

LA-UR-93-3124

*Approved for public release;
distribution is unlimited.*

Title: Nonlocal Models in Continuum Mechanics

Author(s): Norman L. Johnson and Nhan Phan-Thien

Published in: *Advanced Computational Methods for Material Modeling,*
D.J. Benson, R.A. Asaro, Eds., ASME, pp. 59-70, 1993.

Los Alamos

NATIONAL LABORATORY

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Intentionally blank

NONLOCAL MODELS IN CONTINUUM MECHANICS

N. L. Johnson

Fluid Dynamics, Theoretical Division
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

N. Phan-Thien

Department of Mechanical Engineering
The University of Sydney, NSW 2006, Australia

ABSTRACT

The recent appearance of nonlocal methods is examined in the light of traditional continuum mechanics. A comparison of nonlocal approaches in the fields of solid and fluid mechanics reveals that no consistent definition of a nonlocal theory has been used. We suggest a definition based on the violation of the principle of local action in continuum mechanics. From the consideration of the implications of a nonlocal theory based on this definition, we conclude that constitutive relations with nonlocal terms can confuse the traditional separation of the roles between conservation laws and constitutive relations and bring into question the identification of constants in the constitutive equation as material parameters. The diversity of motivations for the nonlocal approaches are presented, resulting primarily from deficiencies in numerical solutions to practical problems. To illustrate these concepts, the history of nonlocal terms in the field of viscoelastic fluids is reviewed. A specific example of a viscoelastic constitutive relation that contains a stress diffusion term is applied to a simple shear flow and found not to be a physical description of any known fluid. We conclude by listing questions that should be asked of nonlocal approaches. [Keywords: nonlocal, nonlinear plasticity, viscoelasticity, constitutive relations, continuum mechanics.]

1. INTRODUCTION

There are repeated examples in the literature that the addition of nonlocal terms to constitutive equations, or more subtly the implied nonlocal terms of some numerical schemes, have resulted in an improved description of physical phenomena. Often these modifications to existing theories are initially empirical, often numerical in nature. In time, as their utility is demonstrated, their use is supported by theoretical considerations. But there has not been the discussion in the literature about the appropriateness of nonlocal constitutive equations within the context of continuum mechanics. Intense activity in the development of nonlocal theories occurs currently in the fields of localized failure in solids and of spectral turbulence models, and to a lesser degree in viscoelastic

fluids. We first consider the meaning of a nonlocal approach within the perspective of traditional continuum mechanics. We then review the motivations for including nonlocal terms, either in constitutive equations or implied in the constitutive equation by the numerical schemes. Finally the lessons learned from viscoelastic fluid modeling are presented, and a specific nonlocal viscoelastic model is examined in detail.

Because viscoelastic fluids exhibit solid-like and fluid-like behavior depending on the time scale of deformation, the governing equations exhibit behavior and numerical challenges that are remarkably similar to those in solid mechanics. As more complex constitutive equations are considered and computational resources increase, the ability to compute solutions to the governing equations in the two fields has become more important. As we shall argue, the difficulties in obtaining realistic numerical solutions have resulted in the introduction of nonlocal approaches over the past 5 years in both fields. And theoretical justifications are being proposed for these numerical necessities. We hope that the examination of the history of nonlocal approaches in viscoelastic fluids will benefit the solid mechanics community.

We have chosen not to include nonlocal turbulence theories in this paper. These approaches are largely motivated by theoretical necessity, not numerical necessity, and are not as appropriate in the comparison to solid mechanics in the following discussions. Furthermore the continuum mechanics concepts applied to nonlocal approaches in this paper, those of conservation equations and constitutive relations, are not typically applied to turbulence theories. Instead, turbulent theories strive to develop system of equations that are universal to Newtonian fluids and not to develop constitutive relations for certain materials. We do note that the following discussions are relevant if the *turbulence conservation equation* are taken as the ensembled-averaged conservation equation of traditional continuum mechanics and the *constitutive relations* are given by the by the auxiliary equations that relate the Reynolds stress to the mean-kinematic variables. An introduction to and a comparison of nonlocal modeling in solid mechanics and turbulence should be consulted for further reference (Chen and Clark, 1991).

2. THE PERSPECTIVE OF TRADITIONAL CONTINUUM MECHANICS

Before nonlocal approaches can be discussed, the relevant concepts used in continuum mechanics are summarized as a reference point. All modeling of materials discussed in this paper is based on a continuum representation of noncontinuous or discrete subunits, whether atoms that make up a solid or polymer fluid, grains in a crystalline solid, or eddies in a turbulent fluid. The continuum assumption reduces these phenomena to a spatially continuous description. The continuum assumption is made out of necessity; the detailed treatment of these systems in their full complexity for applications of practical interest is not possible. The closest that we may model these systems at their fundamental complexity are by massive computer simulations, such as molecular dynamics of solid and fluids or direct numerical simulation of turbulence.

