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Finite Element Methods for Transient Viscoelastic
Free surface Flows

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ABSTRACT: We describe a numerical technique for solving two-dimensional transient free surface flows of viscoelastic fluids of the Oldroyd type. The method is based on a Galerkin principle invoked on deforming finite elements. Two strategies for the temporal discretization are compared in terms of ease of implementation and cost effectiveness: a predictor-corrector scheme in which the computation of the free surface is decoupled from that of velocity and stress fields (Keunings 1986a), and a newly developed implicit scheme in which the free surface and the flow field are calculated simultaneously.

1. INTRODUCTION

The numerical simulation of the flow of highly elastic fluids is the subject of active research (for reviews, see Crochet et al. 1984, Keunings, in preparation). In view of the significant amount of computer resources involved, only a few time-dependent simulations have been described in the literature. The motivations for the development of transient algorithms are many, however. One is of course the large number of applications that are transient in nature. Another stems from recent experiments by Boger (1986) and Lawler et al. (1986) in which complex transitions between steady state and transient regimes have been observed. These transitions may well be typical of complex viscoelastic flows and their prediction requires a transient approach.

In a recent paper, Keunings (1986a) has proposed a numerical procedure for solving a class of transient free surface flows of viscoelastic fluids of the Oldroyd type. The method is based on deforming finite elements combined with a semi-implicit temporal integration scheme. It has been applied successfully to a number of surface-tension-driven flows (Keunings 1986a,b, Bousfield et al. 1986). Such flows lead to evolution problems that can be very stiff, thus imposing severe restrictions on the magnitude of the time steps.

The goal of the present work is to implement a fully implicit scheme into Keunings' algorithm. Also, we enlarge the range of possible applications with the adoption of a technique developed by Kistler and Scri-

ven (1983) for the representation of arbitrarily complex free surface shapes.

2. GOVERNING EQUATIONS

The isothermal flow of an Oldroyd-B fluid is governed by the following equations:

$$\overset{\nabla}{T}_p + \lambda \overset{\nabla}{T}_p = 2\mu_p \underline{D}, \quad (1)$$

$$\rho \frac{Dv}{Dt} = \nabla \cdot (-p\underline{I} + 2\mu_s \underline{D} + \overset{\nabla}{T}_p) + \underline{f}, \quad (2)$$

$$\nabla \cdot v = 0, \quad (3)$$

where $\overset{\nabla}{T}_p$ is the polymer contribution to the stress, λ is a relaxation time, μ_s and μ_p are viscosity coefficients, and the symbol $\overset{\nabla}{\cdot}$ in (1) is the upper-convected derivative (see Crochet et al. 1984).

The set (1-3) is to be solved in terms of $\overset{\nabla}{T}_p$, v , and p in a flow domain Ω . For transient free surface flows, Ω is an unknown function of time $\Omega(t)$. We assume that Ω is two-dimensional (plane or axisymmetric), and that its boundary $\partial\Omega$ is the union of a fixed part $\partial\Omega_f$ and a moving part $\partial\Omega_m(t)$. An additional equation is needed to determine the latter. Conservation of mass yields

$$v \cdot \underline{n} = \frac{\partial}{\partial t} \underline{x}(x_0, t) \cdot \underline{n} \quad \text{on } \partial\Omega_m, \quad (4)$$

where \underline{n} is the normal to the free surface $\underline{x}(t) = \underline{x}(x_0, t)$. If the free surface can be represented by a single-valued function h of time and one spatial coordinate (e.g. x) the kinematic condition (4) reduces to

$$\frac{\partial h}{\partial t} + v_x \frac{\partial h}{\partial x} = v_y, \quad (5)$$

where v_x and v_y are the velocity components evaluated at the free surface. Proper initial and boundary conditions complete the mathematical formulation of the moving boundary problem (1-4).

2. SPATIAL DISCRETIZATION

Spatial discretization of (1-4) is achieved by means of a Galerkin principle invoked on deforming elements (Keunings 1986a). We define finite element approximations for the polymer extra-stress, the velocity, and the pressure as follows

$$\begin{aligned} \underline{T}_p^* &= \sum_i \underline{T}_p^i(t) \phi_i, \quad \underline{v}^* = \sum_j \underline{v}_j^*(t) \psi_j, \\ p^* &= \sum_k p^k(t) \pi_k, \end{aligned} \quad (6)$$

where ϕ_i , ψ_j , π_k are finite element basis functions, and \underline{T}_p^i , \underline{v}_j^* , p^k are time-dependent nodal values. Since nodal motion will occur in the course of the simulation, the basis functions are implicit functions of time. One has for example

$$\psi_j = \psi_j(\underline{x}, \underline{x}_m(t)), \quad (7)$$

where the \underline{x}_m are nodal position vectors.

