Coil-stretch transition and the breakdown of computations for viscoelastic fluid flow around a confined cylinder

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Synopsis

The breakdown of finite element (FEM) computations for the steady symmetric two-dimensional flow of dilute and ultradilute Oldroyd-B fluids around a cylinder in a channel, at Weissenberg numbers Wi = O(1), is shown to arise due to a coil-stretch transition experienced by polymer molecules in the wake of the cylinder in the vicinity of the location of the stress maximum on the centerline. In dilute Oldroyd-B fluids, due to the modification of the flow caused by the presence of the polymer, the coil-stretch transition leads to the stress maximum diverging toward infinity at a finite value of $Wi \approx 0.7$. On the other hand, in ultradilute solutions, the stress maximum approaches infinity only as $Wi \rightarrow \infty$. In FENE-P fluids, the coil-stretch transition leads to the mean extension of the molecules saturating to a value close to the fully-extended length, with the maximum stress remaining bounded with increasing *Wi*. An estimation of the number of finite elements required to achieve convergence for ultradilute Oldroyd-B fluids reveals that obtaining solutions at Wi > 1 is not feasible. © 2008 The Society of Rheology. [DOI: 10.1122/1.2807444]

I. INTRODUCTION

The behavior of polymeric liquids in complex flows is intimately linked to the distribution of molecular conformations in the flow field. Macroscopic field variables such as the stress and velocity are strongly coupled to microscopic quantities such as the stretch and orientation of polymer molecules, and they influence and determine the magnitude of each other. Recent advances in computational rheology have led to the development of micro-macro methods that are capable of resolving information at various length and time scales. However, because of computational cost, most numerical simulations are still

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based on the purely macroscopic approach of continuum mechanics, where the conservation laws of mass and momentum are solved with a constitutive equation that relates the stress to the deformation history, without explicitly accounting for the microstructure [Keunings (2000)]. The simplest constitutive equations capable of capturing some qualitative aspects of the viscoelastic behavior of polymer solutions and melts are the Oldroyd-B and upper convected Maxwell models, respectively. These models have been widely used in the investigation of complex flows since the early days of computational rheology [Owens and Phillips (2002)].

Despite the apparent simplicity of the macroscopic equations, obtaining solutions at industrially relevant values of the Weissenberg number (*Wi*) has proven to be extremely difficult in a range of flow geometries. Careful numerical studies over the past few decades suggest that the principal source of computational difficulties is the emergence of large stresses and stress gradients within narrow regions of the flow domain. Significant efforts have been made to develop grid-based numerical techniques for resolving these stresses and their gradients. In spite of considerable progress, numerical solutions still break down at disappointingly low values of $Wi \sim O(1)$, and it is still not clear whether this is because solutions do not exist at higher values of Wi, or whether it is simply due to the inadequacy of current numerical techniques [Keunings (2000)]. Very recently, Renardy (2006) has shown analytically that in the special case of steady flows with an interior stagnation point, the mathematical structure of the upper convected Maxwell and Oldroyd-B models can be expected to lead to singularities in the viscoelastic stresses and their gradients with increasing Wi.

Nearly two decades ago, Rallison and Hinch (1988) argued in a seminal paper that in the case of the Oldroyd-B model, the inability to compute macroscopic flows at high Weissenberg numbers (the so-called high Weissenberg number problem, or HWNP), has a physical origin in a microscopic phenomenon. The Oldroyd-B model predicts an unbounded extensional viscosity in homogeneous extensional flows at a critical value of *Wi*. The Oldroyd-B constitutive equation can be derived from kinetic theory by representing polymer molecules by Hookean dumbbells. The unphysical behavior in extensional flows is due to the infinite extensibility of the Hookean spring used in the model. By considering the simple example of a stagnation point flow of an Oldroyd-B fluid, Rallison and Hinch showed that when the strain rate is supercritical, infinite stresses can occur in the interior of a steady flow, brought about by the unbounded stretching of polymer molecules. Based on their analysis, they suggested the use of a constitutive equation that is derived from a microscopic model with a nonlinear spring force law (which would impose a finite limit on a polymers extension), as an obvious remedy for the HWNP.

Chilcott and Rallison (1988) examined the benchmark complex flow problems of unbounded flow around a cylinder and a sphere using a dumbbell model with finite extensibility as a means of demonstrating the validity of this analysis. In order to understand the coupling between the polymer extension by flow, the stresses developed in the fluid, and the resultant flow field, they deliberately used the conformation tensor as the fundamental variable instead of the stress. The conformation tensor gives information on the distribution of polymer conformations within the flow field in an averaged sense. Chilcott and Rallison relied on kinetic theory to develop their model and to derive a simple expression relating the conformation tensor along with the mass and momentum conservation laws, Chilcott and Rallison showed that even though there existed highly extended material close to the boundary and in the wake of the obstacle, there no longer was an upper limit to Wi in the range of values accessible in their computations. Because the degree of molecular extension is directly related to the mag-



FIG. 1. Flow domain and boundary conditions for the flow around a cylinder confined between parallel plates.

nitude of stress, the Chilcott and Rallison procedure established a clear connection between high stresses and stress gradients in the flow domain with the configurational and spatial distribution of polymer conformations. Indeed, when simulations were carried out with the polymer length set to infinity rather than a finite value, the downstream structure could not be resolved, and the mean stretch of the polymers in the flow direction continued to grow with increasing *Wi* until the solution failed.

Despite this compelling demonstration of the physical origin of the HWNP, the upper convected Maxwell and Oldroyd-B models continue to be used extensively in computational rheology. The reason for this may be that stresses become large, yet remain bounded; so far, there has been no conclusive demonstration that bounded solutions for the viscoelastic stress do not exist in complex flows at high values of *Wi*. Conversely, by considering the steady flow of upper convected Maxwell and Oldroyd-B fluids around a cylinder confined between two parallel plates (a schematic of the flow geometry is displayed in Fig. 1), Wapperom and Renardy (2005) presented strong numerical evidence that suggests that solutions do exist for Wi > 1, and that current numerical techniques are not able to find them.

The particular benchmark problem of flow around a cylinder between parallel plates was chosen by these authors because even though the geometry has no singularities, the maximum values of Wi for which converged solutions exist are amongst the lowest of all benchmark flows [Alves et al. (2001); Caola et al. (2001); Coronado et al. (2006); Fan et al. (1999); Sun et al. (1999)]. The presence of upstream and downstream stagnation points leads to the development of steep stress boundary layers near the cylinder and in the wake of the cylinder, making the flow a stringent test of any numerical technique. Rather than solving the coupled problem simultaneously for the velocity and conformation tensor fields, for which the existence of solutions at high Wi is unknown, Wapperom and Renardy assumed a Newtonian-like velocity field and solved only for the conformation tensor field. The chosen velocity field has an analytical representation, is very similar to the Newtonian velocity field in the same geometry and the velocity field for an Oldroyd-B fluid at $Wi \sim \mathcal{O}(1)$, and satisfies all the key requirements for the velocity field near the cylinder. The advantage of this approach is that the existence of a solution for an upper convected Maxwell model in such a velocity field is guaranteed at all values of Wi [Renardy (2000)]; hence, failure of a numerical scheme can be attributed purely to numerics. By developing a Lagrangian technique which involves integrating the conformation tensor equation along streamlines using a predictor-corrector method, the authors were able to compute stresses up to arbitrarily large values of Wi (as high as 1024), and as a result, establish conclusively the existence of narrow regions with very high stresses near the cylinder, and in its wake. Moreover, they showed that although the velocity field is known, one of the currently used numerical techniques, the backward-tracking Lagrangian technique, is unable to resolve the extremely thin stress boundary layers even at relatively low values of *Wi*. Because the fully coupled problem and the fixed flow kinematics problem share the same basic dilemma of computing the stress field, Wapperom and Renardy argue that solutions also probably exist for Wi > 1 for the steady flow of upper convected Maxwell and dilute Oldroyd-B fluids around a cylinder confined between parallel plates, but current numerical techniques are unable to find them.

