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A LEAST SQUARES FINITE ELEMENT METHOD FOR VISCOELASTIC FLUID FLOW PROBLEMS

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SUMMARY

Viscoelastic flows remain a demanding class of problems for approximate analysis, particularly at increasing Weissenberg numbers. Part of the difficulty stems from the convective behavior and in the treatment of the stress field as a primary unknown. This latter aspect has led to the use of higher-order piecewise approximations for the stress approximation spaces in recent finite element research. The computational complexity of the discretized problem is increased significantly by this approach but at present it appears the most viable technique for solving these problems. Motivated by recent success in treating mixed systems and convective problems, we formulate here a least squares finite element method for the viscoelastic flow problem. Numerical experiments are conducted to test the method and examine its strengths and limitations. Some difficulties and open issues are identified through the numerical experiments. We consider the use of high degree elements (*p* refinement) to improve performance and accuracy.

KEY WORDS Viscoelastic Least squares Finite elements

INTRODUCTION

The numerical simulation of viscoelastic flows is an important and challenging research topic that has met with limited success during the past two decades. In particular, as the Weissenberg number for a viscoelastic flow problem increases beyond the so-called 'critical' value, most numerical schemes breakdown (e.g. see References 1–6). Clear evidence indicating significant numerical inaccuracy for simulation of flow of second-order fluids at relatively low Weissenberg numbers has been provided by Mendelson *et al.*[7] More recently, Keuning[8] carried out extensive mesh refinement studies to investigate the nature of the problem and sensitivity to the mesh resolution. His results suggest that limit points which are associated with the degradation of the numerical schemes are numerical artifacts, since the limit points decrease significantly as the grid is refined.

Part of the difficulty in approximating these flows stems from the type of the equations. The theoretical analyses of Joseph *et al.*[9] and Dupret and Marchal[10] describe the underlying hyperbolicity and change of type inherent in the viscoelastic flow equations. As the Weissenberg number is increased, the convective terms in the constitutive equations play a more dominant role and the hyperbolicity increases. It is well known that standard Galerkin finite element methods lead to central difference type operators that are not well suited to hyperbolic problems. Petrov–Galerkin and similar strategies (e.g. Taylor–Galerkin methods) introduce numerical dissipation and have been successfully applied to convective problems. For example, Marchal and Crochet[11] have developed a Petrov–Galerkin finite element scheme employing a streamline upwind formulation for viscoelastic flows.

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Using a Petrov–Galerkin or similar strategy does not suffice in itself to produce a convergent method at moderate and high Weissenberg numbers. Recent work has also emphasized the need to have consistent approximation spaces for the respective velocity and stress variables. That is, in the spirit of the consistency theory for velocity and pressure approximations in mixed Navier–Stokes formulations, similar concepts are required here.[12,13] Accordingly, Marchal and Crochet[1] use different discretizations for the piecewise polynomial spaces: for example, each biquadratic velocity element is subdivided into a uniform subgrid to produce the discretization for the piecewise bilinear stresses. Their best results are obtained using a 4×4 submesh and this technique permits computation to high Weissenberg number. It also corroborates the previous statement regarding limit points.

The major detraction to this procedure, however, is the increased computational complexity necessitated by the added discretization for the stresses. Viscoelastic flows generally require fine graded meshes and this restriction for the stress discretization exacerbates the problem. If a similar requirement was made in three dimensions—and this is not yet known—then the practical value of the method would be limited.

For these reasons, alternative computationally less intensive methods that could address this class of problems would be of great significance and value. Least-squares finite element techniques are particularly appealing for several reasons: first, they lead to symmetric discrete systems and are better suited to problems with change of type; secondly, for convective problems they have been shown to be equivalent to Petrov–Galerkin type variational statements; finally, and of greatest importance in the present context, recent studies with mixed systems indicate that the consistency conditions on the approximation spaces can be relaxed.[14–16] This last point suggests that a finer discretization for stresses might not be necessary in a least-squares formulation and has motivated the present study. Since high degree (high p) finite element methods are less sensitive to the consistency issue and offer accurate approximation on coarse grids, we also consider their applicability.

BASIC EQUATIONS

Although the least-squares approach is quite general, for clarity of exposition we will concentrate on the flow of a steady upper-convected Maxwell fluid. This is also a common test case (although physically other models might be preferred). The constitutive equation for an upper-convected Maxwell fluid is defined by

$$\tau_{ij} + \lambda \hat{\tau}_{ij} = 2\eta_0 D_{ij}, \tag{1}$$

where

$$\hat{\tau}_{ij} = \frac{\partial \tau_{ij}}{\partial t} + u_k \frac{\partial \tau_{ij}}{\partial x_k} - \frac{\partial u_i}{\partial x_k}\tau_{kj} - \frac{\partial u_i}{\partial x_k}\tau_{ki} \tag{2}$$

and

$$D_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{3}$$

for velocity u_i, viscosity η_0 and relaxation time λ.