For plane flows, the Galerkin equations read

$$\langle \phi_i; \underline{T}_p^* + \lambda \underline{T}_p^* - 2\mu \underline{D}_p^* \rangle = 0, \quad (8)$$

$$\begin{aligned} \langle \psi_j; \rho \frac{D\underline{v}_j^*}{Dt} - \underline{f} + \langle \nabla \psi_j; -p^* \underline{I} + 2\mu \underline{D}_p^* + \underline{T}_p^* \rangle = \\ \langle \langle \psi_j; \underline{t} \rangle \rangle, \end{aligned} \quad (9)$$

$$\langle \pi_k; \nabla \cdot \underline{v}^* \rangle = 0, \quad (10)$$

where the brackets $\langle ; \rangle$, $\langle \langle ; \rangle \rangle$ denote the L^2 scalar product over $\Omega(t)$ and $\partial\Omega(t)$ respectively, and \underline{t} is the surface traction. Terms marked by an asterisk denote finite element approximations obtained from (6).

Special care is needed in the evaluation of the time derivatives present in (8-9) when nodal motion is allowed. For example,

$$\frac{D\underline{T}_p^*}{Dt} = \sum_i \dot{\underline{T}}_p^i(t) \phi_i + (\underline{v}^* - \underline{v}^g) \cdot \nabla \underline{T}_p^*, \quad (11)$$

where the superscript $\dot{}$ denotes time differentiation, and \underline{v}^g is the grid velocity defined by

$$\underline{v}^g = \sum_m \dot{\underline{x}}_m(t) \theta_m. \quad (12)$$

(the symbol θ_m denotes the m th basis function used in the isoparametric transformation). See Keunings (1986a) for details. The conventional Galerkin method on a fixed mesh ($\underline{v}^g=0$) and the purely Lagrangian approach ($\underline{v}^g=\underline{v}^*$) are particular cases of the present formulation.

The discretization of the free surface remains to be discussed. Keunings (1986a) used the particular form (5) of the kinematic condition and defined a one-dimensional finite element representation for the height function h :

$$h^* = \sum_l h^l \beta_l(x). \quad (13)$$

The set of Galerkin equations (8-10) can then be closed with

$$\langle \beta_l; \frac{\partial h^*}{\partial t} + \underline{v}^* \frac{\partial h^*}{\partial x} - \underline{v}_y^* \rangle = 0, \quad (14)$$

where $\langle ; \rangle$ now denotes the L^2 scalar product over the domain of definition of h . In the present paper, we adopt a more general approach developed by Kistler and Scriven (1983) which rests on the following ideas: (i) the finite element representation of the free surface $\partial\Omega_m(t)$ is used to define the parameterization \underline{x} :

$$\underline{x}(\underline{x}_0, t) = \underline{x}(\underline{x}_{fs}(t)), \quad (15)$$

where \underline{x}_{fs} are the position vectors of the nodes belonging to the moving free surface, (ii) the free surface nodes move along pre-defined spines. Each spine is defined by a base point \underline{x}_b and a direction vector \underline{e}_i ; the motion of a free surface node \underline{x}_{fs} belonging to spine number i is thus given by

$$\underline{x}_{fs}(t) = \underline{x}_b^i + h^i(t) \underline{e}_i = \underline{x}_{fs}(h^i(t)). \quad (16)$$

The set of coefficients $h^i(t)$ provides a discrete representation of the free surface that is independent of any coordinate system; (iii) similarly, the motion of internal nodes \underline{x}_m is related to a spine coefficient h^i :

$$\underline{x}_m(t) = \underline{x}_b^i + c^m h^i(t) \underline{e}_i, \quad (17)$$

where c^m is a constant. The nodal motion is thus anchored to the displacement of the free surface in a way that preserves the initial topology of the element layout. Note that the approach of Keunings (1986a) is a particular case for which the spines are lines $x=\text{constant}$.

