Numerical breakdown at high Weissenberg number in non-Newtonian contraction flows

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Abstract Planar contraction flows of non-Newtonian fluids with integral constitutive models are studied to investigate the problem of numerical breakdown at high Weissenberg or Deborah numbers. Spurious shear stress extrema are found on the wall downstream of the re-entrant corner for both sharp and rounded corners. Moreover, a non-monotonic relation between shear stress and strain rate is found when the Deborah number limit is approached, which correlates with these shear extrema. This strongly suggests that non-monotonicity between shear stress and strain rate may be responsible for the Deborah number limit problem in contraction flow simulations. This non-monotonicity is caused by the inaccuracy of the quadrature, using constitutive equations that do not have shear stress maxima when exactly evaluated. This conclusion agrees with recent analytical findings by others that inaccuracy of the integration along the streamlines – either by numerical integration or asymptotic approximation – makes the problem ill-conditioned, with spurious growth occurring on the wall downstream of the re-entrant corner.

Key words Non-monotonic numerical simulation · Quadrature · UCM

Introduction

Review

Numerical simulation of non-Newtonian contraction flows has been as active research area for nearly two decades. Simulators have been confounded by the so-called high Weissenberg number problem (Keunings 1986), i.e., all of the numerical schemes break down when the Weissenberg number (Bird et al. 1987), We, reaches a certain limit. Two major successes have been achieved by Marchal and Crochet (1987) and King et al. (1988). They increased the We limit by one order of magnitude over existing methods. However, the reasons for the high We problem have not been clearly established.

Recently, Renardy (1993) introduced a new approach using asymptotic analysis of planar flows in the neighborhood of a re-entrant corner; see Fig. 1. He investigated the stress solution very near the corner. He used the upper convected Maxwell (UCM) model (Bird et al. 1987) with a Newtonian velocity field, expecting that the Newtonian velocity and velocity of converged solution are nearly the same. Note that We can be scaled out, which means that the solutions are self-similar no matter how closely the corner is approached. Therefore Renardy’s analysis is independent of We. Some of Renardy’s conclusions are:

1. The normal stress difference is approximately symmetric and shear stress is approximately anti-symmetric about the line \( \theta = 3/4\pi \).
2. Theoretically, the stress goes through a minimum and then a maximum near the downstream wall, i.e., when \( \theta = 3/2\pi \). However, in his numerical results, crude mesh results agree with the theoretical analysis; refined meshes do not have the minimum-maximum
**Renardy’s analysis is important for at least two reasons:**

1. It suggests that the We limit may be caused by an ill-conditioned calculation of stress in the UCM model, when the stress equations are integrated along the streamlines.

2. Many, if not most, computations with integral models use Newtonian velocity as the initial guess; hundreds of iterations may be needed to get convergence. If the result from the first iteration is as spurious as is suggested by Renardy’s analysis, then there is little hope of obtaining the correct solution, even after hundreds of iterations. In a following paper, Renardy (1994) uses a specially constructed, better integration scheme and the spurious bump is removed. So Renardy’s analysis, if it is valid in practice, may have identified the mechanism of the high We problem and suggested a way to avoid it.

Our goal is to verify that Renardy’s analysis is actually applicable to the problem at hand, when a commonly used solution technique is applied to it. In this paper, we use our code to examine both the stress and velocity fields on a downstream wall region when We reaches its limit.

**Numerical strategies of our code**

The numerical code used in this paper was developed and explained in detail in Bernstein et al. (1985, 1994). The code is a parallel computer version (Tsai 1994) of the 1985 code, incorporating many enhancements by Feigl and others over the years; see, for example, Feigl (1991) and Bernstein et al. (1994). The constitutive equations we use are the KBKZ type (Bird et al. 1987). The governing equations are:

\[
\begin{align*}
\rho (\mathbf{u} \cdot \nabla) \mathbf{u} &= \rho \mathbf{f} + \nabla \cdot \mathbf{T} \\
\mathbf{T} &= -\rho \mathbf{I} + \tau \\
\nabla \cdot \mathbf{u} &= 0 \\
\tau(t) &= \int_{-\infty}^{t} M(t-t') [\phi_1(I_1,I_2)(C_i^{-1}(t') - \mathbf{I}) \\
&\quad + \phi_2(I_1,I_2)(I - C_i(t'))] dt' ,
\end{align*}
\]

where \(M(t)\) is the memory function, \(C_i^{-1}\) and \(C_i\) are the Finger and Cauchy strain tensors at a historical time \(t'\), relative to time \(t\), \(I_1\) and \(I_2\) are their traces, respectively. Time \(t = 0\) is typically chosen in steady flow situations.

The weak form of the governing equations can be derived by applying a Galerkin method to equations (1):

\[
\begin{align*}
\int_{\Omega} [\tau \cdot \nabla \mathbf{v}^h + 2\zeta (\nabla \cdot \mathbf{u}^h)(\nabla \cdot \mathbf{v}^h) \\
&+ \rho [(\mathbf{u}^h \cdot \nabla) \mathbf{u}^h] : \mathbf{v}^h - \mathbf{v}^h \cdot \mathbf{f} d\Omega = 0, \quad \forall \mathbf{v}^h \in H_0^1(\Omega) ,
\end{align*}
\]

where \(\zeta\) is a penalty number for incompressibility (Bernstein et al. 1985). \(H_0^1(\Omega)\) is the appropriate space for the test functions, since velocities are imposed on all boundaries for the trial functions, with a ‘predecessor flow’ upstream of the finite domain (Bernstein et al. 1994). The strain is computed by tracking the particle path along the streamlines. With the NRC element (Bernstein et al. 1985), the streamlines and the strains can be calculated analytically in the element. The calculated strain is then substituted into the constitutive equation of (1). The quadrature rule used for integrating the constitutive equation is the composite Simpson’s rule (Feigl 1991; Bernstein et al. 1994):

\[
\begin{align*}
\int_{T}^{0} G(t) dt &= \sum_{j} \frac{\Delta t}{6} \left[ G(t_j) + 4G\left(\frac{t_j + t_{j+1}}{2}\right) + G(t_{j+1}) \right] \\
&\quad + O(\Delta t^4) ,
\end{align*}
\]

where \(\Delta t = t_{j+1} - t_j = |T_j|/n\) and \(n = 1, 2, 3, \ldots, \) \(T_j\) is the cut-off time when the integrand is small enough. It means there are \(n\) subintervals used in the integration before the memory function decays to some \(\varepsilon\), whose value can be used to choose \(T_j\). Note that the left end and right end fall on the boundary of element \(i\). In our code, \(\varepsilon\) is set to 0.01, i.e., the composite Simpson’s rule is used before the memory decays to 0.01, and \(\Delta t\) is fixed.

**Numerical results**

The geometry we use is the canonical 4:1 contraction flow with a parabolic velocity profile on the inlet and outlet. One of the meshes we tested is shown in Fig. 2, where there are total 810 elements. The dimension of the corner mesh is about 0.05 of the width of the down-