The equations governing the steady flow of a two-dimensional Maxwell fluid with velocity (u, v) and pressure p are the momentum equations

$$Re\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) + \frac{\partial p}{\partial x} - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{xy}}{\partial y} = 0, \tag{4}$$

$$Re\left(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)+\frac{\partial p}{\partial y}-\frac{\partial \tau_{xy}}{\partial x}-\frac{\partial \tau_{yy}}{\partial y}=0 \tag{5}$$

and continuity equation

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0. \tag{6}$$

The stress components satisfy the system of equations

$$\tau_{xx}\left(1-2We\frac{\partial u}{\partial x}\right)+We\left(u\frac{\partial \tau_{xx}}{\partial x}+v\frac{\partial \tau_{xx}}{\partial y}\right)-2We\tau_{xy}\frac{\partial u}{\partial y}-2\frac{\partial u}{\partial x}=0, \tag{7}$$

$$\tau_{yy}\left(1-2We\frac{\partial v}{\partial y}\right)+We\left(u\frac{\partial \tau_{yy}}{\partial x}+v\frac{\partial \tau_{yy}}{\partial y}\right)-2We\tau_{xy}\frac{\partial v}{\partial x}-2\frac{\partial v}{\partial y}=0, \tag{8}$$

$$-We\tau_{xx}\frac{\partial v}{\partial x}-We\tau_{yy}\frac{\partial u}{\partial y}+We\left(u\frac{\partial \tau_{xy}}{\partial x}+v\frac{\partial \tau_{xy}}{\partial y}\right)+\tau_{xy}-\frac{\partial u}{\partial y}-\frac{\partial v}{\partial x}=0. \tag{9}$$

Here $Re=\rho UL/\eta_0$ and $We=\lambda U/L$ are the Reynolds and Weissenberg numbers, respectively, for given velocity and length scales U and L. Equations (4)–(9) together with the associated boundary conditions complete the classical mathematical statement of the problem.

LEAST SQUARES FINITE ELEMENT METHOD

For any admissible 'trial' functions, $u, v, p, \tau_{xx}, \tau_{yy}$ and τ_{xy} satisfying the boundary conditions, we may define residuals r_i, $i=1,2,\ldots 6$ for the governing equations (4)–(9). A corresponding least-squares functional may then be defined as

$$I=\frac{1}{2}\int_\Omega (r_1^2+r_2^2+r_3^2+r_4^2+r_5^2+r_6^2)\,\mathrm{d}x\,\mathrm{d}y,$$

where $r_1, r_2, \ldots, r_6$ are obtained by substitution of the admissible trial functions in the respective governing equations on domain Ω.

Taking variations with respect to $u, v, p, \tau_{xx}, \tau_{yy}$ and τ_{xy}, the stationary condition $\delta I=0$ implies

$$\int_\Omega \sum_{j=1}^{6} r_j \delta r_j\,\mathrm{d}x\,\mathrm{d}y=0, \tag{10}$$

where

$$\delta r_j=\frac{\partial r_j}{\partial u}\delta u+\frac{\partial r_j}{\partial v}\delta v+\cdots+\frac{\partial r_j}{\partial \tau_{xy}}\delta\tau_{xy}. \tag{11}$$

From the general form of (10), (11) we see that the stationary condition does yield an equivalent variational statement involving the respective residuals of the governing equations and weight functions that depend on the derivatives of the residual with respect to the field variables. Hence, this is equivalent to a complicated form of Petrov–Galerkin method. (For a related discussion of a simpler class of problems see, e.g. Carey and Jiang[17])

Introducing finite element expansions

$$u_h=\sum_{j=1}^{N} u_j\phi_j(x,y),\ \ldots,\ \tau_{xy}=\sum_{k=1}^{K} \tau_{xy}^k \chi_k(x,y) \tag{12}$$

into the weak statement (10), (11) and setting $\delta u=\phi_i(x,y),\ldots,\delta\tau_{xy}=\chi_l(x,y)$ leads to a nonlinear discrete system of algebraic equations to be solved. In the numerical results shown later we use the same basis for all field variables.

