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On the Numerical Modeling of an Oldroyd-Type Constitutive Equation

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A one-dimensional coupled set of equations consisting of appropriate forms of an equation of motion and a three-constant Oldroyd constitutive equation, used in the description of certain non-Newtonian flows, has been modeled using a finite-difference technique. These one-dimensional equations may be applicable along the centerline of a symmetric almost parallel flow field, where extensive molecular stretching occurs, with the restrictions of zero pressure gradient and zero shear. Mainly, this article differs from previous numerical work on these equations, such as Townsend's work on a four-constant Oldroyd equation, in that the nonlinear convection terms, which did not appear in this earlier work due to the parallel flow being considered, are now present. In comparison with the full set of equations, it is seen that the structure of the motion and constitutive equation used retain the essential characteristics of the complete set. In the equations, the time and spatial derivatives of both velocity and stress were centered so that in the Newtonian limit of zero relaxation and retardation times, the motion equation would reduce to Burgers' equation with the diffusion term time lagged. Stability of the differencing scheme for the constitutive equation dictated that the convective derivative of the deformation rate be time lagged with respect to the convective derivative of the stress. A von Neumann stability analysis was performed on the model equation yielding restrictions on Δt based on the usual viscous condition and, in addition, on the convective inertial and elastic propagation velocities, and also on the time scale of the straining motion. As a test for the proposed scheme an initial-boundary-value problem was formulated. An analytic steady-state solution to the problem can be obtained in Lagrangian coordinates if a constant velocity and a linear stress-deformation rate condition are assumed at the inflow to the flow field. This analytic solution, expressed in Eulerian coordinates, was then used as a check for the iterated steady-state solution.

I. INTRODUCTION

The equations under discussion in this paper are

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{\rho}\frac{\partial \tau}{\partial x}, \tag{1}$$

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$$\tau + \lambda_1 \left[\frac{\partial \tau}{\partial t} + u\frac{\partial \tau}{\partial x} - 2\tau\frac{\partial u}{\partial x}\right] = \eta_0 \left\{\frac{\partial u}{\partial x} + \lambda_2 \left[\frac{\partial^2 u}{\partial t\,\partial x} + u\frac{\partial^2 u}{\partial x^2} - 2\left(\frac{\partial u}{\partial x}\right)^2\right]\right\}, \tag{2}$$

where $u = u(x, t)$ and $\tau = \tau(x, t)$, ρ is a constant density, and λ_1, η_0, and λ_2 are constants which will be identified later. Equation (1) is recognized as a motion equation which, in the limit of zero relaxation and retardation time ($\lambda_1, \lambda_2 \to 0$) in the constitutive equation, reduces to Burgers' equation. Equation (2) is shown in Section II to be similar to the three-constant Oldroyd constitutive equation proposed by Giesekus [3] to model the flow of polymer solutions. These equations are intractable analytically except in the simplest of flow configurations and therefore to obtain solutions a numerical technique must be employed. Here, finite-difference techniques have been used to solve the above one-dimensional set of nonlinear model equations.

Previous numerical modeling of the Oldroyd equation (Townsend [4]) has been in parallel flow fields, thus eliminating the nonlinear convection terms and hence some hyperbolic features of more general forms of the Oldroyd equation which describe the flow in nonparallel geometries.

In the motion equation to be modeled, the time and spatial derivatives of the stress were differenced so that in the Newtonian limit of zero relaxation and retardation times this diffusion term would reduce to a lagged centered spatial difference of the velocity. In the constitutive equation it was found necessary to lag the convective derivative of the velocity gradient with respect to the convective derivative of the stress. Otherwise, the time and spatial derivatives were handled in the same manner as those in the motion equation.

A stability analysis yielded the usual viscous and convective restrictions on Δt. In addition, restrictions on Δt due to the elastic propagation velocity and the time scale of the straining motion were found.

Equations (1) and (2) lend themselves to an exact steady-state solution in Lagrangian coordinates. Thus, an initial-boundary-value problem can be formulated using these equations and the exact solution can be compared with the resulting Eulerian steady-state solution.

It is hoped that the proposed system of differential and difference equations will serve as a basis for future investigators in the numerical modeling of non-Newtonian fluids.

