Chapter 8

Numerical Simulation of Viscoelastic Flow in Some Polymer Processing Applications

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8.1 INTRODUCTION

A wide effort has been undertaken by several research groups over the last few years in order to predict the flow of polymer solutions and polymer melts in forming processes by means of numerical techniques. The non-Newtonian character of the flow under such circumstances is not limited to spectacular phenomena like the extrudate swell or the Weissenberg effect in a torsional flow; dramatic effects like vortex enhancement do also occur within confined boundaries. These phenomena, which typically are of a nonlinear nature, occur at fairly low Reynolds numbers. The amount of elasticity encountered in practical flow situations precludes the use of classical explicit constitutive equations of the hierarchy type, and one wishes to use constitutive equations which can exhibit long-range memory effects.

The difficulty of the task of elaborating a numerical technique is twofold: (i) among the many available constitutive equations, how to make a selection to solve the flow of a particular fluid under specified flow conditions; (ii) for a given constitutive equation, how to extend available techniques to solve Navier-Stokes equations towards the treatment of viscoelastic flow. A large effort has been devoted to an (apparently) simple model, the Maxwell fluid, for qualitative reasons and with the hope of understanding the effect of elasticity upon the flow. The Maxwell fluid has attracted much attention because its constitutive equations contain only two material constants: the constant shear viscosity and the relaxation time; the Maxwell fluid is a perfect candidate if one wishes to separate elastic effects from purely Newtonian effects, without the simultaneous addition of shear-thinning. For relaxation times which are greater than a characteristic time of the flow, the viscometric properties of the Maxwell fluid greatly differ from those of current polymer solutions and polymer melts. It is
thus important to extend the available numerical techniques to more realistic models; in particular, we will devote some attention in the next sections to the flow of a Phan-Thien Tanner fluid, which has suitable properties for the study of flows of an essentially elongational nature. The necessary field and constitutive equations will be reviewed in Section 8.2.

Numerical techniques are unavoidable for solving the flow of such fluids whenever the geometry is nontrivial. Different approaches have been used by various groups: finite differences, finite elements for models of the integral type and of the differential type. A comprehensive review of the numerical simulation of the flow of viscoelastic fluids may be found in Crochet and Walters. Whatever the method used for the numerical integration, an outstanding problem is the limitation of the domain of elasticity where the flow can be solved; it is indeed typical that, beyond some value of the Weissenberg number, which compares the relaxation time of the fluid to a natural time of the flow, the iterative technique used for solving the nonlinear equations breaks down. The reasons behind this lack of convergence are presently unknown. Within the course of a recent investigation, it was found that the addition of a retardation time in the constitutive equation of a fluid of the differential type greatly improves the performance of the numerical method. This improvement will be explained in the present chapter.

The numerical methods used for solving the flow of viscoelastic fluids are the subject of a recent book and will be reviewed only briefly in Section 8.3. Rather, we wish to show in more detail the applicability of the finite element method for solving flows of technical importance in polymer processing. Abrupt contractions, treated in Section 8.4, constitute a good example of the type of flow problems which are encountered in practice; the problem is difficult because re-entrant corners pose severe problems for stress calculation. Moreover, some dramatic effects like those described by Nguyen and Boger have not yet been obtained as a result of numerical simulation. Extrusion problems are ideal as examples of viscoelastic flows; indeed, the large memory effects produce an important swelling ratio for the extrudate. Large swelling ratios have been obtained by Crochet and Keunings, and the results will be summarized in Section 8.5. Another problem of great technical interest is the flow analysis of melt spinning. Theoretical analyses are based upon asymptotic equations which are valid at some distance from the spinneret; they are based upon boundary conditions which may only be confirmed by means of a closer analysis of the flow in the neighbourhood of the spinneret. Such an analysis has been the subject of a recent paper and will be reviewed in Section 8.6.

### 8.2 Constitutive Equations

Polymer solutions and polymer melts may be considered as incompressible viscoelastic fluids; the Cauchy stress $\sigma$ is decomposed as the sum of a pressure
contribution \(- p I\) and an extra-stress tensor \(T\) which is not traceless in most constitutive equations. The momentum and continuity equations are respectively given by

\[
- \nabla p + \nabla \cdot T + f = \rho \ddot{v} \tag{8.1}
\]

\[
\nabla \cdot v = 0 \tag{8.2}
\]

where \(f\) is the body force per unit volume, \(\rho\) is the specific mass and a dot denotes the material time derivative. In the present paper we will only consider axisymmetric motion; for further reference, we note that Equations (8.1) and (8.2) then become

\[
- p_r + T_{rr,r} + T_{rz,z} + (T_{rr} - T_{\theta \theta})/r + f_r = \rho \ddot{v}_r \\
- p_z + T_{rz,r} + T_{zz,z} + T_{rz}/r + f_z = \rho \ddot{v}_z \tag{8.3}
\]

\[
u_r + u/r + w_z = 0 \tag{8.4}
\]

where a comma denotes the spatial derivative, and \(u, w\) are the radial and axial components of the velocity field.

Constitutive equations for the extra-stress tensor \(T\) are needed for closing the system of Equations (8.1) and (8.2). Although full generality would dictate the use of a functional relationship between \(T\) and the strain-history of a material point, one generally adopts an integral model or a differential model, which are both special cases of the simple fluid model.\(1,2\) Details on integral models and related numerical work may be found in Viriyayuthakorn and Caswell\(^3\) and Bernstein et al.\(^4\); we will limit ourselves in the present paper to constitutive equations of the differential type, which establish a tensor relation between the extra-stress tensor \(T\), the rate-of-deformation tensor \(D = (\nabla v + \nabla v^\top)/2\), and their convected time derivatives. The upper- and lower-convected derivatives of the stress tensor \(T\), denoted respectively by \(\dot{T}\) and \(\overset{\wedge}{T}\), are defined by

\[
\overset{\wedge}{T} = \dot{T} - LT - TL^\top \tag{8.5}
\]

\[
\dot{T} = \dot{T} + TL + L^\top T \tag{8.6}
\]

where \(L\) is the velocity gradient tensor, and a dot denotes the material derivative.