The continuum assumption results in fundamental changes in the functional dependence of the dependent state variables on the dynamics of a system and the parameters that are used to

describe a specific material. For example, in an *actual* system the stress at a point depends only on the *current* state of the system in the vicinity of the point (here, and in the discussion that follows, we use *states* to refer to both the kinematic variables and the dependence state variables). There is no reference to previous states of the system, nor to a reference state. An illustration of this ideas occurs in a molecular dynamics simulation of a solid undergoing elastic deformation. The state of stress depends only on the current phase space and intermolecular forces. The parameters that describe a specific material are the parameters in the atomic potentials. This description of the material is essentially local, meaning the current state of the material is only affected by its immediate neighbors. There are no physical mechanisms that produce *action at a distance*. It is noted that the concept of a stress at a point in a discontinuous system of atoms is only meaningful as an ensemble average over many possible phase-space configurations. The application of the continuum assumption results in a simplified description of the system, but at the expense of a loss of information at small length and time scales. The consequence of the loss of information is that the state of stress at a material point in a continuum may now depend on the state at distant material points and on the *history* of states of the system. Furthermore the parameters that describe a specific material are typically continuum material properties, such as the elastic modulus or fluid viscosity. Thus it is the application of the continuum assumption that introduces the possibility of a nonlocal description from an essentially local description of a discrete system.

Traditional continuum mechanics for fluid and solid systems has been founded on the basic premise that there are universal *conservation laws* that apply to all continuum materials. In these integral or differential conservation laws appear state variables of the material, the stress, for example. Theoretical investigations currently focus on development of constitutive relations that specify dependence of the current state of material on the current or past kinematic or state variables. (We note that constitutive relations have many alternative names, such as constitutive equations or rheological equations of state.) The conservation laws are considered inviolate and are not modified to accommodate changes in materials. In order to describe a different material or physical process, material parameters in the constitutive equation are changed or an entirely different constitutive equation is used. Because we are exclusively concerned with mechanical theories, a constitutive equation will be taken to mean the auxiliary equation or equations that are required for the solution of the conservation of momentum equation.

Constitutive equations have traditionally been required to satisfy the following principles that restrict their form (summarized from Crochet *et al.*, 1984; also see Bird *et al.*, 1987a):

1. **Principle of local action.** In determining the stress at a given material point, the motion or stress outside an arbitrary neighborhood of the material point is disregarded. There exists no mechanism for action-at-a-distance.
2. **Principle of two-frame invariance.** The relationship between the stress tensor and the history of motion of a body cannot depend on the particular coordinate system used to describe the stress and the history of motion. Furthermore, constitutive equations must satisfy usual tensorial invariance expected of a physical theory.

3. Principle of invariance under translation or superimposed rigid body motion.

Constitutive equations must have a significance which is independent of absolute motion in space. The superposition of a rigid body motion on a given deformation history cannot have any effect on the stress field other than that arising from the obvious physical effects brought about by the superposed rotational motion.

We note that the principle of two-frame invariance is justified if a material does not have any sub-continuum inertia. Observance of these principles leads to constitutive equations that describe a *simple* material, or in the field of fluid rheology, a *simple fluid*. Oldroyd (1950) used the term *rheological invariance* to describe these three principles.

The motivation for the second and third principles of invariance above are self-evident. The principle of local action is motivated by the resulting simplicity in the constitutive equations and the belief that the current state of stress at a material point should depend only on the history of states of the material point. A further advantage of the assumption of local action is the differentiation of roles of the conservation and constitutive equations. By requiring that constitutive equations satisfy the principle of local action, the conservation law of momentum has the distinct role of describing the kinematic evolution of the neighboring material elements by forces that act between them. The constitutive equation has the role of relating stress at a material point to the history of states of the material point. A *local* constitutive equation requires no additional information beyond its own history of states, time derivatives of states, or spatial gradients of states. If the stress in a constitutive equation did depend on the state at a material point at a distance, then the role of a constitutive equation has changed, and it now shares an equal role with the conservation laws by coupling the evolution of the states of non-adjacent material points.

