

SOME INTEGRATION TECHNIQUES FOR THE ANALYSIS OF VISCOELASTIC FLOWS

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INTRODUCTION

The analysis of steady flows of non-Newtonian fluids with viscoelastic properties often requires the use of extremely elaborate numerical schemes. The difficulties encountered in such analyses are due, in part, to the dependency of the flow on its own history. Thus an iterative procedure is necessary, since some approximation to the velocity field must be known to establish the necessary material parameters.

These history-dependent parameters must be obtained for each particle through an integration along that particle's stream line. In this paper we present some finite element schemes for carrying out such integrations in a very straightforward and efficient manner. These techniques do not constitute a new algorithm for the analysis of viscoelastic flows but can be used within existing algorithms. The procedures appear to be rather general and look promising for a wide range of applications.

CONVECTIVE INTEGRATION

In this section we show how the integration of the first order equations for the material derivative of a scalar variable can be used to obtain functions which are of importance in the analysis of steady flows with applications in viscoelasticity. The governing equation is

$$u_i \frac{\partial A(x)}{\partial x_i} = f(x), \quad \text{in } V \quad (1)$$

with

$$A(x) = \bar{A}, \quad \text{on } \delta_e$$

where u_i are the Cartesian components of the velocity, assumed known, $A(x)$ is the unknown scalar function, and $f(x)$ is the known convected (material) time derivative of $A(x)$. x represents the set of spatial coordinates, x_i fixed in space. A is specified on that segment of the boundary, δ_e , through which the fluid enters the control volume. The requirement for this boundary condition excludes, for the present, consideration of flows having closed streamlines within the control volume.

A finite element approximation for $A(x)$ can be given as

$$A(x) \doteq N_\alpha A_\alpha \quad (2)$$

where N_α are the basis functions associated with node α , and A_α are the nodal values of the approximations to $A(x)$. Repeated subscripts are used to indicate a summation over all nodes. Greek letters will be used to indicate nodal values; lower case Latin letters will indicate components of Cartesian tensors.

The application of Galerkin's method to equation (1) with N_α used as weighting functions gives

$$\int_V N_\beta u_i(x) \frac{\partial N_\alpha}{\partial x_i} A_\alpha \, dV = \int_V N_\beta f(x) \, dV \quad (3)$$

or

$$K_{\beta\alpha} A_\alpha = F_\beta \quad (4)$$

where

$$K_{\beta\alpha} = \int_V N_\beta u_i \frac{\partial N_\alpha}{\partial x_i} \, dV$$

and

$$F_\beta = \int_V N_\beta f \, dV$$

In most cases of practical interest, $u_i(x)$ will be given by a finite element approximation over the same mesh as that used for A_α . However, it is not generally necessary for the order of approximation used for the two functions to be the same.

We now consider three examples of scalar functions for the variable $A(x)$.

Residence time

The residence time of a material particle is that time which has elapsed between the particle's entry into the control volume and the time at its current position. We are concerned here with a residence time *field*, in contrast to the more usual engineering use of the term, which refers only to residence time values on the exit boundary of the domain. Clearly, the material derivative of the residence time is simply unity, hence

$$u_i \frac{\partial R}{\partial x_i} = 1, \quad \text{in } V \quad (5)$$

$$R = 0, \quad \text{on } \delta_e$$

Effective strain

We define the effective strain as the integral of the second invariant of the rate of deformation tensor. This quantity can play a significant role in the analysis of plastic flows of metals during forming processes, where it is the principal variable related to the phenomenon known as work hardening. (Strictly speaking, the effective strain only contains the plastic strain developed within the material. This can be obtained by subtracting the elastic component calculated from the state of stress.) Our governing equation for effective strain is

$$u_i \frac{\partial e_{\text{eff}}}{\partial x_i} = \varepsilon_{ij} \varepsilon_{ij} \quad (6)$$

$$e_{\text{eff}} = 0, \quad \text{on } \delta_e$$

where

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

Entrance co-ordinates

Each particle in a flow field can be considered to carry with it the co-ordinates of the point where it entered the control volume. Hence the material derivative of a particle's entrance co-ordinates is zero, giving us

$$\left. \begin{aligned} u_i \frac{\partial X_e}{\partial x_i} &= 0 \\ u_i \frac{\partial Y_e}{\partial x_i} &= 0 \\ u_i \frac{\partial Z_e}{\partial x_i} &= 0 \end{aligned} \right\} \text{in } V \quad (7)$$

and

$$\left. \begin{aligned} X_e &= x \\ Y_e &= y \\ Z_e &= z \end{aligned} \right\} \text{on } \delta_e$$