One of the simplest examples of fluids of the differential type is the Maxwell fluid, which is defined by the equation

\[
T + \lambda \overset{\wedge}{T} = 2\mu D \tag{8.7}
\]

The Maxwell fluid has a constant shear viscosity, and a first normal-stress difference which is quadratic in the rate of shear. Such behaviour is unrealistic for most polymeric materials, and the interest in studying the Maxwell fluid is essentially qualitative; however, a numerical technique developed for solving the flow of a Maxwell fluid can be extended without major difficulty to the flow of
more realistic fluids, like the White–Metzner fluid\textsuperscript{16} or the Phan Thien–Tanner fluid.\textsuperscript{17} In order to complete the system formed by Equations (8.3) and (8.4), let us consider the explicit form of Equation (8.7) for the case of an axisymmetric flow; we have

\[
\begin{align*}
T_{rr} + \lambda(T_{rr,t} + T_{rr,u} + T_{rr,w}) &= 2\mu u_r, \\
T_{zz} + \lambda(T_{zz,t} + T_{zz,u} + T_{zz,w}) &= 2\mu w_z, \\
T_{\theta\theta} + \lambda(T_{\theta\theta,t} + T_{\theta\theta,u} + T_{\theta\theta,w}) &= 2\mu u/\lambda, \\
T_{rz} + \lambda(T_{rz,t} + T_{rz,u} + T_{rz,w} - u_r T_{rz} - u_z T_{rz}) &= \mu(u_z + w_r).
\end{align*}
\] (8.8)

An inspection of Equations (8.3), (8.4), (8.8) reveals the nature of the problem posed by the Maxwell fluid and related constitutive equations: it is impossible to extract from Equation (8.8) an explicit form of the extra-stress tensor in terms of the velocity field, and one must resort to numerical techniques which differ from those used for solving Navier–Stokes equations.

In later sections we will also study the flow of a fluid proposed by Phan Thien and Tanner,\textsuperscript{17} which has a constitutive equation based on a network theory. In the presence of a single relaxation time, the constitutive equation for the extra-stress tensor $T$ reads

\[
Y(\varepsilon, T\mathbf{T}) + \lambda\{1 - \frac{\xi}{2}\mathbf{T} + \frac{\xi}{2}\mathbf{T}^2\} = 2\mu\mathbf{D}
\] (8.9)

where $\xi$ and $\varepsilon$ are material parameters and $Y(\varepsilon, T)$ is a function related to the rate of creation and destruction of network junctions; the following definition is suggested by Phan Thien:\textsuperscript{18}

\[
Y(\varepsilon, T) = \exp(\varepsilon\lambda/\mu \text{ trace } T)
\] (8.10)

with the aim of describing network rupture effects in strong flows.

The viscosity coefficient $\mu$ and the relaxation time $\lambda$ are evaluated on the basis of linear viscoelastic measurements, while the dimensionless parameters $\xi$ and $\varepsilon$ are determined from nonlinear rheological properties: $\xi$ is related to the ratio of normal stress-differences and governs the amount of shear-thinning in simple shear flow, while $\varepsilon$ is the relevant parameter in steady uniaxial elongation. Values of $\xi \sim 0.2$ and $\varepsilon \sim 0.015$ are typical for low-density polyethylene.\textsuperscript{17,18}

In simple shear flow, the shear stress $T_{xy}$ is related to the shear rate $\dot{\gamma}$ by

\[
T_{xy} = \mu\dot{\gamma}/[1 + \lambda^2\dot{\gamma}^2(2 - \xi)] + O(\varepsilon).
\] (8.11)

It is easy to verify that Equation (8.11) implies an increasing value of $T_{xy}$ as a function of $\lambda\dot{\gamma}$ up to a maximum value at the critical dimensionless shear rate

\[
\lambda\dot{\gamma}_{\text{crit}} = 1/\sqrt{\xi(2 - \xi)},
\]

followed by an asymptotic decrease to zero. The constitutive Equation (8.9) is therefore unacceptable unless $\xi$ takes the values 0 or 2.

The difficulty may, however, be overcome by considering a slight modification
of the constitutive equation. The extra-stress tensor $T$ is split into two separate components

$$ T = T_1 + T_2 $$ (8.12)

where $T_1$ has a constitutive equation identical to Equation (8.9) with a viscosity coefficient $\mu_1$, while $T_2$ has a Newtonian constitutive equation, namely

$$ T_2 = 2\mu_2 D $$ (8.13)

In other words, we may consider that the extra-stress in Equation (8.12) combines the contributions of a viscoelastic fluid and a Newtonian solvent. The fluid response in simple shear flow then becomes

$$ T_{\gamma\gamma} = \{\mu_2 + \mu_1/[1 + \lambda^2 \dot{\gamma}^2 (2 - \xi)]\} \dot{\gamma} + O(\epsilon) $$ (8.14)

and one may verify easily that $T_{\gamma\gamma}$ is an increasing function of $\dot{\gamma}$ whenever

$$ \mu_2 \geq \mu_1 / 8 $$ (8.15)

When $\epsilon$ does not vanish, the Phan Thien–Tanner model predicts a finite elongational viscosity $\eta_T$ for all rates of elongation $\dot{\epsilon}$ in steady uniaxial extension; with the definition of $Y(\epsilon, T)$ given by Equation (8.10), $\eta_T$ starts from the Newtonian value of $3\mu$ for low $\dot{\epsilon}$, increases and then decreases beyond some critical value of $\dot{\epsilon}$.19

It is worth considering the special case obtained by combining Equations (8.9), (8.12) and (8.13) with $\epsilon = 0$; by eliminating $T_1$ and $T_2$ between these three equations, one obtains a differential equation which may be written as follows:

$$ T + \lambda \square T = 2\mu (D + \lambda \star D) $$ (8.16)

where

$$ \mu = \mu_1 + \mu_2; \quad \lambda \star = \lambda \mu_2 / (\mu_1 + \mu_2) $$ (8.17)

and

$$ \square T = (1 - \zeta / 2)\nabla T + \zeta / 2 \hat{T} $$ (8.18)

When $\zeta$ equals 0 or 2, Equation (8.16) becomes a four-constant Oldroyd model of the contravariant or the covariant type, respectively; $\lambda \star$ is then called a retardation time. It was noted by Oldroyd20 that Equation (8.7) implies a rate of deformation tending to infinity when the stress tensor for a material particle is discontinuous in time. The presence of the retardation time in Equation (8.16) cures that defect.