Another advantage of the separation of the roles of the conservation and constitutive equations is that material properties of the continuum material can be defined from constants in the constitutive equation. If the constitutive equation did depend on states of non-adjacent material points, the parameters in the constitutive equation would not be associated with a single material element. Consider two adjacent but different materials; a nonlocal constitutive equation would result in the stress at a point in one of the materials being dependent on the stress or deformation in the other dissimilar material, and therefore the identification of the constants in the constitutive equation could not be associated with just one material. In a similar manner, the evaluation of the constants now depend on the details of deformation throughout the domain and cannot be associated with the a single material history. In Section 5 we shall present specific examples of these points. We can now see how separation of roles of the constitutive and constitutive equations has greatly simplified the treatment of the continuum and consequently been the foundation of traditional continuum mechanics.

3. THE MOTIVATION AND FORM OF NONLOCAL APPROACHES

There is a need to define what is meant by a nonlocal approach. We must state on the outset that the term *nonlocal* has been loosely used in the literature, and no clear guidance or consensus

of what constitutes a nonlocal approach has evolved. In the areas of solid and non-turbulent fluid mechanics, there is sufficient discrepancy as to what constitutes a nonlocal approach as to prohibit a workable definition. Often it would appear that proposed terms in constitutive equations are called nonlocal on the basis of containing spatial gradients which do not normally occur in classical constitutive equations. Consequently theories that are considered nonlocal by this definition could be local theories to researchers in other fields. Until a consensus of the nonlocal approaches is achieved, we submit the following discussion, supplemented by examples of local and nonlocal terms in constitutive equations in the following sections.

A more universal definition of a nonlocal approach is a method that results in a constitutive equation that violates the principle of local action given above. Probably the best example of a nonlocal approach using this definition is the integral constitutive equations in two-point spectral models for turbulence which contain integrals over non-adjacent material points (Clark, 1991). This theory is clearly nonlocal, because the extent to which the non-adjacent points are sampled may be of the size of the domain.

In the fields of solid and non-turbulent fluid mechanics, the determination of whether or not a theory is nonlocal using the above definition may well be determined by the interpretation of *non-adjacent* material points for a given physical system. For example, a newly proposed constitutive equation that includes spatial gradients of kinematic variables that are not traditionally included may be called nonlocal by researchers, because the effects of the deformational history of adjacent material points now affect the stress. In other fields similar spatial gradient terms may have been traditionally used and are considered to be local terms. This may be the current situation between the fields of solids and viscoelastic fluid mechanics. In the next section we will give examples of terms that are considered local in the area of viscoelastic fluids and examine a constitutive equation that is indisputably nonlocal. For completeness we give two examples of a nonlocal term in constitutive equations: in solid mechanics the gradient of the plastic strain in a yield function associated with localization phenomenon (Schreyer, 1990a) and (2) in fluids, the Laplacian of the stress, a stress diffusion term, as presented in the next section.

Why have nonlocal approaches been considered, given their radical departure from the past understanding of continua? In almost all circumstances numerical difficulties or deficiencies in the solution of practical problems have been the motivation. These fall into two categories: (1) the inability to obtain numerically converged solutions in certain parameter ranges, as discussed in the next section or (2) the unphysical results of numerical solutions, as was observed by de Borst (1987) for strain localization or as observed in one-point models in turbulence (Clark, 1991). In addition to numerical motivations, there are theoretical arguments for nonlocal effects, either to include additional physics (Brave *et al.*, 1991; Ottinger, 1992) or to enable existence proofs of solutions (El-Kareh and Leal, 1989).

These modifications of classical constitutive equations are the more easily identified nonlocal approaches. A more obscure occurrence of nonlocal terms is a consequence of certain modifications to the numerical solution method, typically in order to obtain improved convergence or stability.

Some numerical schemes result in an inconsistent solution to the governing equations, i.e., the discrete equations being solved do not approach the governing differential equations in the limit of small time steps and mesh size. Because the equations of motion are inviolate, the additional terms that result in the inconsistent solution must then appear in the constitutive equation. Often these added terms are diffusive in nature and might appear as nonlocal terms in the *apparent* constitutive equation. These occurrences of nonlocal terms are difficult to recognize simply because of the variety of numerical modifications that have been employed and the absence of analysis of consistency of the discrete equations with the governing differential equations.

4. LOCAL AND NONLOCAL MODELS IN VISCOELASTIC FLUIDS

Before we turn to the discussion of nonlocal terms in viscoelastic fluids, we present the functional form of terms in constitutive equations that have been accepted to result in a local theory for viscoelastic fluids (Bird *et al.*, 1987a).