Two uses for the entrance co-ordinates are worth noting. Contour plots of constant X_e , Y_e and/or Z_e represent stream lines for flows without recirculation. In turn, knowledge of the entrance co-ordinates of a particle identifies the stream line with which it is associated.

A second use is in determining the material co-ordinates, which in the present context we take to be the co-ordinates that each particle in the control volume had at some earlier specified time outside the control volume. If the flow of the fluid before entering the control volume is steady in the Lagrangian sense, then it is simple to integrate upstream from a particle's entrance co-ordinates to obtain its earlier position. The range of integration is from the moment of entry back to the specified time, and the moment of entry is the current time less the residence time. It should be noted that a number of problems of practical interest have very simple flow fields prior to entering the control volume, such as rigid body translation or Poiseuille flow.

Example

One of the most significant computational aspects of the integration described above is that the finite element matrix, \mathbf{K} , is not dependent on the specific applications. Therefore, once it has been assembled and factored, all of the above analyses can be conducted with relatively little computer expense. To illustrate the above methods we consider two examples. The velocity fields for both were obtained by finite element analyses of a Newtonian fluid.

Consider first a fluid in plane flow passing through a contraction as shown in Figure 1(a). The flow analysis used a flat entrance velocity profile and included a slip velocity at the wall, which produced a downstream velocity profile as indicated in Figure 1(b). Residence times, as well as various strain and deformation quantities, go to infinity as velocity tends to zero on a non-slip wall, and the present approach clearly has a limitation here. It has been found though that solutions can be obtained for the no-slip case. The singularity at the wall renders results at neighbouring nodes inaccurate, but the solutions may still be adequate for certain applications.

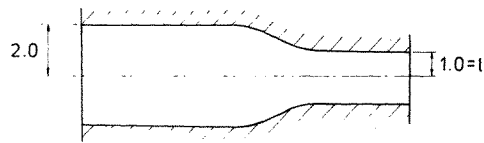


Figure 1(a). Domain of the planar flow contraction problem

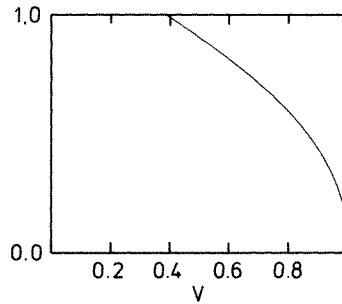


Figure 1(b). Exit velocity profile

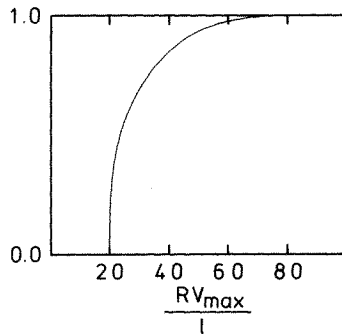


Figure 1(c). Dimensionless residence time profile at exit

The finite element mesh used for the present analysis is shown in Figure 2(a). Quadratic approximations were used for velocity and the convected variables. The residence time field is shown in Figure 2(b). Because of the small wall slip velocity, residence time becomes very large near the downstream wall. Figure 1(c) shows the profile in this vicinity. Stream-lines obtained by plots of constant entrance co-ordinates are shown in Figure 2(c).

