CONNFFESSIT Approach for Solving a Two-Dimensional Viscoelastic Fluid Problem

Kathleen Feigl,* Manuel Laso, and Hans Christian Öttinger

Institut für Polymere, Eidgenössische Technische Hochschule Zürich, ETH-Zentrum, CH-8092 Zürich, Switzerland

Received August 30, 1994; Revised Manuscript Received December 6, 1994[⊗]

ABSTRACT: An innovative approach for numerically solving viscoelastic fluid problems, recently introduced to solve a time-dependent one-dimensional problem, is extended to two-dimensional space for a steady-state problem. Referred to as CONNFFESSIT (Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique), this new approach uses standard finite element techniques for solving the momentum and continuity equations but replaces the integral or differential constitutive equation, traditionally used to compute polymer stresses, with stochastic simulations of polymer dynamics. In CONNFFESSIT, the polymer contribution to the stress tensor is determined from a stochastic simulation of an ensemble of model polymer molecules from whose configurations the polymer stress can be computed as an ensemble average. The problem considered for testing the CONNFFESSIT approach in two dimensions is the steady flow of an Oldroyd-B fluid in an abrupt 4:1 axisymmetric contraction, assuming incompressibility and isothermal conditions. After details of the implementation of the stochastic simulation technique are presented, a comparison is made between the numerical results obtained using the CONNFFESSIT approach and those obtained using the closed-form integral constitutive equation of the Oldroyd-B model. We find excellent agreement in most cases and explain reasons for the sometimes large differences.

1. Introduction

The numerical solution of viscoelastic fluid problems in complex geometries, using primarily finite element techniques, has been an area of extensive research in polymer fluid mechanics. A principal goal of this research has been the ability to simulate accurately on a computer the flow behavior of polymeric fluids during various processing procedures. The success of a particular simulation crucially depends upon the accurate description of the relationship between the strain history experienced by the fluid and the resulting stress. The conventional approach taken in finite element (or finite difference or finite volume) programs is to use a closed-form constitutive equation, given either as a differential equation or as an integral, to describe this relationship and to compute polymer stress.

Recently, a new approach has been introduced for computing polymer stress in finite element programs which is based on stochastic simulations of the polymer dynamics. The polymer stresses are determined from a large ensemble of model polymer molecules, such as bead–spring chains or dumbbells. As with real polymer molecules, the configurations of these model molecules hold the information about the strain history needed to compute the polymer stress. We call this approach of combining standard finite element techniques for solving the momentum and continuity equations with stochastic simulation techniques for computing polymer stress CONNFFESSIT (Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique).

A clear advantage of the CONNFFESSIT approach over conventional finite element programs for solving viscoelastic fluid problems is that CONNFFESSIT allows one to use models from polymer kinetic theory without having or having to derive an equivalent closed-form constitutive equation. CONNFFESSIT can consider models which have no known equivalent, or only an approximate, closed-form constitutive equation, such as the FENE model (finitely-extensible-nonlinear-elastic model). Furthermore, the fact that individual "molecules" are being simulated in CONNFFESSIT makes it possible to include effects such as hydrodynamic interactions and polydispersity. Also, CONNFFESSIT automatically provides information on the configurations of polymer molecules which determine, for example, the mechanical properties of finished plastic products.

The CONNFFESSIT approach has been previously tested in one-dimensional space by solving the start-up of plane Couette flow for several molecular models: upper-convected Maxwell, Oldroyd-B, FENE, FENE-P, Curtiss-Bird, and Doi–Edwards.[1,2] It is the purpose of this paper to extend CONNFFESSIT to steady-state problems in two-dimensional space. We do so by incorporating the stochastic simulation method for stress calculation into an existing finite element program which solves the two-dimensional steady flow of incompressible viscoelastic fluids under isothermal conditions using an integral constitutive equation. As a test problem, the steady flow of an Oldroyd-B fluid in an abrupt 4:1 axisymmetric contraction is solved using CONNFFESSIT. The contraction problem, or die entry problem, is a well-accepted benchmark problem for testing numerical algorithms for viscoelastic flow calculations.

The paper is organized as follows. In section 2 the basic ideas of CONNFFESSIT are introduced. A two-step stochastic simulation technique for computing stress is described along with the finite element method for solving the equations of motion. Details of the stochastic simulation as applied to our test problem are given in section 3. In section 4 we evaluate the performance of the CONNFFESSIT approach by comparing the numerical results obtained using CONNFFESSIT to solve our test problem with the results obtained using a conventional finite element program with the closed-form integral constitutive equation for

* To whom correspondence should be addressed.

[⊗] Abstract published in *Advance ACS Abstracts,* April 1, 1995.

0024-9297/95/2228-3261$09.00/0

the Oldroyd-B model. A summary and conclusions are presented in section 5.

2. CONNFFESSIT Idea

We wish to solve the equations of state for the steady flow of an incompressible viscoelastic fluid under isothermal conditions. Letting $\boldsymbol{u}$ and p denote the velocity and pressure fields, respectively, and ϱ the (constant) density, the equations for the conservation of momentum and mass can be written as

$$\nabla\cdot\boldsymbol{\tau}^{\mathrm{p}} + \eta_{\mathrm{s}}\nabla\cdot\dot{\boldsymbol{\gamma}} - \nabla p = \varrho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} \tag{1}$$

$$\nabla\cdot\boldsymbol{u} = 0 \tag{2}$$

In eq 1 we have written the extra-stress $\boldsymbol{\tau}$ as the sum of a polymer contribution, $\boldsymbol{\tau}^{\mathrm{p}}$, and a Newtonian (or solvent) contribution, $\boldsymbol{\tau}^{\mathrm{s}}$, given by

$$\boldsymbol{\tau}^{\mathrm{s}} = \eta_{\mathrm{s}}\dot{\boldsymbol{\gamma}} = \eta_{\mathrm{s}}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}}) \tag{3}$$

where η_{s} is the viscosity of the solvent fluid and $\dot{\boldsymbol{\gamma}} = (\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}})$ is the rate-of-strain tensor.

The polymer contribution to the stress tensor, $\boldsymbol{\tau}^{\mathrm{p}}$, describes the complex relationship between a fluid's deformation history and its stress response. In the literature one can find many models, or constitutive equations, which have been proposed for the stress–strain relationship of various polymeric liquids (see ref 3 for a review). These models have their derivation either in continuum mechanics or in polymer kinetic theory, or perhaps in both, and they most often appear in closed form either as an integral or as a differential equation. The constitutive equation we consider in this paper is the Oldroyd-B model which can be derived from both continuum mechanics and polymer kinetic theory and may be expressed as the following integral or differential equation, respectively,

$$\boldsymbol{\tau}^{\mathrm{p}} = \frac{\eta_{\mathrm{p}}}{\lambda^2}\int_0^\infty (\boldsymbol{C}_0^{-1}(s) - \boldsymbol{I})\mathrm{e}^{-s/\lambda}\,ds \tag{4}$$

$$\boldsymbol{\tau}^{\mathrm{p}} + \lambda\left[\frac{D\boldsymbol{\tau}^{\mathrm{p}}}{Dt} - (\nabla\boldsymbol{u})^{\mathrm{T}}\cdot\boldsymbol{\tau}^{\mathrm{p}} - \boldsymbol{\tau}^{\mathrm{p}}\cdot\nabla\boldsymbol{u}\right] = \eta_{\mathrm{p}}[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}}] \tag{5}$$

where λ is the relaxation time of the fluid, η_{p} is the polymer viscosity, and $\mathrm{D}(\cdot)/\mathrm{D}t = \partial(\cdot)/\partial t + (\boldsymbol{u}\cdot\nabla)(\cdot)$ is the material derivative. The tensor $\boldsymbol{C}_0^{-1}(s) = (\partial\boldsymbol{x}(s)/\partial\boldsymbol{x}(0))^{-1}\cdot(\partial\boldsymbol{x}(s)/\partial\boldsymbol{x}(0))^{-\mathrm{T}}$ is the relative Finger strain tensor, where $\boldsymbol{x}(0)$ is the point at which stress is being computed and $\boldsymbol{x}(s)$ is the position of the particle, initially at $\boldsymbol{x}(0)$, s time units in the past ($s \geq 0$).

Solving the momentum and continuity equations (eqs 1 and 2) for a given "definition" for $\boldsymbol{\tau}^{\mathrm{p}}$ is the finite element part of CONNFFESSIT. Those who work in the numerical simulation of the flows of viscoelastic fluids, using the finite element method for example, have focused on the use of closed-form integral or differential constitutive equations in their algorithms.

We describe below a way for determining $\boldsymbol{\tau}^{\mathrm{p}}$ in a given flow field which is based at the molecular level and uses stochastic techniques to determine the polymer stresses from a large ensemble of models of polymer molecules. This is the stochastic simulation part of CONNFFESSIT. After this discussion, we describe the essential features of the finite element method used to solve the momentum and continuity equations (eqs 1 and 2) given a definition for $\boldsymbol{\tau}^{\mathrm{p}}$.

Stochastic Simulation. In polymer kinetic theory there are two steps for determining the polymer stresses. The first step is the derivation of a "diffusion equation" for the configurational distribution function.[4] This is a second-order partial differential equation whose solution, the configurational distribution function $\psi(\boldsymbol{q},t)$, is the probability density that the polymer configuration $\boldsymbol{q}$ occurs at time t. The second step is the development of an expression for the stress tensor involving the polymer configurations whose distribution is described by $\psi(\boldsymbol{q},t)$.