The use of the conformation tensor as the fundamental quantity rather than the stress has become common in computational rheology, and the challenge of developing numerical methods capable of resolving steep stresses and stress gradients has been transformed to one of developing techniques capable of resolving rapidly varying conformation tensor fields. In an important recent breakthrough, Fattal and Kupferman (2004) have shown that by changing the fundamental variable to the matrix logarithm of the conformation tensor, stable numerical solutions can be obtained at values of *Wi* significantly greater than ever obtained before. The success of their variable transformation protocol is predicated on their identification of the source of the HWNP as the inability of methods based on polynomial basis functions (such as finite element methods) to adequately represent the exponential profiles that emerge in conformational tensor fields in the vicinity of stagnation points and in regions of high deformation rate.

Hulsen et al. (2005) have recently carried out a stringent test of the log conformation representation by examining the flow of Oldroyd-B and Giesekus fluids around a cylinder confined between parallel plates. {It is worth noting that unlike the Oldroyd-B models prediction of unbounded extensional viscosity at a finite extension rate, the extensional viscosity predicted by the Giesekus model is always finite Bird *et al.* (1987a)]}. For both the fluids, Hulsen et al. (2005) find that with the log conformation formulation, the solution remains numerically stable for values of Wi considerably greater than those obtained previously with standard finite element (FEM) implementations. On the other hand, the two fluids differ significantly from each other with regard to the behavior of the convergence of solutions with mesh refinement. The lack of convergence with mesh refinement is usually seen most drastically in the failure of different meshes to yield a converged value of the maximum that occurs in the polymeric streamwise stress $\sigma_{\rm rr}$ on the centerline in the wake of the cylinder. In the case of the Giesekus model, even at values of Weissenberg number as high as $W_i=100$, mesh convergence is achieved in large parts of the flow domain, with the exception of localized regions near the stress maximum in the wake where convergence is not attained. For the Oldroyd-B model, however, the log conformation formulation fails to achieve mesh convergence in the entire wake region at roughly the same value ($Wi \ge 0.6$) as in previous studies. Moreover, the solution becomes unsteady at some greater value of Wi (depending on the mesh), finally breaking down at even higher Wi. Hulsen et al. (2005) speculate that this failure is probably due to the infinite extensibility of the Hookean dumbbell model that underlies the Oldroyd-B model, and call for further investigations to see if this might lead to the nonexistence of solutions beyond some value of Wi. Thus, after many years of attempting to resolve the HWNP by purely numerical means, its origin still remains a mystery.

In this article, we conclusively establish the connection between the HWNP and the unphysical behavior of the Oldroyd-B model, in the benchmark problem of the steady symmetric two-dimensional flow around a cylinder confined between parallel plates. We consider both dilute and ultradilute solutions (in which the velocity field is decoupled from the conformation tensor and stress field). The examination of the ultradilute case is similar to the earlier work by Wapperom and Renardy (2005) described previously. However, rather than using an ad hoc velocity field, we compute the Newtonian velocity field by the finite element method. We show for both ultradilute and dilute fluids, that when $Wi \approx 1$, polymer molecules flowing along the centerline in the wake of the cylinder undergo a coil-stretch transition; the transition occurs in the vicinity of the location of the maximum in the normal stress component σ_{xx} on the centerline. For ultradilute solutions, with increasing Wi, the molecules stretch without bound; this is accompanied by the stress maximum increasing without bound. However, the stress maximum shows no indication of diverging at all finite Wi. On the other hand, in a dilute solution, the coupling of the stress and velocity fields is shown to lead to the stress maximum diverging toward infinity at a finite value of $Wi \approx 0.7$. Thus, for the first time, evidence is presented of an upper bound in Wi for the existence of solutions for the steady flow of an Oldroyd-B fluid around a cylinder confined between parallel plates. For a UCM fluid, Alves *et al.* (2001) have previously speculated that σ_{xx} may develop a singularity at the position where it reaches a maximum value, based on the asymptotic behavior of highly accurate numerical results obtained by them using a finite volume method. However, they were unable to attribute a precise reason for the occurrence of a singularity.

Computations carried out here for a FENE-P fluid reveal that in this case also, polymer molecules undergo a coil-stretch transition, which is located at the stress maximum. However, with increasing *Wi*, the mean extension of the molecules saturates to a value close to their fully extended length, enabling computations beyond the critical Weissenberg number.

For the ultradilute model, a solution of the equation for the conformation tensor **M** along the centerline in the cylinder wake, valid for arbitrarily large values of Wi, is obtained here using two different techniques. In the first method, the fact that the equation for **M** in the Oldroyd-B and FENE-P models reduces at steady state to a system of ordinary differential equations (ODEs) along the centerline is exploited. In the second method, trajectories of the end-to-end vectors of an ensemble of dumbbells, flowing down the centerline in the wake of the cylinder, are calculated by carrying out Brownian dynamics simulations using the known velocity field. Averages carried out over the ensemble of trajectories lead to macroscopic predictions that are identical to the results obtained by solving the macroscopic model ODEs discussed previously. Comparison of the FEM results with the ODE and BDS results along the centerline in the finite element method. In particular, an estimation of the number of elements in the FEM method required to achieve convergence with increasing Wi reveals that obtaining solutions for Wi > 1 becomes excessively expensive.

The layout of this paper is as follows. In Sec. II, we summarize the governing equations, boundary conditions and the finite element computational method used here for the flow of dilute Oldroyd-B and FENE-P fluids around a cylinder confined between parallel plates. In Sec. III, we describe the two alternative methods by which solutions to the ultradilute models along the centerline in the cylinder wake may be obtained. Results of all three solution methods for ultradilute solutions are first discussed in Sec. IV, followed by a discussion of the predictions of FEM computations for the dilute model. Section V summarizes the main conclusions of this work.

II. DILUTE SOLUTIONS

A. Basic equations

As displayed in Fig. 1, the cylinder axis is in the z-direction perpendicular to the plane of flow. With the assumption of a plane of symmetry along the centerline (y=0), computations are only carried out in half the domain. The cylinder, with radius *a*, is assumed to be placed exactly midway between the plates, which are separated from each other by a distance 2*H*. The blockage ratio is H/a=2, in common with other benchmark flows around a confined cylinder simulations.

All macroscopic length scales are normalized with respect to *a*, velocities with respect to the mean inflow velocity far upstream $\langle v \rangle \equiv Q/H$ (*Q* is the flow rate through the half inflow), macroscopic time scales with respect to $a/\langle v \rangle$, and stresses and pressure with respect to $\eta \langle v \rangle / a$, where $\eta = \eta_s + \eta_{p,0}$ is the sum of the Newtonian solvent viscosity η_s and the zero-shear rate polymer contribution to viscosity $\eta_{p,0}$. The two relevant dimensionless numbers are the Weissenberg number $Wi = \lambda \langle v \rangle / a$, in which λ is a relaxation time, and the Reynolds number $Re = \rho a \langle v \rangle / \eta$, where ρ is the fluid density.