Because of the small slip velocity in this previous example, the material co-ordinates produce an extremely distorted mesh. Therefore, to produce a more pleasing illustration, we chose the problem illustrated in Figure 3. Here a much more uniform velocity field is obtained. Again the flow is planar and a Newtonian fluid was assumed. The finite element mesh is shown in Figure 4(a). Quadratic approximations were used for velocity and linear approximations were used for the convected variables. The residence time field and stream lines are shown in Figures 4(b) and 4(c). The mesh corresponding to the material co-ordinates which the nodes would have had before entering the control volume is shown in Figure 4(d). This mesh was obtained using the assumption that the material enters the control volume with rigid body motion. Note that meshes representing the material

co-ordinates can be used to obtain the displacement functions and hence their gradients and resulting finite strains. Furthermore, these quantities are easily obtained at the quadrature points of the control volume mesh (Figure 4(a)) since the material co-ordinates are given as nodal point values.

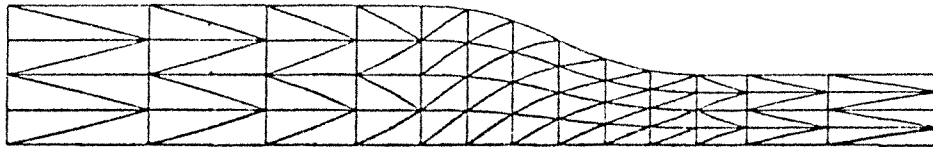


Figure 2(a). Finite element mesh for the problem shown in Figure 1(a)



Figure 2(b). Contours of residence time

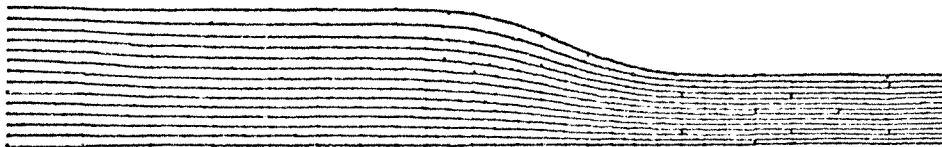


Figure 2(c). Streamlines

CALCULATION OF STRESS IN VISCOELASTIC FLOWS

Differential models

Differential formulations of constitutive equations for viscoelastic fluids involve stress implicitly. To obtain the stress field corresponding to a given flow field it is necessary, therefore, to solve a differential equation with appropriate boundary conditions. Shimazaki and Thompson¹ showed how this could be accomplished for a corotational Maxwell fluid. As in the previous section, the method involves the integration of a first order equation by the

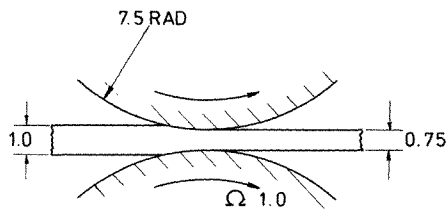


Figure 3. Geometry of a rolling problem

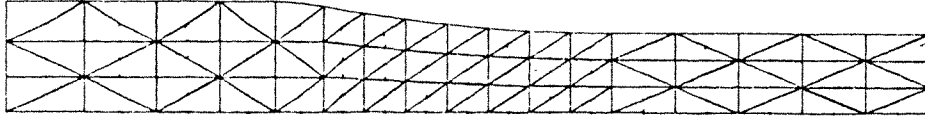


Figure 4(a). Finite element mesh for the problem shown in Figure 3

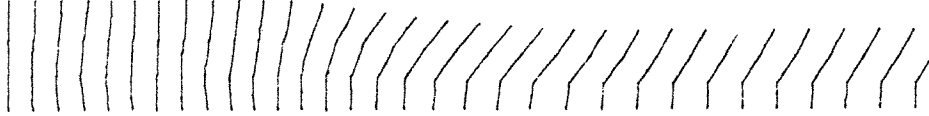


Figure 4(b). Contours of residence time

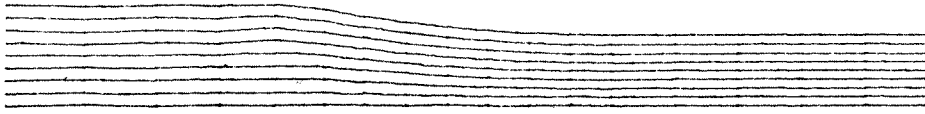


Figure 4(c). Streamlines

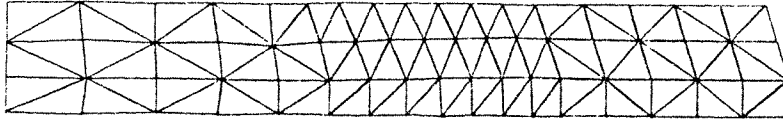


Figure 4(d). Material co-ordinates. Form of the mesh Figure 4(c) before entry to the problem domain