II. Formulation of the Governing Equations

The appropriate one-dimensional set of equations, (1) and (2), can be obtained utilizing the general equation of motion and a three-constant Oldroyd constitutive equation for a dilute polymer solution (Giesekus [3]), with no shear thinning,

$$\frac{\partial u_i}{\partial t} + u^j u_{i,j} = -\frac{1}{\rho} P_{,i} + \frac{1}{\rho} \tau_i{}^j{}_{,j}, \tag{3}$$

$$\tau^{ij} + \lambda_1 \frac{\delta \tau^{ij}}{\delta t} = 2\mu_0(1 + c[\eta]) \left\{ S^{ij} + \frac{\lambda_1}{1 + c[\eta]} \frac{\delta S^{ij}}{\delta t} \right\}, \tag{4}$$

where

$$S^{ij} = \tfrac{1}{2}(u^{i,j} + u^{j,i}),$$

$$\begin{aligned} \frac{\delta(\tau^{ij} - 2\mu_0 S^{ij})}{\delta t} = {} & \frac{\partial}{\partial t}(\tau^{ij} - 2\mu_0 S^{ij}) + (\tau^{ij} - 2\mu_0 S^{ij})_{,k}\, u^k \\ & - u^i{}_{,m}(\tau^{mj} - 2\mu_0 S^{mj}) - u^j{}_{,m}(\tau^{im} - 2\mu_0 S^{im}); \end{aligned}$$

also $u_i = u_i(x_i, t)$ are the components of a general velocity vector, $\tau^{ij}(x_i, t)$ and $\tau_i{}^j(x_i, t)$ are components of a general second-order stress tensor, $S^{ij} = S^{ij}(x_i, t)$ are components of a general second-order strain rate tensor, P is the pressure, ρ is once again the constant density, λ_1 is the relaxation time of the molecules, μ_0 is the dynamic viscosity of the solvent, $[\eta]$ is the intrinsic viscosity due to the presence of the molecules, and c is the concentration of polymer, x_i are the components of the position vector, and t is the time.

Consider a symmetric almost parallel flow field with zero pressure gradient and zero shear. Then from (3) and (4), the equations of interest on the centerline of this flow field would be

$$\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_1}{\partial x} = \frac{1}{\rho} \frac{\partial \tau_{11}}{\partial x}, \tag{5}$$

$$\begin{aligned} & \tau_{11} + \lambda_1 \left[\frac{\partial \tau_{11}}{\partial t} + u_1 \frac{\partial \tau_{11}}{\partial x} - 2\tau_{11} \frac{\partial u}{\partial x} \right] \\ & \quad = 2\mu_0(1 + c[\eta]) \left\{ S_{11} + \frac{\lambda_1}{1 + c[\eta]} \left[\frac{\partial S_{11}}{\partial t} + u_1 \frac{\partial S_{11}}{\partial x} - 2S_{11} \frac{\partial u}{\partial x} \right] \right\}, \end{aligned} \tag{6}$$

where $x = x_1$. Note that in the equation of motion, Eq. (5), $\tau_{12,2}$ and $\tau_{13,3}$ were neglected relative to $\tau_{11,1}$. This approximation should hold on the centerline in regions where extensive stretching of the molecules occurs, since here transverse gradients of the shearing stresses become unimportant relative to $\tau_{11,1}$. Finally, dropping the subscripts and identifying the constants in Eq. (2) gives the system of dimensional equations to be numerically modeled,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{\rho} \frac{\partial \tau}{\partial x}, \tag{7}$$

$$\tau + \lambda_1 \left[\frac{\partial \tau}{\partial t} + u \frac{\partial \tau}{\partial x} - 2\tau \frac{\partial u}{\partial x}\right]$$
$$= 2\mu_0(1 + c[\eta]) \left\{\frac{\partial u}{\partial x} + \frac{\lambda_1}{1 + c[\eta]} \left[\frac{\partial^2 u}{\partial t\, \partial x} + u \frac{\partial^2 u}{\partial x^2} - 2 \left(\frac{\partial u}{\partial x}\right)^2\right]\right\}. \quad (8)$$