1. Any term that includes the kinematic variables, typically the strain or strain-rate tensor. A common example of this type of term is the velocity gradient or strain-rate tensor that appears in the constitutive equation for a Newtonian fluid.
2. Any term that includes gradients, of any order, of the kinematic variables. A example of this is the gradient of the strain-rate in a second order fluid.
3. Certain gradients of the stress. A commonly occurring convective term in viscoelastic constitutive equations is $\mathbf{u} \cdot \nabla \mathbf{S}$ in which \mathbf{u} is the velocity and \mathbf{S} is the polymer contribution to the stress tensor. An example of a constitutive equation with this term is the Maxwell model.
4. Certain inner products of the strain-rate and stress tensor. An example of a constitutive equation with this term is the Jeffreys model.
5. Any term that is a time integral, or multiple time integrals, over the past history of a material point of a kinematic variable or product of kinematic variables. A general integral expression that illustrates many of these terms is contained in the memory integral expansion. This constitutive equation describes the most general functionality of a rheologically invariant, and therefore local, material and includes all of the above examples of constitutive equations for viscoelastic fluids.

This list illustrates the variety of terms that have been considered in local viscoelastic constitutive equations. There are possible functional terms that are missing in this list, for example the Laplacian of the stress, which will be examined later in this section. It would appear that the terms described in items 2 would be the fluid equivalent of the gradient of the plastic strain that is considered to be a nonlocal term in solid mechanics (Schreyer, 1990a). Whether or not the this term actually violates the principle of local action, as required by our suggested definition of nonlocal, cannot be establish without further analysis. Further evidence that these are possibly local theories is the absence of the difficulties that may be associated with a truly nonlocal theory, as presented in the remainder of this paper.

Some observations can be made as to the theoretical support for nonlocal constitutive equations in viscoelastic fluids. A general kinetic theory of polymer liquids (Curtiss *et al.*, 1976; Curtiss and Bird, 1983; and Bird *et al.*, 1987b, Part IV) has been developed that starts with a description of a polymer and solvent as a collection of mass points with arbitrary potentials specifying their interactions. From first principles the conservation laws of classical hydrodynamics are recovered and a general expression for the stress tensor, the constitutive equation, is found. The required assumptions are (1) the construction of a mechanical model for the molecules, (2) the potentials are pair-wise additive (three-body effects are neglected), (3) the variation of the distribution functions over molecular scales is neglected and (4) acceleration terms in the equation of motion of the mass points are neglected. With these few assumptions, the constitutive equations that result from this general kinetic theory are all found to be rheologically invariant. We can then conclude that from a very general kinetic theory description of viscoelastic fluids, nonlocal terms in the constitutive equation do not occur. But in fairness to the emerging field of nonlocal approaches, the development of the general kinetic theory focused on establishing the existing understanding of continuum mechanics, and the possibility of nonlocal contributions has not been examined, except as noted below.

In the rest of this section nonlocal approaches within the field of viscoelastic fluids are presented. It is beyond the scope of this paper to consider the origin of nonlocal terms in the kinetic theory other than to note that it can occur because of relaxation of the third assumption above, as might be expected (Phan-Thien *et al.*, 1990; Brave *et al.*, 1991; Ottinger, 1992).

For more than two decades in the field of viscoelastic fluids, a breakdown or failure of convergence was observed in the numerical solution of flows. For a summary of the conundrum at the time see the review by Crochet *et al.* (1984). The limit was often reached in a region where the solutions, before breaking down, have elastic effects that are no more than perturbations about a Newtonian fluid. This was a dismal time for numerical researchers when all the interesting phenomena in viscoelastic fluids occurred when elasticity dominated the flow.

A dimensionless parameter that describes the relative importance of the elastic contribution is the Weissenberg number, W , the ratio of an elastic time constant to a time constant associated with the flow. (Some researchers use the Deborah number in place of the Weissenberg number; the difference is a minor distinction here). It was found that for Weissenberg numbers in the neighborhood of unity, the numerical methods would break down. This barrier was observed independent of the numerical approach used (finite elements, finite difference, collocation methods), the flow being examined (shearing, elongational, complex flows), and the type of constitutive equation used (differential or integral forms). As the critical value of W was approached, spurious spatial oscillations in the field variables were observed. Stress components were more affected than velocity components, resulting in large and erroneous stress gradients. Typically the spurious oscillations had no physical origin, and their wavelength was dependent on the mesh discretization. Many reasons were attributed to the existence of the limit (Crochet *et al.*, 1984), including improper constitutive models, improper evaluation of the stress particularly along boundaries,

insufficient mesh refinement, improper boundary conditions, and bifurcation of the physical solution as supported by experimental results. Because counterexamples existed for each of these possible explanations, there was no consistent understanding of the limit accepted by the community. The situation was not unlike the considerable theoretical, numerical and experimental controversy surrounding the phenomena of strain softening and localization in solid mechanics in the 1980's (Schreyer, 1990b), which ultimately led to the consideration of nonlocal plasticity.