finite element method. Applied to either a corotational or codeformational Maxwell fluid, it is necessary to solve

$$\left[u_k \frac{\partial \sigma_{ij}}{\partial x_k} - C_1 \left(\frac{\partial u_i}{\partial x_k} \sigma_{kj} + \frac{\partial u_j}{\partial x_k} \sigma_{ik} \right) + C_2 \left(\frac{\partial u_k}{\partial x_i} \sigma_{kj} + \frac{\partial u_k}{\partial x_j} \sigma_{ik} \right) \right] + \frac{G}{\mu} \sigma_{ij} = 2G\epsilon_{ij}, \quad \text{in } V \quad (8)$$

with

$$\sigma_{ij} = \bar{\sigma}_{ij}, \quad \text{on } \delta_e$$

In the above, μ is the viscosity and G is the shear modulus. When $C_1 = C_2 = 0.5$, the term in the brackets is the Jaumann derivative used for the corotational model. When $C_1 = 1$ and $C_2 = 0$, the term is the upper convective derivative, and when $C_1 = 0$ and $C_2 = 1$, it is the lower convective derivative, both given by Oldroyd² and used in the codeformational models.

Substitution of the finite element approximation for stress

$$\sigma_{ij}(x) \doteq N_\alpha(x) \sigma_{\alpha ij} \quad (9)$$

into the above, gives

$$\left[u_k \frac{\partial N_\alpha}{\partial x_k} \delta_{im} \delta_{jp} - C_1 N_\alpha \frac{\partial u_i}{\partial x_k} \delta_{km} \delta_{jp} - C_1 N_\alpha \frac{\partial u_j}{\partial x_k} \delta_{im} \delta_{kp} + C_2 N_\alpha \frac{\partial u_k}{\partial x_i} \delta_{km} \delta_{jp} + C_2 N_\alpha \frac{\partial u_k}{\partial x_j} \delta_{im} \delta_{kp} \right] \sigma_{\alpha mp} + \frac{G}{\mu} [N_\alpha \delta_{im} \delta_{jp}] \sigma_{\alpha mp} = 2G\epsilon_{ij} \quad (10)$$

where δ_{ij} is the Kronecker delta. Applications of Galerkin's method to this equation, with N_β

used as the weighting functions, gives

$$\overline{\mathbf{K}}_{\beta\alpha mipj} \sigma_{\alpha mp} + \mathbf{K}_{\beta\alpha mipj} \sigma_{\alpha mp} = F_{\beta ij} \quad (11a)$$

where

$$\begin{aligned} \overline{\mathbf{K}}_{\beta\alpha mipj} = \int_V N_\beta \left[u_k \frac{\partial N_\alpha}{\partial x_k} \delta_{im} \delta_{jp} - C_1 N_\alpha \frac{\partial u_i}{\partial x_k} \delta_{km} \delta_{jp} \right. \\ \left. - C_1 N_\alpha \frac{\partial u_j}{\partial x_k} \delta_{im} \delta_{kp} + C_2 N_\alpha \frac{\partial u_k}{\partial x_i} \delta_{km} \delta_{jp} + C_2 N_\alpha \frac{\partial u_k}{\partial x_j} \delta_{im} \delta_{kp} \right] dV \end{aligned} \quad (11b)$$

$$\mathbf{K}_{\beta\alpha mipj} = \int_V N_\beta \frac{G}{\mu} N_\alpha \delta_{im} \delta_{jp} dV \quad (11c)$$

$$F_{\beta ij} = \int_V N_\beta 2G \varepsilon_{ij} dV \quad (11d)$$

We shall have further need for $\overline{\mathbf{K}}$ in the next section, when integral formulations of constitutive equations are considered.

