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A CONTINUUM THEORY FOR FIBER SUSPENSIONS

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ABSTRACT

A continuum constitutive equation is obtained for suspensions of rigid rodlike fibers in a viscous Newtonian medium, enabling simultaneous calculation of the kinematics, stress distribution, and fiber orientation distribution. A closure approximation in deriving the equation has little effect in flows where an exact solution for the orientation distribution can be obtained. A finite element procedure is developed for the solution of boundary value problems in complex geometries like those encountered in processing. Special care is required because of a near-singularity at solid boundaries where the kinematical no-slip condition is satisfied.

KEYWORDS

Fiber suspension; constitutive equation; continuum theory; finite element.

INTRODUCTION

The calculation of fiber orientation distributions in the flow of suspensions in complex geometries has been limited to non-interacting systems, where the fiber motion is described by Jeffery's (1922) solution for the motion of an ellipsoid in a Newtonian fluid. Such calculations (e.g., Goettler et al., 1979, 1981; Givler, 1981; Givler et al., 1983; York, 1982) require specification of an initial orientation for each fiber; computation of a statistical orientation distribution function is possible only by repeated calculation for different initial configurations. The statistical orientation distribution function is the meaningful quantity both for experimental measurement of orientation and for determination of physical properties of a solidified shaped object.

We present here a continuum constitutive equation for non-interacting suspensions of rigid rodlike particles in a viscous medium. The equation enables simultaneous calculation of the kinematics, stress distribution, and fiber orientation distribution. The continuum theory incorporates an order parameter that is obtained by statistical averaging over the response of an isolated fiber. Finite-element calculations with the continuum theory provide the detailed mechanics and orientation distribution in complex flow

fields like those that would be used in molding of composites; any initial orientation distribution, including a random distribution, can be specified.

SINGLE PARTICLE EQUATIONS

Lipscomb and Denn (1983) have shown that the equations computed by Jeffery for the fluid stress at a particle are equivalent to the equations for Ericksen's (1960) transversely isotropic liquid (TIL):

$$\underset{\sim}{\tau}_{TIL} = 2\mu_o \underset{\sim}{d} + \mu_1 \underset{\sim}{N} + \mu_2 \underset{\sim}{d}:\underset{\sim}{N}\underset{\sim}{N} + 2\mu_3 (\underset{\sim}{N}\cdot\underset{\sim}{d} + \underset{\sim}{d}\cdot\underset{\sim}{N}) \tag{1}$$

$$\frac{\delta \underline{n}}{\delta t} = \lambda \left[\underset{\sim}{d}\cdot\underline{n} - \underset{\sim}{d}:\underset{\sim}{N}\underline{n}\right] \tag{2}$$

$$\underset{\sim}{d} = \frac{1}{2}\left[\nabla\underset{\sim}{v} + (\nabla\underset{\sim}{v})^{\dagger}\right] \tag{3}$$

$$\underset{\sim}{N} = \underline{n}\underline{n}^{\dagger} \tag{4}$$

Here, the director $\underline{n}$ is a vector of unit magnitude, and $\delta/\delta t$ is the corotational derivative. In the Ericksen theory the director is a vector field with a value at each spatial point.

The equivalence to the Jeffery analysis is based on identifying $\underline{n}$ with the orientation of the axis of revolution of an ellipsoid of revolution. In that case, with η the Newtonian viscosity of the suspending medium and $\mu_1 = 0$, μ_o/η, μ_2/η, μ_3/η and λ can be expressed as unique functions of the aspect ratio, r, as shown in Fig. 1.

The particles are assumed to occupy a volume fraction ϕ. The condition that the particles be non-interacting is

$$\phi r^2 << 1 \tag{6}$$

which is highly restrictive for applications. Particles are to be found in any small volume region with probability ϕ. The stress at the particle is given by Eqs. (1) through (5), while the stress away from the particle is given by $2\eta\underset{\sim}{d}$. The average stress in a small region of fluid containing a single particle is therefore

$$\underset{\sim}{\tau} = 2\eta\underset{\sim}{d} + \phi\underset{\sim}{\tau}_{TIL} \tag{7}$$

It is to be noted that as $r \to 1$, $\mu_o/\eta \to 2.5$ and Eq. (7) reduces to the Einstein equation for the viscosity of dilute suspensions of spheres in a Newtonian fluid. Equation (7) requires specification of the initial spatial distribution of $\underline{n}$; this distribution will usually be known only as a statistical orientation distribution, in which case flow problems must be solved repeatedly for different initial orientations until a sufficient population of solutions has been obtained to compute an ensemble average. This is clearly not a feasible approach.