In 1987 Marchal and Crochet (Marchal and Crochet, 1987; Debbaut *et al.*, 1988) were one of the first to successfully break the Weissenberg number barrier by using a numerical method that resulted in the diffusion of the stress. Because numerical solutions using this method were not consistent with the governing equations, these methods were suspect. Later studies removed the lack of consistency without loss of the range of solution (Basombrío *et al.*, 1991). It is now accepted that the limit on the Weissenberg number was caused by singularities in the discrete equations (Keunings, 1987; Crochet, 1989). Solutions with high Weissenberg numbers remain a challenge in the field. What is of interest here is the history of the nonlocal terms that were proposed in constitutive equations during this time.

In an attempt to validate the use of a stress diffusion and thereby achieve a consistent numerical method, a kinetic theory argument was proposed that resulted in a stress diffusion term in a constitutive equation (El-Kareh and Leal, 1989). By the addition of a stress diffusion term, the resulting set of governing equations were parabolic, instead of hyperbolic, and the first proof of convergence for a viscoelastic fluid for all values of the Weissenberg numbers was presented. Although the numerical necessity for a stress diffusion term has diminished because of improved numerical algorithms, the question of the appropriateness of the nonlocal terms is still relevant. There have been two recent studies that have argued for stress diffusion-like terms in modeling polymer diffusion and migration (Bhave *et al.*, 1991 and Ottinger, 1992). In the rest of this section we consider a nonlocal constitutive equation taken from Phan-Thien *et al.* (1990), a simplified form of the constitutive equation proposed by El-Kareh and Leal (1989).

The standard approach for incompressible viscoelastic fluids is to separate the total stress $\boldsymbol{\sigma}$ into an isotropic pressure contribution, a Newtonian solvent contribution and a polymer contribution, \mathbf{S} :

$$\boldsymbol{\sigma} = -P\mathbf{1} + 2\eta_s\mathbf{D} + \mathbf{S} , \quad (1)$$

where $\mathbf{1}$ is the unit tensor, η_s is the solvent viscosity, \mathbf{L} is the gradient of the velocity, $\mathbf{D} = (\mathbf{L} + \mathbf{L}^\dagger)/2$ is the strain-rate tensor, and $2\eta_s\mathbf{D}$ is the Newtonian contribution.

The constitutive equation for the polymer contribution to the total stress tensor as derived from kinetic theory arguments (Phan-Thien *et al.*, 1990) is:

$$\mathbf{S} + \lambda \left\{ \frac{\partial \mathbf{S}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{S} - \mathbf{L} \cdot \mathbf{S} - \mathbf{S} \cdot \mathbf{L}^\dagger \right\} = 2\eta_p\mathbf{D} + \mathcal{D}\nabla^2\mathbf{S} . \quad (2)$$

in which λ is the relaxation time that is associated with a multisegmented polymer chain, η_p is the polymer-contributed viscosity, and \mathcal{D} is the stress diffusivity coefficient. El-Kareh and Leal (1989)

showed that the stress diffusion term is small, of the order of 10^{-9} of the convective term. With λ and \mathcal{D} taken to be zero, this equation simply describes the polymer viscous contribution to the stress tensor. The constitutive equation (2) differs from that proposed by El-Kareh and Leal only in one aspect: the spring force law used to derive (2) is linear, whereas a non-linear spring force law is required for El-Kareh and Leal's existence proof for all Weissenberg numbers. Without the stress diffusion term, the constitutive equation (2) is the Maxwell model, and the combination of (1) and (2) is the Oldroyd fluid B (Bird *et al.*, 1987a).

Regardless of how small the diffusion term is, the mathematical structure of (2) is fundamentally changed from a hyperbolic to parabolic equation. Furthermore, (2) requires boundary conditions for \mathbf{S} , or gradients of \mathbf{S} , or a combination of both, to be prescribed throughout the boundary of the domain, as illustrated below. Specific difficulties that arise by the addition of the stress diffusion term are covered in the next section but can be motivated here by a simple argument.