This system can be solved iteratively using various methods. In the present studies we have considered both successive approximation and Newton iteration in conjunction with incremental continuation in the Weissenberg number. For example, in the successive approximation scheme, the residuals for iterate n are linearized using the previous iterate (iterate $n-1$) as

$$
\begin{aligned}
r_1^n&=Re\left(u^{n-1}\frac{\partial u^n}{\partial x}+v^{n-1}\frac{\partial u^n}{\partial y}\right)+\frac{\partial p^n}{\partial x}-\frac{\partial \tau_{xx}^n}{\partial x}-\frac{\partial \tau_{xy}^n}{\partial y},\\
r_2^n&=Re\left(u^{n-1}\frac{\partial v^n}{\partial x}+v^{n-1}\frac{\partial v^n}{\partial y}\right)+\frac{\partial p^n}{\partial y}-\frac{\partial \tau_{xy}^n}{\partial x}-\frac{\partial \tau_{yy}^n}{\partial y},\\
r_3^n&=\frac{\partial u^n}{\partial x}+\frac{\partial v^n}{\partial y},\\
r_4^n&=(-2We\,\tau_{xx}^{n-1}-2)\frac{\partial u^n}{\partial x}+We\left(u^{n-1}\frac{\partial \tau_{xx}^n}{\partial x}+v^{n-1}\frac{\partial \tau_{xx}^n}{\partial y}\right)-2We\,\tau_{xy}^{n-1}\frac{\partial u^n}{\partial y}+\tau_{xx}^n,\\
r_5^n&=(-2We\,\tau_{yy}^{n-1}-2)\frac{\partial v^n}{\partial y}+We\left(u^{n-1}\frac{\partial \tau_{yy}^n}{\partial x}+v^{n-1}\frac{\partial \tau_{yy}^n}{\partial y}\right)-2We\,\tau_{xy}^{n-1}\frac{\partial v^n}{\partial x}+\tau_{yy}^n,\\
r_6^n&=-We\,\tau_{xx}^{n-1}\frac{\partial v^n}{\partial x}-We\,\tau_{yy}^{n-1}\frac{\partial u^n}{\partial y}+We\left(u^{n-1}\frac{\partial \tau_{xy}^n}{\partial x}+v^{n-1}\frac{\partial \tau_{xy}^n}{\partial y}\right)+\tau_{xy}^n-\frac{\partial u^n}{\partial y}-\frac{\partial v^n}{\partial x}.
\end{aligned}
\tag{13}
$$

Then, the variations with respect to new iterate values are

$$
\begin{aligned}
\delta r_1^n&=Re(u^{n-1}\delta u_x+v^{n-1}\delta u_y)-\delta p_x-\delta(\tau_{xx})_x-\delta(\tau_{xy})_y,\\
\delta r_2^n&=Re(u^{n-1}\delta v_x+v^{n-1}\delta v_y)-\delta p_y-\delta(\tau_{xy})_x-\delta(\tau_{yy})_y,\\
\delta r_3^n&=\delta u_x+\delta v_y,\\
\delta r_4^n&=(-2We\,\tau_{xx}^{n-1}-2)\delta u_x+We(u^{n-1}\delta(\tau_{xx})_x+v^{n-1}\delta(\tau_{xx})_y)-2We\,\tau_{xy}^{n-1}\delta u_y+\delta\tau_{xx},\\
\delta r_5^n&=(-2We\,\tau_{yy}^{n-1}-2)\delta v_y+We(u^{n-1}\delta(\tau_{yy})_x+v^{n-1}\delta(\tau_{yy})_y)-2We\,\tau_{xy}^{n-1}\delta u_x+\delta\tau_{yy},\\
\delta r_6^n&=-We\,\tau_{xx}^{n-1}\delta v_x-We\,\tau_{yy}^{n-1}\delta u_y+We(u^{n-1}\delta(\tau_{xy})_x+v^{n-1}\delta(\tau_{xy})_y)+\delta\tau_{xy}-\delta u_y-\delta v_x,
\end{aligned}
\tag{14}
$$

where $\delta u,\ldots,\delta\tau_{xy}$ are the basis functions indicated previously.