The discretized kinematic condition is then

$$\langle \theta_m; \dot{y}^* \cdot \dot{n}^* - \dot{x}(h^i(t)) \cdot \dot{n}^* \rangle = 0 \quad (18)$$

where the integration is performed over the moving boundary $\partial\Omega_m(t)$, and the weights θ_m are the basis functions used in the isoparametric transformation.

3. TEMPORAL DISCRETIZATION

Equations (8-10) and (18) constitute a set of first-order differential equations of the form

$$A(\dot{I}, \dot{V}, \dot{H}, \dot{I}, \dot{V}, \dot{P}, \dot{H}) = 0, \quad (19)$$

$$B(\dot{H}, \dot{H}, \dot{V}) = 0, \quad (20)$$

where I, V, P are vector of nodal values of the polymer extra-stress, the velocity, and the pressure, respectively; H denotes the set of coefficients h^i which define the free surface in (16). These coefficients appear in (19) through the boundary condition at the free surface, the definition of the flow domain, and the rate of deformation of the finite elements, as explained above.

If we define a global unknown vector $Z = (I, V, P, H)$, the set (19-20) can be written in the concise form

$$C(\dot{Z}, Z) = 0. \quad (21)$$

We shall define and compare two strategies for the temporal integration of (21).

One, developed by Keunings (1986a), is based on the decoupled solution of (19-20). The method developed in the present work consists of a fully implicit solution of the coupled problem (21).

Let Z_n be the solution vector at time $t=t_n$. The solution Z_{n+1} at time $t_{n+1}=t_n+\Delta t_n$ is obtained after completion of the following steps:

3.1 Decoupled scheme (Keunings, 1986a)

- [1] Prediction: $Z_{n+1}^{\text{pred}} = Z_n + \Delta t_n \dot{Z}_n$
- [2] Relocation of the nodes of the finite element mesh by means of (17)
- [3] Correction of the flow field: solution of (19) on the predicted mesh by means of the first-order implicit Euler scheme. The resulting non-linear set of algebraic equations is solved by Newton's method with predicted values as first estimates.
- [4] Correction of the free surface: solution of (20) with the velocity

field found in step [3].

- [5] Computation of the time derivative \dot{Z}_{n+1} , to be used at the next time step, by inversion of Euler's rule.

3.2 Implicit scheme

- [1] Prediction as in [1] above
- [2] Relocation of nodes as in [2] above
- [3] Correction of the flow domain and the flow field: solution of the coupled problem (21) by means of the implicit Euler scheme; solution of the algebraic equations by a full Newton scheme.
- [4] Computation of \dot{Z}_{n+1} as in [5] above.

The following remarks should be made:

- R1. The first time step requires a slightly different treatment (see Keunings, 1986a).
- R2. The magnitude of the time step can be computed during the course of the simulation on the basis of the difference between predicted and corrected values and a user-specified level of local time discretization errors (see e.g. Gresho et al. 1980).
- R3. For both semi and fully implicit schemes, the most costly operation in terms of computer time lies in step [3] which involves the evaluation of an intricate Jacobian matrix and the solution of a large linear system.
- R4. Although we have not shown it explicitly in this brief presentation, the Jacobian matrix used in the implicit scheme 3.2 is much more complex to derive than that of the decoupled scheme 3.1. The reason for this is the need for the evaluation of the derivatives of the residuals with respect to the free surface coefficients H . How this is done is explained in detail by Kistler and Scriven (1983).
- R5. In the present work, the Jacobian matrix is built and factorized at each time step. This fact, together with the use of predicted values as first estimates, has ensured a fast convergence of the iterative process in all the simulations we have performed so far. One or two Newton's iterations are usually sufficient to achieve full convergence.
- R6. In view of its implicit character, the coupled scheme 3.2 is expected to be more stable than the decoupled algorithm 3.1 (it is indeed A-stable).

4. NUMERICAL RESULTS

The decoupled scheme 3.1 has been applied successfully to a number of surface-tension-driven viscoelastic flows, including the leveling of disturbances in thin films (Keunings and Bousfield 1986) and the breakup of axisymmetric jets (Keunings 1986a, Bousfield et al. 1986). At the time of this writing, we have completed the coding of the coupled scheme 3.2 for the particular case of a Newtonian fluid. The implementation of the Oldroyd-B fluid is underway.