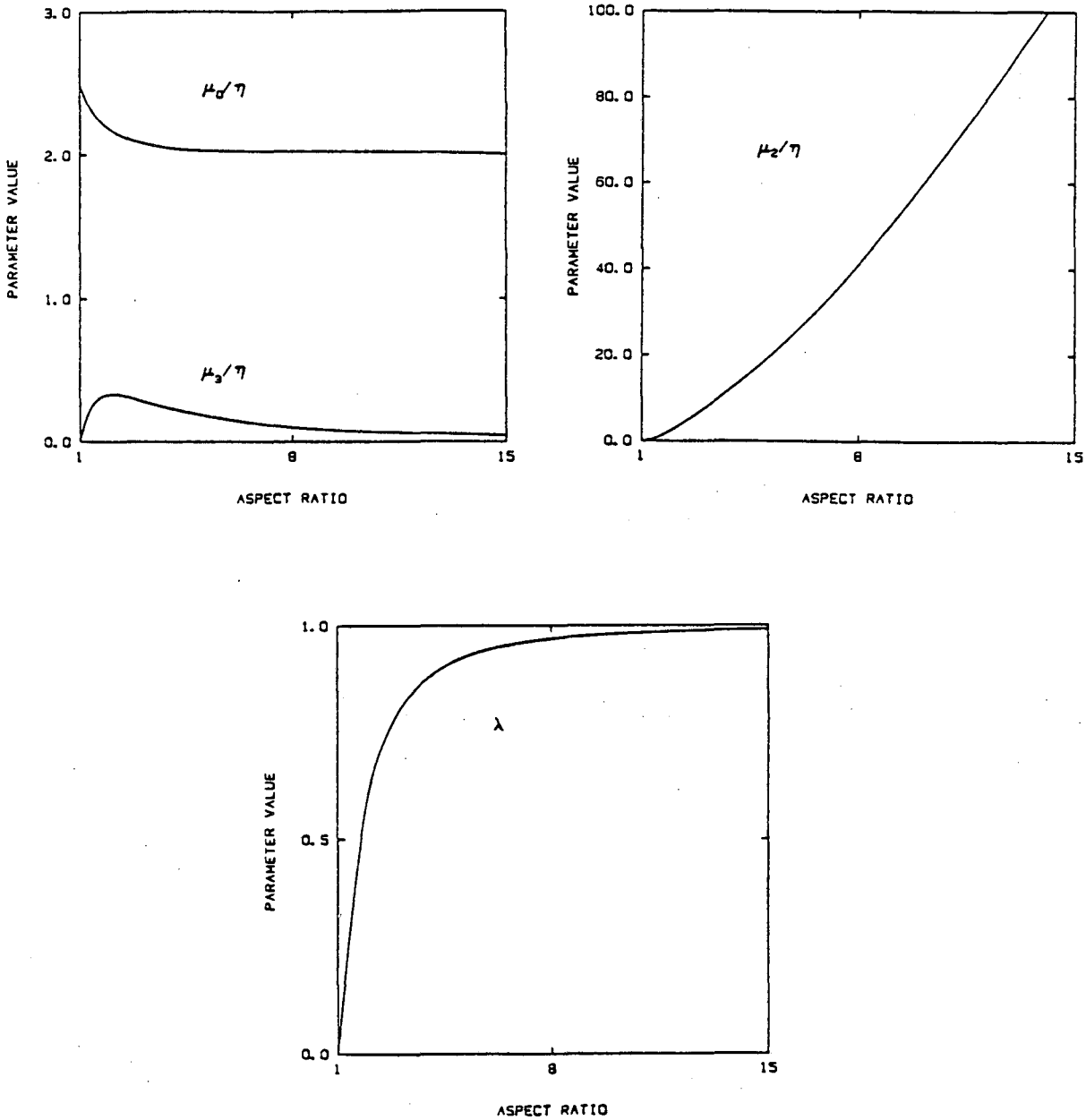

Fig. 1. Parameters for transversely isotropic fluid as functions of particle aspect ratio.