Using this iterative linearization in (10), (11), the element matrix contributions to the system for nodal vector $\mathbf{U}_e^{\mathrm{T}}=(u,v,\tau_{xx},\ldots\tau_{xy},p)_e$ can be written in the compact form

$$
\mathbf{K}_e^{n-1}=\int_{\omega_e}(\mathbf{A}_{n-1}\phi_x+\mathbf{B}_{n-1}\phi_y+\mathbf{C}\phi)_e^{\mathrm{T}}(\mathbf{A}_{n-1}\phi_x+\mathbf{B}_{n-1}\phi_y+\mathbf{C}\phi)_e\,\mathrm{d}x\,\mathrm{d}y,
\tag{15}
$$

where n is the iterate, e is the element index, and the same basis $\{\phi_i\}$ has been taken for all field variables. The matrices in (15) are

$$
\mathbf{A}_{n-1}=\begin{bmatrix}
Re\,u & 0 & -1 & 0 & 0 & 1\\
0 & Re\,u & 0 & -1 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0\\
-2We\,\tau_{xx}-2 & 0 & We\,u & 0 & 0 & 0\\
0 & -2We\,\tau_{xy} & 0 & 0 & We\,u & 0\\
0 & -We\,\tau_{xx} & 0 & We\,u & 0 & 0
\end{bmatrix}_{n-1}
$$

$$\mathbf{B}_{n-1}=\begin{bmatrix} Re\,v & 0 & 0 & -1 & 0 & 0 \\ 0 & Re\,v & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -2We\,\tau_{xy} & 0 & We\,v & 0 & 0 & 0 \\ 0 & -2We\,\tau_{yy}-2 & 0 & 0 & We\,v & 0 \\ -We\tau_{yy}-1 & 0 & 0 & We\,v & 0 & 0 \end{bmatrix}_{n-1}$$

$$\mathbf{C}=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{16}$$

The second approach is Newton–Raphson iteration of the nonlinear discretized system. Recalling the form of the least-squares variational statement in (10), (11) and noting the dependence of $r_1, r_2, \ldots, r_6$ on $u, v, \tau_{xx}, \tau_{xy}, \tau_{yy}$ and p, we obtain

$$\begin{aligned}
\int_\Omega \left(r_1 \frac{\partial r_1}{\partial u} + r_2 \frac{\partial r_2}{\partial u} + r_3 \frac{\partial r_3}{\partial u} + r_4 \frac{\partial r_4}{\partial u} + r_5 \frac{\partial r_5}{\partial u} + r_6 \frac{\partial r_6}{\partial u} \right) \mathrm{d}x\,\mathrm{d}y &= 0, \\
\int_\Omega \left(r_1 \frac{\partial r_1}{\partial v} + r_2 \frac{\partial r_2}{\partial v} + r_3 \frac{\partial r_3}{\partial v} + r_4 \frac{\partial r_4}{\partial v} + r_5 \frac{\partial r_5}{\partial v} + r_6 \frac{\partial r_6}{\partial v} \right) \mathrm{d}x\,\mathrm{d}y &= 0, \\
\int_\Omega \left(r_1 \frac{\partial r_1}{\partial \tau_{xx}} + r_4 \frac{\partial r_4}{\partial \tau_{xx}} + r_6 \frac{\partial r_6}{\partial \tau_{xx}} \right) \mathrm{d}x\,\mathrm{d}y &= 0, \\
\int_\Omega \left(r_1 \frac{\partial r_1}{\partial \tau_{xy}} + r_2 \frac{\partial r_2}{\partial \tau_{xy}} + r_4 \frac{\partial r_4}{\partial \tau_{xy}} + r_5 \frac{\partial r_5}{\partial \tau_{xy}} + r_6 \frac{\partial r_6}{\partial \tau_{xy}} \right) \mathrm{d}x\,\mathrm{d}y &= 0, \\
\int_\Omega \left(r_2 \frac{\partial r_2}{\partial \tau_{yy}} + r_5 \frac{\partial r_5}{\partial \tau_{yy}} + r_6 \frac{\partial r_6}{\partial \tau_{yy}} \right) \mathrm{d}x\,\mathrm{d}y &= 0, \\
\int_\Omega \left(r_1 \frac{\partial r_1}{\partial p} + r_2 \frac{\partial r_2}{\partial p} \right) \mathrm{d}x\,\mathrm{d}y &= 0.
\end{aligned} \tag{17}$$

Let us denote this system as

$$\mathbf{g}(\mathbf{U})=0. \tag{18}$$

Then the iteration is: given starting iterate $\mathbf{U}^0$, for $n=0,1,2,\ldots$ compute

$$\mathbf{J}_n \delta \mathbf{U}_n = -\mathbf{g}_n, \tag{19}$$

where $\mathbf{J}_n$ is the Jacobian matrix at $\mathbf{U}_n$, $\mathbf{g}_n=\mathbf{g}(\mathbf{U}_n)$ and $\delta\mathbf{U}_n=\mathbf{U}_{n+1}-\mathbf{U}_n$. The performance of Newton iteration was superior in the numerical experiments, so results with this method alone are discussed in the next section.

