sphere benchmark problem, graphically depicted in Figure 4(a), is defined as follows. The sphere with radius $R$ is located at the centerline of the tube with radius $R_c$. The tube wall moves parallel to the centerline with a velocity $V$ in the positive $z$-direction. The ratio of the cylinder radius $R_c$ and the sphere radius $R$ is $\beta = (R_c/R) = 2$. The Weissenberg number is defined as

$$Wi = \frac{\lambda V}{R}$$  \hspace{1cm} (22)

The drag $F_0$ on a sphere falling in an unbounded Newtonian medium is given by

$$F_0 = 6\pi \eta RV$$  \hspace{1cm} (23)

It is customary to compare the so-called drag correction factor given by

$$K(Wi) = \frac{F(Wi)}{F_0}$$  \hspace{1cm} (24)

where $F$ is the drag on the cylinder as a function of the Weissenberg number.

Figure 4(b) depicts an overview of currently available results, with the restriction that only reference is made to studies that report drag correction factors beyond a Weissenberg number of 2, while results on the finest mesh available are included. The $\tau_{zz}$ stress distribution is depicted in Figure 5 and illustrates the difficulty of computing viscoelastic flows even for a geometry having no geometrical singularity. Steep stress boundary layers are formed near...
The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

Figure 5. Distribution of the $\tau_{zz}$ stress component as a function of the Weissenberg number.

curved boundaries. Moreover, rapid changes in stress fields are observed at the wake of the sphere, which emanate from the wake of the sphere. These steep stress gradients require the use of highly refined meshes.

Convergent results up to reasonably high values of the Weissenberg number (larger than 2) have been obtained for the falling-sphere-in-a-tube benchmark problem using a variety of methods, including EVSS, DEVSS, and explicitly elliptic momentum equation (EEME) based methods, as well as $hp$ methods, provided that sufficiently refined meshes have been used.

It is unclear at this point whether results at even higher values of the Weissenberg number can be obtained with second or higher-order methods when more refined meshes are used, although this may indeed be expected on the basis of previous experience. Nevertheless, it is fair to state that significant progress has been made over the past decade. Petera (2002), who also studied the falling-sphere benchmark problem, has reached Weissenberg numbers up to 6.6. However, a careful analysis of the stress levels obtained by Petera show that the values obtained differ a factor 4 with the results obtained by other authors, explaining the difference in the maximum achieved Weissenberg number (Fan, 2003). Comparing the drag correction factor for different numerical methods only is insufficient to judge the quality of the numerical solution. It is more appropriate to compare the stress in the wake of the sphere for the different models. Moreover, if a time-marching scheme is used, special attention has to be given to demonstrate that the steady state has been reached; in particular, for these high Weissenberg numbers (Hulsen, Peters and van den Brule, 2001).

3.4 Application to polymer processing

The viscoelastic flow of polymer melts has been investigated in several nominally two-dimensional geometries, such as contraction flows (Schoonen, 1998; Verbeeten, 2001), flows past a confined cylinder and the cross-slot flow (Peters et al., 1999; Verbeeten, Peters and Baaijens, 2002). Using the stress-optical rule, the computed stress fields may be compared to birefringence measurements. Clearly, accuracy, stability, and robustness of the computational scheme is a prerequisite for such an exercise, but the quality of the predictions largely depends on the ability of the constitutive model to predict the rheological behavior of the polymer melt. In recent years, a number of constitutive models have been developed that are able to quantitatively describe rheological measurements in both shear and elongation. On the basis of the pom-pom model (McLeish and Larson, 1998), the XPP model was developed by Verbeeten, Peters and Baaijens (2001) that quantitatively describes rheological data of a number of commercial polymer melts. This model is applied to the analysis of the flow past a confined cylinder and the cross-slot flow.

To characterize the strength of the different flows, the Weissenberg number is defined as

$$Wi = \frac{\bar{\lambda} \bar{u}_{2D}}{\bar{h}}$$

(25)
Here, $\lambda$ denotes the viscosity averaged relaxation time for the material and $\bar{u}_{2D}$ is the two-dimensional mean velocity and $h$ a characteristic length of the flow geometry. A spectrum of relaxation time is necessary to quantitatively capture the rheological data of polymer melts.