An exact steady-state solution to these equations can be found. (The form of Eqs. (7) and (8) and the following exact solution are due to J. L. Lumley in a private communication.) First the nondimensional counterparts to (7) and (8) can be found by scaling with respect to some characteristic velocity and length scale u_s and l, respectively,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{\partial w}{\partial x} + 2\alpha \frac{\partial^2 u}{\partial x^2}, \quad (9)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} - 2w \frac{\partial u}{\partial x} + \frac{w}{T} = -2\epsilon \left[\frac{\partial^2 u}{\partial t\, \partial x} + u \frac{\partial^2 u}{\partial x^2} - 2 \left(\frac{\partial u}{\partial x}\right)^2\right], \quad (10)$$

where $w = \tau - 2\mu_0(1 + c[\eta])\, u_x$, $\alpha = (1 + c[\eta])/R_s$, $R_s = \rho u_s l/\mu_0$, $T = u_s\lambda_1/l$, $\epsilon = c[\eta]/R_s$. If a steady-state condition is assumed the motion equation can be integrated immediately and gives

$$u^2/2 = w + 2\alpha(\partial u/\partial x) + \text{const.} \quad (11)$$

The constant can be identified if we assume no stretching at the inflow, $w(x = 0) = 0$ and, in addition, unit inflow velocity and prescribed strain rate. Substituting the appropriate value for the constant into Eq. (11) gives

$$\frac{(u^2 - 1)}{2} = w + 2\alpha \left(\frac{\partial u}{\partial x} - \frac{\partial u}{\partial x}\bigg|_{x=0}\right). \quad (12)$$

Transforming now to Lagrangian coordinates, where $d/dt = u(\partial/\partial x)$, gives for (10) and (12), respectively,

$$\left(\frac{d}{dt} + \frac{1}{T}\right)\left(\frac{w}{u^2}\right) = \epsilon \frac{d^2}{dt^2} \left(\frac{1}{u^2}\right), \quad (13)$$

$$\left(\frac{d}{dt} + 2 \frac{\partial u}{\partial x}\bigg|_{x=0} - \frac{1}{2\alpha}\right)\left(\frac{1}{u^2}\right) = \frac{1}{\alpha} \left(\frac{w}{u^2}\right) - \frac{1}{2\alpha}. \quad (14)$$

Combining these two equations yields the second-order linear differential equation,

$$\left[\left(1 - \frac{\epsilon}{\alpha}\right) \frac{d^2}{dt^2} + \left(2 \frac{\partial u}{\partial x}\bigg|_{x=0} - \frac{1}{2\alpha} + \frac{1}{T}\right) \frac{d}{dt}\right.$$
$$\left. + \frac{1}{T} \left(2 \frac{\partial u}{\partial x}\bigg|_{x=0} - \frac{1}{2\alpha}\right)\right]\left(\frac{1}{u^2}\right) = - \frac{1}{2\alpha T}. \quad (15)$$

The solution can immediately be written as

$$\frac{1}{u^2} = \left(1 - 4\alpha \frac{\partial u}{\partial x}\bigg|_{x=0}\right)^{-1} + A_0 e^{\beta_1 t} + B_0 e^{\beta_2 t}, \tag{16}$$

where

$$\binom{\beta_1}{\beta_2} = \left\{-2 \frac{\partial u}{\partial x}\bigg|_{x=0} + \frac{1}{2\alpha} - \frac{1}{T} \pm \left[\left(2 \frac{\partial u}{\partial x}\bigg|_{x=0} - \frac{1}{2\alpha} - \frac{1}{T}\right)^2 + \frac{4\epsilon}{\alpha}\left(2 \frac{\partial u}{\partial x}\bigg|_{x=0} - \frac{1}{2\alpha}\right)\right]^{1/2}\right\}\left[2\left(1 - \frac{\epsilon}{\alpha}\right)\right]^{-1}$$

and

$$A_0 = \left[2 \frac{\partial u}{\partial x}\bigg|_{x=0} \Big/ (\beta_1 - \beta_2)\right]\left[2\alpha\beta_2\left(1 - 4\alpha \frac{\partial u}{\partial x}\bigg|_{x=0}\right)^{-1} - 1\right],$$

$$B_0 = \left[2 \frac{\partial u}{\partial x}\bigg|_{x=0} \Big/ (\beta_1 - \beta_2)\right]\left[-2\alpha\beta_1\left(1 - 4\alpha \frac{\partial u}{\partial x}\bigg|_{x=0}\right)^{-1} + 1\right].$$

In this study, the case to be considered is $4\alpha(\partial u/\partial x)|_{x=0} < 1$, which, depending on the sign of the gradient, corresponds to either a decelerating or an accelerating flow field. Since α can be interpreted as the ratio of extension forces to inertial forces, the above case would correspond to dominant inertial forces in an accelerating flow field. For the purpose of this investigation, then, only a Lagrangian accelerating velocity field will be examined, thus restricting $(\partial u/\partial x)|_{x=0}$ to positive values. In addition, the parameter T was taken to be unity so as to ensure a maximum effect. For certain values of A_0 and B_0 the solution for $1/u^2$ in Eq. (16) has a zero, which implies that $u \to \infty$ at some point in the flow. Since the objective here is to effectively numerically model the various terms in (7) and (8), only flow fields, narrowed so as not to include the singular point, will be considered. Recalling that the solution in Eq. (16) is expressed in terms of a Lagrangian system, this solution must be transformed back to the Eulerian frame before a comparison can be made with the numerical results.