The selection of a non-dimensional parameter for evaluating the amount of elasticity of the flow is not obvious. The $Weissenberg number$ $We$ usually denotes the group $\lambda V / L$, where $\lambda$ is the relaxation time, $V$ is a characteristic velocity of the flow and $L$ is a characteristic length. A more crucial parameter is the product,
called by some the Deborah number $D_e$, of the relaxation time $\lambda$ and a characteristic wall shear-rate $\dot{\gamma}_w$. For a Maxwell fluid, the product $\lambda \dot{\gamma}_w$ is also the ratio of the first normal stress-difference $N_1$ to twice the shear stress on the wall $\tau_w$; the ratio $S_R = N_1/2\tau_w$ is called the recoverable shear. In the present paper, we will use the recoverable shear for evaluating the elasticity in the flow of Maxwell and Oldroyd-B fluids. For a Phan Thien–Tanner fluid, the problem is complicated by the fact that when $\lambda \dot{\gamma}_w$ increases, the recoverable shear first increases and then decreases. Before one compares solutions obtained by various authors, it is essential to verify that they use the same non-dimensional parameters for evaluating the elasticity of the flow.

8.3 NUMERICAL METHOD

For solving the flow of fluids of the differential type, it has become standard with several research groups\textsuperscript{5–9} to use a mixed formulation of the problem, where the unknowns are the extra-stress components, the velocity components and the pressure; the procedure was initiated by Kawahara and Takeuchi.\textsuperscript{21} Let $T^*, v^*$ and $p^*$ denote the respective finite element interpolations for $T$, $v$ and $p$; one writes

$$T^* = \sum T^{(i)} \phi_i, \quad v^* = \sum v^{(i)} \psi_i, \quad p^* = \sum p^{(i)} \pi_i$$  \hspace{1cm} (8.19)

where the $T^{(i)}$'s, $v^{(i)}$'s and $p^{(i)}$'s are nodal values, and $\phi_i, \psi_i, \pi_i$ are the associated shape functions. The problem now consists of discretizing the field Equations (8.1) and (8.2) together with the constitutive equations, which we temporarily assume to be given by Equation (8.7).

The Galerkin formulation is used for obtaining the discrete form of the constitutive equations and of the continuity equation, i.e.

$$\langle \phi_i, T^* + \lambda T^* - 2\mu D^* \rangle = 0$$  \hspace{1cm} (8.20)

$$\langle \pi_i, \nabla \cdot v^* \rangle = 0$$  \hspace{1cm} (8.21)

where the brackets denote the $L^2$-scalar product. When a Newtonian velocity field is inserted in Equation (8.20), one finds that the extra-stress components calculated from the resulting linear system are devoid of spurious oscillations, even for high values of $\lambda$. Let us replace the momentum Equations (8.1) by their weak formulation,

$$\langle -pI + T, \nabla \psi_i \rangle + \langle \psi_i, \rho \dot{v} \rangle = F^{(i)}$$  \hspace{1cm} (8.22)

where $F^{(i)}$ is the nodal force vector associated with the node $i$. In a first formulation which we call MIX1, the system of Equations (8.20), (8.21) is closed by the addition of the Galerkin form of the momentum equations,

$$\langle -p^*I + T^*, \nabla \psi_i \rangle + \langle \psi_i, \rho \dot{v}^* \rangle = F^{(i)}$$  \hspace{1cm} (8.23)
There is, however, another possible formulation, still based on Equations (8.20), (8.21) which we call MIX2. From Equation (8.7) we write

$$\mathbf{T} = 2\mu \mathbf{D} - \lambda \mathbf{T}^\nabla$$  \hspace{1cm} (8.24)

and by substitution in Equation (8.22) we obtain

$$\langle -p^* \mathbf{I} + 2\mu \mathbf{D}^*, \nabla \psi_i \rangle - \langle \lambda \mathbf{T}^*, \nabla \psi_i \rangle + \langle \psi_i, \rho \nabla \mathbf{v}^* \rangle = \mathbf{F}^{(i)}$$  \hspace{1cm} (8.25)

It has been shown elsewhere$^5$ that the method MIX1 requires piecewise polynomials of the same degree for $\phi_i$ and $\psi_i$ in Equation (8.19). A difficulty with MIX1 is its high cost due to the large number of nodal stress.$^5$ $^7$ The method MIX2 may be used with a lower degree for the $\phi_i$'s than the $\psi_i$'s,$^8$ $^9$ or with the same order.$^5$ It has been shown$^{12}$ that both suffer from the same major defect which will be made explicit in the next section: when the elasticity increases, spatial oscillations appear in the various fields, although the iterative technique for solving the nonlinear system is still converging; the iterative technique then diverges beyond some critical value of the elasticity. Unfortunately, the domain of elasticity where the method converges is much smaller than the domain of practical interest. The reasons for the appearance of the oscillations and the lack of convergence are unclear, since in particular the form of Equation (8.20) for the constitutive equations does not generate oscillations when they are not coupled with the momentum equations.