The cross-slot geometry is particularly challenging because regions with steady shear and steady elongation and combination thereof are present. A typical example of a comparison of predicted and experimental birefringence patterns is found in Figure 6. Steady shear is observed in the upstream and down-stream channel, while steady planar stagnation point is shown, the top quarter depicts the experimental result. The bottom half of the image depicts the predicted birefringence profile. Excellent agreement between computed and measured birefringence is found. Verbeeten, Peters and Baaijens (2002) have shown that for this particular flow, the XPP model outperforms other models that are frequently used to analyze viscoelastic flows of polymer melts.

4 TIME DEPENDENT FLOWS

The most direct extension to unsteady flows of the mixed formulations discussed above are based on an implicit temporal discretization as first used by Northey, Armstrong and Brown (1992) and later by many others. By introducing a selective implicit/explicit treatment of various parts of the equations, a certain decoupling at each time step of the set of equations may be achieved to improve computational efficiency. For instance, Singh and Leal (1993) first applied the three-step operator splitting methodology developed by Glowinski and Pironneau (1992) to viscoelastic flows, later followed by Saratimo and Piau (1994) and Luo (1996). In the first and third step, a generalized Stokes problem is obtained, while in the second step a convection–diffusion type of problem needs to be solved. This offers the possibility to apply dedicated solvers to subproblems of each fractional time step.

In order to obtain an efficient time-marching scheme, we consider an operator splitting method to perform the temporal integration. The major advantage of operator splitting methods is the decoupling of the viscoelastic operator into parts that are ‘simpler’ and can be solved more easily than the full problem. Hence, if we write equation (20) to (21) as

$$\frac{\partial x}{\partial t} = A(x) = A_1(x) + A_2(x)$$

the $\theta$-scheme is defined following Glowinski and Pironneau (1992):

$$\frac{x^{n+1} - x^n}{\theta \Delta t} = A_1(x^{n+\theta}) + A_2(x^n)$$

$$\frac{x^{n+1} + \theta x^n}{(1 - 2\theta) \Delta t} = A_1(x^{n+\theta}) + A_2(x^{n+1-\theta})$$

$$\frac{x^{n+1} - x^{n+1-\theta}}{\theta \Delta t} = A_1(x^{n+\theta}) + A_2(x^{n+1-\theta})$$

with time step $\Delta t$ and $\theta = 1 - (1/\sqrt{2})$ in order to retain second-order accuracy. The remaining problem is to define the separate operators $A_1$ and $A_2$. In essence, we like to choose $A_1$ and $A_2$ in such a way that solving equation (27) to (29) requires far less computational effort as compared to solving the implicit problem while the stability envelope of the time integrator remains sufficiently large. If the simplified problem $A_1 = \beta A$ and $A_2 = (1 - \beta)A$ is considered, the stability envelopes are plotted in Figure 7 for different values of $\beta$. The arrows point towards the region of the complex plane for stable time integration. Obviously, setting $\beta = 0$ yields only a small portion of the complex plane whereas $0.5 \leq \beta \leq 1.0$ results in a scheme that is unconditionally stable. On the basis of the argument that we split the

![Figure 6. Comparison of the predicted and measured birefringence pattern in the cross-slot flow device.](image)
A unconditionally stable for this special choice of $\beta$ and it can be seen that for $0.5 \leq \beta \leq 1.0$ this $\theta$-scheme is unconditionally stable for this special choice of $A_1$ and $A_2$.

Figure 7. Stability envelope of the $\theta$-scheme for $A_1 = \beta A$ and $A_2 = (1 - \beta)A$ with $\mu$ the spectrum of $A$. Regions for stable time integration are indicated by the arrows for different values of $\beta$ and it can be seen that for $0.5 \leq \beta \leq 1.0$ this $\theta$-scheme is unconditionally stable for this special choice of $A_1$ and $A_2$.

viscoelastic operator into a kinematic problem and a transport problem for the advection of polymer stress, we can define $A_1$ and $A_2$ from the approximate location of the governing eigenvalues. For instance, the viscous (Stokes) problem has eigenvalues that are essentially real and negative. The absolute value has the tendency to grow very fast with mesh refinement (for a one-dimensional diffusion problem using a low-order finite element method, $\text{max}(|\mu|) = O(N^2)$ with $N$ the number of grid points) and it is convenient to define $A_1$ as the kinematic problem for given polymer stress. On the other hand, the eigenspectrum of the remaining advection operator in the CE is located close to the imaginary axis (however not on the imaginary axis due to the introduction of Petrov–Galerkin weighting functions later on) and we define $A_2$ as the transport of extra stress. One possible definition of the $\theta$-scheme ($A_1$ and $A_2$) is