The complete set of nondimensional governing equations for a dilute polymer solution, described by the Oldroyd-B or FENE-P models, is

$$\nabla \cdot \mathbf{v} = 0 \quad (\text{Mass balance}), \tag{1}$$

$$Re \mathbf{v} \cdot \nabla \mathbf{v} - \nabla p - \nabla \cdot \boldsymbol{\tau}_{s} - \nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \quad (\text{Momentum balance}), \tag{2}$$

$$\partial \mathbf{M} / \partial t + \mathbf{v} \cdot \nabla \mathbf{M} - \boldsymbol{\kappa} \cdot \mathbf{M} - \mathbf{M} \cdot \boldsymbol{\kappa}^{T} = -1/Wi\{f(\operatorname{tr} \mathbf{M})\mathbf{M} - \mathbf{I}\}$$
 (Conformation tensor),

(3)

$$\tau_{\rm s} = 2\beta {\rm D}$$
 (Solvent stress), (4)

$$\boldsymbol{\sigma} = \frac{(1-\beta)}{Wi} \{ f(\operatorname{tr} \mathbf{M})\mathbf{M} - \mathbf{I} \} \quad (\text{Polymer stress}).$$
 (5)

In these equations, $\kappa = (\nabla \mathbf{v})^T$ is the transpose of the velocity gradient, $\mathbf{D} = 1/2$ ($\kappa^T + \kappa$) is the rate of deformation tensor, and the parameter $\beta = (\eta_s / \eta)$ is the viscosity ratio. Hereafter, Re=0, as usual in benchmarks for the Oldroyd-B model. The form of the function $f(\text{tr } \mathbf{M})$ depends on the microscopic model used to derive the equation for the evolution of the conformation tensor, and is consequently different in the Oldroyd-B and FENE-P models. For the Oldroyd-B model $f(\text{tr } \mathbf{M})=1$. For the FENE-P model, the function $f(\text{tr } \mathbf{M})$ is [Pasquali and Scriven (2004)]

$$f(\operatorname{tr} \mathbf{M}) = \frac{b-1}{b-\operatorname{tr} \mathbf{M}/3},\tag{6}$$

where b is the finite extensibility parameter. Note that the definition of b used here is different from the definition of the finite extensibility parameter given in Bird *et al.* (1987b), which is widely used in the literature. This is elaborated further in Sec. III B.

B. Boundary conditions and computational method

The set of governing equations [Eqs. (1)-(5)] are solved with the boundary conditions shown in Fig. 1. The location of the inflow and outflow boundaries coincides with that chosen by Sun *et al.* (1999), who showed that the flow is insensitive to further displacement of the open boundaries in the range of Weissenberg numbers examined. A no-slip

TABLE I. Meshes used in the finite element simulations for computing viscoelastic flow around a cylinder.

Mesh	M1	M2	M3	M4	M5
Number of elements	2311	5040	8512	16425	31500

boundary condition is imposed on the cylinder surface and the channel walls. Fully developed flow is assumed at both inflow and outflow boundaries, with the velocity prescribed at both boundaries. Here, $\langle v \rangle = 1$ for the prescribed velocity field. The boundary conditions on the conformation tensor are imposed only at the inflow boundary following the method in Xie and Pasquali (2004). At the symmetry line, $\mathbf{tn}:(\boldsymbol{\tau}_s + \boldsymbol{\sigma}) = 0$ and $v_y = 0$ is imposed, where **t** and **n** are the unit vectors tangential and normal to the symmetry line, respectively.

The governing equations are discretized by using the DEVSS-TG/SUPG mixed finite element method [Pasquali and Scriven (2002)]. The DEVSS-TG formulation involves the introduction of an additional variable, the velocity gradient κ . Continuous biquadratic basis functions are used to represent velocity, linear discontinuous basis functions to represent pressure, and continuous bilinear basis functions are used for the interpolated velocity gradient and conformation tensor. The DEVSS-TG/SUPG spatial discretization results in a large set of coupled nonlinear algebraic equations, which are solved by Newton's method with analytical Jacobian and first order arc-length continuation in *Wi* [Pasquali and Scriven (2002)]. Five different meshes are used for the FEM calculations. Details of the different meshes used in this work are given in Table I, and the mesh M2 is displayed in Fig. 2. The important distinction among the five meshes is the density of elements on the cylinder surface and in the wake of the cylinder.

III. ULTRADILUTE SOLUTIONS

Since the velocity field for an ultradilute solution is determined completely by the solvent stress, it is identical to the velocity field for a Newtonian fluid. The ultradilute conformation tensor and velocity fields are simply obtained by solving the governing equations with the parameter β set equal to unity. As can be seen from Eq. (5), this implies σ =0, leading to Eqs. (1) and (2) being identical to the mass and momentum balances for a Newtonian fluid. The same FEM formulation described previously for the solution of the dilute case can consequently also be used to obtain the ultradilute conformation tensor and Newtonian velocity fields when β =1.

In such an an ultradilute solution, the conformation tensor field corresponds to the average configurations of polymer molecules in a predetermined velocity field. Note that



FIG. 2. Mesh M2 used in the finite element simulations.

the choice of value for *Wi* has no influence on the velocity field (which is determined once and for all for the specified geometry), but can significantly affect the conformation tensor field, as will subsequently be seen.

The polymer contribution to the stress tensor cannot be obtained from a solution of the macroscopic equations, where it is assumed to be zero. In this case, the dimensionless stress predicted by the microscopic models, $\sigma^* = \{f(\operatorname{tr} \mathbf{M})\mathbf{M} - \mathbf{I}\}$, is reported. This is similar to the evaluation of the polymer contribution to the stress in a homogenous simple shear or extensional flow, where the velocity field is prescribed *a priori*.

The FEM formulation does not give mesh-converged results for the conformation tensor field for an ultra-dilute solution beyond a critical *Wi*. Yet, an accurate solution to the conformation tensor equation along the centerline in the wake of the cylinder can be computed at arbitrary *Wi* by the two methods discussed below.

A. System of ODEs

By the requirements of symmetry along the centerline, the velocity field must have the form, $v_x = g(x)$, $v_y = 0$, and the components of the velocity gradient tensor must satisfy $\kappa_{xy} = \kappa_{yx} = 0$. Incompressibility requires $\kappa_{xx} = -\kappa_{yy}$; therefore, the flow along the centerline is planar extensional in character. Substituting this velocity field into the evolution equation for the conformation tensor [Eq. (3)] leads at steady state to a system of ODEs in the independent variable *x*, for the diagonal components of the conformation tensor **M**. In the case of the Oldroyd-B model, these equations are decoupled. Here, we are only interested in the equation for M_{xx} , which is

$$\frac{d\mathbf{M}_{xx}}{dx} = -\frac{\left[1 - 2\lambda\kappa_{xx}(x)\right]}{\lambda v_x(x)}\mathbf{M}_{xx} + \frac{1}{\lambda v_x(x)}.$$
(7)

Here, $W_{i=\lambda}$, because in dimensionless units $\langle v \rangle = 1$ and a=1. Equation (7) is a first order linear ODE for M_{xx} that can be integrated straightforwardly once an initial condition is prescribed. At the downstream stagnation point (x=1), the polymer molecules are at equilibrium ($\mathbf{v} = \boldsymbol{\kappa} = 0$); therefore $M_{xx} = 1$. However, as can be seen from the form of Eq. (7), this boundary condition cannot be used since $v_x=0$ at the stagnation point. This difficulty can be overcome by estimating the velocity field asymptotically close to the stagnation point. While Phan-Thien (1984) has previously obtained exact solutions for the plane and axisymmetric stagnation flows of an Oldroyd-B fluid, our interest in the ultradilute limit is in the Newtonian flow field. For an unbounded flow of a Newtonian fluid near a stagnation point on the surface of a two-dimensional body, the assumption of a quadratic velocity field, asymptotically close to the stagnation point, is exactly valid for Stokes flow, and is consistent with the accepted numerical solution for Hiemenz flow [Pozrikidis (1997)]. The approximate Newtonian velocity field postulated by Wapperom and Renardy (2005) for the flow around a confined cylinder is also of the form $v_x = k(x)$ $(-1)^2$ [see also Renardy (2000)], with k=4, in the limit as $x \to 1$ (from previous). The assumption of a quadratic velocity field, with k=4.178, fits well the Newtonian velocity field close to the downstream stagnation point obtained by the FEM solution. For a quadratic velocity field, Eq. (7) admits an analytical solution for M_{yy} :

$$M_{xx} = 1 + 2\alpha(x-1) + 3\alpha^2(x-1)^2 + 3\alpha^3(x-1)^3 + 1.5\alpha^4(x-1)^4,$$
(8)

where $\alpha = 2k\lambda$. The analytical value of M_{xx} at x = 1.01 is used here as the boundary condition to integrate Eq. (7), with a fourth-order Runge–Kutta method. The functions $v_x(x)$ and $\kappa_{xx}(x)$ are obtained by interpolating the Newtonian FEM solution, at each of the values of x where they are required for the purpose of integration.