Our stochastic simulation algorithm for computing the polymer stresses follows this two-step procedure. Its theoretical foundation lies in the fact that the diffusion equation has associated with it an equivalent stochastic differential equation. The relationship between diffusion equations, which are referred to as Fokker–Planck equations in mathematical stochastics, and stochastic differential equations is well-known. Briefly stated, the polymer dynamics described by the diffusion equation for $\psi(\boldsymbol{q},t)$ can be thought of as a Markovian stochastic process, $\boldsymbol{Q}(t)$, whose transition probabilities satisfy the diffusion equation and which solves a stochastic differential equation whose coefficients at any time depend only on the current configuration of polymer molecules.[5,6]

We can write one general form of the diffusion equation for $\psi(\boldsymbol{q},t)$ and an equivalent stochastic differential equation for $\boldsymbol{Q}(t)$ (in the absence of external forces) respectively as

$$\frac{\partial}{\partial t}\psi(\boldsymbol{q},t) = -\frac{\partial}{\partial\boldsymbol{q}}\cdot[\boldsymbol{A}(\boldsymbol{q},t)\,\psi(\boldsymbol{q},t)] + \frac{1}{2}\frac{\partial}{\partial\boldsymbol{q}}\cdot\left[\frac{\partial}{\partial\boldsymbol{q}}\cdot\{\boldsymbol{D}(\boldsymbol{q},t)\,\psi(\boldsymbol{q},t)\}\right] \tag{6}$$

$$\mathrm{d}\boldsymbol{Q}(t) = \boldsymbol{A}(\boldsymbol{Q}(t),t)\,\mathrm{d}t + \boldsymbol{B}(\boldsymbol{Q}(t),t)\cdot\mathrm{d}\boldsymbol{W}(t) \tag{7}$$

where $\boldsymbol{A}(\boldsymbol{q},t)$ and $\boldsymbol{W}(t)$ are d-component column vectors, $\boldsymbol{D}(\boldsymbol{q},t)$ is a positive semidefinite $d \times d$ matrix, and $\boldsymbol{B}(\boldsymbol{q},t)$ is a $d \times d$ matrix such that $\boldsymbol{D}(\boldsymbol{q},t) = \boldsymbol{B}(\boldsymbol{q},t)\cdot\boldsymbol{B}^{\mathrm{T}}(\boldsymbol{q},t)$. The components $W_i(t)$ of $\boldsymbol{W}(t)$ are independent Wiener processes, that is, Gaussian processes with mean $\langle W_i(t)\rangle = 0$ and covariance given by $\langle W_i(t)\,W_j(t')\rangle = \delta_{ij}\min(t,t')$.

The time discretization of the stochastic differential equation (eq 7) provides us with the first step of our stochastic simulation technique. If we partition time into intervals $[t_i,t_{i+1})$ where $t_i < t_{i+1}$, $i = 0,1,2,\ldots$ and let $\boldsymbol{Q}_i$ be the approximation to $\boldsymbol{Q}(t)$ at $t = t_i$, then eq 7 can be discretized as

$$\boldsymbol{Q}_{i+1} - \boldsymbol{Q}_i = \boldsymbol{A}(\boldsymbol{Q}_i,t_i)\Delta t_i + \boldsymbol{B}(\boldsymbol{Q}_i,t_i)\cdot\boldsymbol{W}_i\sqrt{\Delta t_i} \tag{8}$$

where $\Delta t_i = t_{i+1} - t_i$. Here, the d components of each increment $\boldsymbol{W}_i$ of the Wiener process are independent standard Gaussian random variables and for different time steps $i \neq j$ the Gaussian vectors $\boldsymbol{W}_i$ and $\boldsymbol{W}_j$ are independent. The details of the crucial relationship between diffusion equations and stochastic differential equations, and the Brownian dynamics used to obtain the stochastic difference equation (eq 8), can be found in refs 7–9.

For a given model of the polymer molecules, the stochastic difference equation (eq 8) is used to simulate the configurations of these model molecules at each time t_i starting from a given probability distribution function of configurations at t_0. In this study, we use Hookean dumbbells in a suspending medium to model the polymer molecules; this model can be shown to lead to the

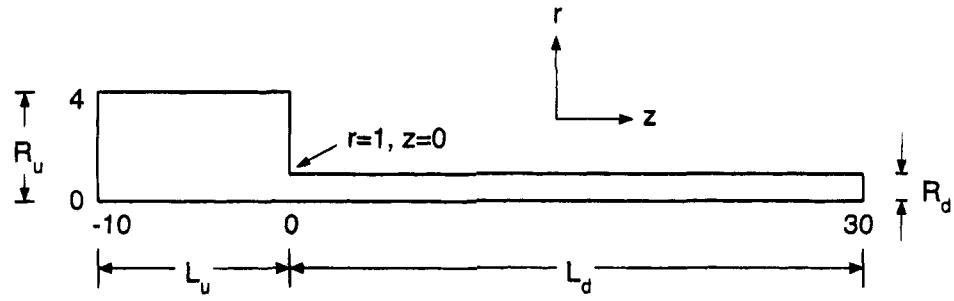

Figure 1. Die entry domain.

closed-form Oldroyd-B constitutive equation, eq 5 (and eq 4 in integral form), derived from continuum mechanics.[4] Each Hookean dumbbell "molecule" consists of two identical beads with friction coefficients ζ connected by an elastic spring obeying Hooke's spring law with spring constant H. Letting $\boldsymbol{F}^{(c)} = H\boldsymbol{q}$ denote the connector force, the diffusion equation and equivalent stochastic differential equation corresponding to this molecule model are found by taking

$$\boldsymbol{A}(\boldsymbol{q},t) = \kappa(t)\cdot\mathbf{q} - \frac{2}{\zeta}\boldsymbol{F}^{(c)}(\boldsymbol{q}) \tag{9}$$

$$\boldsymbol{B}(\boldsymbol{q},t) = 2\sqrt{\frac{kT}{\zeta}}\boldsymbol{\delta} \tag{10}$$

$$\boldsymbol{D}(\boldsymbol{q},t) = \frac{4kT}{\zeta}\boldsymbol{\delta} \tag{11}$$

in eqs 6 and 7, where $\kappa(t)$ is the (position-dependent) transposed velocity gradient tensor characterizing the flow field, $\boldsymbol{\delta}$ is the unit tensor, and T and k are the absolute temperature and Boltzmann constant.

By eq 8, the configuration of each Hookean dumbbell at time t_{i+1} is then described by the stochastic difference equation

$$\boldsymbol{Q}^*_{i+1} = \boldsymbol{Q}^*_i + \mathcal{K}_i\cdot\boldsymbol{Q}^*_i\,\Delta t_i - \frac{1}{2}\boldsymbol{Q}^*_i\frac{\Delta t_i}{\lambda_H} + \boldsymbol{W}_i\sqrt{\frac{\Delta t_i}{\lambda_H}} \tag{12}$$

where the vectors $\boldsymbol{Q}^*_i$ and $\boldsymbol{W}_i$ have three components each, $\boldsymbol{Q}^*_i = \boldsymbol{Q}_i[H/(kT)]^{1/2}$ is the dimensionless connector vector between the two beads of the dumbbell at time t_i, and $\lambda_H = \zeta/(4H)$ is the relaxation time of the dumbbells. Also, $\mathcal{K}_i$ is a 3×3 matrix representing the known transposed velocity gradient used to advance the dumbbell from its position at t_i to its position at t_{i+1} in the simulation; in our CONNFFESSIT program we took $\mathcal{K}_i$ to be the average of the (known) transposed velocity gradient at the positions occupied by the dumbbell at simulation times t_i and t_{i+1}, *i.e.* $\mathcal{K}_i = (\kappa_i + \kappa_{i+1})/2$. Simulating the configurations of a large ensemble of dumbbells via eq 12 comprises the first step of our two-step procedure for stress calculation.

In the second step of our procedure these configurations are used to compute the polymer stresses using the Kramers form for the stress tensor for the Hookean dumbbell model[4]

$$\boldsymbol{\tau}^p(t) = -nkT(\boldsymbol{\delta} - \langle\boldsymbol{Q}^*(t)\,\boldsymbol{Q}^*(t)\rangle) \tag{13}$$

where n is the dumbbell number density and $\langle\boldsymbol{Q}^*(t)\,\boldsymbol{Q}^*(t)\rangle$ represents the position-dependent ensemble average of $\boldsymbol{Q}^*(t)\,\boldsymbol{Q}^*(t)$. (We note that the sign convention we use here for the stresses is the opposite of that used in refs 3 and 4.) The number of dumbbells in the ensemble determines the accuracy with which the polymer stresses in a given flow field are calculated.

In summary, through eqs 12 and 13, we have defined our general two-step stochastic simulation algorithm for polymer stress calculation. The details of the algorithm for our particular two-dimensional problem—the axisymmetric die entry problem—are discussed in section 3. We now describe the application of the finite element method for solving the equations of motion, eqs 1 and 2.

Finite Element Method. The finite element method is a well-established technique for the numerical solution of a wide range of engineering problems, including problems in fluid dynamics. It is a type of Rayleigh–Ritz or Galerkin method in which the original continuous problem is expressed in a variational, or weak, form. Once in this form, it is assumed that the solution can be approximated by a linear combination of so-called "trial" functions. These functions are chosen to be basis functions for the underlying finite dimensional vector space so that the coefficients in this expression represent the solution of the equations at specific points in the problem's domain. This approximation reduces the continuous weak equations to a discrete system of algebraic equations which can then be solved by a computer.

The particular finite element procedure used by CONNFFESSIT in the two-dimensional test problem considered here was taken from a finite element program developed by Bernstein, Malkus, et al.[10–12] This program, referred to as FLUCODE, was developed for solving steady flow problems of incompressible viscoelastic fluids under isothermal conditions using a K-BKZ or Rivlin-Sawyers integral constitutive equation. It has been previously used to solve a 4:1 axisymmetric contraction problem (see ref 12), and the results were found to be in agreement with those of Dupont and Crochet,[13] Goublomme,[14] and Luo and Mitsoulis[15] for the same integral constitutive equation. It has also been used to simulate the die entry behavior of a low-density polyethylene melt.[16]

The CONNFFESSIT program we used for our test problem was formed by replacing the integral constitutive equation in FLUCODE with the stochastic simulation technique for polymer stress calculation. We outline some of the main steps of the finite element method in terms of its application in FLUCODE and CONNFFESSIT.

The finite element method is applied to the penalty method formulation of the system (eqs 1 and 2) obtained by replacing the incompressibility condition (eq 2) with the penalty equation $p = -(1/\epsilon)\nabla\cdot\boldsymbol{u}$, where ϵ is a small penalty parameter. The fluid is thus treated as being slightly compressible. The penalty method is a popular technique used in numerical methods for solving two- or three-dimensional incompressible fluid problems

since it eliminates not only the incompressibility condition (eq 2) but also pressure as an unknown.