In the transformation to Lagrangian coordinates, the initial displacement of the material point was zero, allowing the displacement of a material fluid element to be given by

$$x(t) = \int_0^t u[x(s)]\, ds, \tag{17}$$

or, if the variables are a set of discrete points,

$$x(t_i) = \sum_{q=1}^{i} u[x(t_q)](t_{q+1} - t_q). \tag{18}$$

One can then write for the Eulerian velocity,

$$u(x_l) = [x(t_l) - x(t_{l-1})]/\Delta t. \tag{19}$$

Now, the unknown variable $x(t_l)$ must be determined, and this is related to the known Lagrangian velocity in Eq. (16) by

$$x(t_l) = \int_0^{t_l} u(s)\, ds. \tag{20}$$

Since the values for $u(s)$ can be determined from Eq. (16), the integral in Eq. (20) can be evaluated. This was done using Simpson's rule and Newton's 3/8 rule (IBM 370/168 subroutine DQSF).

III. The Differencing Scheme

The differencing scheme which was used was applied to the nondimensional counterparts of (7) and (8), which can be written as

$$u_t + uu_x = \tau_x\,, \tag{21}$$

$$\tau + T[\tau_t + u\tau_x - 2\tau u_x] = 2\alpha u_x + (2T/R_s)[u_{xt} + uu_{xx} - 2u_x^2], \tag{22}$$

for ease of comparison with the exact steady-state solution. If the velocity is defined at the mesh point of the Cartesian computational grid covering the flow field under consideration and the stress is defined at points midway between the velocities, the following explicit difference scheme (Gatski [2]) can be used to model (21) and (22).

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} + \frac{u_j^{n}(\mu\delta u_j^{n})}{\Delta x} = \frac{\delta\tau_j^{n}}{\Delta x}, \tag{23}$$

$$\begin{aligned} \tau_{j+1/2}^{n+1} &+ T\left[\frac{\tau_{j+1/2}^{n+1} - \tau_{j+1/2}^{n-1}}{2\Delta t} + \frac{\mu u_{j+1/2}^{n}(\mu\delta\tau_{j+1/2}^{n})}{\Delta x} - \frac{2\tau_{j+1/2}^{n}(\Delta_+ u_j^{n})}{\Delta x}\right] \\ &= \frac{2\alpha(\Delta_+ u_j^{n})}{\Delta x} + \frac{2T}{R_s}\left[\frac{(\Delta_+ u_j^{n}) - (\Delta_+ u_j^{n-2})}{2\Delta t\, \Delta x}\right. \\ &\quad \left. + \frac{\mu u_{j+1/2}^{n-1}(\mu\delta\Delta_+ u_j^{n-1})}{\Delta x} - \frac{2(\Delta_+ u_j^{n-1})^2}{\Delta x^2}\right], \end{aligned} \tag{24}$$

where

$$\delta\tau_j{}^n = \tau^n_{j+1/2} - \tau^n_{j-1/2}, \qquad \mu\delta u_j{}^n = (u^n_{j+1} - u^n_{j-1})/2,$$

$$\mu u^n_{j+1/2} = (u^n_{j+1} + u_j{}^n)/2, \qquad \mu\delta\tau^n_{j+1/2} = (\tau^n_{j+3/2} - \tau^n_{j-1/2})/2,$$

$$\Delta_+ u_j{}^n = u^n_{j+1} - u_j{}^n, \qquad \mu\delta\Delta_+ u_j^{n-1} = (u^{n-1}_{j+2} - u^{n-1}_{j+1} - u_j^{n-1} + u^{n-1}_{j-1})/2,$$

and here subscripts and superscripts refer to the spatial and temporal grid points, respectively. The truncation error of the difference approximations (23) and (24) to the system (21) and (22) is $O(\Delta t, \Delta x^2)$.