\[
A_1 = - \begin{bmatrix}
-\nabla \cdot \left( \tau + \alpha \eta \left( D - (G + G^T) \right) \right) + \nabla p \\
\nabla \cdot u \\
G^T - \nabla u
\end{bmatrix}
\]

and

\[
A_2 = - \begin{bmatrix}
\lambda (u \cdot \nabla \tau - G \cdot \tau - \tau \cdot G^T) + \tau - \eta(G + G^T) \\
0 \\
0 \\
0
\end{bmatrix}
\]

(30)

On the basis of the above definitions for $A_1$ and $A_2$, the kinematic (elliptic saddle point) problem for $u, \rho, G$ is updated implicitly in the first (equation (27)) and last (equation (29)) step of the $\theta$-scheme, whereas the transport of polymeric stress is updated explicitly.

A similar strategy is employed in the implicit/explicit Newton-like implementation of the DG method by Baaijens (1994b), which allows the elimination of the extra stresses on the element level at each time step. The resulting set of equations has the size of a Stokes problem in the regular velocity-pressure setting.

Notice that, rather than solving the steady flow problem as such, one may use a time-marching procedure to approach steady state as a limiting case. In particular, the splitting of the set of equations as is achieved in the $\theta$-scheme is of interest to reduce memory requirements as each of the subproblems is significantly smaller than the full coupled set of equations.

4.1 Linear stability analysis of complex flows

The computational analysis of the stability of viscoelastic flows has proven to be a major challenge. This is amply demonstrated by Brown et al. (1993) and Szady et al. (1995), who computed the linear stability of a plano-Couette flow of the upper-convected Maxwell to access the numerical stability of a number of mixed finite element formulations. Theoretical results have shown that this inertialless flow is stable for any value of the Weissenberg number. Methods based on a Galerkin, EEME, and EVSS formulation in combination with either SUPG or SU demonstrated a limiting Weissenberg beyond which the numerical solution became unstable. It is for this reason that the EVSS-G/SUPG and EVSS-G/SU formulations in which introduced for which no limiting Weissenberg number was found within the range of Weissenberg numbers and mesh resolutions examined.

Simulation and prediction of transient viscoelastic flow phenomena probably represent the most challenging task of computational rheology today. For instance, the study of the stability of polymer solutions in complex flows, such as the flow around a cylinder (Sureshkumar et al., 1999) or the corrugated channel flow (Sureshkumar, 2001), has gained attention.

The development of numerical tools that are able to handle these dynamic flow phenomena (i.e. the transition from steady to transient flows as dictated by the stability problem) requires a number of important issues to be addressed properly. First of all, the CE that relates the polymer stress to the fluid deformation (and deformation history) needs to be defined. While most present research focused on the stability behavior of the UCM model (e.g. Gorodtsov and Leonov, 1967; Renardy, 2000),
there has been much less interest on how the choice of constitutive model affects the predicted stability of a given polymer melt flow (Ho and Denn, 1977; Ganpule and Khorami, 1999; Grillet et al., 2002). This is an important issue when the dynamics of polymer melt flows are predicted using numerical simulations. Grillet et al. (2002) and Bogaers et al. (2002) have shown that this is not a trivial task since generally accepted models for polymer melts can behave very different in terms of their stability characteristics.

Bogaers et al. (2002) introduced an extension of the commonly used three-step $\theta$-scheme described above, which shows superior stability behavior. The idea is to eliminate the stress from the hyperbolic equation and to substitute it in the momentum equation yielding a modified momentum equation:

Problem 4 ($\theta$-Bogaers 1a) Given the base flow $(u, \tau)$ at time $t = t_n$ the solution is found at $t = t_n + \Delta t$ by

\[
\begin{align*}
\frac{\tau^{n+0} + \theta \Delta t}{\theta \Delta t} - \tau^n + u^{n+0} \Delta t \cdot \nabla \tau^n & = -G^{n+0} \cdot \mathbf{\tau}^{n+0} \cdot \mathbf{\tau}^n \\
& - \nabla \cdot (G^{n+0} + (G^{n+0} \mathbf{\tau}^{n+0} \mathbf{\tau}^n)) + \frac{1}{\kappa} (\omega \theta^{n+0} \Delta t + (1 - \omega) \tau^n) \\
& - \eta (G^{n+0} + (G^{n+0} \mathbf{\tau}^{n+0} \mathbf{\tau}^n)) \mathbf{\tau}^n = 0 \\
\n\n\n\end{align*}
\]