When the present authors started working on the Phan Thien–Tanner model, they found that the addition of a viscous component, as in Equations (8.12) and (8.13), was mandatory in order to avoid unstable flows. It was soon realized, however, that the decomposition expressed by Equation (8.12) would lead to an important increase of the domain of $S_R$ where the iterative numerical technique converges; moreover, it was found that the enlargement of the domain of convergence due to the presence of a viscous term would also apply for the Oldroyd-B fluid given by

$$\mathbf{T} = \mathbf{T}_1 + \mathbf{T}_2, \quad \mathbf{T}_1 + \lambda \mathbf{T}_1^\nabla = 2\mu_1 \mathbf{D}, \quad \mathbf{T}_2 = 2\mu_2 \mathbf{D}$$  \hspace{1cm} (8.26)

It is easy to design a mixed finite-element method for solving the flow of an Oldroyd-B fluid. One selects $\mathbf{T}_1$ instead of $\mathbf{T}$ as the unknown stress tensor; in place of the system consisting of Equations (8.20) and (8.23) we write

$$\langle \phi_i, \mathbf{T}_1^* + \lambda \mathbf{T}_1^\nabla - 2\mu_1 \mathbf{D}^* \rangle = 0$$  \hspace{1cm} (8.27)

$$\langle -p^* \mathbf{I} + 2\mu_2 \mathbf{D}^* + \mathbf{T}_1^*, \nabla \psi_i \rangle + \langle \psi_i, \rho \nabla \mathbf{v}^* \rangle = \mathbf{F}^{(i)}$$  \hspace{1cm} (8.28)

where we have used in Equation (8.22) the substitution

$$\mathbf{T} = 2\mu_2 \mathbf{D} + \mathbf{T}_1$$  \hspace{1cm} (8.29)
We note that, in principle, it is no longer necessary to introduce a method of the type MIX2 if we wish to use polynomials of lower degree for the stresses than for the velocity components, in view of the term $\mu_2 \mathbf{D}^*$ appearing in the momentum equations. Similar techniques apply when one uses the constitutive relation for $T_1$ given by Equation (8.9).

The boundary conditions which are necessary for solving a problem consist of those used for solving Navier–Stokes equations; in addition, when the boundary contains an entry section, one must specify the deformation history of the material points by imposing the extra-stress field on a line which crosses the streamlines. For solving the nonlinear algebraic system, we use Newton's method together with successive incrementations of the relaxation time $\lambda$. In the examples given below, we use 6-node triangular and 9-node quadrilateral isoparametric elements, with first-degree polynomials for the pressure and second-degree polynomials for the extra-stress and velocity components. We also note that the approximation for the stress and velocity components and the pressure are $C^0$-continuous.

### 8.4 DIE-ENTRY FLOW

In the present section, we will study the flow of a viscoelastic fluid in a four-to-one axisymmetric contraction. The abrupt contraction is typical of several problems of technical interest; the flow is difficult to solve on account of the stress singularity at the re-entrant corner. The numerical prediction of the flow is of genuine interest in rheology because the available experimental data on the flow behaviour have left many questions unanswered. Some molten polymers exhibit a dramatic corner vortex growth when the elasticity of the flow increases, while some others do not; a solution of polyacrylamid in glucose also shows vortex growth. It is hoped that the use of several constitutive equations for solving the problem will eventually lead to a better understanding of the subject.

Good results on die-entry flow have been obtained by Viriayuthakorn and Caswell using their finite-element method for solving the flow of fluids of the integral type; they were able to obtain converging solutions up to $S_R = 2$ on the downstream channel wall. Their results were obtained on a refined mesh; to establish a valid comparison, we have used the same mesh shown in Figure 8.1.

![Figure 8.1](image_url)

**Figure 8.1** Finite element mesh used for solving the die-entry flow
However, since our finite-element code accepts triangular and quadrilateral isoparametric elements, we have not divided the quadrilateral elements into four triangles as was done by Viriyayuthakorn and Caswell; it was suggested by Gartling et al.\textsuperscript{23} that, for solving the Navier–Stokes equations, the performance of the Lagrangian element is essentially equivalent to the performance obtained when the quadrilateral is divided in four triangles. The mesh contains 129 elements, 577 nodes and 3623 degrees of freedom.

The use of method MIX1 or method MIX2 for solving the flow of a Maxwell

\[ w \]

\[ -10 -6 -2 0 2 6 10 z \]

\[ (a) \]

\[ w \]

\[ -10 -6 -2 0 2 6 10 z \]

\[ (b) \]

Figure 8.2 Centreline axial velocity as a function of the axial coordinate: (a) Newtonian fluid; (b) Maxwell fluid, \( S_\text{r} = 1 \)
fluid defined by Equation (8.7) leads to a pattern which has been observed in solving several other problems, and which may be summarized as follows: (i) the highest attainable value of $S_R$ depends significantly upon the finite-element mesh; (ii) beyond some critical value of $S_R$, the velocity and stress fields exhibit spatial oscillations which follow the element pattern, while the pressure and the stream function remain acceptable; (iii) the iterative method ceases to converge beyond some value of $S_R$. With the mesh shown in Figure 8.1, it was found impossible, with MIX1, to solve the problem beyond $S_R = 1$. A sensitive quantity in the flow through a contraction is the axial velocity profile along the axis of symmetry. Figure 8.2(a) shows a graph of this for the Newtonian case; with a unit mean velocity in the downstream channel, the axial velocity climbs sharply from a value of 0.125 to 2. The source of the problem with the Maxwell fluid is evident in Figure 8.2(b), the values of the axial velocity at the mid-side nodes are not aligned with those at the vertices, and convergence is lost for higher values of $S_R$.

The behaviour of the algorithm in solving the contraction problem is entirely different when we consider the flow of an Oldroyd-B fluid (Equation (8.26)) rather than the Maxwell fluid (Equation (8.7)) while using the same mesh. In the present case, convergence can be obtained easily for values of $\lambda \gamma_w$ in the downstream channel as high as 4. In view of Equation (8.15), we use a ratio $\mu_2/\mu_1 = 1/8$, and the corresponding value of $S_R$ is $32/9$. In Figure 8.3, we show graphs of the centreline axial velocity for the Newtonian case and for $S_R = 16/9, 24/9$ and $32/9$; spatial oscillations appear when $S_R = 32/9$, which are presumably due to the insufficient length of the downstream channel. An overshoot of the centreline velocity may be observed in Figure 8.3; the value of the overshoot and its distance from the contraction as a function of $S_R$ is shown in Table 8.1. Viriyayuthakora and Caswell observed an overshoot of 2.5% at $z = 1$ for $S_R = 2$.