IV. Stability of the Finite-Difference Equations

A von Neumann stability analysis was performed on the linearized set of difference equations corresponding to (23) and (24),

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} + \frac{u_0(\mu\delta u_j{}^n)}{\Delta x} = \frac{\delta\tau_j{}^n}{\Delta x}, \tag{25}$$

$$\begin{aligned} \tau^{n+1}_{j+1/2} &+ T\left[\frac{\tau^{n+1}_{j+1/2} - \tau^{n-1}_{j+1/2}}{2\Delta t} + \frac{u_0(\mu\delta\tau^n_{j+1/2})}{\Delta x} - \frac{2\tau_0(\Delta_+ u_j{}^n)}{\Delta x}\right] \\ &= \frac{2\alpha(\Delta_+ u_j{}^n)}{\Delta x} + \frac{2T}{R_s}\left[\frac{(\Delta_+ u_j{}^n) - (\Delta_+ u_j^{n-2})}{2\Delta t\,\Delta x}\right. \\ &\quad \left. + \frac{u_0(\mu\delta\Delta_+ u_j^{n-1})}{\Delta x} - \frac{2S_0(\Delta_+ u_j^{n-1})}{\Delta x}\right], \end{aligned} \tag{26}$$

where u_0 is a local mean velocity and S_0 and τ_0 are a local mean strain rate and stress, respectively. The eigenvalues of the resulting amplication matrix from the above equations were made to satisfy the condition $|\xi_i| < 1$, where ξ_i are the roots of the characteristic equation of the amplification matrix. However, with a multilevel difference scheme the characteristic equation is a high-order polynomial. One possible method of extracting conditions on Δt from the characteristic equation is the following.

A set of $2k$ conditions, developed by Cohn [1], on the real coefficients of a kth order polynomial $f(\xi)$ for the eigenvalues to lie within the unit circle are given as

$$f(1) \geqslant 0, \qquad (-1)^k f(-1) \geqslant 0, \qquad |A_s + \hat{A}_s| \geqslant 0,$$

and

$$|A_s - \hat{A}_s| \geqslant 0, \qquad s = 1, 2, \ldots, k-1, \tag{27}$$

where

$$A_s = \begin{pmatrix} a_k & a_{k-1} & \cdots & a_{k-s+1} \\ 0 & a_k & \cdots & a_{k-s+2} \\ \vdots & \vdots & & \vdots \\ 0 & \cdots 0 & \cdots & a_k \end{pmatrix}, \qquad \hat{A}_s = \begin{pmatrix} 0 & 0 & \cdots a_0 & a_0 \\ & 0 & \cdots a_0 & a_1 \\ \vdots & \vdots & & \vdots \\ & a_0 & \cdots a_{s-3} & a_{s-2} \\ a_0 & a_1 & \cdots a_{s-2} & a_{s-1} \end{pmatrix}.$$

Applying the above conditions to the characteristic equation yields necessary and sufficient conditions for the eigenvalues to lie within the unit circle. Now consider the characteristic equation obtained from (25) and (26):

$$\begin{aligned}
&[2\Delta t + T]\,\xi^4 + \left[4u_0\left(\frac{\Delta t}{\Delta x}\right)(\Delta t + T)\sin\gamma\right] i\xi^3 \\
&\quad - \left[(2\Delta t + T) + T\left(1 - \frac{16\Delta t}{\Delta x^2}\,\frac{\sin^2(\gamma/2)}{R_s}\right)\right. \\
&\quad \left. + 4\left(\frac{\Delta t}{\Delta x}\right)^2 \left(u_0{}^2 T \sin^2\gamma - 8(\alpha + T\tau_0)\sin^2\frac{\gamma}{2}\right)\right] \xi^2 \\
&\quad - \left[64\,\frac{T}{R_s}\left(\frac{\Delta t}{\Delta x}\right)^2 S_0 \sin^2\frac{\gamma}{2} + 4Tu_0\left(\frac{\Delta t}{\Delta x}\right)\left(1 - \frac{8\Delta t}{R_s\,\Delta x^2}\right) i \sin\gamma\,\sin^2\frac{\gamma}{2}\right]\xi \\
&\quad + T\left[1 - \frac{16\Delta t}{R_s\,\Delta x^2}\sin^2\frac{\gamma}{2}\right] = 0,
\end{aligned} \tag{28}$$

where γ is a wavenumber times Δx, following the usual procedure in the von Neumann analysis, and $i = \sqrt{-1}$. Since the analysis only holds for real coefficients it is necessary to split it into two parts. The first consists of analyzing Eq. (28) with $\tau_0 = S_0 = 0$,