The above equations can be used for the analysis of the generalized Maxwell model, if this is written as

$$\sigma_{ij} = \sum_N \sigma_{ij}^{(N)} \quad (12a)$$

$$\overline{\sigma}_{ij}^{(N)} + \frac{G^{(N)}}{\mu^{(N)}} \sigma_{ij}^{(N)} = 2G^{(N)} \varepsilon_{ij}, \quad \text{in } V \quad (12b)$$

where

$$\sigma_{ij}^{(N)} = \overline{\sigma}_{ij}^{(N)}, \quad \text{on } \delta_e \quad (12c)$$

Here, and subsequently the box over the stress is used to indicate the derivative as expressed in equation (8). It is necessary to specify $\sigma_{ij}^{(N)}$ on δ_e which can be done provided the material enters the control volume with a simple viscometric flow which has existed for a sufficiently long time.

Because the material parameters $G^{(N)}$ and $\mu^{(N)}$ appear on the left-hand side of equation 12(b), it is necessary to assemble and factor the finite element matrix for each N . This could prove costly for large N , in which case the approach for the generalized Maxwell model outlined in the next section might be preferable.

Integral models

We next consider the evaluation of stress during steady-flow when an integral formulation of the constitutive equation is used. We begin by considering a general quasi-linear single integral model:

$$\sigma_{ij}(t) = \int_{t'=-\infty}^{t'=t} \psi(t-t') \mathbf{B}_{im} \mathbf{B}_{jp} \varepsilon_{mp}(t') dt' \quad (13)$$

where the specific form of the transformation tensor \mathbf{B} depends on the objective frame of reference used, and the integration is the inverse of the convected differentiation indicated by the symbol $\overline{\sigma}_{ij}$. Equation (13) is a consequence of Boltzman's superposition principle, and must be carried out with respect to a given material particle, which we could call particle

(t, x) indicating that at time t it is at position x . t' is an earlier time, when the particle was at position x' . Equation (13) is derived from the simpler statement

$$\bar{\sigma}_{ij}^{\square}(t, t') = \psi(t - t') \varepsilon_{ij}(t') \quad (14)$$

It is important to note that equation (14) does not give the *current* rate of stress change, but only that part of it which is due to the rate of deformation $\varepsilon_{ij}(t')$ which took place at t' .

We now consider the relationship between t, t' and the residence time, R . In equations (13) and (14), an important factor is the difference, $(t - t')$, the lapsed time. In the integration for particle (t, x) , this lapsed time is simply the difference between the residence time value R at x , and the value R' at x' , an upstream point on the streamline through x . For steady flow, therefore, we may write equation (14) as

$$\bar{\sigma}_{ij}^{\square}(x, x') = \psi(R - R') \varepsilon_{ij}(x') \quad (15)$$

The finite element equation for the solution of equation (15) is

$$\bar{\mathbf{K}}_{\beta\alpha, ipj}^{\square} \sigma_{\alpha mp}^* = F_{\beta ij} \quad (16a)$$

where $\bar{\mathbf{K}}^{\square}$ is defined by equation 11b and here

$$F_{\beta ij} = \int_V N_{\beta} \psi(R - R') \varepsilon_{ij} dV \quad (16b)$$

The pseudo-stresses σ_{ij}^* coincide with the true stresses corresponding to the given velocity field at the node(s) where residence time has the value R used in equations (16), and indeed at all points on the contour of residence time R . If we eschew the interpolation procedure which this comment suggests, then it seems that in general a solution is required for each and every node of the FE mesh. However, the cost may not be as great as at first appears. Because R occurs only on the right-hand side of the equation, the same LDU factored $\bar{\mathbf{K}}^{\square}$ matrix may be used for each solution. Further, when we look at specific forms of the relaxation modulus $\psi(t - t')$ we find that it is often unnecessary to solve for each and every nodal residence time.

Consider, for example, the generalized Maxwell fluid:

$$\sigma_{ij} = \sum_N \int_{t'=-\infty}^{t'=t} 2G^{(N)} e^{-(t-t')/\lambda^{(N)}} B_{im} B_{jp} \varepsilon_{mp} dt' \quad (17)$$

with summation over N .