Let Ω denote the domain on which we solve the system of equations along with associated boundary conditions, and let V be an appropriately defined vector space of scalar functions. The continuous weak equations are formed by multiplying the momentum equation (eq 1) by so-called "weight" functions $\boldsymbol{w} \in V^2$ (in the spirit of the method of weighted residuals) which vanish on the boundary of the domain Ω, integrating over Ω, and integrating the stress and pressure terms by parts. The weak formulation of the problem can then be stated as follows: find $\boldsymbol{u} \in V^2$ satisfying prescribed boundary conditions such that

$$\int_\Omega \Big[(\boldsymbol{\tau}^p + \eta_s \dot{\gamma}) : \nabla \boldsymbol{w} + \frac{1}{\epsilon} (\nabla \cdot \boldsymbol{u})(\nabla \cdot \boldsymbol{w}) + \varrho[(\boldsymbol{u} \cdot \nabla)\boldsymbol{u}] \cdot \boldsymbol{w} \Big] \, d\Omega = 0 \quad (14)$$

for all $\boldsymbol{w} \in V^2$ which vanish on the boundary (the pressure p has been replaced by the penalty equation). The left-hand side of eq 14 is referred to as the residual. In our algorithm, an iterative procedure is used which decouples the stress calculation from the momentum equation. In each iteration the polymer stresses $\boldsymbol{\tau}^p$ (as well as the Newtonian stress $\boldsymbol{\tau}^s$ in eq 3, if present) are computed from the known velocity field of the previous iteration using an appropriate definition of $\boldsymbol{\tau}^p$. These stress values are then used in the residual (eq 14) to obtain an update to the velocity field. The procedure is repeated until specified convergence conditions are satisfied.

Each component of the solution $\boldsymbol{u}$ of eq 14 is approximated by a continuous piecewise polynomial in the following manner. The domain is triangulated, or partitioned, into small nonoverlapping regions. In each small region, the velocity $\boldsymbol{u}$ is assumed to be a polynomial, and across region boundaries continuity is enforced. The type of "finite element" we use to discretize eq 14 in our algorithm is the NRC or crossed-triangle macro-element[17] described as follows. The domain is triangulated by quadrilaterals, each of which is then divided into four triangles formed by the diagonals of the quadrilateral. The velocity is assumed to be linear in each triangle, while the pressure and stress are assumed to be constant in each triangle. The set of vertices of the triangles are the "nodes" of our finite element mesh. These are the points in the domain at which we solve the discretized system of equations.

Let $\{\boldsymbol{x}_k\}$, $k = 1, ..., N$, be the set of nodes of the mesh at which we want to determine the velocity. At each of these nodes, k, let $\phi^{(k)}$ represent the continuous "global shape function" with the property that $\phi^{(k)}(\boldsymbol{x}_l) = \delta_{kl}$. For our finite elements, $\phi^{(k)}(\boldsymbol{x})$ is a linear polynomial in triangles having $\boldsymbol{x}_k$ as a vertex and vanishes for all $\boldsymbol{x}$ in triangles not containing $\boldsymbol{x}_k$. The set $\{\phi^{(k)}\}$, $k = 1, ..., N$, is the set of basis functions for the N-dimensional finite element vector space $V^h \subset V$ in which we approximate each component of the solution. We can then write the approximate solution $\boldsymbol{u}^h$ as

$$\boldsymbol{u}^h(\boldsymbol{x}) = \sum_{k=1}^{N} \bar{\boldsymbol{u}}_k \phi^{(k)}(\boldsymbol{x}) \quad (15)$$

where $\{\bar{\boldsymbol{u}}_k\}$, $k = 1, ..., N$, is the set of nodal velocities we wish to determine. Approximating the weight functions $\boldsymbol{w}$ in the weak equations (eq 14) also by a linear combination of the $\phi^{(k)}$ yields a discrete system of algebraic equations described by

$$\boldsymbol{Q}(\boldsymbol{u}^h) + \boldsymbol{C}\boldsymbol{u}^h + \boldsymbol{N}(\boldsymbol{u}^h) = 0 \quad (16)$$

in which the contribution to each of these terms from node k is

$$[\boldsymbol{Q}(\boldsymbol{u}^h)]_k = \int_\Omega [\tau^p_{ji}(\boldsymbol{u}^h) + \tau^s_{ji}(\boldsymbol{u}^h)] \phi^{(k)}_j \boldsymbol{e}_i \, d\Omega \quad (17)$$

$$[\boldsymbol{C}\boldsymbol{u}^h]_k = \int_\Omega \frac{1}{\epsilon} u^h_{j,j} \phi^{(k)}_{,i} \boldsymbol{e}_i \, d\Omega \quad (18)$$

$$[\boldsymbol{N}(\boldsymbol{u}^h)]_k = \int_\Omega \varrho u^h_j u^h_{i,j} \phi^{(k)} \boldsymbol{e}_i \, d\Omega \quad (19)$$

where $\boldsymbol{e}_i$, $i = 1, 2$, is the ith standard basis vector in R^2. For a given definition of $\boldsymbol{\tau}^p$, the system given in eq 16 is solved for the nodal velocities $\{\bar{\boldsymbol{u}}_k\}$, $k = 1, ..., N$, in eq 15. The stresses $\boldsymbol{\tau}^p$ and $\boldsymbol{\tau}^s$ needed to compute the term $\boldsymbol{Q}(\boldsymbol{u}^h)$ in the residual are computed at the centroid of each triangle of the mesh. Once convergence is achieved, an L^2 projection is used to transform the stress (and pressure) fields from the space of values that are constant on each triangle to the space of bilinear stresses based at the corner nodes of the macroelement.

Details of the finite element technique we used, including modifications to our finite element for axially symmetric flow, can be found in refs 10–12.

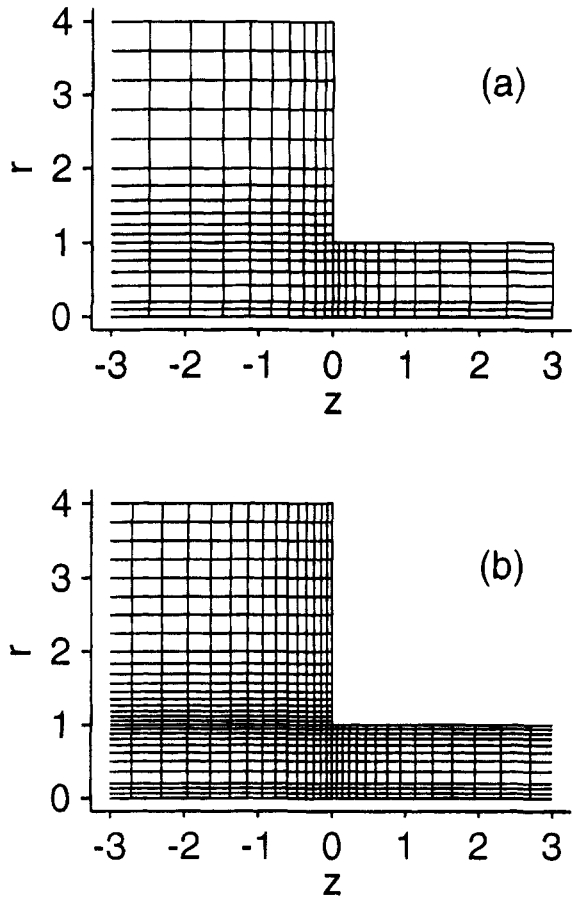

Figure 2. Portions of the finite element meshes used, $0 \le r \le 4$, $-3 \le z \le 3$. Both meshes were used for FLUCODE calculations, with mesh b used to confirm the results of mesh a. Mesh a was used for the CONNFFESSIT calculation.

3. Test Problem and Procedure

We test the CONNFFESSIT technique described in the previous section by solving the 4:1 axisymmetric

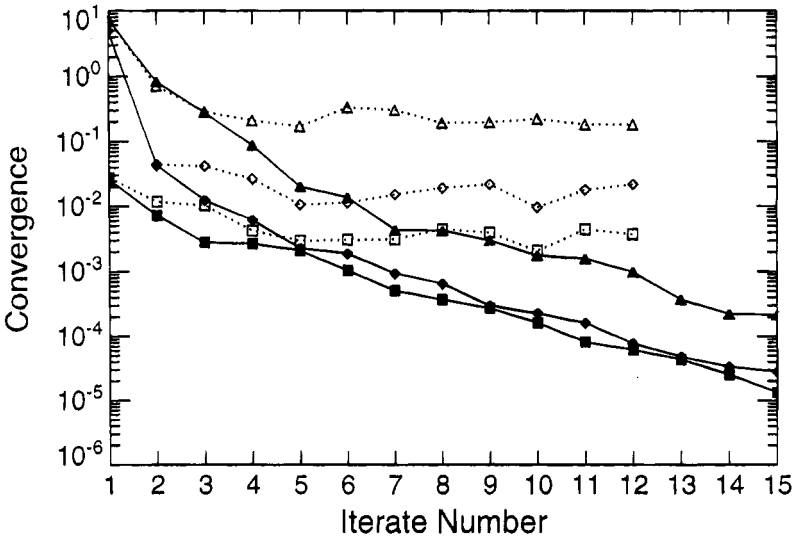

Figure 3. Convergence behavior of FLUCODE (solid symbols) and CONNFFESSIT (hollow symbols): relative norm of changes in velocity (□); relative norm of changes in polymer stresses (◇); maximum component of residual in absolute value (△).