In Figure 8.4 we compare the streamlines of the Newtonian flow with those of the viscoelastic flow with $S_R = 32/9$. The normalized stream function takes the value unity on the axis of symmetry and vanishes on the wall of the die. We show the streamlines with increments of 0.1 in the main flow, and increments of 0.002 in the main vortex. One observes a moderate enlargement of the corner vortex when $S_R$ increases, while the intensity of the vortex gets larger; the intensity of the corner vortex climbs from a value of $10^{-3}$ in the Newtonian case to $7 \times 10^{-3}$ when $S_R = 32/9$, with a maximum value of 1 for the stream function. It is clear that

<table>
<thead>
<tr>
<th>$S_R$</th>
<th>0</th>
<th>8/9</th>
<th>16/9</th>
<th>24/9</th>
<th>32/9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overshoot (%)</td>
<td>—</td>
<td>0.7</td>
<td>2.15</td>
<td>3.35</td>
<td>4.21</td>
</tr>
<tr>
<td>$z$</td>
<td>—</td>
<td>1</td>
<td>1.25</td>
<td>1.25</td>
<td>1.75</td>
</tr>
</tbody>
</table>
Figure 8.3 Centreline axial velocity as a function of the axial coordinate; Oldroyd-B fluid with $S_R = 16/9, 24/9, 32/9$

Figure 8.4 Streamlines for the flow on an Oldroyd-B fluid: (a) $S_R = 0$; (b) $S_R = 32/9$
the numerical results do not exhibit the large vortex growth observed in the flow of some polymeric solutions and polymer melts.

An important global quantity in die-entry flow is the value of the entry-pressure loss. Let \( p_0 \) and \( p_L \) be the pressures calculated respectively in the entry section of the large tube and in the exit section of the small tube, and let \( \Delta p \) be the pressure loss which would be calculated on the basis of fully developed Poiseuille flow in both tubes. The entry-pressure loss is defined by

\[
\delta p_{en} = (p_0 - p_L - \Delta p)(2\tau_w) \tag{8.30}
\]

where \( \tau_w \) is the wall-shear stress in the downstream tube. Figure 8.5 shows the value of \( \delta p_{en} \) as a function of \( S_R \), together with the values reported by Viriyayuthakorn and Caswell. The fact that \( \delta p_{en} \) becomes negative is not surprising. Indeed, the existence of a fully developed Poiseuille flow in the exit section involves the appearance of normal stresses \( T_{zz} \) which exert a traction on the fluid. If we compare the average value of these tractions to the wall-shear stress in a tube of radius \( R \) we obtain

\[
\left[ \int_0^R T_{zz}2\pi r\,dr/\pi R^2 \right]/2\tau_w = S_R/2 \tag{8.31}
\]

If we take these tractions into account in calculating the entry-pressure loss, we find little difference between the Newtonian and the viscoelastic cases; this may be observed in Figure 8.5 where we have also plotted the value of \( (\delta p_{en} + S_R/2) \) as a function of \( S_R \).

It is of course deceptive that so little difference is obtained between the Newtonian flow in a contraction and the flow of a Maxwell fluid under the same conditions. It may be shown easily that the stress-field is greatly affected by the elasticity of the flow, but the kinematics remain essentially unaffected. In a recent publication,\(^{19}\) we have shown that the use of another fluid model i.e. the Phan Thien–Tanner fluid, may induce dramatic changes in the flow kinematics. We will now report briefly on some of these results.

Referring back to Equations (8.9) and (8.10), we will use here the parameters \( \varepsilon = 0.015 \) and \( \xi = 0.2 \); the values have been used by Phan Thien and Tanner\(^{17}\) for

![Figure 8.5 Entry pressure loss as a function of \( S_R \). Present paper: crosses; Viriyayuthakorn and Caswell 1980: dotted circles](image-url)
modelling the behaviour of low-density polyethylene. When \( \xi \) differs from 0 or 2, we have seen in Section 8.2 that a viscous component must be included in the constitutive equations. As for the Maxwell fluid, we select a ratio of 1/8 for \( \mu_2/\mu_1 \). It must be pointed out that the behaviour of the Phan Thien–Tanner fluid differs greatly from that of the Maxwell fluid; the former is indeed shear-thinning, and its elongational properties differ considerably from those of the latter.

The non-dimensional parameter \( S_R = N_1/2\tau_w \) is not a good indicator of the elasticity of the flow of the Phan Thien–Tanner fluid; in Figure 8.6, we find that \( S_R \) plotted against \( \lambda \dot{\gamma}_w \) goes through a maximum. We will rather use a Weissenberg number defined by

\[
We = \lambda \bar{V}/D
\]  

(3.32)

where \( \lambda \) is the relaxation time in Equation (8.9), \( \bar{V} \) is the mean downstream velocity, and \( D \) is the downstream diameter. We note that, for a Maxwell fluid, \( We = \lambda \dot{\gamma}_w/8 \).

We have been able to obtain a solution for the flow in the abrupt contraction for values of \( We \) up to 1.75. The finite element mesh is shown in Figure 8.1. It was necessary, however, to increase the length of the last few downstream elements; the memory effects are such that a length of 20 radii is necessary in order to obtain a fully developed flow at the exit.

This time, the flow kinematics are greatly affected by the elasticity of the flow. Figure 8.7 shows a graph of the centreline axial velocity as a function of the axial coordinate \( z \) for various values of \( We \). One may observe the appearance of large
Figure 8.7 Centreline axial velocity as a function of the axial coordinate for various values of the Weissenberg number; Phan Thien–Tanner fluid.