$$\frac{d\mathbf{M}_{xx}}{dx} = -\frac{1}{\lambda v_x(x)} \left\{ \frac{b-1}{b-\operatorname{tr} \mathbf{M}/3} - 2\lambda \kappa_{xx}(x) \right\} \mathbf{M}_{xx} + \frac{1}{\lambda v_x(x)},$$

$$\frac{d\mathbf{M}_{yy}}{dx} = -\frac{1}{\lambda v_x(x)} \left\{ \frac{b-1}{b-\operatorname{tr} \mathbf{M}/3} - 2\lambda \kappa_{yy}(x) \right\} \mathbf{M}_{yy} + \frac{1}{\lambda v_x(x)},$$

$$\frac{d\mathbf{M}_{zz}}{dx} = -\frac{1}{\lambda v_x(x)} \left\{ \frac{b-1}{b-\operatorname{tr} \mathbf{M}/3} \right\} \mathbf{M}_{zz} + \frac{1}{\lambda v_x(x)}.$$
(9)

It is difficult to solve these equations analytically even with the assumption of a quadratic velocity field close to the stagnation point. Since $\kappa_{xx}(x) \ll 1$ at x=1.01, the equilibrium initial conditions, $M_{xx}=1$, $M_{yy}=1$, and $M_{zz}=1$, are used as the boundary conditions, though these values are strictly correct only at the stagnation point x=1. It turns out, however, that the conformational tensor fields along the centerline, downstream of the stagnation point, are insensitive to a variation by a few percent in the boundary values chosen for the diagonal components of **M** close to the stagnation point. (For instance, identical results are obtained if the boundary conditions for the Oldroyd-B model at x = 1.01, are used instead.)

B. Brownian dynamics simulations

The conformation along the centerline in the cylinder wake can also be computed by exploiting the connection between the macroscopic and microscopic models. For both the Oldroyd-B and FENE-P fluids, the microscopic model is a dumbbell, with the spring force obeying the linear expression, $\mathbf{F}^{(s)} = H\mathbf{Q}$, in the former case, and the nonlinear expression;

$$\mathbf{F}^{(s)} = \frac{H}{(1 - \langle Q^2 \rangle / Q_0^2)} \mathbf{Q},\tag{10}$$

in the latter. Here, $\langle (.) \rangle$ denotes an ensemble average, *H* is the spring constant, **Q** is the connector vector between the beads, and Q_0 is the fully extensible length of the spring [Bird *et al.* (1987b)]. The variable that is common to the two levels of description is the conformation tensor;

$$\mathbf{M} = \frac{1}{(\langle Q^2 \rangle_{\rm eq}/3)} \langle \mathbf{Q} \mathbf{Q} \rangle, \tag{11}$$

where $\sqrt{\langle Q^2 \rangle_{eq}}$ is the root mean square end-to-end vector at equilibrium. For a Hookean dumbbell, $\sqrt{\langle Q^2 \rangle_{eq}/3} = \sqrt{k_B T/H}$ (with k_B being the Boltzmanns constant and T the temperature), while for a FENE-P spring

$$\langle Q^2 \rangle_{\rm eq} = \frac{3Q_0^2(k_{\rm B}T/H)}{Q_0^2 + 3(k_{\rm B}T/H)}.$$
 (12)

Note that the finite extensibility parameter is defined here by $b=Q_0^2/\langle Q^2 \rangle_{eq}$. In the Bird *et al.* definition, the microscopic length scale used to nondimensionalize Q_0 is the Hookean dumbbell length scale $\sqrt{k_B T/H}$.

A packet of fluid with an ensemble of dumbbells, starting close to the stagnation point and traveling down the centerline with velocity $v_x(x)$, experiences the local velocity gradient at each position *x*. In this case, the variation with time of $\mathbf{M} = \langle \widetilde{\mathbf{Q}} \widetilde{\mathbf{Q}} \rangle$, where, $\widetilde{\mathbf{Q}} = \mathbf{Q} / \sqrt{\langle \langle Q^2 \rangle_{eq}/3 \rangle}$, would be equivalent to the variation of **M** with *x* in the macroscopic models. The ensemble average $\langle \widetilde{\mathbf{Q}} \widetilde{\mathbf{Q}} \rangle$ can be obtained by integrating the stochastic differential equation (SDE),

$$d\tilde{\mathbf{Q}} = \left\{ \boldsymbol{\kappa}(t) \cdot \tilde{\mathbf{Q}} - \frac{1}{2Wi} f(\langle \tilde{Q}^2 \rangle) \tilde{\mathbf{Q}} \right\} dt + \frac{1}{\sqrt{Wi}} d\tilde{\mathbf{W}},$$
(13)

which governs the stochastic dynamics of Hookean or FENE-P dumbbells subject to the time varying velocity gradient $\kappa(t)$ [Öttinger (1996)]. Here, \tilde{W} is a nondimensional Wiener process, and

$$f(\langle \tilde{Q}^2 \rangle) = \begin{cases} 1 & \text{for Hookean dumbbells,} \\ (b-1)/(b-\langle \tilde{Q}^2 \rangle/3) & \text{for FENE-P dumbbells} \end{cases}$$
(14)

is the same function for the FENE-P model as in Eq. (6), with $\langle \tilde{Q}^2 \rangle$ taking the place of tr **M**.

The velocity gradient $\kappa_{xx}(t)$ for a packet of fluid traveling down the centerline in the wake of the cylinder can be found in a straightforward way since $v_x(x)$ and $\kappa_{xx}(x)$ are known for a Newtonian fluid. Since $dx/dt=v_x(x)$, the integral,

$$t = \int_{1+\delta}^{x} dx' \frac{1}{v_x(x')} \equiv h(x),$$
 (15)

gives t as a function of x for a material particle. Clearly, $\kappa_{xx}(t) = \kappa_{xx}(h^{-1}(t))$. The fluid packet starts its journey slightly downstream of the stagnation point [represented by 1 + δ in the lower limit of the integral in Eq. (15)].

The velocity field $v_x(x)$ and the velocity gradient $\kappa_{xx}(x)$ along the centerline, computed using the FEM formulation with the M5 mesh, are displayed in Fig. 3. Note the quadratic nature of the velocity close to the stagnation point. The position x of a fluid packet as a function of time t, calculated using Eq. (15), is displayed as the dashed green line. Consistent with the boundary conditions for the ODE for M_{xx} before, we use δ =0.01. Clearly, a material particle spends a significant time close to the stagnation point before rapidly accelerating away from it, and for a significant fraction of this time, it is subjected to a strong time-dependent velocity gradient (indicated by the dashed black line).