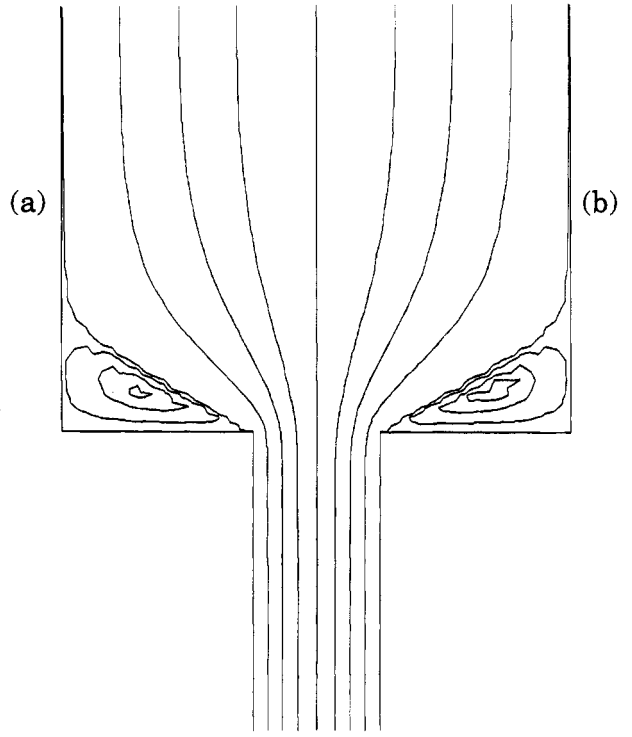

Figure 4. Streamline patterns for the Oldroyd-B model ($R_d = 1$, $\lambda_H = 1$, $\eta_0 = \eta_s + \eta_p = 1$, $\eta_s/\eta_p = 1$, $\varrho = 0.1$) for $S_R \approx 5$: (a) integral constitutive equation (FLUCODE); (b) CONNFFESSIT.

contraction (or die entry) problem for the Oldroyd-B model. The contraction domain is shown in Figure 1. The upstream tube (*i.e.* the reservoir) and the downstream tube (*i.e.* the die) are chosen to be long enough so that, for the flow rates we consider, the flow near the inlet and outlet boundaries of the domain is Poiseuille flow. Setting the radius of the downstream tube, R_d, to be one unit, we take $R_u = 4R_d$, $L_u = 10R_d$, and $L_d = 30R_d$, where R_u is the radius of the upstream tube and L_u and L_d are the lengths of the upstream and downstream tubes, respectively. The length of our downstream tube falls within the range of lengths that have commonly been used for the 4:1 die entry problem (*e.g.*, $L_d = 20R_d$ in refs 18 and 19; $L_d = 30R_d$ in refs 15, 20, and 21; $L_d = 50R_d$ or $60R_d$ in refs 13, 22, and 23).

Table 1. Relative Error in Extra-Stresses τ_{rz} and $\tau_{zz} - \tau_{rr}$

	percentage of nodes	
rel error (%)	τ_{rz}	$\tau_{zz} - \tau_{rr}$
0.1	6.3	2.7
1.0	50.3	20.0
2.0	66.6	29.4
3.0	75.3	39.1
4.0	79.0	49.4
5.0	81.0	59.3
10.0	88.9	76.9
15.0	91.1	82.6
20.0	93.0	84.9

The velocity boundary conditions we impose in the problem are the ones which are usually imposed for the die entry problem (see, for example, refs 13, 15, and 18–23): no slip along the walls of the domain and fully-developed Poiseuille flow along the inlet and outlet boundaries. The velocity values we fix at nodes along inlet and outlet boundaries are determined by solving one-dimensional Poiseuille flow problems under the condition that the flow rate is the same along both boundaries.

The parameters in the problem are fixed as follows. Without loss of generality, the units of length, time, and mass are fixed so that the radius of the downstream tube is $R_d = 1$, the relaxation time is $\lambda \equiv \lambda_H = 1$, and the total viscosity is $\eta_0 = \eta_s + \eta_p = 1$. We then set the density to $\varrho = 0.1$ and $\eta_s/\eta_p = 1$. We considered the flow at one flow rate, characterized by the stress ratio $S_R = N_1/(2\tau_w) \approx 5$, where N_1 is the first normal stress difference in the far downstream tube and τ_w is the shear stress along the wall of the downstream tube.

Before testing the CONNFFESSIT technique, we first solved our problem using the finite element program FLUCODE. Two finite element meshes were used, portions of which are shown in Figure 2. The first mesh contained 622 rectangular macro-elements (each of which was divided into four triangles) and 700 corner nodes (*i.e.* vertices of the quadrilaterals), with the size of the corner rectangular element being 0.11 × 0.10. This was the mesh to be used when solving the problem with CONNFFESSIT. The second mesh used by FLUCODE was more refined and was used to confirm the

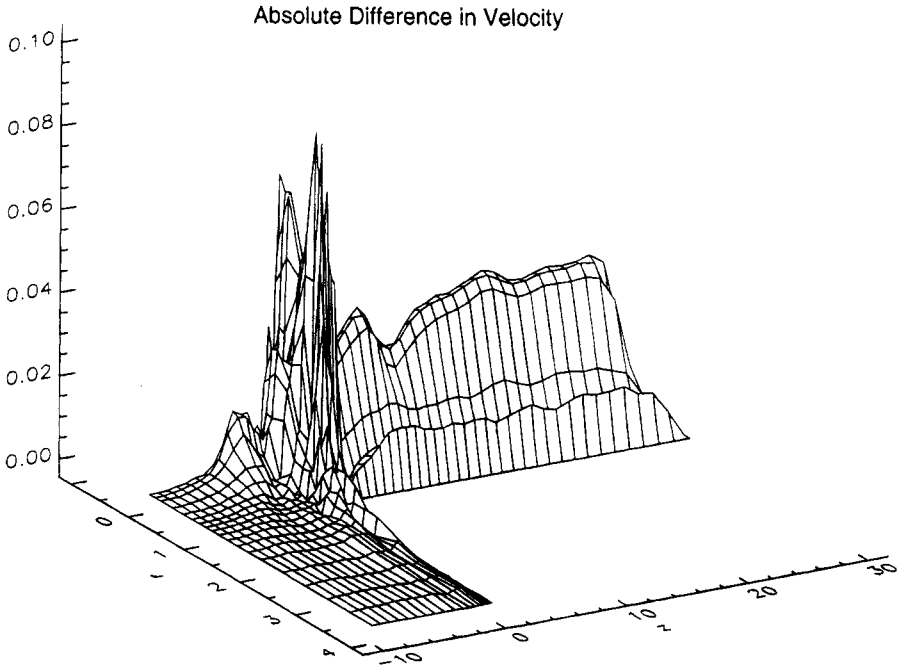

Figure 5. Norm of the difference in velocity throughout the die entry domain.

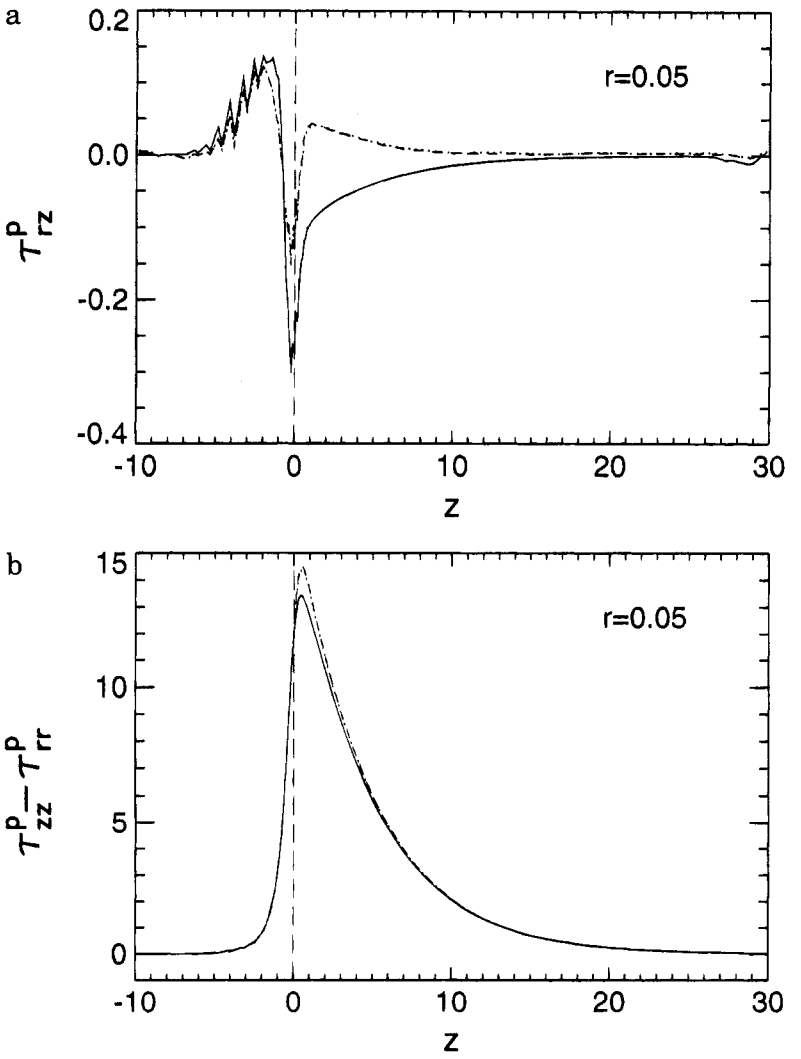

Figure 6. Comparison of polymer stresses at triangle centroids along $r = 0.05$; (a) τ^p_{rz}; (b) $\tau^p_{zz} - \tau^p_{rr}$. (Solid line represents FLUCODE; dashed and dotted lines represent CONNFFESSIT.)

validity of the results from the first mesh. It contained 1333 macro-elements and 1440 corner nodes, with more refinement taking place near the reentrant corner (the size of the corner element in this case was 0.05 × 0.07).

We then replaced the integral constitutive equation in the FLUCODE program with the Brownian dynamics simulation for polymer stress computation described in eqs 12 and 13 and solved the problem via CONNFFESSIT (using the first mesh described above). The procedure for implementing the stochastic simulation technique was as follows. In each iteration we chose a set of open streamlines from the known velocity field of the previous iteration which stretched from inlet to outlet boundary. One feature of the crossed-triangle macroelement is that for a given flow field the portion of a streamline in any triangle is known analytically, and therefore the streamlines can be determined quickly and exactly (to within machine accuracy). The set of streamlines, numbering approximately 100, was chosen so that at least three streamlines passed through each triangle not in the vortex region (except for some triangles in the Poiseuille flow upstream where only two streamlines passed). We sent $N = 20\,000$ dumbbells along each of these streamlines starting from the inlet boundary and traversing the entire domain until they reached the outlet boundary. Because we are using the Oldroyd-B model, there is no migration of dumbbell "molecules" between streamlines. The number of dumbbells passing through each triangle ranged from 60 000 (except for those triangles mentioned above in which two streamlines, and hence 40 000 dumbbells, passed) to approximately 1 000 000, with the average typically being between 160 000 and 200 000, depending on the velocity field. Since the density of the streamlines is greater in the smaller downstream tube, there are more streamlines, and hence more dumbbells, passing through triangles in the die.