$$\begin{aligned}
&[2\Delta t + T]\,\zeta^4 - \left[4u_0\left(\frac{\Delta t}{\Delta x}\right)(\Delta t + T)\sin\gamma\right]\zeta^3 \\
&\quad + \left[(2\Delta t + T) + T\left(1 - \frac{16\Delta t}{\Delta x^2}\,\frac{\sin^2(\gamma/2)}{R_s}\right)\right. \\
&\quad \left. + 4\left(\frac{\Delta t}{\Delta x}\right)^2\left(u_0{}^2 T\sin^2\gamma - 8\sin^2\frac{\gamma}{2}\right)\alpha\right]\zeta^2 \\
&\quad - \left[4Tu_0\left(\frac{\Delta t}{\Delta x}\right)\left(1 - \frac{8\Delta t}{\Delta x\,R_s}\sin^2\frac{\gamma}{2}\right)\sin\gamma\right]\zeta \\
&\quad + \left[T\left(1 - \frac{16\Delta t}{R_s\,\Delta x^2}\sin^2\frac{\gamma}{2}\right)\right] = 0,
\end{aligned} \tag{29}$$

where $\zeta = i\xi$, and the second consists of analyzing Eq. (28) with $u_0 = 0$,

$$[2\Delta t + T]\,\xi^4 - \Big[(2\Delta t + T) + T\Big(1 - \frac{16\Delta t}{\Delta x^2}\,\frac{\sin^2(\gamma/2)}{R_s}\Big) - 32\Big(\frac{\Delta t}{\Delta x}\Big)^2(\alpha + T\tau_0)\sin^2\frac{\gamma}{2}\Big]\,\xi^2 - \Big[64\,\frac{T}{R_s}\Big(\frac{\Delta t}{\Delta x}\Big)^2 S_0 \sin^2\frac{\gamma}{2}\Big]\,\xi + T\Big[1 - \frac{16\Delta t}{R_s\,\Delta x^2}\sin^2\frac{\gamma}{2}\Big] = 0. \quad (30)$$

The above equations would then yield a total of 16 conditions. Fortunately many conditions are redundant, and from the remaining conditions, restrictions on Δt can be extracted by arranging each of the conditions of (27) in powers of $\Delta t/T$. From these, rather restrictive conditions on Δt are found,

$$\frac{\Delta t}{\Delta x^2} \leqslant \frac{1}{16\alpha + |\,u_0\,|\,\Delta x}, \qquad \frac{\Delta t}{\Delta x^2} \leqslant \frac{1}{8\,|\,\tau_0\,|^{1/2}\,\Delta x},$$
$$\frac{\Delta t}{\Delta x^2} \leqslant \frac{1}{4\,|\,S_0\,|\,\Delta x^2 + (8/R_s)}, \qquad \tau_0 \leqslant \frac{2S_0}{R_s} - \frac{\alpha}{T}. \quad (31)$$

The first three of these conditions can combine to form the further inequality

$$\Delta t/\Delta x^2 < 1/[16\alpha + |\,u_0\,|\,\Delta x + 8\,|\,\tau_0\,|^{1/2}\,\Delta x + 4\,|\,S_0\,|\,\Delta x^2 + (8/R_s)]. \quad (32)$$

Of course the most restrictive of these conditions depend on the magnitude of the parameters involved. The terms appearing in (32) can be easily identified; 16α and $8/R_s$ are simply viscous conditions, $|\,u_0\,|$ represents the C–F–L condition for the scheme, $4S_0$ is rather unique and requires that the time step be less than the mean deformation rate of the fluid motion, and, finally, $8\,|\,\tau_0\,|^{1/2}$ can be considered as an elastic propagation velocity analogous to the usual C–F–L condition. The last of conditions (31) can be shown to be the criterion for the decay of a small-amplitude harmonic disturbance introduced into the linearized differential system of equations, (21) and (22). However, the main contribution to $\Delta t/\Delta x^2$ comes from the terms containing α and R_s. Using only these terms in inequality (32), an estimate for critical Δt can be made for the two sample computations presented in Section VI. For the values of R_s, $c[\eta]$, and Δx given in the figures the linear stability analysis would predict a critical value of Δt of approximately 2.5×10^{-4} (a value of 2.0×10^{-4} was used in the actual computation). Test runs indicated, however, that for the case $c[\eta] = 1.0$ a stable computation could be carried out at a value of Δt about 3.5 times greater than the predicted value, and for the case $c[\eta] = 0$ a value of Δt about 2 times greater than that predicted could be used.

These results indicate that although the linear stability analysis underestimates the critical value of Δt it does provide for a reasonable and stable starting value for it.