Problem 5 ($\theta$-Bogaers 1b) The second step of the $\theta$-scheme using the quantities at time level $t = t^{n+0}\Delta t$ to determine intermediate values at $t = t^{n+1}\Delta t$ by

\[
\begin{align*}
\frac{\tau^{n+1} + (1-\theta)\Delta t}{1 - 2\theta \Delta t} - \tau^n + u^{n+0} \Delta t \cdot \nabla \tau^n & = -G^{n+0} \cdot \mathbf{\tau}^{n+0} \mathbf{\tau}^n \\
& - \nabla \cdot (G^{n+0} \tau^{n+0} + (G^{n+0} \mathbf{\tau}^{n+0} \mathbf{\tau}^n)) + \frac{1}{\kappa} (\omega \theta^{n+0} \Delta t + (1 - \omega) \tau^n) \\
& + \frac{1}{\kappa} \eta (G^{n+0} + (G^{n+0} \mathbf{\tau}^{n+0} \mathbf{\tau}^n)) = 0 \\
\end{align*}
\]

The third step of the $\theta$-scheme is equal to the first step, but now using the quantities at $t = t^{n+1}\Delta t$, which are updated to $t = t^{n+1}\Delta t$.

The above decoupling of the constitutive relation from the remaining equations provides a very efficient time integration technique that is second-order accurate for linear stability problems. The efficiency becomes even more evident when real viscoelastic fluids are modeled for which the spectrum of relaxation times is approximated by a discrete number of viscoelastic modes. For simplicity, the procedure is described for the UCM model. However, if nonlinear models like the PTT, Giesekus, or the XPP model are considered, as is common for polymer melts, a generalization of the $\theta$-scheme is readily obtained.

An illustration of the effectiveness of the DEVSS-G/SUPG($\theta$) formulation relative to, for instance, the DEVSS-G/DG formulation is demonstrated in Figure 8. This shows the $L_2$ norm of the perturbation of the velocity field in the stability analysis of the planar Couette flow employing the UCM model. This flow is known to be stable and the $L_2$ norm of the perturbation should decay at a rate proportional to $1/(2\nu e)$; see Gorodtsov and Leonov (1967). Clearly, the instability predicted by the DEVSS-G/DG method is nonphysical and a numerical artifact. Details of this analysis may, for example, be found in Grillet et al. (2002).

5 INTEGRAL AND STOCHASTIC CONSTITUTIVE MODELS

The conventional approach in the simulation of viscoelastic fluid flow has been to start from a closed-form CE. In the early days, the CE was based on continuum mechanics only (see Figure 9). These models contain limited information on the structure of the polymer and are thus insufficient to ultimately base polymer processing designs directly on the polymer architecture. Therefore, the microstructural modeling became popular in the last two decades. The focus has been on finding models that contain microstructural information of the polymer but remain simple enough that they still can be written as a closed-form CE. Examples are the FENE-P model for dilute polymer solutions (a differential model) and the Doi–Edwards integral model with the so-called independent alignment approximation (IAA). A comprehensive overview of both approaches can be found in Bird, Armstrong and Hassager (1987a) and Bird et al. (1987b).

A basic problem with finding a closed-form CE is the approximations that have to be made in the kinetic theory to arrive at such an equation. Therefore, a technique has been introduced by Laso and Öttinger (1993), to avoid the problems described above, by simply bypassing the need for a CE. The essential idea of this so-called Calculation of Non-Newtonian Flow: Finite Elements & Stochastic Simulation Technique (CONNFFESSIT) approach is to combine traditional finite element techniques and Brownian dynamics simulations that solve the kinetic theory equations of the polymer. In contrast to a conventional finite element approach, however, the polymer contribution to the stress,
The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

Figure 8. Stability analysis of the planar Couette flow using the DG method and the SUPG formulation using the θ-scheme. A color version of this image is available at http://www.mrw.interscience.wiley.com/ecm

Figure 9. Overview of the modeling of the flow of viscoelastic fluids. The traditional approach starts from pure continuum mechanics whereas the more modern approach uses models based on microstructural theory. Closed-form constitutive equations from both approaches are either in differential or integral form. The latest simulations that avoid closed-form constitutive equations are based on stochastic integration techniques, such as Brownian dynamics.