CONTINUUM THEORY

Let $f(\underline{n})\, d\underline{n}$ denote the number of particles per unit volume with orientation between $\underline{n}$ and $\underline{n} + d\underline{n}$. The ensemble average of any quantity ψ is defined

$$\langle\psi\rangle = \int_{\underline{n}} \psi f(\underline{n})\, d\underline{n} \tag{8}$$

It then follows from Eqs. (1) and (7) that the statistically-averaged continuum extra-stress is

$$\underset{\sim}{\tau} = 2(\eta+\phi\mu_o)\, \underset{\sim}{d} + \phi\mu_2 \underset{\sim}{d}:\langle\underset{\sim}{N}\underset{\sim}{N}\rangle + 2\phi\mu_3\, (\langle\underset{\sim}{N}\rangle\cdot\underset{\sim}{d} + \underset{\sim}{d}\cdot\langle\underset{\sim}{N}\rangle) \tag{9}$$

An equation for $\langle\underset{\sim}{N}\rangle$ is obtained by pre- and post-multiplying Eq. (2) by $\underline{n}$ and statistically averaging to obtain

$$\frac{\delta\langle\underset{\sim}{N}\rangle}{\delta t} = \lambda\, (\underset{\sim}{d}\cdot\langle\underset{\sim}{N}\rangle + \langle\underset{\sim}{N}\rangle\cdot\underset{\sim}{d} - 2\underset{\sim}{d}:\langle\underset{\sim}{N}\underset{\sim}{N}\rangle) \tag{10}$$

These equations are equivalent to those derived by Brenner (1972) in the limiting case of negligible Brownian motion; specific results for shear flow in this limit are given by Hinch and Leal (1972). It is to be noted that trace $\langle\underset{\sim}{N}\rangle = 1$.

Equations (9) and (10) contain the average $\langle\underset{\sim}{N}\underset{\sim}{N}\rangle$. Closure is obtained by approximating $\langle\underset{\sim}{N}\underset{\sim}{N}\rangle$ by $\langle\underset{\sim}{N}\rangle\langle\underset{\sim}{N}\rangle$; the coefficient of the approximation must be unity to maintain the condition of a unit trace. The final constitutive equation is thus

$$\underset{\sim}{\tau} = 2(\eta+\phi\mu_o)\underset{\sim}{d} + \phi\mu_2\underset{\sim}{d}:\langle\underset{\sim}{N}\rangle\langle\underset{\sim}{N}\rangle + 2\phi\mu_3(\langle\underset{\sim}{N}\rangle\cdot\underset{\sim}{d} + \underset{\sim}{d}\cdot\langle\underset{\sim}{N}\rangle) \tag{11}$$

$$\frac{\delta\langle\underset{\sim}{N}\rangle}{\delta t} = \lambda\, (\underset{\sim}{d}\cdot\langle\underset{\sim}{N}\rangle + \langle\underset{\sim}{N}\rangle\cdot\underset{\sim}{d} - 2\underset{\sim}{d}:\langle\underset{\sim}{N}\rangle\langle\underset{\sim}{N}\rangle) \tag{12}$$

Appropriate initial conditions for $\langle\underset{\sim}{N}\rangle$ are

random in space : $\langle\underset{\sim}{N}\rangle = \frac{1}{3}\underset{\sim}{I}$

random in a plane : $\langle\underset{\sim}{N}\rangle = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$\langle\underset{\sim}{N}\rangle$ is uniquely specified at solid surfaces in steady flow by Eq. (12), with $\partial\langle\underset{\sim}{N}\rangle/\partial t$ set to zero.

It is important to note that $\langle\underset{\sim}{N}\rangle$ cannot be formed from the dyad product $\underline{n}\underline{n}^{\dagger}$ of any vector $\underline{n}$, so there is no "equivalent fiber" whose motion represents the ensemble average.