The configurational distribution function for the Hookean dumbbell model is Gaussian both at equilibrium, and in the presence of a homogeneous flow field [Bird *et al.* (1987b)]. Since a Gaussian distribution is completely determined by its second moments, the initial distribution function at x=1.01 can be calculated for the known velocity gradient κ_{xx} , using the analytical solution for M_{xx} in Eq. (8) (and a similar expression for M_{yy} ; $M_{zz}=1$). For Hookean dumbbells, the SDE [Eq. (13)] is integrated forward in time here, using a second order predictor-corrector Brownian dynamics simulation (BDS) algorithm [Öttinger (1996)], with an initial ensemble of connector vectors distributed according to the Gaussian distribution at x=1.01, subjected to the time dependent velocity gradient $\kappa_{xx}(t)$ for t>0.

The distribution function is also Gaussian in the case of the FENE-P model, and as a result, the initial distribution function at x=1.01 can in principle be determined using the second moments obtained by solving the set of governing equations [Eq. (9)]. However,



FIG. 3. Velocity (v_x) and velocity gradient (κ_{xx}) for an ultradilute solution (or a Newtonian fluid) along the center line in the wake of the cylinder, computed using the FEM formulation with the M5 mesh. The dashed green line is the position *x*, as a function of time, of a material particle traveling downstream starting close to the stagnation point. The dashed black line is the time dependent velocity gradient $\kappa_{xx}(t)$ used for carrying out BDS of the ultradilute models. The dot-dashed line is the velocity profile for a dilute Oldroyd-B model at Wi=0.6.

we adopt the simpler procedure of using a Gaussian distributed initial ensemble with equilibrium second moments, $M_{xx}=1$, $M_{yy}=1$, and $M_{zz}=1$, at x=1.01, since the solution of the SDE downstream of the stagnation point is found to be insensitive to the choice of the initial distribution. (For instance, identical results are obtained if the initial distribution of Hookean dumbbells at x=1.01, is used instead.) The BDS algorithm for FENE-P dumbbells is identical to the one used to integrate the SDE for Hookean dumbbells, with the additional feature of having to evaluate $\langle \tilde{Q}^2 \rangle$ at every time step.

IV. RESULTS AND DISCUSSION

A. Ultradilute solutions

Figure 4 shows that mesh convergence in the cylinder wake cannot be attained at Wi=1 for an ultradilute polymer solution. The profile of the dimensionless polymer contribution to stress shows two maxima, one on the cylinder wall, and a second in the wake, typical for viscoelastic flow around a confined cylinder. As Wi increases further, the maximum in the wake grows significantly and becomes dominant. Like in the case of dilute solutions, mesh convergence worsens with increasing Wi.

Figure 5 compares the conformation components computed by FEM as well as by solving the ODEs, Eqs. (7) and (9), and by integrating (using BDS) the SDE, Eq. (13), for the Oldroyd-B and FENE-P models. The excellent agreement of the FEM results with the other two solution techniques (except for the Oldroyd-B model at Wi=1.3) shows that the FEM results are accurate at the Weissenberg numbers that have been displayed. The departure of FEM predictions, at Wi=1.3, for the Oldroyd-B model [Fig. 5(b)], is clear proof of the breakdown of FEM computations for Wi>1.

Important insight into the source of computational difficulties can be obtained by considering the nature of the maximum in the M_{xx} component in the wake of the cylinder. For an ensemble of dumbbells that start near the stagnation point (where the velocity gradient κ_{xx} is negligibly small), and then travel downstream to the region of fully



FIG. 4. The dimensionless polymer contribution to stress, σ_{xx}^* , along the cylinder wall and along the centerline in the cylinder wake, at *Wi*=1.0, for an ultradilute solution of an Oldroyd-B fluid computed by FEM formulation. The inset shows the lack of mesh convergence in the vicinity of the stress maximum in the cylinder wake.

developed flow (where $\kappa_{xx}=0$), the M_{xx} component of the conformation tensor initially has a value close to unity, and ultimately returns to a value of unity. Since $\kappa_{xx}>0$ at intermediate values of x, it is clear that M_{xx} must attain a maximum at some point $x = x^*$ along the centerline in the wake of the cylinder. Indeed all computations of flow around a confined cylinder report the occurrence of a maximum, and failure to attain mesh convergence is usually observed most noticeably at the maximum.

At the maximum (where $dM_{xx}/dx=0$), Eq. (7) implies that

$$M_{xx}|_{x=x}^{*} = \frac{1}{1 - 2\lambda \kappa_{xx}|_{x=x}^{*}}.$$
(16)

Clearly, if $\lambda \kappa_{xx} = 0.5$ at $x = x^*$, the maximum value of M_{xx} will be unbounded. One can see from the dotted curve in Fig. 3 that for values of $\lambda = \mathcal{O}(1)$, there are many points along the centerline in the cylinder wake where $\lambda \kappa_{xx}$ can be greater than 0.5. However, as manifest from Eq. (16), the real issue is whether $\lambda \kappa_{xx} = 0.5$ at $x = x^*$.

Figure 6(a) displays $\lambda \kappa_{xx}|_{x=x}^*$ as a function of Wi for an ultradilute Oldroyd-B fluid, obtained with the three different solution techniques. Interestingly, $\lambda \kappa_{xx}|_{x=x}^*$ first approaches 0.5 at $Wi \approx 1$, where computational difficulties with the FEM method are first encountered. While the ODE solution and BDS can be continued to higher Wi, FEM computations (indicated by the crosses) are no longer accurate beyond Wi=1, breaking down completely by Wi=1.55. This is related, as will be discussed in greater detail shortly, to the inability of the FEM solution to resolve the very large stresses that arise as $\lambda \kappa_{xx}|_{x=x}^*$ approaches 0.5. Figure 6(b) shows that the approach of $\lambda \kappa_{xx}|_{x=x}^*$ to the critical value is approximately linear in Weissenberg number for small values of Wi, becoming a power-law ($Wi^{-4.59}$), for $Wi \ge 0.5$. Thus, though $\lambda \kappa_{xx}|_{x=x}^* \to 0.5$ asymptotically, it

never equals or exceeds the critical value. This implies that M_{xx} (and, consequently, σ_{xx}^{+}) will increase without bound as *Wi* increases, but will never become singular. In the case of the FENE-P model, $\lambda \kappa_{xx}|_{x=x}^{+*}$ approaches and exceeds 0.5 with increas-

ing Wi, as shown in Fig. 7, for a range of values of the finite-extensibility parameter b.



FIG. 5. The M_{xx} component of the conformation tensor, computed using FEM, ODE and BDS, for an ultradilute solution of Oldroyd-B and FENE-P (*b*=55) fluids. (a) *Wi*=0.8, (b) *Wi*=1.3, (c) *Wi*=1.5, and (d) *Wi*=2.0. The BDS results are obtained by averaging over 10⁶ dumbbell trajectories. The FEM results are computed using the M5 mesh. For the Oldroyd-B model, at *Wi*=1.3, the FEM results at the maximum are approximately 6% different from the ODE or BDS values.

The value 0.5 is not significant for the FENE-P model since, as can be seen from Eq. (9), $M_{xx}|_{x=x^*} \rightarrow (b - \text{tr } \mathbf{M}/3)/(\text{tr } \mathbf{M}/3-1)$ as $\lambda \kappa_{xx}|_{x=x^*} \rightarrow 0.5$. Hence, $M_{xx}|_{x=x^*}$ remains finite as long as b is finite.