Remarks

Since we are interested in simplifying the treatment of the stresses, the following results all involve the same choice of basis functions and discretization for all variables. It is easy to verify that the Jacobian matrix in (19) is symmetric.

NUMERICAL RESULTS

The first numerical example was the developing flow of an upper convected Maxwell fluid in the entrance region of a planar channel. The geometry and boundary conditions are shown in Figure 1. Our main purpose was to explore the applicability of the least-squares method with equi-interpolation. Accordingly, we began with the simplest choice of C^0 bilinear elements. The problem was solved on a uniform 32×8 discretization of bilinear elements at Weissenberg number $We=0{\cdot}5$ and produced good results. The calculation was repeated on a coarse uniform 16×4 grid again at $We=0{\cdot}5$. The coarse grid result was unsatisfactory since mass conservation was poorly modeled. Hence, it appears that the problem and formulation are particularly sensitive to the grid resolution. There were no apparent problems (such as oscillations, etc.), however, in using equi-interpolation of all field variables even with bilinear elements.

The degree k of the element basis was increased to 9- node biquadratics and the problem again solved on the coarse uniform 16×4 grid. Note that the identical basis is again used for all variables on a single grid. Once again a solution is obtained but now the results are accurate with mass well conserved as indicated by the equispaced section plots of $u, v, p, \tau_{xx}, \tau_{yy}$ and τ_{xy} in Figure 2 for Weissenberg number $We=0{\cdot}5$. Here $i=0$ corresponds to the inlet and $i=8$ to the outlet. Similar section plots for $We=1{\cdot}2$ are shown in Figure 3. These results compare favorably with those in Reference 16. The results for flows above $We=0{\cdot}3$ were obtained by using incremental continuation in We. That is, the solution at $We=0{\cdot}3$ was used as a starting iterate with increments of 0·01 and so on up to the final value of interest. We also remark that the results shown for $We=1{\cdot}2$ do not quite correspond to the convergent limit as can be seen from the profiles in Figure 3(a). These results indicate that a longer channel would be required to match the asymptotic downstream boundary condition for flow at $We=1{\cdot}2$. It is also instructive to compare the present results with those available in the literature for this type of problem. For example, a polyethylene melt flow is considered in Reference 18 for the same channel geometry using a 12×3 mesh and a collocation finite element method with bi-cubic Hermite polynomials. Convergent results were obtained for this formulation up to approximately $We=1{\cdot}06$ for a model of a High Density Polyethylene Melt and $We=2{\cdot}69$ for a model of a Low Density Polyethylene Melt.

The second example is the stick-slip problem. The domain is of size 64×1 with stick-slip point at $x=4$. Upstream, the flow is taken as fully developed. On the axis of symmetry $y=1$, we set $\partial u/\partial y=0$. Figure 4 shows the geometry and boundary conditions for this test problem. There is a strong singularity at the stick-slip point so this is a more demanding test. We began solving the problem with bilinear elements on a series of graded meshes, but the continuity constraint again was poorly satisfied. We then successively increased the degree of the finite element basis functions in a p formulation until at $p\geqslant 6$ we obtained a satisfactory solution. The results shown are for a severely graded mesh with $p=7$. (The total number of nodes is 1590 and the downstream element near the singular point is of size similar to that in Reference 11). Plots of τ_{xx} on the wall for