The right-hand side can be split and written in terms of residence times as previously

$$\sigma_{ij} = \sum_N 2G^{(N)} e^{-R/\lambda^{(N)}} H_{ij}^{(N)} \quad (18a)$$

where

$$H_{ij}^{(N)} = \int_{R'=-\infty}^{R'=R} e^{R'/\lambda^{(N)}} B_{im} B_{jp} \varepsilon_{mp} dR' \quad (18b)$$

We can now regard $H_{ij}^{(N)}$ as a field variable, governed by

$$\bar{H}_{ij}^{\square(N)} = e^{R/\lambda^{(N)}} \varepsilon_{ij}$$

The corresponding finite element equations are

$$\bar{\mathbf{K}}_{\beta\alpha m ipj}^{\square} H_{\alpha mp}^{(N)} = F_{\beta ij} \quad (19a)$$

where \square is defined by equation 11(b) and now

$$F_{\beta ij} = \int_V N_{\beta} e^{R'/\lambda^{(N)}} \varepsilon_{ij} dV \quad (19b)$$

Boundary values for $\mathbf{H}^{(N)}$ must be specified on δ_e which can be done if the upstream flow is sufficiently simple. Note that one solution must now be obtained for each relaxation time $\lambda^{(N)}$, rather than one for each node. For most problems of practical interest N will not exceed 3 or 4. Once the $H_{ij}^{(N)}$ values are obtained, the stresses can be calculated via equation 18(a).

The techniques described above may be extended in obvious ways to non-linear single integral models, where the relaxation modulus incorporates functions of the rate of deformation tensor invariants.

SOLUTION ALGORITHMS FOR STEADY STATE VISCOELASTIC FLOW ANALYSES

Algorithms currently in use for solving the non-linear equations governing flow of viscoelastic liquids can be placed into two general categories. The first contains the mixed finite element methods, which solve the momentum equation and the constitutive equation simultaneously for velocity and stress.^{3,4,5} The equations are linearized by using the solution from the previous iteration to evaluate the dependent parameters. Because these methods use differential forms of constitutive theories, it appears that they will not be practical for complex fluids such as the generalized Maxwell fluid. Clearly, the repeated solution method discussed above for this fluid would not be suitable if a mixed method were used.

The second category includes those methods which solve the momentum equation and the constitutive equation separately. Thus, the momentum equation is solved for velocity with values for stress obtained from the solution of the constitutive equations and *vice versa*. Both finite differences⁶ and finite elements^{1,7,8} have been employed for the solution of the momentum equation. The constitutive equation has been solved by the finite element method when a differential form is used,^{1,8} and when integral models are used, it has been solved by numerically integrating along streamlines.^{6,7} The method based on equation (16) appears to incorporate both approaches.

A difficulty arises when using integral models. This stems from the fact that for the solution of the momentum equation, one must have a linearized expression for stress in terms of velocity. In general, such linearisations are not easily obtained from integral expressions.

Work on this phase of the research has just begun; therefore we outline only briefly a possible general approach. The derivative of the stress at time t is

$$\square \sigma_{ij} = \int_{t'=-\infty}^{t'=t} \frac{d\psi(t-t')}{dt} B_{im} B_{jp} \varepsilon_{mp}(t') dt' + \psi(0) \varepsilon_{ij}(t) \quad (20)$$

The integral has the units of rate of change of stress and we write it as $\square \bar{S}_{ij}$. If equation (20) is multiplied by some characteristic time (or relaxation time), Λ , we can write

$$\sigma_{ij} = -\Lambda \psi_0 \varepsilon_{ij} + \Lambda \square \bar{\sigma}_{ij} - \Delta \sigma_{ij} \quad (21a)$$

where

$$\Delta\sigma_{ij} = (\Lambda \overset{\square}{S}_{ij} - \sigma_{ij}) \quad (21b)$$

We now have our desired expression. The first terms on the right-hand side are linear in velocity and can be retained on the left hand side of the momentum equation. The last terms must go on the right hand side of the momentum equation as a pseudo body force.