Before discussing the dependence of $M_{xx}|_{x=x^*}$ and $\sigma_{xx}^*|_{x=x^*}$ on $\lambda \kappa_{xx}|_{x=x^*}$, it is interesting to first consider the dependence of the location of the maximum, $x=x^*$, and $\kappa_{xx}|_{x=x^*}$, on *Wi*. Figure 8(a) shows that for the Oldroyd-B model, the location x^* of the maximum in M_{xx} continuously moves downstream away from the stagnation point in the cylinder wake, with increasing *Wi*. Simultaneously, Fig. 8(b) indicates that the value of $\kappa_{xx}|_{x=x^*}$ continuously decreases. This is consistent with the behavior of κ_{xx} as a function of *x* displayed in Fig. 3. With increasing *Wi*, the product $\lambda \kappa_{xx}|_{x=x^*}$ (with λ increasing and $\kappa_{xx}|_{x=x^*}$ decreasing) tends to 0.5 in the manner depicted previously in Fig. 6(a).

For a FENE-P fluid, the location of the maximum in M_{xx} and the value of κ_{xx} at $x = x^*$, display intriguing behavior with increasing Wi, as shown in Fig. 8. For each value of b, beyond some threshold value of Wi, both quantities attain constant values. As a consequence, beyond this threshold value, the product $\lambda \kappa_{xx}|_{x=x^*}$ increases linearly with Wi, as can be seen clearly in Fig. 7, enabling a straightforward mapping between $\lambda \kappa_{xx}|_{x=x^*}$ and Wi to be made.

The steep increase in $M_{xx}|_{x=x}^*$ and $\sigma_{xx}^*|_{x=x}^*$ for the Oldroyd-B model, as $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$, is displayed in Figs. 9(a) and 9(b). For the FENE-P model, there is a point of



FIG. 6. (a) Dependence of the nondimensional strain rate $\lambda \kappa_{xx}$ on Wi, at the location $x = x^*$ of the maximum in M_{xx} in the cylinder wake, for an ultradilute Oldroyd-B fluid. Inset shows $\lambda \kappa_{xx}|_{x=x^*}$ approaching 0.5, computed from the ODE solution, for Wi > 1.5. (b) $\lambda \kappa_{xx}|_{x=x^*}$ approaches the critical value 0.5 as a power-law with increasing Wi. The FEM results are for the M5 mesh and BDS results are obtained by averaging over 10⁶ individual Brownian trajectories of Hookean dumbbells.

inflection at $\lambda \kappa_{xx}|_{x=x} = 0.5$, after which the curves increase much more gradually with increasing $\lambda \kappa_{xx}|_{x=x} = 0.5$, after which the curves for the Oldroyd-B and FENE-P models are strikingly reminiscent of the well-known extensional viscosity versus strain rate curves for these models, commonly used to display the unphysical behavior of the Oldroyd-B model [Bird *et al.* (1987b), Owens and Phillips (2002)]. As is well known, in that case, the onset of the steep increase in stress is attributed to the occurrence of a coil-stretch transition, leading to an unbounded stress in the Oldroyd-B model, but a bounded stress in the FENE-P model. While the former is because of the infinite extensibility of the Hookean spring in the Hookean dumbbell model, the latter is because of the existence of a upper bound to the mean stretchability of the spring in the FENE-P model. It can be conjectured, consequently, that in the present instance also, polymer molecules



FIG. 7. Dependence of the nondimensional strain rate $\lambda \kappa_{xx}$, at the location $x = x^*$ of the maximum in M_{xx} in the cylinder wake, on *Wi*, for a FENE-P fluid.

undergo a coil-stretch transition in the wake of the cylinder, in the vicinity of the location of the stress maximum, giving rise to a stress that increases without bound as *Wi* increases.

The breakdown of the FEM computations for the Oldroyd-B model is clearly related to the steep increase in $M_{xx}|_{x=x}^*$ and $\sigma_{xx}^*|_{x=x}^*$, as $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$. [Fig. 9(b) indicates that the stress maximum increases by five orders of magnitude as *Wi* increases from 0.1 to 4]. Since an accurate solution is known for any value of *Wi* through the integration of the ODEs and BDS, the error in the FEM computation can be estimated using

error =
$$\frac{(M_{xx}^{\text{ODE}}|_{x=x}^* - M_{xx}^{\text{FEM}}|_{x=x}^*)}{M_{xx}^{\text{ODE}}|_{x=x}^*} \times 100.$$
(17)

Error estimates obtained in this manner are displayed in Fig. 10(a) for the Oldroyd-B model. The error remains small (<1%) at low Wi, but increases sharply to approximately 8% as $Wi \ge O(1)$. The value of Wi^* , the Weissenberg number up to which the error is less than 1%, depends on the degree of mesh refinement, and a clear improvement in Wi^* can be observed with increased mesh refinement. However, to obtain mesh converged results for Wi > 0.7 (with error <1%), an approximately 100-fold increase in mesh density and hence, approximately ~100 fold increase in computational time is required.

In the case of the FENE-P model, the error in $M_{xx}|_{x=x}^*$ is small even at relatively large values of *Wi* since the chains are close to their fully extended length, and it is difficult to see a clear pattern in the change in error with mesh refinement, unlike in the case of the Oldroyd-B model above. However, the error in the $M_{yy}|_{x=x}^*$ component reveals a more systematic behavior, as displayed in Fig. 10(b), with a decrease in error with increasing mesh refinement.

The infeasibility of carrying out conventional FEM computations for the confined flow around a cylinder of an ultradilute Oldroyd-B fluid, for Wi > 1, is revealed in Fig. 11, where the exponential increase in the number of elements required to attain an error less than 1%, with increasing Wi, can be clearly observed. For the FENE-P model, the rate of increase in the number of elements required for an error less than 1% is significantly



FIG. 8. The dependence on Wi of (a) the location x^* of the maximum in M_{xx} , and (b) the strain rate $\kappa_{xx}|_{x=x^*}$, for ultra-dilute solutions of Oldroyd-B and FENE-P models. Results displayed are solutions of the respective ODEs.

lower than that for the Oldroyd-B fluid. The Mesh 4 curve in Fig. 10(b) even seems to suggest that there might be a degree of mesh refinement beyond which, for the FENE-P model, one can compute at any Wi with an error less than 1%. However, this trend is not easily discernible in Fig. 11, and additional mesh refinement may be required before a firm conclusion can be drawn. Further, a change of variable to the matrix logarithm of the conformation tensor, may lead to mesh converged results at significantly higher vales of Wi.

The reason polymer molecules undergo a coil-stretch transition as they travel down the centerline in the cylinder wake is because of the extended period of time they spend in the neighborhood of the stagnation point, which leads to a significant accumulation of strain. The Hencky strain ϵ at any instant *t*, calculated from the expression ϵ = $\int_0^t dt' \kappa_{xx}(t')$, is displayed in Fig. 12. A very large Hencky strain of roughly eight units is



FIG. 9. Coil-stretch transition in the cylinder wake for an ultradilute solution. Dependence of the polymer stretch (M_{xx}) and stress (σ_{xx}^*) , at $x=x^*$, on $\lambda \kappa_{xx}|_{x=x^*}$. The lines are ODE solutions and the symbols are FEM results on mesh M5.

built up by the time the molecules approach x^* . For a material element of unit length at t=0, this corresponds to a ratio of final to initial length of roughly 3000. The behavior of individual molecules as they are subject to this degree of straining can be obtained, for an ultradilute solution, from the Brownian dynamics simulations carried out here since one can calculate the trajectories of dumbbells as they are convected by the flow field down the centerline, subjected to the local strain rate.

In this context, it is instructive to calculate the size of individual dumbbells relative to a macroscopic feature, such as the length of an element in the finite element mesh. In the nondimensionalization scheme used here, however, since the macroscopic length scale is the cylinder radius a, and the microscopic length scale for Hookean dumbbells is $\sqrt{\langle Q^2 \rangle_{eq}/3}$, direct comparison is difficult unless one has estimates of these length scales.