Figure 8.8 Axial velocity profile at the contraction and exit sections; Phan Thien–Tanner fluid, $We = 1$.
Figure 8.9 Streamlines for the flow of a Phan Thien–Tanner fluid:
(a) $We = 1$; (b) $We = 1.75$

velocity overshoots near the contraction section when $We$ increases; a more detailed view of this is depicted in Figure 8.8 where we have plotted the axial velocity profile at the contraction and exit sections, for $We = 1$. Simultaneously, we obtain a significant vortex growth as shown in Figure 8.9 for $We = 1$ and 1.75, which should be compared with the Newtonian case in Figure 8.4. In Figure 8.10, we plot the vortex intensity as a function of $We$; the vortex intensity gives the ratio of the recirculating flow rate to the total flow rate in the contraction. For comparison, we also show the corresponding curve for the Oldroyd-B fluid.

The present example is the first instance where important elastic effects are
calculated in a contraction flow. The use of a White–Metzner fluid in a previous publication\textsuperscript{24} did not reveal similar effects. It has also been shown that after an initial decrease, the pressure drop increases with the flow rate. The numerical results have been confirmed on more refined meshes.

8.5 DIE EXIT FLOW

In the present section, we consider the extrusion of a viscoelastic fluid from a tube to a free jet, with the associated die-swell phenomenon. We will not elaborate on the description of the problem, which is available in Chapter 10. Again the problem is of genuine interest because the normal stresses associated with the viscoelastic flow together with the memory effects must necessarily produce the swelling of the free jet. The die-swell calculation for an Oldroyd-B fluid has been the subject of a recent paper,\textsuperscript{11} where the reader will find more details than in the present summary. The die-swell problem involves a stress singularity at the edge which renders the numerical solution particularly difficult. For the circular die swell of a Maxwell fluid, no results were available beyond $S_R = 3/4$, for an integral\textsuperscript{25} as well as a differential\textsuperscript{5} representation of the constitutive relations. It has also been shown\textsuperscript{26} that the maximum attainable value is related to the coarseness of the mesh. It was found\textsuperscript{11} that the use of an Oldroyd-B fluid rather than a Maxwell fluid considerably enlarges the domain of $S_R$ where the die-exit flow can be calculated.
When the memory of the fluid increases, the assumption of a fully developed Poiseuille flow at the entry may not be made unless the tube is sufficiently long. To reach a value of \( S_R = 4 \) and obtain results which are essentially equivalent to those obtained at the exit of a tube of infinite length, it is necessary to use a tube length equal to 16 radii; moreover, the important swelling of the free jet when \( S_R = 4 \) requires a jet length of the same magnitude. The mesh used for our calculations is shown in Figure 8.11; it contains three rows of quadrilateral elements, 75 elements, 357 nodes and 2246 degrees of freedom. For a given value of \( S_R \), the location of the free surface is obtained by an iterative process;\textsuperscript{6} three to four iterations on the free surface are usually sufficient. The present results are again based on an Oldroyd-B fluid for which \( \mu_2/\mu_1 = 1/8 \).

The main result of the calculation is shown in Figure 8.12 which gives the swelling ratio as a function of the recoverable shear; the same figure shows the theoretical curve obtained by Tanner\textsuperscript{27} for a Maxwell fluid. The dashed vertical line shows the limit of previous numerical calculations for a Maxwell fluid.\textsuperscript{6,25} The curve of Figure 8.12 has been confirmed by calculations with shorter entry lengths and a denser mesh up to \( S_R = 3 \); we have not verified on a denser mesh whether the change of curvature observed in Figure 8.12 depends upon the mesh used for the calculation.

Figure 8.13 shows the deformed mesh, the streamlines and the axial velocity.
Figure 8.13: Deformed mesh, streamlines and contour lines of axial velocity for (a) $\lambda_{yw}=2$ and (b) $\lambda_{yw}=4.5$. 

CIRCULAR DIE

$\lambda_{yw}=4.5$

$\lambda_{yw}=2$

(a)  (b)
contours for $S_R = 16/9$ and $S_R = 4$; for such high values of $S_R$, the results are still remarkably smooth as compared to those of previous calculations.

It is possible to obtain from the numerical results the pressure loss at the exit as a function of the elasticity of the flow. Let $p_0$ be the pressure calculated in the entry section and $\Delta p$ the pressure loss which would be calculated in the tube if the flow were fully developed up to the exit section. The exit-pressure loss is defined by

$$\delta p_{ex} = (p_0 - \Delta p)/(2\tau_w)$$  \hspace{1cm} (8.33)

We may combine $\delta p_{ex}$ with $\delta p_{en}$ defined by Equation (8.30) and calculate the Couette correction for the flow in a capillary, defined by

$$C = \delta p_{en} + \delta p_{ex}$$  \hspace{1cm} (8.34)

Figure 8.14 shows the graphs of $\delta p_{ex}$ and of $C$ as functions of $S_R$.

### 8.6 MELT SPINNING

In this section we consider the process of continuous drawing of viscoelastic fluids (melt spinning) shown schematically in Figure 8.15. A molten filament is extruded from a small hole in the spinneret plate into ambient air; the filament is drawn by a take-up device that induces a continuous decrease of the cross-section diameter and a corresponding increase of the axial velocity.