V. Initial and Boundary Conditions

The initial choice of values was dependent only on the transient phenomenon desired. Here only accelerating velocity fields were considered. Therefore, initially, a linearly increasing strain rate field was chosen, thus making the initial velocity profile parabolic. As for the initial stress, these values were chosen so that the boundary condition at inflow, $\tau(0, 0) = 2\alpha[\partial u(x, 0)/\partial x]|_{x=0} = 2\alpha$ was satisfied, and in the remainder of the flow field $\tau(x, 0) > 2\alpha[\partial u(x, 0)/\partial x]$.

Considering now the boundary conditions, the inflow condition on the velocity is

$$u_0{}^n = 1.0, \tag{33}$$

and on the stress and velocity gradient is

$$\tau_B{}^n = 2\alpha \left.\frac{\partial u}{\partial x}\right|_B, \qquad \text{i.e.,} \qquad w(0, t) = 0. \tag{34}$$

Since the stress and strain rate are defined at locations one-half mesh spacing from the boundary, it was necessary to take an arithmetic mean of these quantities about the inflow boundary point $x = 0$. This type of average necessitates a knowledge of the velocity and stress exterior to the flow domain under consideration. In addition, the spatial stress gradients in the constitutive equation require a knowledge of an exterior stress point in the calculation at the first interior point of the flow domain. At each time level these two unknowns can be expressed in terms of known values within the flow field by simultaneously solving the boundary condition (34) with the motion equation at the boundary; the resulting expressions are

$$u_{-1}^n = u_1{}^n - [4\Delta x/(4\alpha + \Delta x)]\, \tau_{1/2}^n, \tag{35}$$

$$\tau_{-1/2}^n = [(4\alpha - \Delta x)/(4\alpha + \Delta x)]\, \tau_{1/2}^n. \tag{36}$$

The only remaining boundary condition to be satisfied is the inflow deformation rate condition, $[\partial u(x, t)/\partial x]|_{x=0} = 1$. Recalling Eqs. (9) and (10), this slope condition, along with the inflow velocity condition, allowed this system of equations to be solved more easily than would have been possible had an inflow and outflow condition on velocity been specified; but in the numerical computation, either set of conditions should be equally applicable. In doing the computation, the specification of an inflow and outflow velocity was chosen. The inflow condition has already been mentioned; now, the outflow condition must be considered.

Since the Eulerian velocity profile can be calculated (Section II) up to the singular point in the velocity profile, consider the outflow boundary as being located near the singular point but at a point where the velocity is real and finite. Then, assuming small transient deviations of the calculated boundary velocity, the outflow velocity need only be obtained for the particular boundary point from the Eulerain velocity profile.

As with the inflow boundary, exterior values of the velocity and stress are needed at the outflow boundary, specifically in the nonlinear convection terms in the constitutive equation. Here there is no boundary condition on stress and strain rate and the only equation available is the motion equation subject to the above assumption on small transient deviations of boundary velocity. The additional relation which is needed is found from an extrapolation of strain rate values. The fastest convergence was achieved by using the simple mean of a five-point spatial extrapolation and a three-point time extrapolation. This average value of the strain rate then allows the exterior velocity point to be found and substitution of the value into the motion equation at the outflow boundary allows the stress to be calculated at the exterior point, i.e.,

$$\tau_{J/2}^{n} = \tau_{-J/2}^{n} + u_J{}^n[(u_{J+1}^{n} - u_{J-1}^{n})/2], \tag{37}$$

where J is the grid location of the outflow boundary.

VI. Sample Computations

Using (23) and (24), test runs were made with R_s and $c[\eta]$ varied. Since the results for the accelerating velocity field being considered were qualitatively similar for different values of the solvent Reynolds number R_s, with the flow field becoming narrower as the Reynolds number increases thus decreasing the size of Δt, a representative value of $R_s = 10.0$ was chosen. For this value of R_s, two values for $c[\eta]$ were used. The first is $c[\eta] = 1.0$, which should allow for substantial elastic behavior of the fluid, and the second is $c[\eta] = 0$, which should yield a Newtonian behavior of the fluid since the constitutive equation is solved by the usual linear relationship between stress and strain rate.