In most cases, the simulation time step was taken to be $\Delta t_i = 0.01\lambda_H$. The exceptions were in triangles with residence times $\delta t < 0.1$, in which case we set $\Delta t_i = \delta t/10$. Therefore, we ensure that at least 10 time steps were taken in each triangle. At each time step, we computed the corresponding polymer stresses from the simulation (eqs 12 and 13). The polymer stresses at the centroid of each triangle were taken to be the weighted average of these values over all streamlines passing through the triangle. The weighting factors in the averaging were the residence times of dumbbells along the streamlines. It is another feature of our finite element that these residence times can be determined analytically (using so-called "drift functions"[10-12]).

The procedure described above gives us the polymer stresses in triangles which lie outside the vortex region. It is possible to compute the polymer stresses in triangles lying within the vortex region in the same manner, if we choose a set of closed streamlines along which to send the dumbbells. However, velocities and velocity gradients were generally so small in the vortex region that the magnitudes of the polymer stresses in this region were within the simulation's error. We therefore used Newtonian stress values in triangles in the vortex region and thus saved the CPU time which would have been required to compute stress along additional (closed) streamlines. The rule of switching to Newtonian values whenever the stress is small enough (within the simulation's error) could have been applied to any triangle in our domain, without loss in accuracy of the simulation, but we used it only in the vortex region. We also note that the FLUCODE program was used to test the effect of replacing Oldroyd-B stresses with Newtonian stresses in triangles in the vortex region and we found no significant difference in the solution for the flow rate under consideration.

The initial distribution of configurations which the dumbbells have along the inlet boundary is fixed according to the history of the dumbbells in the predecessor flow, that is, the flow in the region upstream of the inlet boundary (outside the domain on which the problem is solved). Since we assume fully-developed Poiseuille flow in the upstream tube, the predecessor flow is the Poiseuille flow which is defined by the fixed velocity values prescribed on the inlet boundary.

As a first test of CONNFFESSIT, we took the converged velocity field from FLUCODE as the initial velocity field for the CONNFFESSIT program. A set of 102 open streamlines was chosen from this initial velocity field. Each streamline was defined by the r component of its point of intersection with the inlet boundary. In all subsequent iterations, this set of r values defining the streamlines did not need to be updated (although the streamlines themselves changed slightly, due to the difference in velocity fields). After this first test of the CONNFFESSIT program we then took the initial velocity field to be Stokes flow. For this initial velocity field we needed 112 streamlines. This set consisted of the 102 streamlines, defined by the r values, used in the first test of CONNFFESSIT, plus 10 additional streamlines which were needed due to the much smaller vortex associated with Stokes flow. After the first iteration of our velocity–stress iteration procedure, the vortex grew and we were again able to use the streamlines defined by the original set of 102 r values.

4. Results

We judge the performance of the CONNFFESSIT algorithm by comparing its results for our die entry problem with the results obtained using the conventional finite element program FLUCODE. Before doing so, we make the following two comments. First, it is important to describe under what conditions we call our solution converged. We used three quantities to measure convergence: (*i*) the relative norm of the change in the velocity field between two consecutive iterations, (*ii*) the relative norm of the change in the polymer stresses between two consecutive iterations, and (*iii*) the maximum magnitude of the components of the residual. In FLUCODE the solution was considered to be converged when all three quantities were below 10^{-5}. Due to the stochastic nature of the simulation, we did not expect to obtain this degree of convergence with CONNFFESSIT. For each of the two initial velocity fields given above, we ran CONNFFESSIT through at least 10 velocity–stress iterations. This was sufficient to conclude that our solution had converged as much as it would. For each initial velocity field, the relative norm of the change in the velocity field and the polymer stresses did not decrease below the order of 10^{-3} and 10^{-2}, respectively, while the maximum magnitude of the components of the residual did not decrease below the order 10^{-1}. The convergence behavior of both methods is given in Figure 3, which shows the three convergence terms defined above as a function of the iteration number (the FLUCODE calculation was carried beyond the number of iterations shown in the figure). The curves for CONNFFESSIT correspond to the solution when the initial velocity field was Stokes flow. (The value for the relative change in polymer stresses for iteration 1 corresponds to the relative difference between the Newtonian stresses and the polymer stresses computed in the first iteration.)

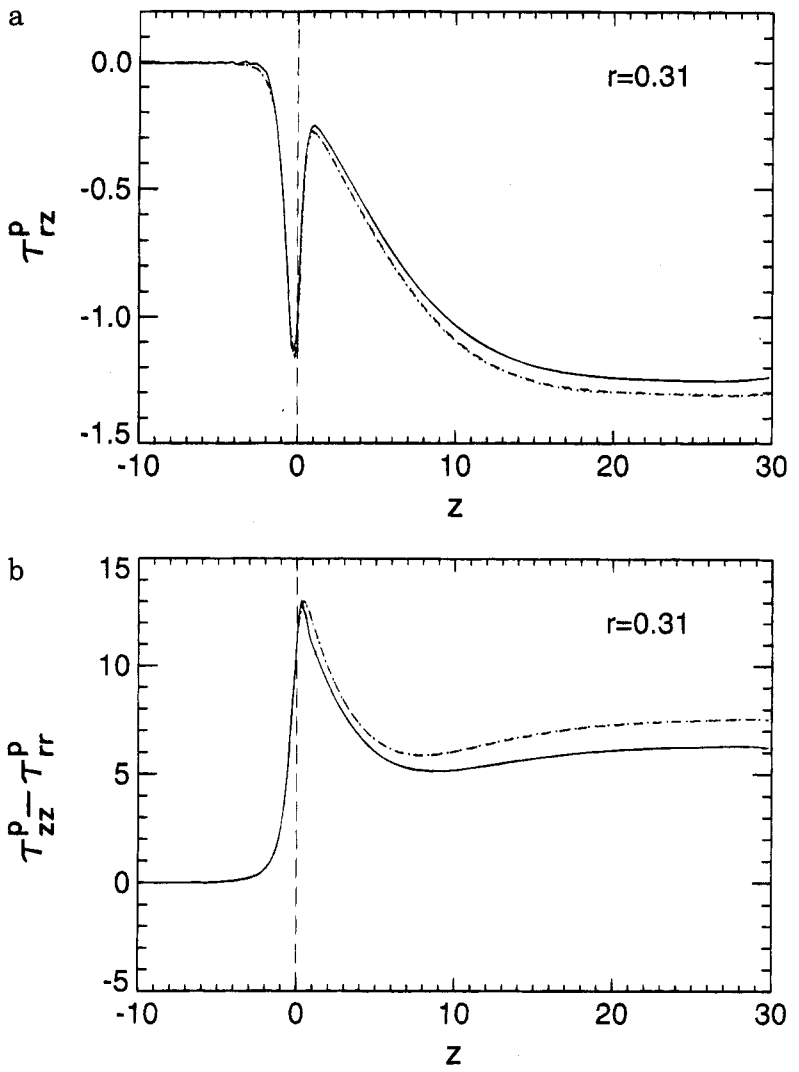

Figure 7. Comparison of polymer stresses at triangle centroids along $r = 0.31$: (a) τ^p_{rz}; (b) $\tau^p_{zz} - \tau^p_{rr}$. (Solid line represents FLUCODE; dashed and dotted lines represent CONNFFESSIT.)

The second comment is that, as should be the case, the results of CONNFFESSIT were independent of our choice of initial velocity field; there was no significant difference between the CONNFFESSIT results produced when Stokes flow was taken as the initial velocity field and those produced when the converged velocity field of the FLUCODE program was taken as the initial velocity field. The CONNFFESSIT results reported below were produced when Stokes flow was used as the initial velocity field.

Velocity Field. Our first point of comparison between CONNFFESSIT and the FLUCODE program is the velocity field. Figure 4 shows the streamline patterns produced from the two algorithms for the same set of stream function values. They are virtually identical. In particular, the size of the vortex, or secondary flow region, is the same. The velocity fields are compared quantitatively in Figure 5, where we show the (absolute) L^2 norm of the difference in the velocity fields throughout the entire domain. (Inflow and outflow velocities along the center line are approximately $u_z = 0.3$ and $u_z = 5.0$, respectively.) The figure shows that the largest absolute difference occurs near the reentrant corner. This is also where the largest *relative* difference in the velocity fields occurs (excluding the vortex region where velocities are very small and where CONNFFESSIT uses Newtonian stress values in the calculations). The maximum relative difference is approximately 7%. There also appears to be a large absolute difference along the center line in the downstream tube ($z > 0$), but the velocity is the largest in this region and the relative difference is at most 1%.

Stress Field. Values of the extra-stress $\tau = \tau^p + \tau^s$ determined by FLUCODE and CONNFFESSIT were also compared at the nodes of the mesh (after the transformation from stress values at the triangles' centroids to stress values at nodes). In most cases the agreement was excellent. The comparison of values of τ_{rz} and $\tau_{zz} - \tau_{rr}$ is summarized in Table 1. Each row of the table shows the percentage of nodes at which the relative error in τ_{rz} (column 2) and $\tau_{zz} - \tau_{rr}$ (column 3) is less than a specified value (column 1). For example, there is less than a 10% relative error in values of τ_{rz} at 88.9% of all nodes, while this degree of agreement is achieved in the $\tau_{zz} - \tau_{rr}$ values at 76.9% of nodes. The relative error in τ_{rz} and $\tau_{zz} - \tau_{rr}$ exceeds 20% at 7.0% and 15.1% of the nodes, respectively. At the majority of these nodes, this large error is attributed to the small magnitude (order 10^{-2} or lower) of τ_{rz} or $\tau_{zz} - \tau_{rr}$. The remaining nodes at which this large error occurs lie (with few exceptions) either in the vortex region (where CONNFFESSIT uses Newtonian stress values), close to the reentrant corner, or along the center line near the die entry.