Theoretical analyses of melt spinning have been reviewed by Petrie\textsuperscript{13} and Denn;\textsuperscript{14} most of them are founded upon so-called thin-filament equations derived
from the same basic argument: it is assumed that the rate of change of the filament curvature is small and the axial velocity profile is uniform in each filament cross-section. These equations are not valid close to the spinneret and are usually assumed to apply downstream from the position of maximum extrudate swell. For a given flow-rate, the initial data required for solving the thin-filament equations are the filament area, and for viscoelastic fluids the ratio of axial to transverse extra-stresses. Fisher et al.\textsuperscript{28} have shown by means of a finite element method that the thin-filament equations of a Newtonian liquid become valid within one filament diameter of the spinneret. In the present section, we extend this numerical approach to a class of viscoelastic fluids described by the Phan Thien–Tanner model. Calculations reported here are valid for low-speed, isothermal spinning. However, since we are mainly interested in the extrusion region close to the spinneret exit, where temperature changes are small and inertial forces negligible, the conclusions regarding initial conditions for the thin-filament equations may also be applicable to the high-speed, non-isothermal case. A more detailed account of the results presented here is available elsewhere.\textsuperscript{15}

The axisymmetric flow geometry and the boundary conditions are described in Figure 8.16. The spinneret is a cylindrical tube of diameter $d_0$ in which the fluid
flows with an average axial velocity \( w_0 \) and a flow rate \( Q = \pi d_0^2 w_0 / 4 \). A take-up device imposes a force \( F \) at some distance downstream from the extrusion section. In the present paper, we assume low-speed spinning, in which case this force is constant along the axis. This enables us to focus our attention on the extrusion region by imposing the force \( F \) as a boundary condition at an arbitrary section of the filament. The spinneret is chosen long enough so that a fully developed Poiseuille flow may be imposed in the entry section, in terms of the components of the velocity \( \mathbf{v} \) and the elastic extra-stress \( \mathbf{T} \). We impose in the end section an axial contact force based on the assumption that the Cauchy stress is uniform and equals the drawing force \( F \) divided by the cross-section. It is also assumed that the shear stress \( \sigma_{rz} \) is much smaller than \( \sigma_{zz} \), so that the tangential contact force may be neglected in the end section. Finally, normal and tangential contact forces vanish on the free surface, while the fluid is assumed to adhere to the spinneret wall.

Figure 8.17 shows a typical mesh used for the calculations; it contains both triangular and quadrilateral elements. Wide elements are needed downstream since for a large drawing force the radius of the fibre becomes quite small. As in the die swell problem, the final shape of the free surface is found by successive approximations.

In view of the simplifying assumptions that we have just made, the drawing process of a Newtonian fluid is governed by a single dimensionless parameter which we define as follows:

\[
B = \frac{4F}{3\pi \mu d_0 w_0}
\]  
(8.35)

In the non-Newtonian case, we need an additional dimensionless group that determines the elastic character of the flow. A convenient choice is the recoverable shear on the wall of the spinneret where the flow is fully developed,

\[
S_R = N_1 / 2\tau_w
\]  
(8.36)

which remains valid as long as the fluid does not exhibit shear-thinning. In the
numerical simulation, we consider a spinneret of unit radius, \( d_0 = 2 \), a unit average velocity, \( w_0 = 1 \), and a unit shear viscosity, \( \mu = 1 \). Various combinations of the parameters \( B \) and \( S_R \) are obtained by imposing values of the drawing force \( F \) and the relaxation time \( \lambda \).

We first examine the results obtained for the Newtonian fluid \((S_R = 0)\) for which we have been able to reach a value of \( B = 1.5 \) with the mesh shown in Figure 8.17. Let us define the physical parameters which may be obtained as a result of the calculations. The draw ratio \( Dr \) is defined by

\[
Dr = \frac{w_F}{w_0}
\]  

(8.37)

where \( w_F \) is the velocity in the end section and \( w_0 \) is the mean velocity in the spinneret. The maximum swelling ratio \( Sw \) is given by

\[
Sw = \frac{d_{\text{max}}}{d_0}
\]  

(8.38)

where \( w_{\text{max}} \) is the maximum diameter along the fibre and \( d_0 \) is the spinneret diameter. The dimensionless location \( z/d_0 \) of the maximum diameter is denoted by \( z_s \).

Table 8.2 shows the values of \( Dr, Sw \) and \( z_s \) as a function of the dimensionless drawing force \( B \). We find that the magnitude of the extrudate swell decreases and its location approaches the spinneret exit when the drawing force increases. High values of the draw ratio are obtained which lead to very thin elements near the end section. One must keep in mind that the temporal stability of such flows is not being considered here. Indeed, earlier investigations have shown that the thin filament solutions are unstable under the influence of infinitesimal perturbations beyond a draw ratio of 20 in the Newtonian case.\(^{29}\)

In order to compare our numerical results with the corresponding thin-filament solution, we determine the position of the section where the velocity profile may be considered as uniform. We calculate within each section the relative difference between each nodal velocity and the mean velocity, and consider that the profile is uniform when the maximum departure from the mean is less than 5\%. The value \( z_{\text{un}} \) is the ratio of the abscissa of the section where

<table>
<thead>
<tr>
<th>Table 8.2 Characteristic values for a Newtonian fluid as a function of the dimensionless drawing force ( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B )</td>
</tr>
<tr>
<td>( Dr )</td>
</tr>
<tr>
<td>( Sw )</td>
</tr>
<tr>
<td>( z_s )</td>
</tr>
</tbody>
</table>
uniformity occurs to the initial diameter $d_0$. It is found that $z_{un} = 0.6$ in all cases, except for $B = 1.5$, where $z_{un} = 0.9$. Thus, the transition between the viscometric spinneret flow to the elongational extrusion flow takes place over an axial distance less than one spinneret diameter, which is consistent with previous results.\(^{28}\)

The thin-filament solution for the axial velocity $w$, referred to an arbitrary origin $z_{or}$, is given by\(^{13}\)

$$\frac{w}{w_{or}} = \exp(B(z - z_{or})/d_0)$$ \quad (8.39)

where $w_{or} = w(z_{or})$; the origin is usually selected in the section of maximum swelling. Table 8.3 gives the values of the mean velocity $\bar{w}$ obtained numerically, compared with the thin filament solutions $w_x$ and $w_{un}$ defined by Equation (8.39) with $z_{or}/d_0 = z_x$ and $z_{un}$ respectively. The agreement is excellent as long as the origin for the thin-filament solution is taken at $z_{un}$.