6 GOVERNING EQUATIONS

The governing momentum equations are as stipulated by equation (2) and (1). As before, we will use the Oldroyd-B model.

As an example of an integral model derived from microstructural theory, we will use the well-known Doi–Edwards model with (IAA) by Doi and Edwards (1986), in which only the longest relaxation time of the original Doi–Edwards spectrum, the reptation time, here denoted by \( \lambda \), is retained. The polymer stress \( \tau \) in this model is proportional to the orientation tensor \( S \),

\[
\tau = 5G_0 S
\]  

(37)

The constant \( G_0 \) is the elastic modulus, \( G_0 = nk_BT \), where \( n \) is the number of tube segments per unit volume, \( k_B \) denotes Boltzmann’s constant, and \( T \) denotes the absolute temperature. The orientation tensor \( S \) is an integral over the deformation history:

\[
S(t) = \int_{-\infty}^{t} \mu(t; t') \hat{Q}(t; t') \, dt'
\]  

(38)

where the weight factor \( \mu(t; t') = \exp[-(t - t')/\lambda]/\lambda \) and \( \hat{Q}(\vec{x}; t; t') \) is a tensor representing the orientation of tube segments that were created at time \( t' \) and surviving at the current time \( t \). Using Currie’s approximation (Currie,
1982), the tensor $\hat{Q}(\vec{x}, t; t')$ can be fully expressed in terms of the Finger tensor $B(x, t; t')$:

$$\hat{Q} = \frac{1}{(I_B - 1 + 2\sqrt{I_B} + 13/4)} \left[ B - \frac{B^{-1}}{\sqrt{I_B} + 13/4} \right]$$

(39)

In this expression $I_B$ denotes the trace of $B$ and $I_{B_B}$ denotes the second invariant of $B$,

$$I_B = \frac{1}{2}(I_B^2 - I_{B^2})$$

(40)

As example of a stochastic model, we use the Hookean dumbbell. In this model, a polymer solution is considered as a suspension of noninteracting elastic dumbbells consisting of two Brownian beads with friction coefficient $\zeta$ connected by a linear spring. The configuration of a dumbbell, that is, the length and orientation of the spring connecting the two beads, is indicated by a vector $Q$. The spring force can thus be written as $F^{(c)} = HQ$, where $H$ is the spring constant. It is possible to describe this model in terms of a distribution function and a diffusion equation (the Fokker–Planck equation); see Bird et al. (1987b). It turns out that the model can be closed and the stress is given by the Oldroyd-B equation with a relaxation time $\lambda = \zeta/4H$ and $\eta = nkT\lambda$. An alternative, but equivalent, approach for generating the configuration distribution is to make use of a stochastic differential equation. This approach for generating the configuration distribution is the result of a stochastic process acting on the individual dumbbells. In order to compute the extra stress in every point of the domain.

7 THE DEFORMATION FIELDS

METHOD

In integral type models, such as the Doi–Edwards model given by equations (37) to (39), we need to find the Finger tensor $B_{i'}(t)$ at all past times $t'$. The time evolution of the Finger tensor $B_{i'}(t)$ for a fixed particle and fixed reference time $t'$ is governed by

$$\dot{B}_{i'} = L \cdot B_{i'} + B_{i'} \cdot L^T$$

(44)

where $L = (\nabla u)^T$. The initial condition is $B_{i'}(t') = I$, where $I$ is the unity tensor. In principle, equation (44) must be solved for all particles and all reference times $t' < t$ in order to compute the extra stress in every point of the domain.

Particle tracking can be avoided by introducing a field variable $B_{i'}(\vec{x}, t)$ and solving equation (44) in a Eulerian frame:

$$\frac{\partial}{\partial t} B_{i'} + u \cdot \nabla B_{i'} = L \cdot B_{i'} + B_{i'} \cdot L^T$$