If we simplify (2) for $\lambda = 0$, that is, for no elasticity, the dependence of the stress on its boundary values and gradients can be made explicit by recasting (2) using the Green function representation:

$$S_{kl}(\mathbf{y}) = \int_{\partial\Omega} S_{ijkl}^*(\mathbf{x}, \mathbf{y}) \frac{\partial S_{ij}}{\partial x_m}(\mathbf{x}) n_m dA(\mathbf{x}) - \int_{\partial\Omega} \frac{\partial S_{ijkl}^*}{\partial x_m}(\mathbf{x}, \mathbf{y}) n_m S_{ij}(\mathbf{x}) dA(\mathbf{x}) + \frac{2\eta_p}{\mathcal{D}} \int_{\Omega} D_{ij}(\mathbf{x}) S_{ijkl}^*(\mathbf{x}, \mathbf{y}) dV(\mathbf{x}), \quad (3)$$

where Ω is the flow domain, $\partial\Omega$ is its boundary, \mathbf{n} is the outward unit vector on $\partial\Omega$, and $S_{ijkl}^*(\mathbf{x}, \mathbf{y})$ is the Green function that satisfies

$$\mathcal{D}\nabla^2 S_{ijkl}^* - S_{ijkl}^* = -\delta_{ijkl}\delta(\mathbf{x} - \mathbf{y}) \quad (4)$$

in which δ_{ijkl} is equal to unity if all subscripts are equal, and zero otherwise.

We see from the two integral terms in (3) that the stress at any point specifically depends on the stress gradients and stress on the bounding domain. In the absence of the diffusion term ($\mathcal{D} \equiv 0$), the stress at a material point depends only on the current strain-rate at that material point. The dependence of the stress on the stress boundary conditions is not a surprising result for a parabolic diffusion equation but is a surprising result for a constitutive equation. Normally the dependence of the stress on boundary values, or for that matter on the state at neighboring points, is achieved by application of the conservation of momentum equation. With the inclusion of a stress diffusion term in the constitutive equation, the state of stress is now directly coupled with the state of stress over the entire domain, and the traditional understanding of the distinct role of the constitutive equation and conservation laws is lost, as presented in Section 2. Because the stress at a point depends on non-adjacent material points, we conclude that (2) is a nonlocal model. The consequences of this will be illustrated in detail in the next section. But given that the stress of a material point now depends on its distant neighbors, and possibly on a different

material or deformational history, the identification of the constants in the constitutive equation as material parameters cannot be made.

This analysis of the nonlocal nature of (2) suggests that a more precise determination of a nonlocal theory is the demonstration that a constitutive equation, in the absence of the conservation equation, depends on information far removed from its application. Possibly the Green's function analysis or similar mathematical tools may provide a general method to realize this definition of nonlocal.

5. A FLOW EXAMPLE FROM VISCOELASTIC FLUIDS

We now consider the behavior of the fluid described by (2) as it undergoes steady-state shearing deformation between two parallel plates, separated by a distance d . The lower plate is held stationary and the upper plate is moved with a uniform speed U . We make the standard assumption that the flow is uni-directional with a velocity field $\mathbf{u} = \{u(y), 0, 0\}$. We further assume that only three stress components are non-zero (S_{xx} , S_{xy} and S_{yy}); this is clearly an additional assumption to the uni-directional flow assumption, because non-zero boundary conditions on the other stress components will still result in uni-directional flow. At the lower plate of the channel ($y = 0$), the boundary condition on the velocity is $u = 0$, and at the upper plate ($y = d$), $u = U$.

It is convenient to set

$$\mathcal{D} = \epsilon^2 d^2, \quad (5)$$

and normalize all distances with respect to d , all velocities with respect to U , and all stresses and pressure (S_{xx} , S_{xy} , S_{yy} and P) with respect to $\eta U/d$, where $\eta = \eta_s + \eta_p$ is the total shear viscosity in the Maxwell case; ϵ is a dimensionless diffusion length scale.

The governing equations are

$$\frac{\partial P}{\partial x} = (1 - \beta) \frac{d^2 u}{dy^2} + \frac{dS_{xy}}{dy}, \quad (6)$$

$$\frac{\partial P}{\partial y} = \frac{dS_{yy}}{dy}, \quad (7)$$

$$S_{xx} - 2W \frac{du}{dy} S_{xy} = \epsilon^2 \frac{d^2 S_{xx}}{dy^2}, \quad (8)$$

$$S_{xy} - W \frac{du}{dy} S_{yy} = \beta \frac{du}{dy} + \epsilon^2 \frac{d^2 S_{xy}}{dy^2}, \quad (9)$$

$$S_{yy} = \epsilon^2 \frac{d^2 S_{yy}}{dy^2}, \quad (10)$$

where $W = \lambda U/d$ is the Weissenberg number, and $\beta = \eta_p/\eta$ is the dimensionless polymer-contributed viscosity. Eqns. (6) and (7) are the x and y terms of the combination of the conservation of momentum equation at steady state, $\nabla \cdot \boldsymbol{\sigma} = 0$ and (1). Eqns. (8)-(10) are the xx , xy , and yy terms of the tensor equation (2).