In order to evaluate more directly the performance of our stochastic simulation technique, we consider the

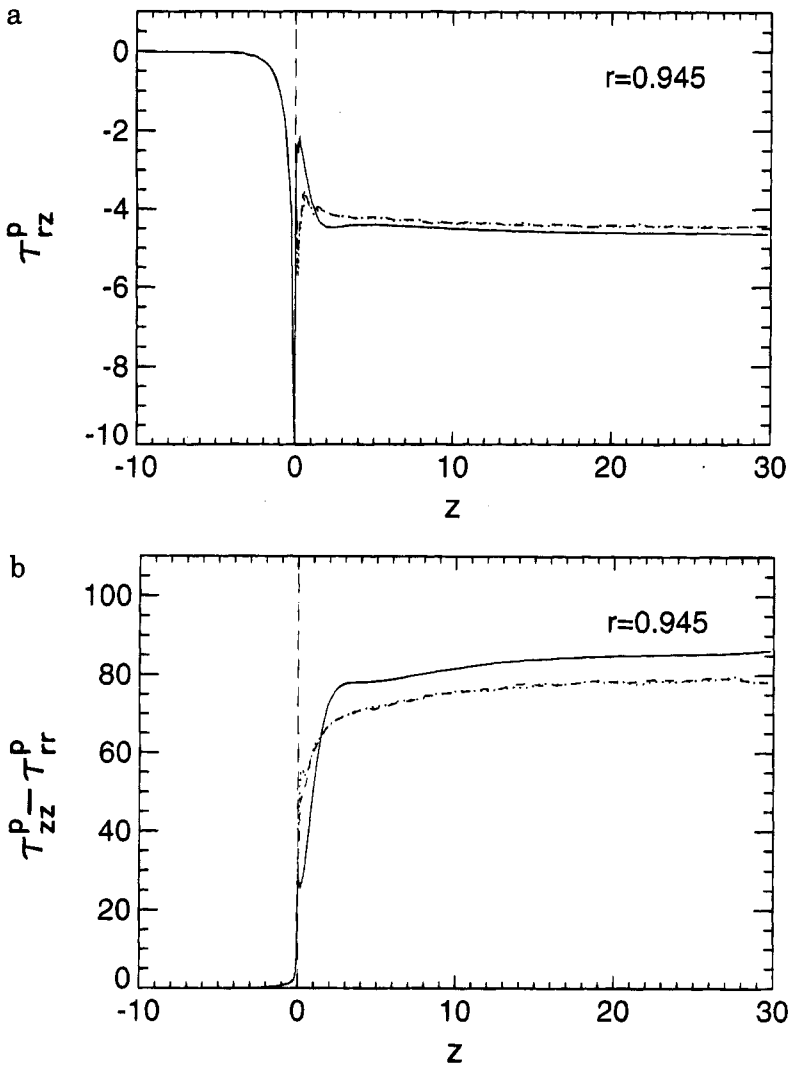

Figure 8. Comparison of polymer stresses at triangle centroids along $r = 0.945$: (a) τ^p_{rz}; (b) $\tau^p_{zz} - \tau^p_{rr}$. (Solid line represents FLUCODE; dashed and dotted lines represent CONNFFESSIT.)

values of the polymer stresses τ^p assigned to the centroid of each triangle. In other words, we make the comparison in the absence of the solvent contribution $\tau^s = \eta_s(\nabla u + (\nabla u)^T)$ and before applying the L^2 projection from the space of piecewise constant stresses, based on the triangles, to the space of bilinear stresses, based on the corner nodes of each macroelement. We again found that in most triangles the agreement between FLUCODE and CONNFFESSIT was excellent. Rather than illustrating this excellent agreement, we choose to focus below on areas in which there are significant differences and to investigate the reasons for these differences.

For graphical convenience we represent the polymer stresses as functions of z for a fixed value of r corresponding to centroids of triangles. Figures 6–8 show the graphs of τ^p_{rz} and $\tau^p_{zz} - \tau^p_{rr}$ as functions of z along the entire length of our domain ($-10 \le z \le 30$) for three fixed values of r. The die entry is located at $z = 0$ with $z < 0$ and $z > 0$ corresponding to the upstream and downstream tubes, respectively. Each graph contains three curves, representing the values from FLUCODE (solid line) and the values from the last two iterations of CONNFFESSIT (dashed and dotted line). We graph the stresses from the last two iterations of CONNFFESSIT in order to illustrate that, with few exceptions, these stochastically computed values do not significantly change between iterations; in fact, the curves almost completely coincide. The exceptions are close to the reentrant corner in Figure 8b, where differences in the CONNFFESSIT values are visible. These differences do not indicate that we need to perform more iterations of CONNFFESSIT in order to obtain a more converged solution. Inspection of the last five iterations of CONNFFESSIT show that the changes in polymer stresses are not systematic; instead the polymer stresses fluctuate.

We wish to point out that the jagged appearance of the curves of τ^p_{rz} before the die entry for fixed $r = 0.05$ in Figure 6 is due to the type of velocity approximation our finite element uses in elements along the center line in axisymmetric geometry (see ref 12 for a discussion) and is not due to the stochastic simulation technique. Indeed, it is an indication of the strength of the stochastic simulation that CONNFFESSIT is able to reproduce such behavior.

The largest discrepancies between FLUCODE and CONNFFESSIT occur in the far downstream tube in Figure 7b, where the relative difference is approximately 20%, and immediately after die entry in Figures 6a and 8a,b, where the relative difference can exceed 70%. Other differences apparent in the graphs—in Figure 6b immediately after the die entry and in the far downstream tube in Figures 7a and 8a,b—are less than 10%.

The large differences in polymer stress values in a triangle stem from large variations in τ^p along the

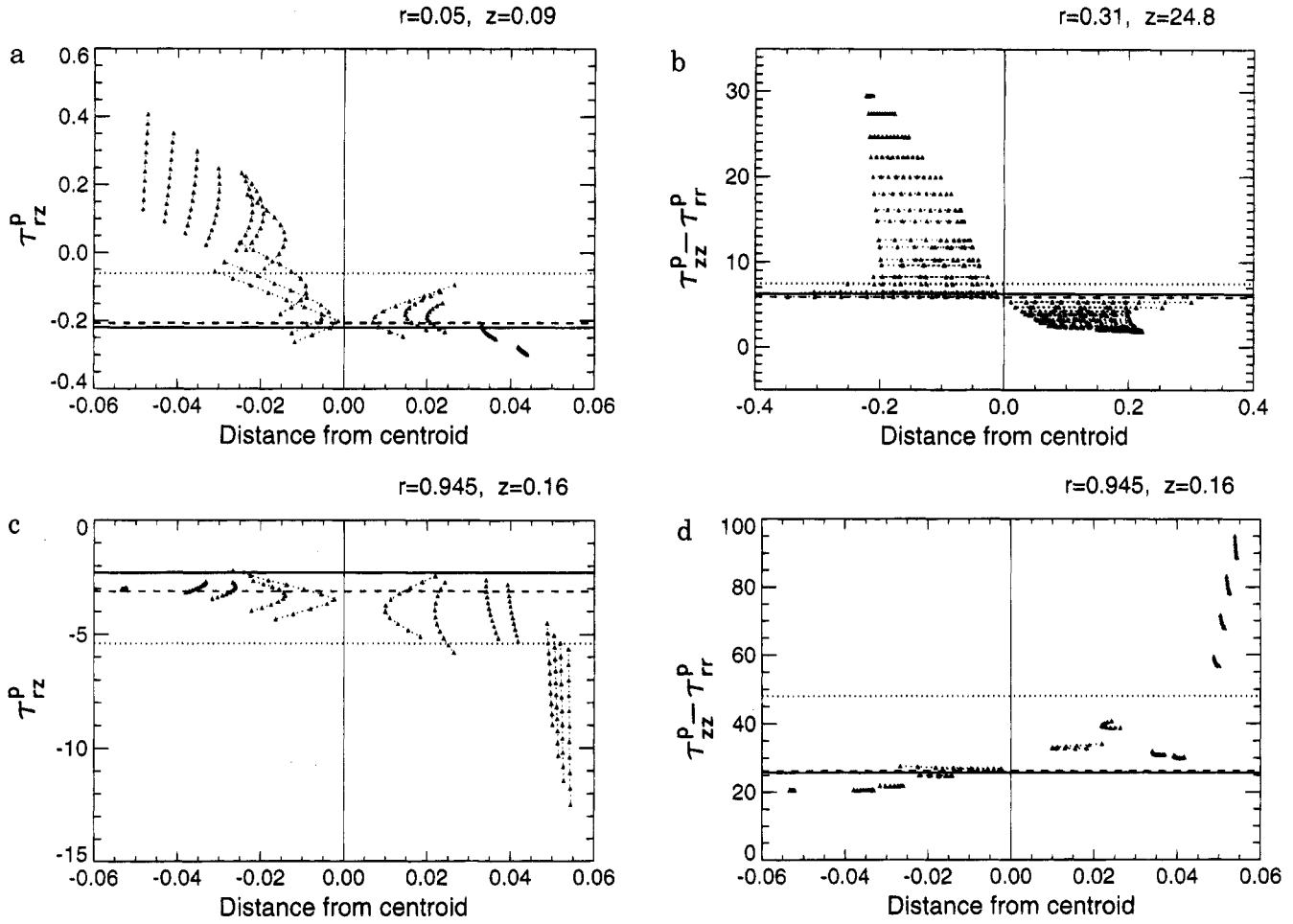

Figure 9. Polymer stress values from CONNFFESSIT along all streamlines passing through the triangle with the specified centroid (triangle symbols connected by dotted lines) as a function of distance from the centroid. The average centroidal value computed by CONNFFESSIT is indicated by the dotted horizontal line; the centroidal values computed by FLUCODE using its velocity field and the velocity field of CONNFFESSIT are indicated by solid and dashed horizontal lines, respectively.

various streamlines which pass through the triangle and from the type of averaging of these values that CONNFFESSIT uses to assign values of τ^p at the triangle's centroid. We illustrate this for a few triangles in which the difference in centroidal values of τ^p_{rz} or $\tau^p_{zz} - \tau^p_{rr}$ is very large (over 20%). However, the same explanation applies for smaller differences, such as the less than 7% difference seen downstream in Figure 7a. For each of three triangles, Figure 9 shows the values of τ^p_{rz} or $\tau^p_{zz} - \tau^p_{rr}$ computed by CONNFFESSIT along all streamlines passing through the triangle. The stress value at the point corresponding to each integration time step is graphed as a function of the point's distance from the triangle's centroid. (Negative and positive distances are used to indicate points with r coordinate respectively less than or greater than that of the centroid.) Each stress value is plotted as a triangular symbol and a dotted line is used to connect values along the same streamline. CONNFFESSIT's centroidal average of these stress values is indicated by a horizontal dotted line, while a solid horizontal line indicates the centroidal stress value from FLUCODE. Since the velocity fields produced by CONNFFESSIT and FLUCODE are not identical (see Figure 5), we also indicate by a dashed horizontal line the stress value computed by FLUCODE using the velocity field of CONNFFESSIT.