Note that it has not yet been necessary to define the characteristic time. Therefore, it can be chosen so as to minimize the length of the vector $\Delta\sigma_{ij}$, and hence reduce the corrective term represented by the pseudo body force.

For a Maxwell fluid

$$\psi(t-t') = 2Ge^{-(t-t')/\Lambda} \quad (22a)$$

$$\frac{d\psi}{dt} = -\frac{1}{\Lambda} 2Ge^{-(t-t')/\Lambda} \quad (22b)$$

$$\begin{aligned} \overset{\square}{S}_{ij} &= \int_{t'=-\infty}^{t'=t} -\frac{1}{\Lambda} 2Ge^{-(t-t')/\Lambda} B_{im} B_{jp} \varepsilon_{mp} dt' \\ &= -\frac{1}{\Lambda} \sigma_{ij} \end{aligned} \quad (22c)$$

If $\Lambda = \lambda$, then equation 21(a) becomes

$$\sigma_{ij} = \frac{1}{\lambda} 2G\varepsilon_{ij} - \lambda \overset{\square}{\sigma}_{ij} \quad (22d)$$

which is the differential form of the constitutive equation of the Maxwell fluid.

Unfortunately, the evaluation of $\overset{\square}{S}_{ij}$ will, in general, require additional finite element solutions, thereby nearly doubling the cost of the stress analysis. However, these new solutions only require additional right-hand sides to be used in the general equation for stress, equation (16).

EXAMPLE

To illustrate the calculation of stress by the above procedures we chose the problem of expanding radial flow shown in Figure 5(a). This choice was made because once the assumption of radial flow is imposed, the flow field is determined by continuity and is independent of the constitutive equation, thus eliminating the need to iterate to correct stress and velocity fields. The problem was treated both as a plane flow problem, with the mesh illustrated in Figure 5(b), and as an axisymmetric problem, with the mesh shown in Figure 5(c).

A corotational Maxwell fluid was assumed with both the shear modulus and viscosity specified as unity. The velocity, assumed known, was taken as

$$u_r = \frac{1.6}{r}$$

For the following definition of the Weissenberg number, we therefore have

$$W_e = \frac{\mu u_a}{Gr_a} = 1.6$$

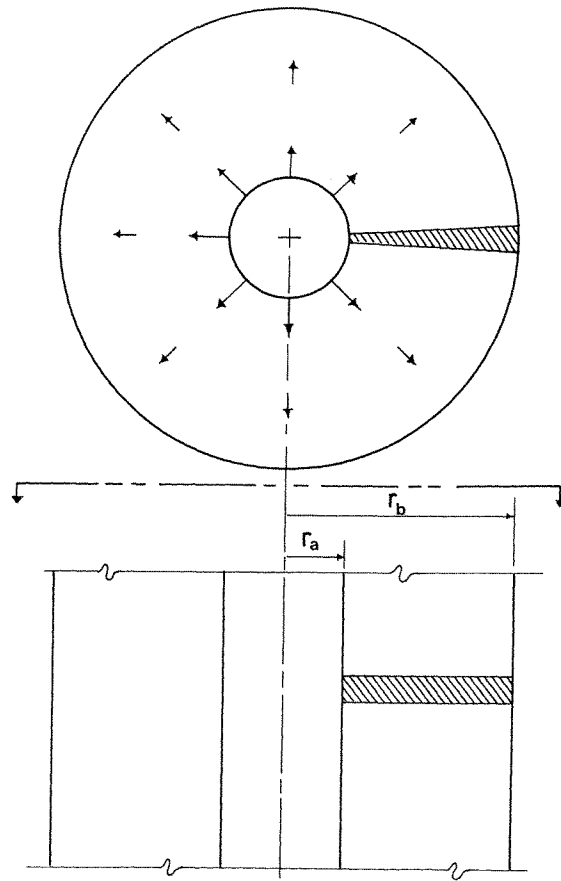


Figure 5(a). Geometry of the radial flow problem. The hatched area in the upper view shows the domain of the finite element problem treated as a planar flow in Cartesian co-ordinates; in the lower view the hatched area is the domain of the axisymmetric version of the problem