The selection of a non-trivial test problem is difficult when dealing with transient free surface flows. We have chosen to solve a transient version of the planar die swell problem which could be studied with Keunings' code as well as with ours (recall that the former is limited to free surfaces that can be represented by a single-valued height function). Steady-state die swell calculations have been reviewed by Tanner (1985). For creeping Newtonian extrusion from a planar die, the swelling ratio is about 20%; it decreases when inertia forces come into play. Much larger values (of the order of 100%) have been observed and computed with viscoelastic fluids (see e.g. Crochet and Keunings 1982). To our knowledge, no time-dependent die swell computation has ever been reported in the literature, even for Newtonian liquids.

A typical flow geometry is shown in Fig.1 together with the finite element mesh used in the calculations. The boundary of the flow domain consists of a plane of symmetry, a fully developed flow section, the die wall, the free surface, and a downstream section. The boundary conditions are (i) a specified pressure in the upstream section, (ii) no-slip at the die wall, no traction along the free surface and in the downstream section, (iii) symmetry conditions at the plane of symmetry. We use nine-node isoparametric Lagrangian elements to discretize the flow domain. For a Newtonian fluid, the set of unknown fields reduces to the velocity, the pressure, and the free surface representation. We use C^0 - P^2 basis functions for the velocity, C^0 - P^1 for the pressure; as mentioned above, the discretization of the free surface is C^0 - P^2 . The mesh shown in Fig.1 contains 682 nodal values for the velocity, 96 for the pressure, and 19 degrees of freedom for the free surface. Note that the mesh is refined near the exit lip where the stress is singular. This singularity is integrable for a Newtonian fluid; recent results on viscoelastic singularities and their implications

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in numerical computations are described in Lipscomb et al. (1986) and Keunings (1986b).



Fig.1 Planar extrusion: geometry and finite element mesh.

The results of a transient simulation of the planar extrusion problem are depicted in Fig.2. The initial condition is the steady-state solution obtained with a pressure drop equal to 30 (we have specified $\mu_p = \lambda = 0$, $f = 0$, $\mu_s = 1$, $\rho = 1$; the die half-width is 1.) This steady-state solution corresponds to a Reynolds number of 3.5 based on the die half-width. The initial swelling ratio is 13%. At time $t = 0$, the pressure drop is decreased to 10. The steady-state solution corresponding to that pressure drop leads to a Reynolds number equal to 1 and 19.3% of extrudate swell. Both steady-states have been computed with the time-independent version of our implicit code, which computes the flow field and the free surface simultaneously by means of Newton's method.

Even though the initial and final states do not differ appreciably in this numerical experiment, the transient is quite interesting, as seen in Fig.2. One observes that the extrudate continuously shrinks, the thinnest point being transported downstream. This behavior is the result of conservation of mass: the decrease in pressure drop reduces the upstream flow velocity before that downstream. As a result, the extrudate must thin (we have also studied the effect of an increase in pressure drop. In this case, conservation of mass implies that the extrudate continuously thickens in the form of a bulge moving downstream; this bulge keeps on growing as long as there is fluid to accelerate downstream.) In the present case, the thinnest point leaves the integration domain before breakup of the extrudate sheet occurs. After that, the extrudate thickness starts to grow towards the final steady-state solution. Another look at this interesting transient is provided in Fig.3 where we show the evolution of the extrudate half-thickness at the downstream section. These numerical results have been obtained with both semi and fully implicit methods (no difference can be noted at the scales used in Fig.2 and 3.). In both cases, the time step was selected such that the rela-