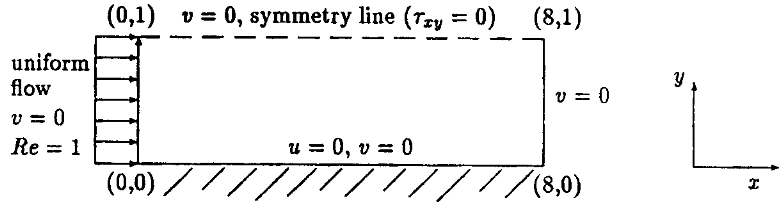

Figure 1. Domain and boundary conditions for developing flow test problem

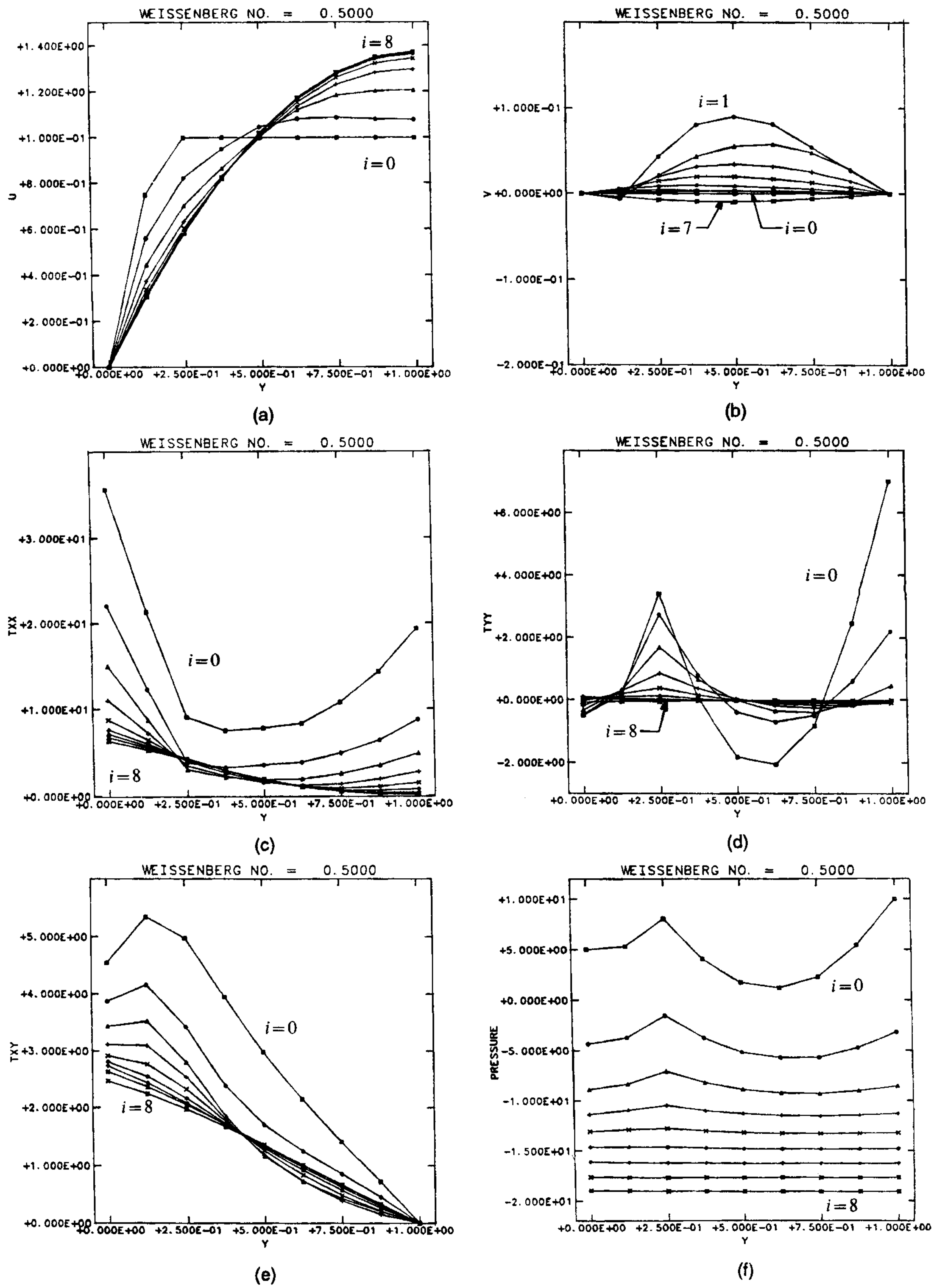

Figure 2. Profiles of $u, v, p, \tau_{xx}, \tau_{yy}, \tau_{xy}$ at equispaced sections x_i, $i=0, 1, 2, \ldots 8$, for developing flow at $We=0{\cdot}5$