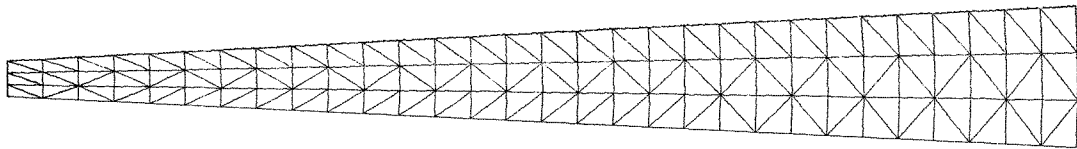


Figure 5(b). Finite element mesh for the planar version of the radial flow problem

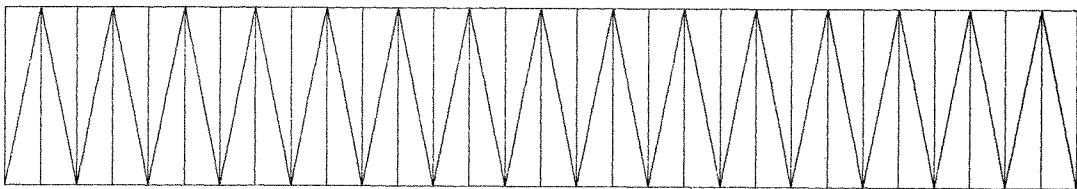


Figure 5(c). Finite element mesh for the axisymmetric version of the radial flow problem

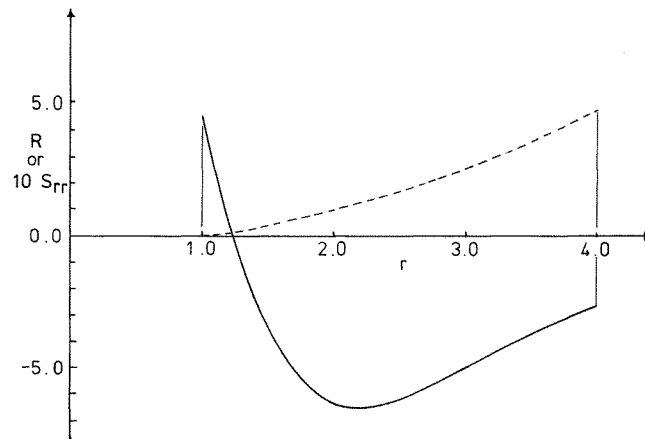


Figure 6. Residence time and radial component of stress versus radius

The extra stress in the entering material ($r_a = 1.0$) was specified as

$$\begin{bmatrix} S_{rr} & S_{r\theta} & S_{rz} \\ S_{r\theta} & S_{\theta\theta} & S_{\theta z} \\ S_{rz} & S_{\theta z} & S_{zz} \end{bmatrix} = \begin{bmatrix} +0.45 & 0 & 0 \\ 0 & -0.45 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

This same stress specification was used for the plane flow problem. However, it was given in terms of its rectangular Cartesian components which differed from node to node.

The velocity was specified exactly at each node from which quadratic approximations were made for use in the calculations of residence time and stress. Both the residence time and stress were calculated using triangular elements.

The constitutive equation was used in its integral form. The method outlined for the generalized Maxwell fluid was used for both the plane flow and axisymmetric analyses. In addition, the node by node approach, outlined for use with a general relaxation function, was used for the axisymmetric case. Both axisymmetric analyses gave identical results. It has been shown previously¹ how for this radial flow problem S_{rr} is given by an initial value ordinary differential equation, and a solution was obtained by a fourth order Runge-Kutta method. Results from all three present analyses were within plotting accuracy of the Runge-Kutta solution. The residence time field and the radial component of stress are shown in Figure 6.

CONCLUSION

We have shown in this paper several integration techniques which should prove useful in the analysis of flows of viscoelastic fluids. The culmination of these techniques is the ability to calculate the stress field associated with a given flow field for a wide range of constitutive equations. However, the methods do not apply to regions of fluid flow which are completely contained within the control volume. Stagnation points and other regions where the velocity goes to zero such as no-slip boundaries, are also excluded. Continued research is being conducted to develop methods for incorporating these regions into the analysis.

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