FIG. 10. Percentage error in FEM computations of (a) $M_{xx}|_{x=x}^*$ for an ultradilute Oldroyd-B solution, and (b) $M_{yy}|_{x=x}^*$ for an ultradilute FENE-P fluid, as a function of *Wi*. The error is calculated based on the results of the ODE solutions.

Here, we use the experimental data of McKinley *et al.* (1993), who investigated the flow around a confined cylinder (with radius 3.188×10^{-3} m) of a 1.2 million molecular weight Polyisobutelene solution, to obtain a typical estimate of these length scales. For these molecules, the equilibrium size can be shown to be $\sqrt{\langle Q^2 \rangle_{eq}} = 0.0497 \ \mu$ m. Defining a dimensionless length in the flow direction by

$$Q_x^* = \frac{\tilde{Q}_x \sqrt{\langle Q^2 \rangle_{\text{eq}}/3}}{aL_m |_{x=x}^*},$$
(18)

where $L_m|_{x=x^*}$ is the nondimensional length of the element at $x=x^*$, the relative length of individual molecules in the flow direction can be calculated from the BDS trajectories as a function of strain.



FIG. 11. The number of elements as a function of the Weissenberg number Wi^* , up to which the error remains less than 1%, for the Oldroyd-B and FENE-P models. The inset displays the same data as a log-log plot.

Figure 13 display Q_x^* as a function of ϵ , for an ensemble of 100 dumbbell trajectories, at various values of *Wi*. Nearly all the dumbbells appear to remain close to their initial state of extension until approximately five strain units, beyond which several of the dumbbells undergo rapid extension, which is more pronounced as *Wi* increases. The rapid extension of the dumbbell spring represents the physical unraveling of a polymer molecule from a coiled to a stretched state, and the results in Fig. 13 are inline with the notion that a coil-stretch transition occurs as the molecules experience the maximum strain. As expected, the molecules relax back to their equilibrium configurations once the strain rate downstream of the maximum becomes zero.



FIG. 12. Hencky strain accumulated by a fluid element as it travels along the centerline from the neighborhood of the stagnation point in the cylinder wake.



FIG. 13. The length of individual polymer molecules relative to the size of an element of the M5 mesh, at $x = x^*$, at various values of *Wi*, for an ultradilute Oldroyd-B fluid. The experimental data of McKinley *et al.* (1993) is used to obtain an estimate of the equilibrium size of the molecules and the cylinder radius.

The use of the local element size to achieve nondimensionalization strikingly reveals that the magnitude of some of the molecules is large enough to span several elements. The possibility of polymer length scales becoming comparable to the mesh size in finite element simulations, under certain circumstances, was foreseen earlier by Öttinger [Öttinger (1995)]. Kinetic theory models, such as the Hookean dumbbell model, are typically built on the assumption of homogeneous fields, with negligible variation on the length scale of individual molecules. The data in Fig. 13 suggests that the extensive use of the unphysical Oldroyd-B model in complex flow simulations is questionable, and highlights the need to derive more refined models that are valid in nonhomogeneous fields.

B. Dilute solutions

In the case of dilute solutions, the coupling of the velocity and the conformation tensor (and stress) fields, makes it impossible to obtain error estimates, or to calculate the trajectories of individual dumbbell molecules convected along the centerline by the flow, using the procedures adopted here for the case of ultradilute solutions. Nevertheless, the key insight of the previous section can be exploited because the value of the maximum in the M_{xx} component in the cylinder wake, for the Oldroyd-B model, is still given by Eq. (16), even though the velocity field $v_x(x)$ is not predetermined.

Since the velocity field for a dilute solution changes with each change in W_i , $\lambda \kappa_{xx}|_{x=x}^*$ has to be found at various values of W_i by integrating the full system of equations for the velocity and conformation tensor fields using the FEM formulation. A typical velocity profile for a dilute solution at $W_i=0.6$ is shown in Fig. 3 as the dot-dashed line. (At this value of W_i , it can be seen that the velocity profile is not significantly different from that for an ultradilute solution.)

Figure 14(a) indicates that for various values of β , $\lambda \kappa_{xx}|_{x=x}^*$ for a dilute solution approaches the critical value of 0.5 at a smaller value of *Wi* than in the ultradilute case. While at low *Wi*, dilute solution results are close to those for ultradilute solutions, the rapid departure of dilute solution values of $\lambda \kappa_{xx}|_{x=x}^*$ from ultradilute values, as



FIG. 14. Dependence of $\lambda \kappa_{xt}|_{x=x}^*$ on (a) Wi for dilute and ultra-dilute solutions, and (b) on Wi⁻¹ for dilute solutions. The M4 mesh has been used for FEM computations.

 $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$, is clearly visible in the logarithmic scale of the figure inset. For an ultradilute solution, it was seen earlier in Fig. 6(b) that $\lambda \kappa_{xx}|_{x=x}^*$ approached 0.5 asymptotically as a power law. On the other hand, Fig. 14(b) suggests a linear dependence of $\lambda \kappa_{xx}|_{x=x}^*$ on Wi^{-1} for dilute solutions, with slightly different dependences for the various values of β . This change in the dependence of $\lambda \kappa_{xx}|_{x=x}^*$ on Wi is significant evidence for the modification of the flow by the presence of the polymer, which is not apparent when only the velocity profiles are compared, as in Fig. 3.

Other manifestations of the coupling of the polymer stress and velocity fields in a dilute solution are indicated in Fig. 15, where the dependence of the location of the stress maximum (x^*) , and the velocity gradient $(\kappa_{xx}|_{x=x}^*)$ on Wi, is displayed. In contrast to the ultradilute case, where x^* continuously moves away from the stagnation point, Fig. 15(a) indicates that for dilute solutions x^* remains constant beyond a threshold value of Wi. The behavior of x^* at Wi beyond which mesh convergence has been obtained (i.e., Wi



FIG. 15. The dependence on *Wi* of (a) the location x^* of the maximum in M_{xx} , and (b) the strain rate $\kappa_{xx}|_{x=x^*}$, for ultradilute and dilute Oldroyd-B fluids. The M4 mesh has been used for FEM computations.

>0.6), has also been displayed for β =0.59. Curiously, for such Wi, x^* appears to move toward the stagnation point. This behavior can also be discerned in the results reported earlier by Alves *et al.* (2001) at these Weissenberg numbers. The behavior of $\kappa_{xx}|_{x=x}^*$ as a function of Wi displayed in Fig. 15(b), provides a clue to the origin of the difference between dilute and ultradilute solutions in the approach of $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$ with increasing Wi, seen earlier in Fig. 14(a). Unlike in the ultradilute case, where $\kappa_{xx}|_{x=x}^*$ is a continuously decreasing function of Wi, the modification of the flow caused by the presence of the polymer appears to slow down the decrease of $\kappa_{xx}|_{x=x}^*$. A crucial consequence of this difference is that $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$ at a finite value of Wi, with obvious implications for carrying out computations beyond this limiting value of Wi. This is discussed further shortly in the context of Fig. 17, after first considering the dependence of M_{xx} on $\lambda \kappa_{xx}|_{x=x}^*$.



FIG. 16. Coil-stretch transition in the cylinder wake for a dilute solution. Variation of the polymer stretch M_{xx} at the location of the stress maxima with $\lambda \kappa_{xx}|_{x=x}^*$, for (a) Oldroyd-B and FENE-P models for the viscosity ratio β =0.59, and (b) Oldroyd-B model for various values of β . The M4 mesh is used for the Oldroyd-B model and the M3 mesh is used for the FENE-P model in FEM computations.