(45)

with an initial condition

$$B_{i'}(x, t') = I$$

(46)

for the complete field. Note, that $t'$ is still fixed and we have to solve equation (45) for all reference times $t' < t$. The field variable $B_{i'}(\vec{x}, t)$ for fixed $t'$ is called a deformation field in Peters, Hulsen and van den Brule (2000a). DFs (labelled by their creation time $\tau$) are independent Gaussian variables with zero mean and variance $\Delta t$. Once the configurations are known, the stress can be estimated by

$$\tau \approx -nkT I + nH \frac{1}{N_d} \sum_{i=1}^{N_d} Q_i Q_i$$

(43)

where $N_d$ is the number of dumbbells and $Q_i$ represents the $i$th dumbbell in the ensemble.
The original deformation fields method (DFM) as described above has some serious drawbacks, such as removal and creation of fields and unsteady fields even if the flow is steady. These drawbacks are related to the labeling of fields by the absolute reference (creation) time \( t' \). Therefore, in Hulsen, Peters and van den Brule (2001) an improved DFM is developed that uses the age \( \tau = t - t' \) as independent variable instead of \( t' \):

\[
B(x, t, \tau) = B_{t'-\tau}(x, t)
\]

(47)

The equation for \( B(x, t, \tau) \) now contains an extra term compared to the equation for \( B(x, t, \tau) \):

\[
\frac{\partial B}{\partial t} + \frac{\partial B}{\partial \tau} + u \cdot \nabla B = L \cdot B + B \cdot L^T
\]

(48)

where \( u \) and \( L \) are functions of \((x, t)\) only and thus independent of \( \tau \). Instead of solving a \( n \)-dimensional hyperbolic equation for each \( t' < t \), we now have to solve a \( n+1 \)-dimensional hyperbolic equation. Also the initial condition equation (46) for each field has now turned into the boundary condition:

\[
B(x, t, 0) = I
\]

(49)

We usually assume that at the start \((t = 0)\) the fluid has been at rest for a long time and the initial condition

\[
B(x, 0, \tau) = I
\]

(50)

is valid. Once we have \( B(x, t, \tau) \), we can compute the stress by integrating over the \( \tau \)-co-ordinate.

8 BROWNIAN CONFIGURATION FIELDS

In order to solve a flow problem, it is necessary to find an expression for the stress at a specified position \( x \) at time \( t \). For the stochastic model, we have to convect a sufficiently large number of dumbbells through the flow domain until they arrive at \( x \) at time \( t \). Neglecting center-of-mass diffusion, these dumbbells all experienced the same deformation history but were subjected to different and independent stochastic processes.

However simple in theory, a number of problems have to be addressed in practice. For instance, if we disperse a large number of dumbbells into the flow domain we not only have to calculate all their individual trajectories but, to calculate the local value of the stress, we must every time step also sort all the dumbbells into cells (or elements). Once these problems are solved, it is possible to construct a transient code to simulate a nontrivial flow problem. We used a different approach that overcomes the problems associated with particle tracking. Instead of convecting discrete particles specified by their configuration vector \( Q_i \) an ensemble of \( N_f \) continuous configuration fields \( Q(x, t) \) is introduced. Initially, the configuration fields are spatially uniform and their values are independently sampled from the equilibrium distribution function of the Hookean dumbbell model. After start-up of the flow field, the configuration fields are convected by the flow and are deformed by the action of the velocity gradient, by elastic retraction, and by Brownian motion in exactly the same way as a discrete dumbbell. The evolution of a configuration field is thus governed by

\[
dQ(x, t) = \left( -u(x, t) \cdot \nabla Q(x, t) + L(x, t) \cdot Q(x, t) \right)
\]

\[
- \frac{2H}{\xi} Q(x, t) \right) \, dt + \sqrt{\frac{4kT}{\xi}} \, dW(t)
\]

(51)

The first term on the RHS of equation (51) accounts for the convection of the configuration field by the flow. It should be noted that \( dW(t) \) only depends on time and hence it affects the configuration fields in a spatially uniform way. For this reason, the gradients of the configuration fields are well defined and smooth functions of the spatial coordinates. Of course, the stochastic processes acting on different fields are uncorrelated.

From the point of view of the stress calculation, this procedure is completely equivalent to the tracking of individual dumbbells: An ensemble of configuration vectors \( \{Q_i\} \) with \( i = 1, N_f \) is generated at \((x, t)\), which all went through the same kinematical history but experienced different stochastic processes. This is precisely what is required in order to determine the local value of the stress. The fields \( Q_i \) are called Brownian configuration fields Hulsen, van Heel and van den Brule (1997). In Öttinger, van den Brule and Hulsen (1997), it is shown that the BCF approach can be regarded as an extremely powerful extension of variance reduction techniques based on parallel process simulation.