EXACT SOLUTIONS

Equation (2) can be solved analytically for flows in which the kinematics are specified, in which case $\langle \underset{\sim}{N} \rangle$ can be computed for a given initial orientation distribution by a tedious but straightforward integration over orientation space. This enables direct comparison to the solution of Eq. (12) obtained by numerical integration, and an evaluation of the error introduced by the closure approximation. Figures 2 and 3 show results for plane shear and bi-axial extension, respectively, with r = 10. Agreement between the exact solution and the approximate continuum theory is excellent, and improves with increasing particle aspect ratio.

FINITE ELEMENT SOLUTION

A Galerkin finite-element program has been developed for solution of Eqs. (11) and (12), together with the continuity and Cauchy momentum equations, in complex two-dimensional and axi-symmetric three dimensional geometries. The program uses a mixed method, with linear shape functions for the pressure and orientation and quadratic shape functions for the velocities. Results for the orientation distribution in plane shear and biaxial extension for random far-field conditions agree well with the direct numerical integration of Eq. (12). Computed contours of the independent components of the orientation distribution function for biaxial extension and the mesh used are shown in Fig. 4.

Difficulties in obtaining numerical accuracy for finite-element solutions in pressure-driven flow near solid boundaries or a plane of symmetry point up an interesting deficiency in this and any continuum theory based on particles of zero effective length. Since the velocity vector vanishes at the solid surface, it follows from Eq. (12) that $\langle \underset{\sim}{N} \rangle$ takes on a constant value; $\langle N_{11} \rangle$ equals $(1-\lambda)/2$ along the wall, for example, for Poiseuille flow in the 2-direction. There will always exist streamlines arbitrarily close to the wall for which the residence time is sufficient for the non-zero values of $\langle \underset{\sim}{N} \rangle$ to take on all values because of rotation. Thus, arbitrarily large gradients which cannot be resolved by any numerical scheme must occur near a wall. Similar problems arise along the centerline. The problem is masked in the calculations of York (1983) because the residence times along all streamlines for which the orientation distribution is calculated are too short for particle rotation to occur.

The cause of the mathematical problem is the failure of the continuum theory to account properly for the interaction of particles of finite size with a wall and with the flow field arbitrarily close to the center plane; cf. Batchelor (1970). The problem is analogous to the breakdown of the continuum no-slip condition near a moving contact line. There are two possible numerical resolutions. The first is to use the known asymptotic behavior of Eq. (12) in the shear field adjacent to the wall as the boundary condition on a restricted finite-element domain for the solution of Eq. (12). The second is to note that interactions with the wall should retard rotations in much the same manner as letting r approach infinity ($\lambda \to 1$); thus λ can be set equal to unity at the wall and allowed to decrease to the value corresponding to the proper value of r over a short distance, ideally comparable to one particle length. Orientation in the bulk fluid will be unaffected by this artifact. Similarly, the derivative of $\langle \underset{\sim}{N} \rangle$ normal to a line or plane of symmetry can be set to zero to force the orientation along

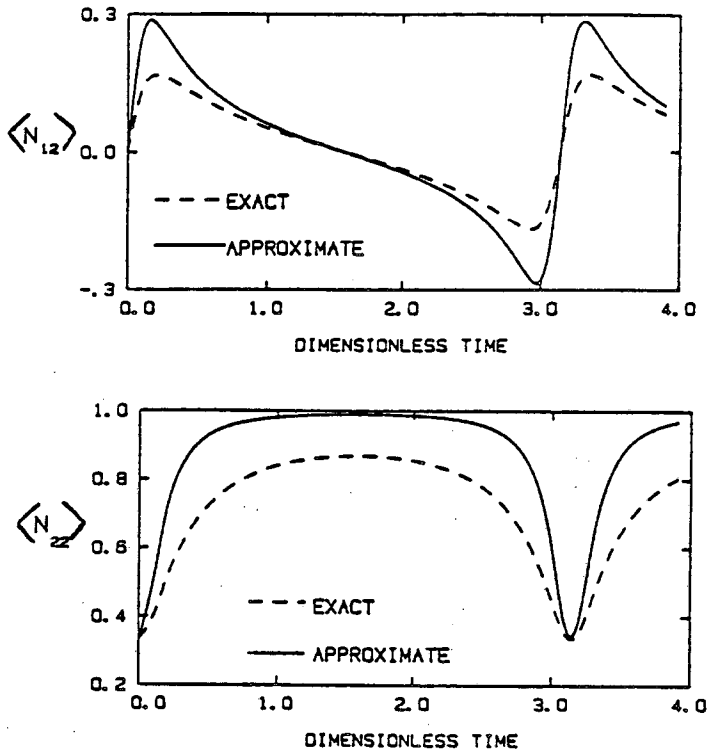

Fig. 2. Exact solution for components of $\langle \underset{\sim}{N} \rangle$ compared to approximate continuum theory, plane shear, r = 10. (dimensionless time = $t\dot{\gamma}/(r+r^{-1})$)