As can be seen clearly from Fig. 16(a), M_{xx} increases steeply for the Oldroyd-B model as $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$, with M_{xx} appearing to become unbounded in this limit. For the FENE-P fluid on the other hand, the curves for M_{xx} exhibit a point of inflection at $\lambda \kappa_{xx}|_{x=x}^*=0.5$, before leveling off to the fully stretched value corresponding to the respective value of *b*. Since both ultradilute and dilute Oldroyd-B fluids (regardless of the value of β) must satisfy Eq. (16) at the location of the maxima, the various cases are plotted, together with a dashed curve representing Eq. (16), in Fig. 16(b). Interestingly, for $\beta=0.2$ and 0.59, the data appear to depart from Eq. (16) for values of Wi > 0.55, even though a comparison of the stress maxima for various meshes indicates mesh convergence up to Wi=0.6. Representing the data in this manner might consequently serve as a



FIG. 17. Variation of the inverse polymer stretch M_{xx}^{-1} for the Oldroyd-B model at the location of the stress maxima in the cylinder wake with inverse Weissenberg number Wi^{-1} at various values of β .

more stringent test of mesh convergence. Indeed, this is the reason why only data in the range $0.4 \le Wi \le 0.54$ have been used to carry out the linear fit in Fig. 14(b).

The similarity of the shapes of the curves in Fig. 16(a) to the curves in Fig. 9 and to the well-known extensional viscosity versus strain rate curves for the Oldroyd-B and FENE-P models suggests that even for a dilute solution, there occurs a coil-stretch transition in the vicinity of the location of the stress maximum in the cylinder wake, and this coil-stretch transition is the source of problems encountered with FEM computations for the flow of an Oldroyd-B fluid around a confined cylinder.

For the Oldroyd-B model, since $M_{xx}^{-1} = 1 - 2 \lambda \kappa_{xx}|_{x=x}^{+*}$ at the location of the stress maximum in the cylinder wake [from Eq. (16)], it follows for dilute solutions that a linear dependence of $\lambda \kappa_{xx}|_{x=x}^{+*}$ on Wi^{-1} implies a linear dependence of M_{xx}^{-1} on Wi^{-1} . Substituting for β =0.59, the expression obtained by fitting the numerical data for $\lambda \kappa_{xx}|_{x=x}^{+*}$ versus Wi^{-1} into Eq. (16), leads to M_{xx}^{-1} =0.168 Wi^{-1} -0.245. On the other hand, for ultradilute solutions, M_{xx}^{-1} has a power law dependence on Wi^{-1} [see Fig. 6(b)]. The mesh converged numerical data for M_{xx}^{-1} at the location of the stress maximum, at various values of β , are shown in Fig. 17, as a function of Wi^{-1} . As can be seen, the simulation data appear to lie on the curve fits. In particular, in the scale of the present figure, the curve fit for β =0.59 also seems to provide a reasonable fit to the simulation data for the other values of β .

For dilute solutions, the linear dependence of M_{xx}^{-1} on Wi^{-1} implies that $M_{xx} \rightarrow \infty$ at a finite value of Wi, whereas, for ultradilute solutions, as pointed out earlier, the power law dependence implies $M_{xx} \rightarrow \infty$ only as $Wi \rightarrow \infty$. The exact value of the limiting Weissenberg number for different values of β is difficult to estimate because of the large errors that arise in the computations in the neighborhood of this Weissenberg number. Nevertheless, the existence of a limiting Wi close to 0.7 clearly appears to be the case for all values of β . This is a fundamental difference between dilute and ultradilute solutions brought about by the modification of the flow due to the presence of the polymer. To our knowledge, there are currently no mesh converged results for the flow of Oldroyd-B fluid around confined cylinders, reported for values of $Wi \ge 0.7$, and the results in Fig. 17 suggest the reason why this might be the case. The expectation by Wapperom and Re-

nardy (2005), based on their analysis of ultradilute solutions, that dilute Oldroyd-B fluids should in principle be computable to arbitrary Wi is in fact not the case due to the coupling of the velocity and stress fields that exists in dilute solutions.

V. CONCLUSIONS

The steady symmetric flow around a cylinder confined between parallel plates of ultradilute and dilute polymer solutions modeled by the Oldroyd-B and FENE-P constitutive equations, has been considered with a view to understand the origin of computational difficulties encountered in numerical simulations.

FEM computations of ultradilute Oldroyd-B solutions are shown to breakdown at Wi = O(1), as has been observed previously for dilute solutions (see Fig. 4). Two alternative numerical means of obtaining a solution along the centerline in the cylinder wake that are accurate for arbitrarily large Wi for both the Oldroyd-B and the FENE-P models, have been developed. These solution techniques are useful to evaluate the value of Wi up to which the FEM computations are accurate (see Fig. 5), and to estimate the error in the FEM results (see Fig. 10).

The steep increase in M_{xx} and σ_{xx}^* that occurs in the vicinity of Wi = O(1) necessitates the use of increasingly refined meshes for increasing values of Wi. The number of elements required to maintain the error in M_{xx} less than 1% is shown to increase exponentially with increasing Wi for ultradilute Oldroyd-B fluids, making it practically infeasible to obtain solutions at Wi > 1 (see Fig. 11).

A material element of an ultradilute solution is shown to accumulate nearly eight units of Hencky strain as it travels downstream from the stagnation point in the wake of the cylinder, due to the extended time it spends in the vicinity of the stagnation point (see Fig. 12). This strain leads to polymer molecules undergoing a large extension in the flow direction, with their magnitude large enough to span several elements in the local finite element mesh (see Fig. 13).

An analysis of the nature of the maximum in M_{xx} in the cylinder wake suggests that the maximum becomes unbounded if the nondimensional strain rate at the location of the stress maximum, $\lambda \kappa_{xx}|_{x=x}^*$ approaches the critical value of 0.5, for both ultradilute and dilute Oldroyd-B fluids. Computations reveal that for ultradilute solutions, $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$ as a power-law in Wi [see Figs. 6(a) and 6(b)]. On the other hand, for dilute solutions, $\lambda \kappa_{xx}|_{x=x}^* \rightarrow 0.5$ linearly in Wi^{-1} [see Figs. 14(a) and 14(b)]. For dilute solutions, this implies that $M_{xx} \rightarrow \infty$ at a finite value of $Wi \approx 0.7$, while for ultradilute solutions, $M_{xx} \rightarrow \infty$ only as $Wi \rightarrow \infty$ (see Fig. 17). For ultradilute and dilute FENE-P liquids, on the other hand, M_{xx} increases relatively rapidly as $\lambda \kappa_{xx}|_{x=x}^*$ approaches 0.5, but levels off and remains bounded for higher values of $\lambda \kappa_{xx}|_{x=x}^*$ (see Figs. 9 and 16). The shape of the curves are strongly suggestive of the occurrence of a coil-stretch transition in the cylinder wake.

It is appropriate to emphasize here that the results obtained in this work are limited to steady symmetric two-dimensional flow around a confined cylinder. Even though the stresses become singular in this particular scenario, a different type of solution to the Oldroyd-B model might arise in a dynamical situation, which is probably asymmetric and time-dependent.

Several issues that must be addressed in the future can be tackled fruitfully with the framework developed here. For instance, the nature and structure of stress boundary layers in the vicinity of the cylinder can be examined for ultradilute solutions along lines similar to the analysis here. It would also be of great interest to examine if a coil-stretch transition is the source of computational difficulties encountered in the numerical simu-

lation of other benchmark complex flows of Oldroyd-B fluids. Further, the existence of a coil-stretch transition suggests that a model with conformation dependent drag might reveal the existence of coil-stretch hysteresis in the cylinder wake.

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