There is a clear effect of the variations in stress values on CONNFFESSIT's average value. The figure shows that stress values along streamlines farthest from the centroid differ significantly from those closer to the centroid which are generally in good agreement with FLUCODE's centroid stress value. As a result, the averaging process of CONNFFESSIT "pulls" the computed average stress value away from FLUCODE's centroidal value. The effect is particularly dramatic in Figure 9d where the stress values along the streamlines closest to the wall (those in the upper right portion of the graph) are 2–4 times larger than those along streamlines closer to the centroid.

A broader message is conveyed by Figure 9, namely that the centroidal polymer stress values computed by CONNFFESSIT in a given triangle can strongly depend upon the distribution of the prechosen streamlines passing through the triangle. Of course, it is not the natural implementation of CONNFFESSIT to send dumbbells along a selected set of streamlines in a steady-state flow situation, such as we have done. It would have been more natural either to send each dumbbell along a randomly selected streamline in steady flow or to let the dumbbells swim throughout the fluid and to consider the flow's time evolution from rest. The former approach was not taken for reasons of numerical efficiency; constructing so many streamlines would be too time-consuming. The latter approach is the approach taken in a forthcoming paper in which CONNFFESSIT is used to solve the two-dimensional start-up flow between eccentric cylinders. Nevertheless, we find that the method of implementation presented

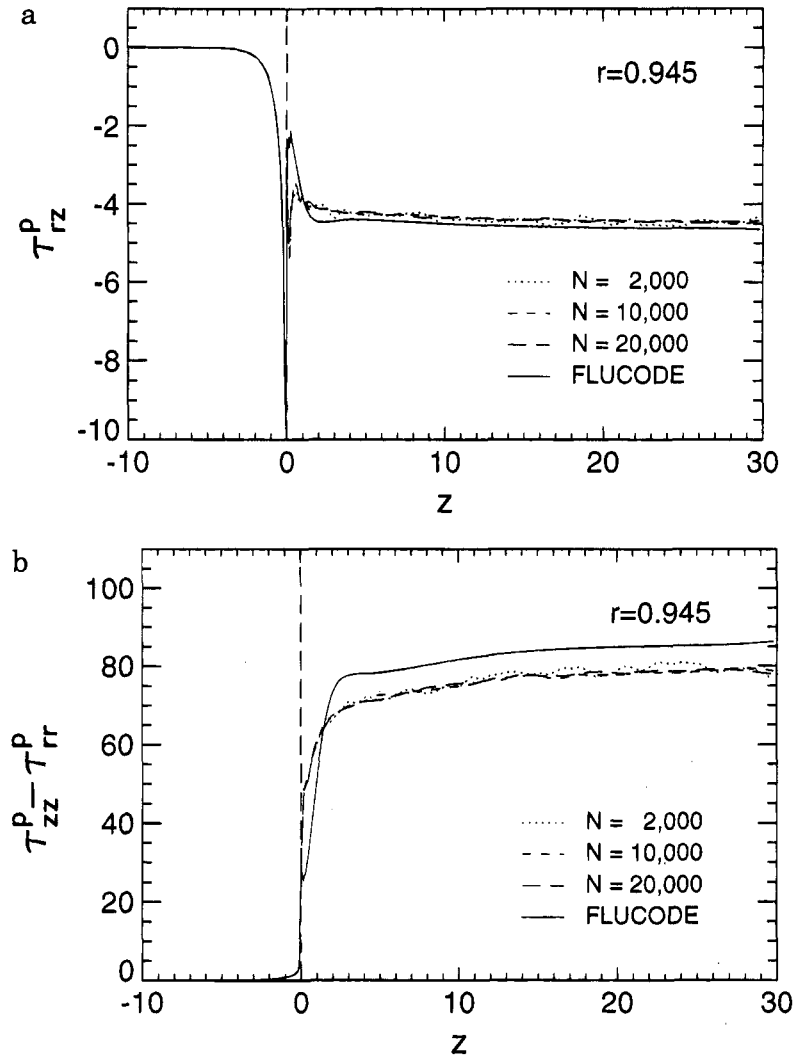

Figure 10. Comparison of polymer stresses along the line $r = 0.945$ for different values of N (number of dumbbells along each streamline): (a) τ_{rz}^p; (b) $\tau_{zz}^p - \tau_{rr}^p$. The curve for each N represents values from the last iteration of CONNFFESSIT.

in this paper performed extremely well.

We also expect that with mesh refinement the differences we see between the two methods will be reduced since the variations in velocity gradient, and hence stress, within a triangle should be reduced. Investigation into this is an area for future research.

Effect of the Number of Dumbbells. We conclude by looking at the effect that reducing the number of dumbbells along each streamline has on the solution. We considered the cases of $N = 10\,000$ and $N = 2000$ dumbbells and compared the results from these cases to the results presented above for $N = 20\,000$.

We found that the results for $N = 10\,000$ were, for the most part, indistinguishable from the results for $N = 20\,000$, in terms of the velocity field, the stress field, and the convergence. When only $N = 2000$ dumbbells were used along each streamline, there were some noticeable effects on the results. There was a slight increase in the residual (although it was of the same order of magnitude, 10^{-1}, as for the other two cases), and in some regions of the domain, although not in all, there were obvious differences in the polymer stresses.

One region where differences occurred was along the line $r = 0.945$. Figures 10–12 illustrate the effect of N on polymer stresses along this line. In Figure 10 the values of τ_{rz}^p and $\tau_{zz}^p - \tau_{rr}^p$ are graphed. The curve for each N represents values from the last iteration of CONNFFESSIT. One can clearly see the differences in the downstream tube between the values for $N = 2000$ dumbbells and the values for $N = 10\,000$ and $N = 20\,000$ dumbbells. While results from the last two are almost identical, there are more pronounced fluctuations when only $N = 2000$ dumbbells are used along each of the streamlines.

These differences are reduced if we compare the mean values of polymer stresses over the last few iterations of CONNFFESSIT. This is illustrated in Figure 11 where, for each N, the mean values of τ_{rz}^p and $\tau_{zz}^p - \tau_{rr}^p$ have been computed over the last five iterations of CONNFFESSIT. Fluctuations are still present, but they are smaller, and better overall agreement is obtained.

Finally, Figure 12 indicates the error in polymer stresses associated with each N (estimated from the last five iterations of CONNFFESSIT) along the line $r = 0.945$ in the downstream tube. As expected, the error increases as N decreases. The figure shows that the increase in error in going from $N = 20\,000$ dumbbells along each streamline to $N = 10\,000$ is small, particularly when compared with the increase in error when the number of dumbbells is reduced to $N = 2000$. This observation is consistent with the comparison of polymer stress values made in Figure 10.

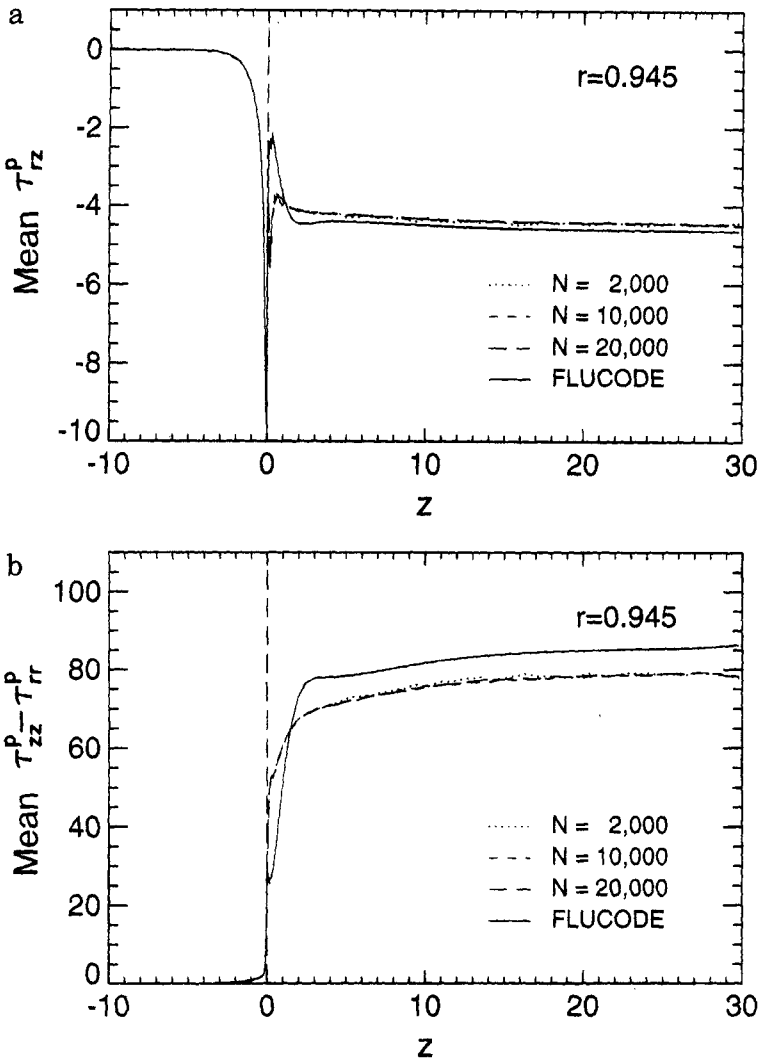

Figure 11. Comparison of the mean values of polymer stresses along the line $r = 0.945$ for different values of N: (a) τ^p_{rz}; (b) $\tau^p_{zz} - \tau^p_{rr}$. The curve for each N represents the mean values over the last five iterations of CONNFFESSIT.