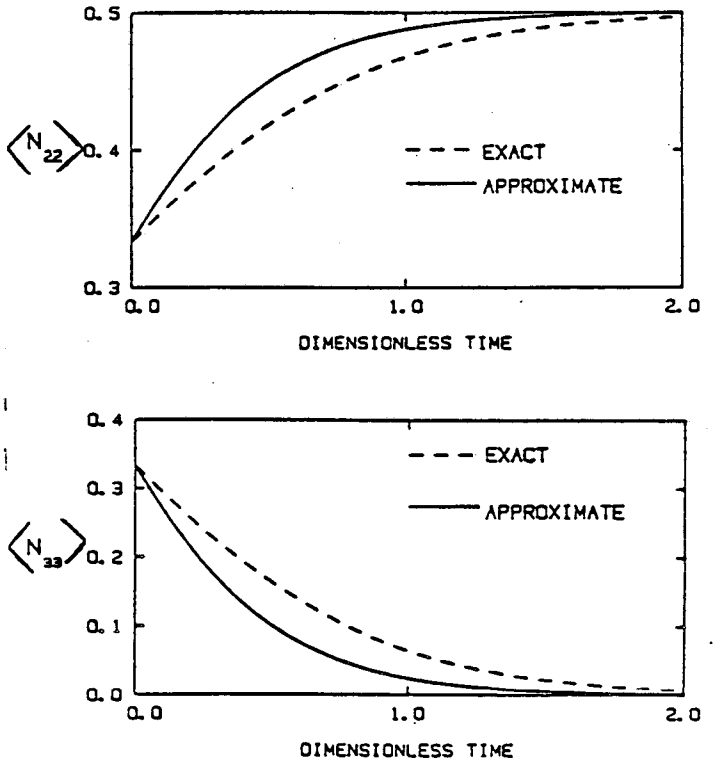

Fig. 3. Exact solution for components of $\langle \underset{\sim}{N} \rangle$ compared to approximate continuum theory, biaxial extension, r = 10. (dimensionless time = $t\lambda\dot{\Gamma}$)

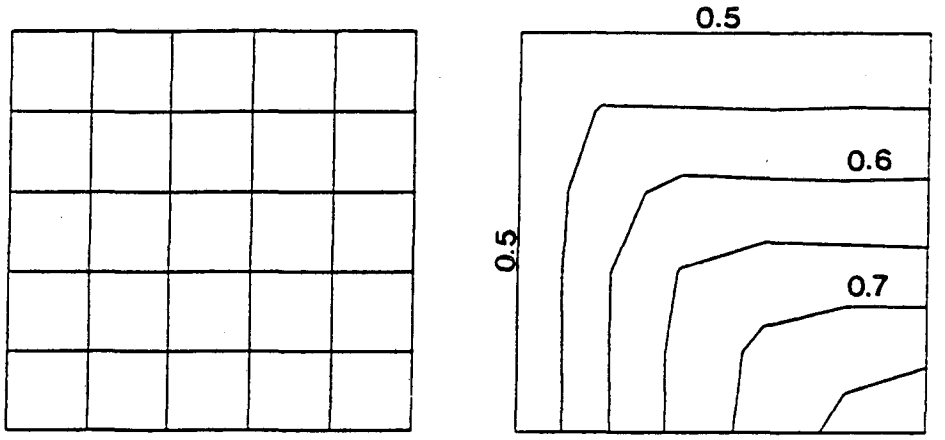

Fig. 4. Mesh and $\langle N_{11} \rangle$ of $\langle \underset{\sim}{N} \rangle$ from finite-element solution, biaxial extension, r = 10. (Note: $\langle N_{12} \rangle = 0$)

that shear-free line or plane to correspond to the orientation in the immediate neighborhood.

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