A velocity profile at various times for $R_s = 10.0$, $c[\eta] = 1.0$ is given in Fig. 1a. The transient behavior of the velocity at certain points in the flow field is shown in

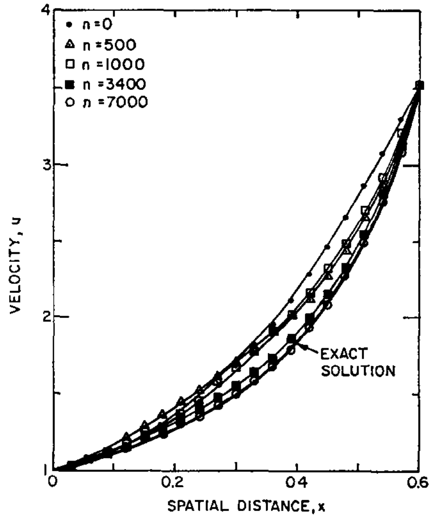

FIG. 1a. Velocity profiles for $R_s = 10.0$, $c[\eta] = 1.0$, with $\Delta x = 3.0 \times 10^{-2}$, and $\Delta t = 2.0 \times 10^{-4}$.

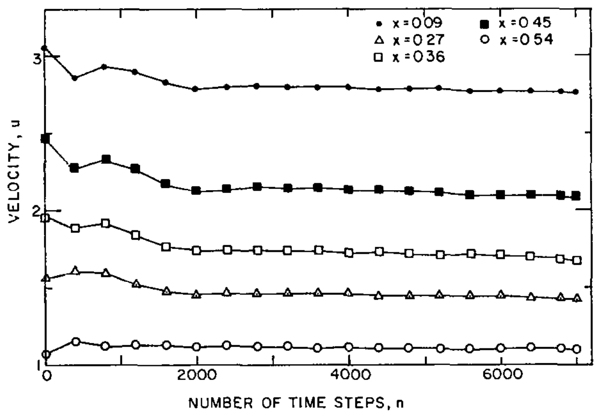

FIG. 1b. Variation of velocity with time for $R_s = 10.0$, $c[\eta] = 1.0$, with $\Delta x = 3.0 \times 10^{-2}$ and $\Delta t = 2.0 \times 10^{-4}$.

Fig. 1b. For the case $R_s = 10.0$ and $c[\eta] = 0$, similar results are shown in Figs. 2a and 2b. It is easily seen that the velocity profile for $c[\eta] = 0$ approaches the steady-state value more rapidly than for the case $c[\eta] = 1.0$; in addition, the oscillatory behavior of the transient vanishes for $c[\eta] = 0$, as would be expected from the form of Eq. (15).

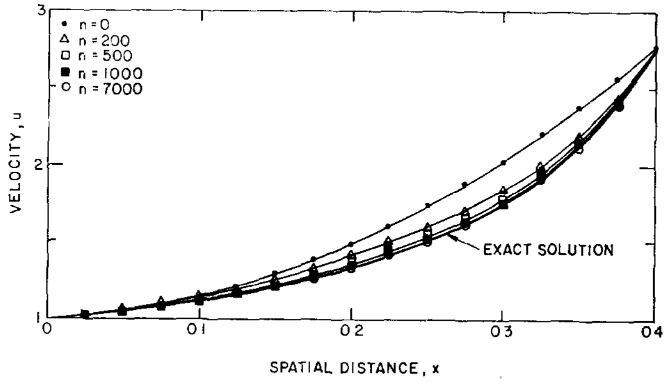

FIG. 2a. Velocity profile for $R_s = 10.0$, $c[\eta] = 0.0$, with $\Delta x = 2.5 \times 10^{-2}$ and $\Delta t = 2.0 \times 10^{-4}$

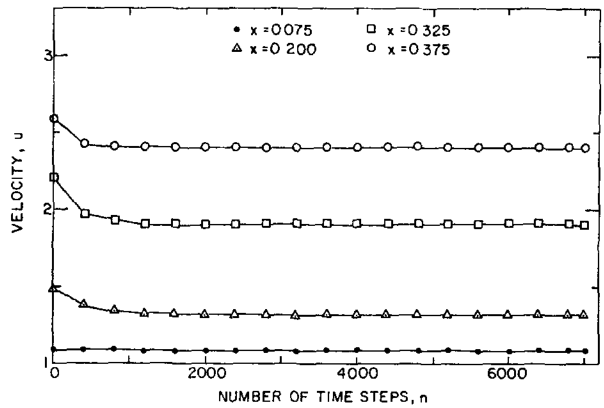

FIG. 2b. Variation of velocity with time for $R_s = 10.0$, $c[\eta] = 0.0$, with $\Delta x = 2.5 \times 10^{-2}$ and $\Delta t = 2.0 \times 10^{-4}$.

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