The boundary conditions are

$$\text{at } y = 0, \quad u = 0, \quad S_{xx} = S_{xx}^{(0)}, \quad S_{xy} = S_{xy}^{(0)}, \quad S_{yy} = S_{yy}^{(0)}, \quad (11)$$

$$\text{at } y = 1, \quad u = 1, \quad S_{xx} = S_{xx}^{(1)}, \quad S_{xy} = S_{xy}^{(1)}, \quad S_{yy} = S_{yy}^{(1)}, \quad (12)$$

where $S_{ij}^{(0)}$ and $S_{ij}^{(1)}$ are prescribed stresses at the boundaries, to be specified later. *The unusual specification of the stress on a prescribed velocity boundary cannot be overemphasized.* They result from the addition of the stress diffusion term in (2).

Equation (10) is uncoupled from the rest and has the solution

$$S_{yy} = a_1 \exp(y/\epsilon) + b_1 \exp(-y/\epsilon), \quad (13)$$

where a_1 and b_1 are to be determined from the boundary conditions for S_{yy} .

In the absence of a pressure gradient in the x -direction, u is determined by solving a quasi-linear differential equation

$$(1 - \beta) \frac{d^4 u}{dy^4} - \left[1 + \frac{Wi}{\epsilon^2} S_{yy} \right] \frac{d^2 u}{dy^2} - \frac{du}{dy} \frac{dS_{yy}}{dy} = 0, \quad (14)$$

subjected to the boundary conditions $u(0) = 0$, $u(1) = 1$. Clearly, the velocity profile may not be linear, despite the fact that a linear velocity profile is the universal solution for all simple materials and is experimentally observed at steady state for all fluids. (We note that a nonlinear velocity profile can occur if the concentration of the polymer is allowed to vary across the gap (Bhave *et al.*, 1991).)

Without much loss of generality, we assume that the boundary conditions for S_{yy} are homogeneous (these boundary conditions are also consistent with the Maxwell equation). Then, $S_{yy} \equiv 0$, (14) changes from quasi-linear to linear, and the closed-form solution for u and S_{xy} is given by

$$\begin{aligned} u(y) = & y + a_2 \left\{ \exp\left(\frac{y}{\epsilon\sqrt{1-\beta}}\right) - 1 - \left[\exp\left(\frac{1}{\epsilon\sqrt{1-\beta}}\right) - 1 \right] y \right\} \\ & + b_2 \left\{ \exp\left(\frac{-y}{\epsilon\sqrt{1-\beta}}\right) - 1 - \left[\exp\left(\frac{-1}{\epsilon\sqrt{1-\beta}}\right) - 1 \right] y \right\}, \end{aligned} \quad (15)$$

$$\begin{aligned} S_{xy}(y) = & \beta + a_2 \left\{ \beta - \beta \exp\left(\frac{1}{\epsilon\sqrt{1-\beta}}\right) - \sqrt{1-\beta} \epsilon \exp\left(\frac{y}{\epsilon\sqrt{1-\beta}}\right) \right\} \\ & + b_2 \left\{ \beta - \beta \exp\left(\frac{-1}{\epsilon\sqrt{1-\beta}}\right) + \sqrt{1-\beta} \epsilon \exp\left(\frac{-y}{\epsilon\sqrt{1-\beta}}\right) \right\}, \end{aligned} \quad (16)$$

where a_2 and b_2 are constants to be determined from the boundary conditions for S_{xy} . The stress component S_{xx} can be solved knowing u and S_{xy} .

The total shear stress in the fluid is given by $\sigma_{xy} = (1 - \beta) du/dy + S_{xy}$. The total shear stress is constant throughout the channel, as required by the steady-state momentum equation, and is given by

$$\sigma_{xy}(y) = 1 + a_2 \left\{ 1 - \exp\left(\frac{1}{\epsilon\sqrt{1-\beta}}\right) \right\} + b_2 \left\{ 1 - \exp\left(\frac{-1}{\epsilon\sqrt{1-\beta}}\right) \right\}. \quad (17)$$

In traditional rheometry that uses this type of shearing flow, the wall velocity is specified and the shear stress (by a force measurement) is measured and a relation such as (Eq. 17) is used to evaluate material parameters in the model. But here, we find that the total shear stress can depend on the boundary conditions for S_{xy} , which can be given independent of the boundary velocity. Thus, conventional rheometry cannot be performed with this type of fluid.