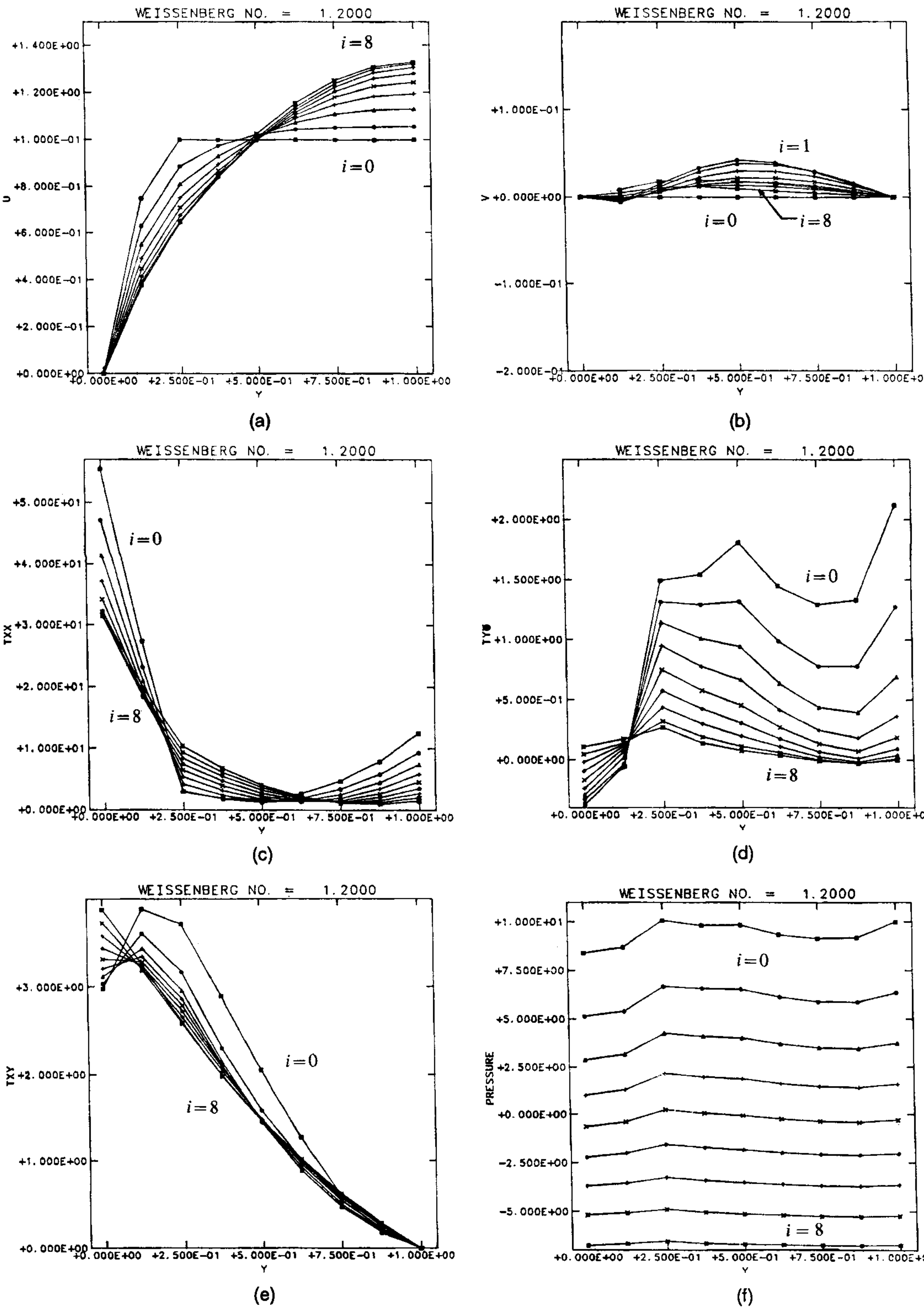

Figure 3. Section profiles for developing flow at $We = 1{\cdot}2$

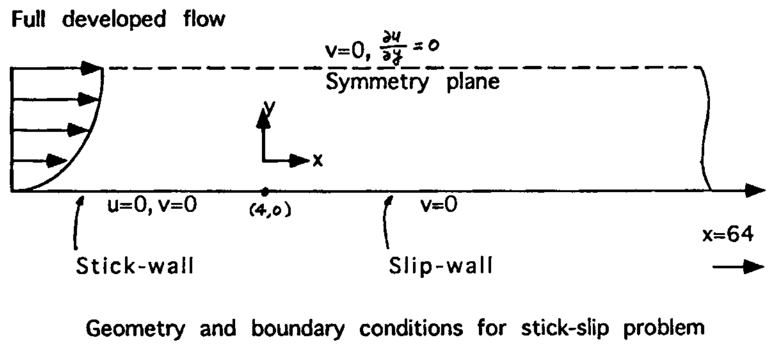

Figure 4. Domain and boundary conditions for stick–slip test problems

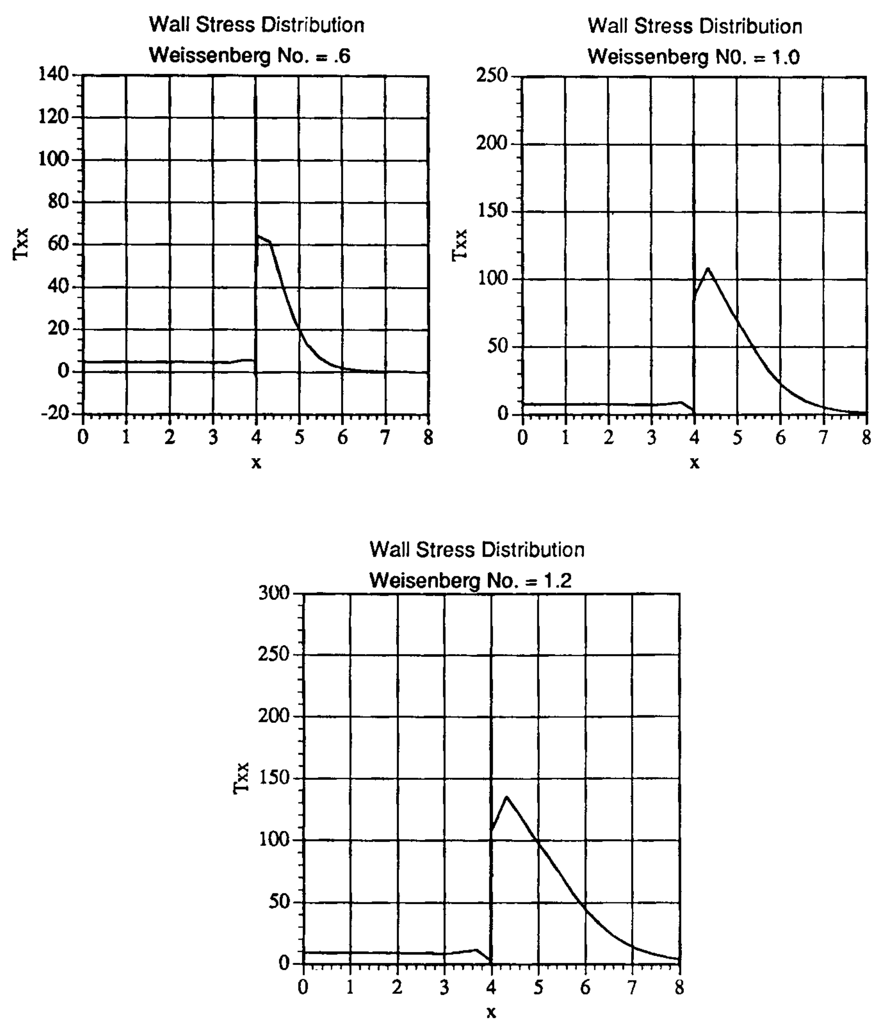

Figure 5. Plots of τ_{xx} along wall at We=0·6, 1·0 and 1·2

Weissenberg numbers equal to 0·6, 1·0 and 1·2 are shown in Figures 5 (a)–(c). The peak stress levels are comparable to those reported by Marchal and Crochet[11] for an Oldroyd-B fluid. We remark that Marchal and Crochet specify fully developed flow downstream and we use the results of a related one-dimensional problem to obtain an additional upstream stress boundary condition (to accommodate the hyperbolicity). In the least-squares treatment, we specify only the fully developed velocity profile upstream. The results for flows above $We = 0{\cdot}05$ were obtained by using incremental continuation in We. Even the continuation problem is sensitive, and for convergence we used small Weissenberg number increments that decreased from 0·01 to 0·001 as We increased. Note that $We = 1{\cdot}2$ does not correspond to the convergent limit of this problem. However, the very small Weissenberg increment (0·001) required to get a convergent solution makes further computation to higher We inefficient and future work needs to be directed to this issue.

CONCLUDING REMARKS

A new least-squares finite element method has been formulated for viscoelastic flows and some exploratory numerical experiments conducted. Equal-order bases are used for all six field variables (including the stresses) which is a departure from standard practice with the Galerkin finite element method. Results on sufficiently fine grids with bilinear elements for a developing flow of an upper-convected Maxwell fluid are satisfactory. On a coarser grid, mass conservation is not well approximated with bi-linears but biquadratics and higher degree elements still give good results. The more difficult stick–slip problems gave rise to the same problems related to mass conservation. A high p solution was achieved for a moderate range of Weissenberg numbers. There are several open theoretical questions and practical issues (such as the scaling of residuals in the least-squares functional, error analysis, high p conditioning, and continuation techniques) that warrant further study and are now being considered.[17,18]

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