Finally, we comment on the efficiency of our CONNFFESSIT program. When $N = 20\,000$ dumbbells were sent along each of our 102 streamlines, the amount of CPU time required for computing the polymer stresses in one iteration was approximately 8.7 h on a CRAY Y-MP computer. Reducing the number of dumbbells along each streamline by half, to $N = 10\,000$, also reduced the CPU time by approximately half and, as noted above, did not appreciably affect the results. Further reduction to $N = 2000$ dumbbells along each streamline reduced the CPU time to under 1 h. In view of this increased efficiency, the differences resulting from using only $N = 2000$ dumbbells along each streamline may be considered insignificant. For comparison, we note that computing the polymer stresses in one iteration using the integral form of the Oldroyd-B model implemented in FLUCODE required less than 8.5 min of CPU time on the CRAY Y-MP computer.

5. Conclusions

A two-dimensional test problem for the CONNFFESSIT approach for solving viscoelastic fluid problems has been presented. The test problem considered was the steady flow of an incompressible Oldroyd-B fluid, under isothermal conditions, in a 4:1 axisymmetric contraction domain. The contraction problem (or the die entry problem) has long served as a benchmark problem for viscoelastic flow calculations. By integrating an ensemble of 20 000 Hookean dumbbells along each of approximately 100 open streamlines, predefined by specifying their r coordinates along the inlet boundary, the polymer contribution to the stress tensor was computed using Brownian dynamics and a weighted averaging technique. The r values defining the streamlines were chosen so that each triangular element was traversed by at least three streamlines (except possibly in the Poiseuille flow upstream where at least two streamlines passed through each triangle). Within the vortex region, Newtonian stress values were used since the magnitude of the stresses here were generally within the simulation's error.

The CONNFFESSIT program we used was formed by replacing the conventional integral constitutive equation of an existing finite element program for solving steady-state incompressible viscoelastic fluid problems (under isothermal conditions) with a specified stochastic simulation technique for polymer stress calculation. We evaluated the performance of the CONNFFESSIT approach for the axisymmetric die entry problem by comparing its results with those of the conventional finite element program. We found that our CONNFFESSIT program performed very well. There was good agreement between the velocity fields produced by each of the two algorithms, and in most cases the

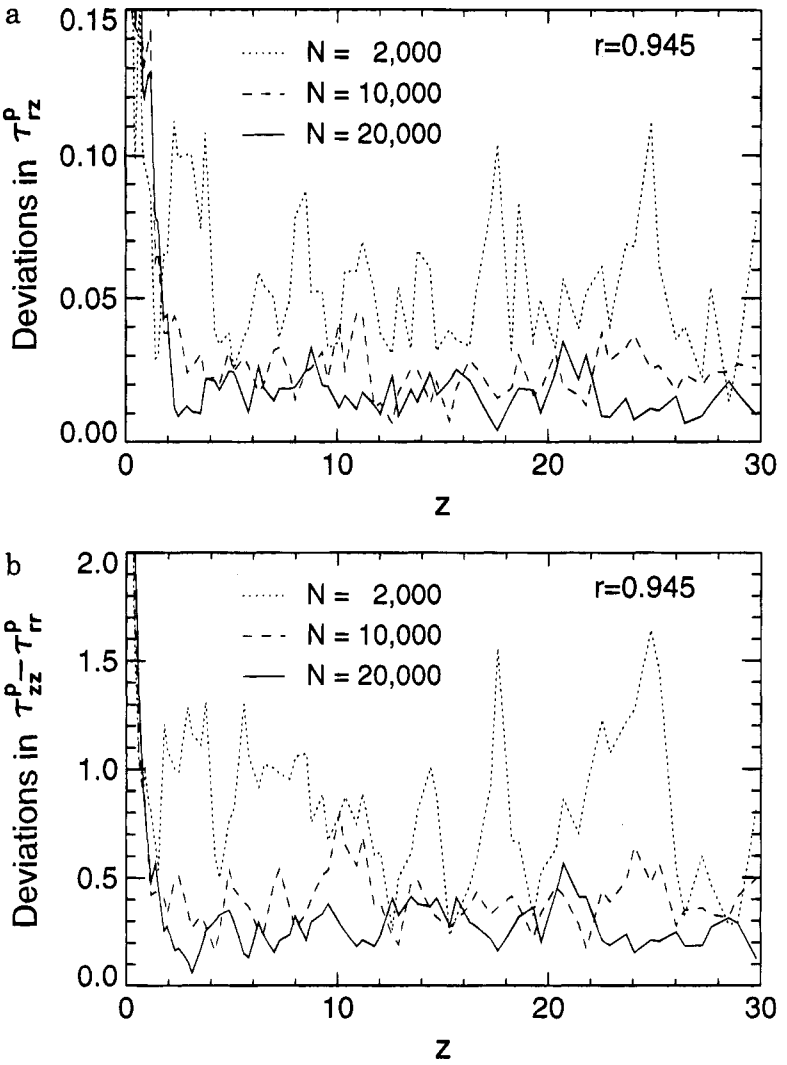

Figure 12. Comparison of the errors associated with each N (based on the last five iterations of CONNFFESSIT) along the line $r = 0.945$ in the downstream tube: (a) τ^p_{rz}; (b) $\tau^p_{zz} - \tau^p_{rr}$.

agreement between the stress fields was also excellent. In triangles where there were large differences in polymer stress values, we found that these differences were the result of large variations in stress values along the streamlines passing through the triangle and the averaging of these values to get centroidal stress values. The degree to which these differences might be reduced with mesh refinement is an area still to be investigated.

Finally, we looked at the effect that the number of dumbbells had on the solution. We found that reducing the number of dumbbells along each of our streamlines by half, from $N = 20\,000$ to $N = 10\,000$, did not significantly change the CONNFFESSIT results, and decreased the CPU time by about half. Larger differences were found in some areas of the domain when only $N = 2000$ dumbbells were used along each streamline.

This paper establishes that the CONNFFESSIT approach can successfully be used to solve complex two-dimensional viscoelastic fluid problems. A disadvantage of this approach over numerical algorithms which use integral or differential constitutive equations is that it requires much more computer memory and CPU time, particularly for large ensembles. However, the program is highly vectorizable (90–95%) and is well-suited for parallelization. Among its many advantages are included in the following: (*i*) The method is able to consider kinetic theory models without the need to develop an equivalent closed-form constitutive equation; it is not even necessary that one exists. (*ii*) It is easy to switch from one model to another by replacing the subroutine controlling the stochastic simulation. (*iii*) Effects such as polydispersity, polymer migration, polymer diffusivity, and hydrodynamic interactions can be treated in a straightforward manner since the motion of individual "molecules" is simulated. (*iv*) It is easy to take chemical reactions into account and, hence, to treat flows in chemical reactors or the combination of polymer synthesis and processing. (*v*) Although we considered here a steady-state problem, CONNFFESSIT is well-suited for time-dependent problems.

In addition, the CONNFFESSIT approach offers the possibility of replacing boundary conditions which one might impose for stress with conditions on the local polymer dynamics and, in this sense, consider interactions between polymer molecules and boundaries.

Acknowledgment. This work was supported by the Swiss National Foundation for Scientific Research (Grant No. 20-36073.92). The authors are grateful for the generous allocations of CPU time on the CRAY Y-MP at ETH and the NEC SX-R24 at the CSCS in Manno.

References and Notes

(1) Laso, M.; Öttinger, H. C. *J. Non-Newtonian Fluid Mech.* **1993**, *47*, 1.
(2) Laso, M.; Öttinger, H. C. In *Proceedings of the XXII Winter Meeting on Statistical Physics*, Cuernavaca, Mexico; de Haro, M. L., Varea, C., Eds.; World Scientific: Singapore, 1994.
(3) Bird, R. B.; Armstrong, R. C.; Hassager, O. *Dynamics of Polymeric Liquids*, 2nd ed.; John Wiley & Sons: New York, 1987; Vol. 1.
(4) Bird, R. B.; Curtiss, C. F.; Armstrong, R. C.; Hassager, O. *Dynamics of Polymeric Liquids*, 2nd ed.; John Wiley & Sons: New York, 1987; Vol. 2.
(5) Gardiner, C. W. *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*; Springer: Berlin, 1983.
(6) Kallianpur, G. *Stochastic Filtering Theory*; Springer: New York, 1980.
(7) Fixman, M. *J. Chem. Phys.* **1978**, *69*, 1527.
(8) Öttinger, H. C. *Makromol. Chem., Macromol. Symp.* **1992**, *56*, 117.
(9) Öttinger, H. C. *Stochastic Processes in Polymeric Fluids*; Springer: Berlin, 1995.
(10) Bernstein, B.; Kadivar, M. K.; Malkus, D. S. *Comput. Methods Appl. Mech. Eng.* **1981**, *27*, 279.
(11) Bernstein, B.; Malkus, D. S.; Olsen, E. T. *Int. J. Num. Methods Fluids* **1985**, *5*, 43.
(12) Bernstein, B.; Feigl, K.; Olsen, E. T. *J. Rheol.* **1994**, *38*, 53.
(13) Dupont, S.; Crochet, M. J. *J. Non-Newtonian Fluid Mech.* **1988**, *29*, 81.
(14) Goublomme, A. Ph.D. Thesis, Université Catholique de Louvain, Louvain-La-Neuve, Belgium, 1992.
(15) Luo, X.-L.; Mitsoulis, E. *J. Rheol.* **1990**, *34*, 309.
(16) Feigl, K.; Öttinger, H. C. *J. Rheol.* **1994**, *38*, 847.
(17) Nagtigaal, J.; Parks, D. M.; Rice, J. R. *Comput. Methods Appl. Mech. Eng.* **1974**, *4*, 153.
(18) Boger, D. V.; Crochet, M. J.; Keiller, R. A. *J. Non-Newtonian Fluid Mech.* **1992**, *44*, 267.
(19) Debae, F.; Legat, V.; Crochet, M. J. *J. Rheol.* **1994**, *38*, 421.
(20) Luo, X.-L.; Mitsoulis, E. *Int. J. Num. Methods Fluids* **1990**, *11*, 1015.
(21) Park, H. J.; Mitsoulis, E. *J. Non-Newtonian Fluid Mech.* **1992**, *42*, 301.
(22) Marchal, J. M.; Crochet, M. J. *J. Non-Newtonian Fluid Mech.* **1987**, *26*, 77.
(23) Debbaut, B.; Marchal, J. M.; Crochet, M. J. *J. Non-Newtonian Fluid Mech.* **1988**, *29*, 119.

MA9461153