The thin-filament equations for a Newtonian fluid require that the ratio of average extra-stresses $\bar{T}_{zz}/\bar{T}_{rr}$ be $-2.0$. The computed ratio is shown in Figure 8.18 for $B = 0.25$ and 1; although there is a large deviation in the region of velocity rearrangement, the ratio of $-2.0$ is reached and maintained beyond $z_{un}$. Finally, we show in Figure 8.19 the axial velocity contourlines for $B = 0.25$ and 1. These lines become essentially straight at one spinneret diameter downstream from the exit section, where the thin-filament approximation becomes valid.

Let us now turn to the viscoelastic cases; for the Oldroyd-B fluid, and to a good approximation for the Pian Thien–Tanner fluid with $\zeta = 0$, the recoverable shear is given by

$$S_R = (8\lambda w_0/d_0)(\mu_1/\mu)$$ \quad (8.40)

while for the Maxwell fluid we have

$$S_R = 8\lambda w_0/d_0$$ \quad (8.41)

The major difference between the Newtonian and the viscoelastic results is depicted in Figure 8.20, where we show the draw ratio $Dr$ as a function of the dimensionless force $B$ for various sets of material parameters. The terminal point of each curve represents the higher value of $B$ reached with the numerical scheme.
When the parameter $\varepsilon$ vanishes in the constitutive Equation (8.9), the corresponding curves of $Dr$ as a function of $B$ seem to approach asymptotically a limiting value $\lim (Dr)$ when the drawing force increases. This is consistent with a result by Denn et al.\cite{30} which states that the thin filament equations for a Maxwell fluid lead to the relation

$$Dr \leq 1 + \frac{8}{S_R d_o} \frac{L}{d_0}$$

(8.42)

provided that the product $BS_R$ is large and the ratio $T_{rr}/T_{zz}$, evaluated at the
origin for the thin-filament equations, is small: $L$ denotes the axial distance from the origin to the point of imposition of the force. This bound is a consequence of the fact that a Maxwell fluid can reach infinite stresses at a finite extension rate. A similar bound does not appear for the Phan Thien–Tanner model with $\varepsilon > 0$. Table 8.4 gives, for the Maxwell and Phan Thien–Tanner fluids at $S_R = 0.5$, the values of $Dr$ as a function of $B$; the Newtonian results are also included for comparison. The Maxwell fluid always remains below the limiting value of $\lim (Dr) = 81$ given by the asymptotic solution Equation (8.42).

The ratio $-T_{zz}/T_{rr}$ is an essential initial datum for the non-Newtonian thin-filament equations. Our calculations indicate that the ratio is only weakly dependent on $S_R$, but is a strong function of $B$. In all cases, we have observed the relation

$$0 \leq -\frac{T_{rr}}{T_{zz}}(z_{un}) \leq 0.2 \quad \text{for} \quad B \geq 1.25 \quad (8.43)$$

so that a vanishing value normally used for this ratio as an initial condition for the
Table 8.4 Draw ratio as a function of dimensionless force;  
N: Newtonian fluid; M: Maxwell fluid ($S_R = 0.5$); PTT: Phan Thien–Tanner fluid ($S_R = 0.5, \varepsilon = 0.015, \xi = 0$).

<table>
<thead>
<tr>
<th>B</th>
<th>0.50</th>
<th>1.00</th>
<th>1.50</th>
<th>2.00</th>
<th>2.50</th>
<th>2.75</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>9.4</td>
<td>120</td>
<td>1440</td>
<td>----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>M</td>
<td>8.7</td>
<td>34</td>
<td>50.4</td>
<td>59.6</td>
<td>65.3</td>
<td>67.4</td>
</tr>
<tr>
<td>PTT</td>
<td>8.8</td>
<td>35.6</td>
<td>56.4</td>
<td>72</td>
<td>86.6</td>
<td>94.5</td>
</tr>
</tbody>
</table>

Figure 8.21 Computed swelling ratio as a function of recoverable shear

thin-filament equations is acceptable. High swelling ratios can be obtained with the numerical simulation. Figure 8.21 shows the swelling ratio $S_w$ as a function of the recoverable shear $S_R$ for the Oldroyd-B fluid, at a fixed value of $B = 0.25$. On the same figure, we show the analytical curve obtained by White and Roman,\textsuperscript{31} based on Tanner's theory.\textsuperscript{27} The agreement is good up to $S_R = 2$; beyond that value, the analytical solution underestimates the actual swell. The final mesh and the axial velocity contour lines are depicted in Figure 8.22 for an Oldroyd-B fluid, with $B = 0.25$ and $S_R = 4$. A significant extrudate swell is observed together with very little net drawdown over five spinneret diameters. The position of maximum swell moves only from $0.35d_0$ to $0.85d_0$ as $S_R$ is changed from 0 to 4, but the velocity does not become uniform until $1.75d_0$ at $S_R = 4$. A velocity overshoot is present near the exit section.
In conclusion, the calculations show that the thin-filament equations become valid for the viscoelastic liquids within two diameters of the spinneret, and they generally support use of a vanishing initial ratio for the transverse to axial extrastresses. The maximum swell is adequately predicted by the White–Roman theory,\textsuperscript{31} up to a recoverable shear of 2. But since the point of maximum swell can occur as much as one diameter upstream of the point of uniform velocity, it is not evident that the White–Roman equation provides any advantage over use of the spinneret area and velocity as initial conditions for the thin-filament equations.

8.7 CONCLUSIONS

The calculation of the flow of viscoelastic fluids presents very difficult problems. They may not be attributed to the form of the constitutive equations \textit{per se}; rather, they are a consequence of the coupling between the momentum and the constitutive equations. The symptoms of the problems are spatial oscillations of the field variables which lead to an eventual lack of convergence of the iterative technique.

In the present paper, we have shown that a slight modification of the constitutive equations allows an important increase in the range of elasticity where numerical solutions can be found. The presence of a retardation time, which is theoretically well founded, introduces some damping in the momentum equations and removes the oscillations. It is then possible to solve problems of technical interest within a reasonable range of Weissenberg numbers.
REFERENCES