In the remainder of this paper, we prefer to scale the length of the configuration vector with \( 1/(kT) \), which is one-third of the equilibrium length of a dumbbell. The relevant equations thus become

\[
\tau = nkT(-I + c) = \frac{\eta}{\lambda}(-I + c)
\]

(52)

where \( c \) is the conformation tensor, which is dimensionless and reduces to the unity tensor at equilibrium. The closed-form CE for the Hookean dumbbell (=Oldroyd-B equation) can now be written as

\[
c + \lambda \frac{\nabla}{\xi} = I
\]

(53)
The equation for the evolution of the configuration fields becomes

\[ d\tilde{Q}(x, t) = \left(-u(x, t) \cdot \nabla \tilde{Q}(x, t) + L(x, t) \cdot \tilde{Q}(x, t) \right) - \frac{1}{2\lambda} \tilde{Q}(x, t) \, dt \quad + \sqrt{\frac{T}{\lambda}} dW(t) \]  

Finally, the conformation tensor field follows from

\[ c(x, t) = \frac{1}{N_f} \sum_{i=1}^{N_f} \tilde{Q}_i(x, t) \tilde{Q}_i(x, t) \]  

From now on the tildes are dropped and it is understood that \( Q \) is a dimensionless quantity.

9 NUMERICAL METHODS

9.1 Spatial discretization

For the spatial discretization of the system of equations, we will use the finite element method. In order obtain a better stability and extend the possible stress space, we use the DEVSS formulation of Guenette and Fortin (1995b) for the discretization of the linear momentum balance and the continuity equation. The DG formulation will be used to discretize the closed-form CEs, the convection equation for the DFs and the equation for the configuration fields. In the DG formulation, the interpolation functions are discontinuous across elements, leading to a minimal coupling between elements. This means that in our time-stepping scheme the convected variables at the next time step can be computed at the element level. In this way, we avoid solving a large number of coupled equations.

In this work, we use quadrilateral elements with continuous biquadratic polynomials for the velocity, discontinuous linear polynomials for the pressure and continuous bilinear polynomials for the projected velocity gradients and discontinuous bilinear polynomials for \( c, B, \) and \( Q \).

9.2 Time discretization

For the time discretization of the convection equations, we use explicit schemes. For the CE and the equation for the configuration fields we use an explicit Euler scheme, whereas for the DF we use a second-order Adams–Bashforth scheme for stability (Hulsen, Peters and van den Brule, 2001). At each step we find the convected quantity at the next time level \( r^{n+1} \), that is, \( c^{n+1}, B^{n+1} \) or \( Q^{n+1} \), by solving the equations at the element level. From these values we can compute the polymer stress \( \tau^{n+1} \). The nonlinear inertia terms are also treated in an explicit way, which leads to a system matrix for solving \( (u^{n+1}, p^{n+1}, H^{n+1}) \) that is symmetrical and LU decomposition is performed at the first time step. Since this matrix is constant in time, solutions at later time steps can be found by back substitution only. This results in a significant reduction of the CPU time.

10 RESULTS

We consider the planar flow past a cylinder of radius \( a \) positioned between two flat plates separated by a distance \( 2H \). The ratio \( a/H \) is equal to 2 and the total length of the flow domain is \( 30a \). The flow geometry is shown in Figure 10.

Rather than specifying inflow and outflow boundary conditions, we take the flow to be periodical. This means that we periodically extend the flow domain such that cylinders are positioned \( 30a \) apart. The flow is generated by specifying a flow rate \( Q \) that is constant in time. The required pressure gradient is computed at each instant in time. We assume no-slip boundary conditions on the cylinder and the walls of the channel. Since the problem is assumed to be symmetrical we only consider half of the domain and use symmetry conditions on the center line, that is, zero tangential traction.

The dimensionless parameters governing the problem are the Reynolds number \( \text{Re} = \rho U a/\eta \), the Weissenberg number \( Wi = \lambda U / \eta \), and the viscosity ratio \( \eta_e/\eta \), where \( U = Q/2H \) is the average velocity and \( \eta \) is the zero-shear-rate viscosity of the fluid. For an Oldroyd-B fluid/Hookean dumbbell, we have \( \eta = \eta_e + \eta \) and, for the Doi–Edwards model, it is given by \( \eta = \eta_e + G_\eta \lambda \). We will define the dimensionless drag coefficient by \( K = F_x/\eta U \) where \( F_x \) is the drag force per unit length on the cylinder.