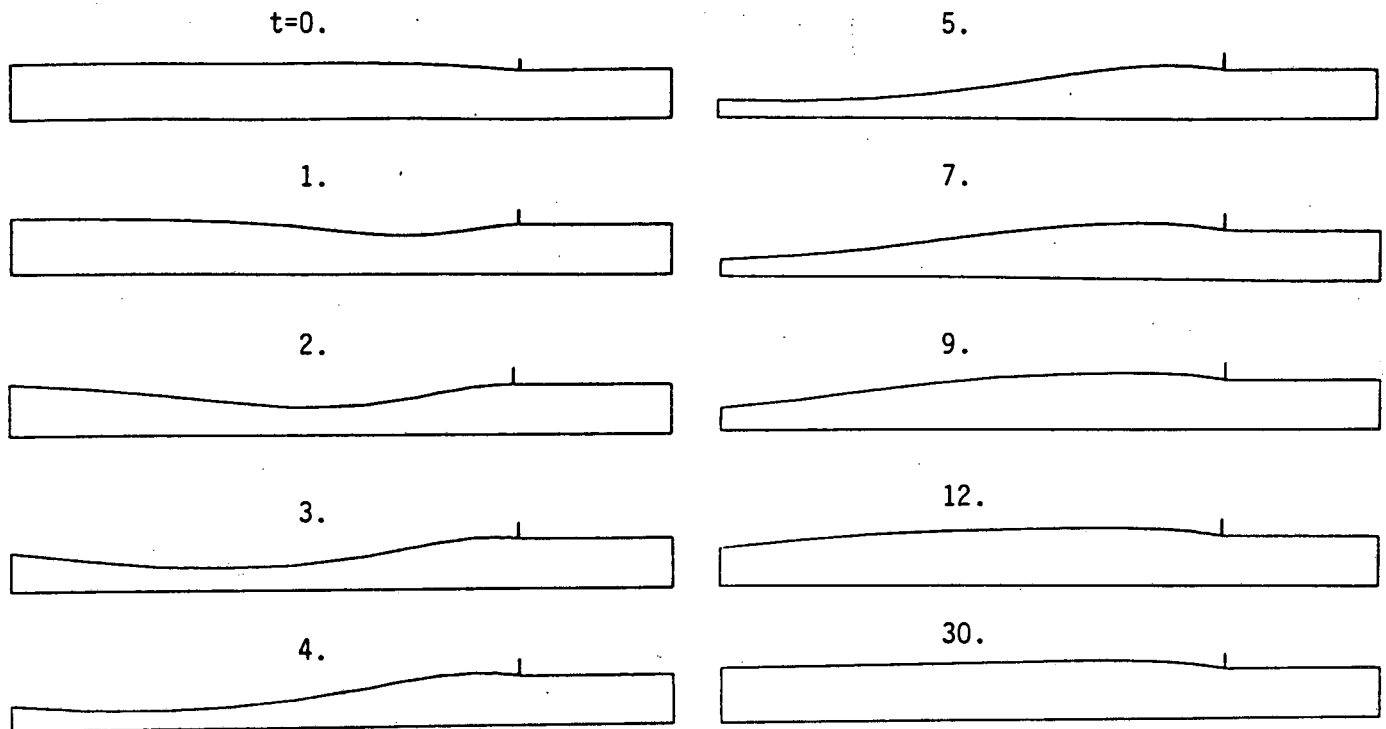


Fig.2. Simulation of a transient extrusion problem. The flow goes from right to left. The initial solution is the steady state for a pressure drop of 30. At time $t=0$, the pressure drop is suddenly decreased to 10. Several snapshots of the deforming flow domain are shown. At time $t=30$, the flow has reached a new steady state.

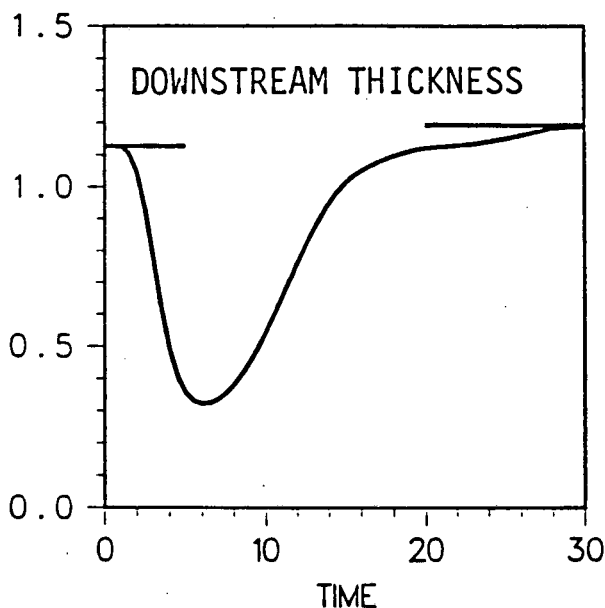


Fig.3. Evolution of the extrudate half-thickness at the downstream section.

tive difference between predicted and corrected values be always less than 0.001. The time step varied between 0.01 and 0.05 for both schemes, and one Newton iteration was generally sufficient to achieve convergence. The cost of one iteration is 0.63 CPU seconds on a CRAY X-MP (one processor) for the semi-implicit code, and 70 CPU seconds on a VAX 8650 for the implicit technique. In order to test our formulation and implementation of the Jacobian matrix of the coupled scheme 3.2, a few time steps have been solved without the associated prediction. The convergence of the iterative scheme was found to be quadratic, as expected with Newton's method.

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