First we show some results for the Oldroyd-B and Hookean dumbbell model for which we take \( \text{Re} = 0.01 \) and \( \eta_e/\eta = 1/9 \). The dimensionless drag coefficient at a Weissenberg number of \( Wi = 0.6 \) until \( tU/a = 7 \) is shown in Figure 10.

![Figure 10. Geometry of the cylinder between two flat plates. The flow is from left to right.](image-url)
The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

Figure 11. The drag on the cylinder for $Wi = 0.6$ as a function of time for the Oldroyd-B and the Hookean dumbbell.

Figure 11. We have a good agreement between the Oldroyd-B model and the Hookean dumbbell, although the latter model shows fluctuations that are typical for stochastic models. Increasing the number of BCF $N_f$ reduces the fluctuations and the drag coefficient seems to converge to a curve slightly below the macroscopic curve. The reason for the slightly different drag coefficient is due to the coarseness of the mesh. In Hulsen, van Heel and van den Brule (1997), it is shown that the BCF method is convergent with mesh refinement.

To show that the BCF method leads to smooth functions in space, we have plotted contours of $c_{xx}$ in Figure 12 for both the Oldroyd-B and the Hookean dumbbell model. We see that the agreement is excellent.

Now we show some results for the Doi–Edwards model with IAA and a single relaxation time. We take $Re = 0$ and $\eta_e = 0.05\eta$ for stability reasons (see Peters et al., 2000b). The dimensionless drag coefficient at a Weissenberg number of $Wi = 0.6$ until $tU/a = 4$ is shown in Figure 13. Also shown is the dimensionless drag coefficient for an Oldroyd-B model with the same value of $\eta_e$, $\eta$, and $\lambda$. The drag of the Doi–Edwards model for larger times is much lower than the Oldroyd-B model due to shear-thinning in the Doi–Edwards model.

11 CONCLUSIONS AND DISCUSSION

We have reviewed a number of mixed finite element methods to solve viscoelastic flow problems. Today, the method of choice appears either the DEVSS(-G)/DG or the DEVSS(-G)/SUPG formulation. The use of the ‘-G’ formulation appears mandatory if the stability of viscoelastic flows is examined, and therefore is also recommended for time-dependent flow analysis. The key advantage of the DEVSS(-G)/DG method is its relative efficiency due to possibility to eliminate the extra stress variables on an element-by-element level. Moreover, the DG method appears to be more robust in the presence of geometrical singularities (Baaijens, 1998). The limitation of this method, however, is its inability to correctly predict the stability of viscoelastic flows. For this purpose, the DEVSS-G/SUPG formulation is superior.

We have also reviewed two methods that are the building blocks for implementation in fluid mechanics codes of models that start from microstructural concepts: the DFM method and the BCF method. The DFM method is for implementation of integral models and the BCF method
The Use of Mixed Finite Element Methods for Viscoelastic Fluid Flow Analysis

Figure 13. The drag on the cylinder for \( Wi = 0.6 \) as a function of time for the Doi–Edwards model and an Oldroyd-B model with the same parameters.

is for implementation of stochastic models. Both methods seem to behave excellently in a time-dependent Eulerian frame.

We have only discussed the basic techniques using the most elementary models. However, both the DF and BCF method can be applied to much more advanced models. For example, the DF method has been applied to complex models for melts such as the Mead–Larson–Doi model (Peters et al., 2000b), the Marrucci–Greco–Ianniruberto model (Wapperom and Keunings, 2000) and the integral pom-pom model (Wapperom and Keunings, 2001). The BCF method has been applied to models for which closure is not possible, such as the FENE (finitely extensible nonlinear elastic) model (van Heel, Hulsen and van den Brule, 1998) and a model for fiber suspensions (Fan, Phan-Thien and Zheng, 1999a). Also, the linear stability of flows for a FENE model has been studied using the BCF method (Somasi and Khomami, 2000). In a recent development, the DF method and the BCF method have been combined to study complex flows of the stochastic model of Öttinger for polymer melts (Gigras and Khomami, 2002). No doubt, that more developments can be expected in the near future.

12 RELATED CHAPTERS

(See also Chapter 9 of Volume 1, Chapter 2, Chapter 4 of this Volume)

REFERENCES