Plots of the velocity and the various components of the polymer contribution to the stress are given in Phan-Thien *et al.* (1990). Except for one choice of boundary conditions, the polymer stress shows steep boundary layers at the walls, and the velocity profile is not linear. Because the stress is not normally specified at a prescribed-velocity boundary, we have no physical guidance as to what to choose for the boundary conditions. A choice of boundary conditions that results in a linear velocity profile and constant polymer shear stress is when the polymer stresses are chosen such that they satisfy the Maxwell constitutive equation, i.e., (2) with the diffusion term omitted. For this simple shearing flow these are given by

$$S_{xx} = 2W_i \frac{du}{dy} S_{xy} , \quad (18)$$

$$S_{xy} = \beta \frac{du}{dy} , \quad (19)$$

$$S_{yy} = 0 . \quad (20)$$

For this choice of boundary conditions, a_2 and b_2 are exactly zero, and the diffusion term has no effect on the solution. Aside from the observation that this choice of boundary conditions results in a linear velocity profile for this flow, there is no physical guidance why this choice should be used in other flows.

The simple example given in this section shows that constitutive equations with stress diffusion terms that are applied across the domain may result in: (1) an unphysical description of real fluid, (2) additional boundary conditions that have uncertain physical meaning, and (3) constants in the constitutive equation that can no longer be identified as material parameters.

6. CONCLUSIONS

One immediate conclusion from the comparison of local and nonlocal theories from solid and fluid mechanics is the need for an accepted definition of what constitutes a nonlocal constitutive equation. A discussion of the issues and of the relative experience of researchers in the various fields must occur before a consensus will be reached. The present situation is fraught with potential misunderstandings from semantic differences alone. We have suggested a definition based on the violation of the principle of local action used in continuum mechanics. Even with this definition there is ambiguity as to the extent of a local effect. As we have illustrated with a specific example from viscoelastic fluids, a more precise definition may be the mathematical demonstration that the constitutive equation, in the absence of the conservation equation, depends on information far removed from its application.

Once a definition has been accepted by the continuum mechanics community, we can inquire about the appropriateness of nonlocal theories. In summary, a few general recommendations can

be made. Foremost there is the need to reach a consensus as to implications of the fundamental changes to continuum mechanics if nonlocal terms are included in constitutive equations. The example presented from viscoelastic fluids clearly demonstrates that the separation of the roles of conservation laws and constitutive relations can be lost because of the effect of the nonlocal constitutive equation in coupling the states of stress of non-adjacent material points. The meaning of material parameters in a constitutive equation is consequently ambiguous. As a counter example to this concern, Schreyer (1990a) evaluates the constants in a nonlocal model by comparison with experiments without difficulty.

One issue that must be considered in the application of nonlocal theories is the need for additional boundary conditions as required by the higher spatial gradients of strain or stress. In the example presented from viscoelasticity, the original presentation of the nonlocal terms used a more abstracted quantity, the configurational tensor instead of the stress tensor (El-Kareh and Leal, 1989), and the boundary conditions were chosen somewhat arbitrarily, with the recognition by the researchers that other choices were equally possible. It was not until a correspondence was made between the configurational tensor and the stress tensor that the unreasonableness of the additional boundary conditions became apparent (Phan-Thien *et al.*, 1990). We conclude that not only does the issue of boundary conditions need to be considered, the additional boundary conditions must be cast in physically meaningful way. Again as a counter example, in the analysis by Schreyer (1990a) additional boundary conditions proved not to be necessary, because the nonlocal term only applied in part of the domain, in the region of localized strain away from specified boundaries.

Finally there is need in proposing new numerical schemes to consider if these are consistent with the governing differential equations. If not, then it may be more forthright to include the useful effects of the scheme into the constitutive equation. Analysis of the appropriateness of the additional terms can be more easily understood and completed, as illustrated by the viscoelastic example presented.

ACKNOWLEDGMENTS

The authors wish to thank Drs. R. M. Brannon, P. J. Dotson and D. Oscar for helpful suggestions. Funding for this work was sponsored by the U.S. Department of Energy under contract W-7405-ENG-36 with the University of California and by the Australian Research Grant Scheme.

REFERENCES

- Basombrío, F. G., Buscaglia, G. C., and Dari, E. A., 1991, "Simulation of Highly Elastic Fluid Flow Without Numerical Diffusivity," *Journal of Non-Newtonian Fluid Mechanics* **39**, pp. 189–206.
- Bhave, A. V., Armstrong, R. C., and Brown, R. A., 1991, "Kinetic Theory and Rheology of Dilute, Nonhomogeneous Polymer Solutions," *Journal of Chemical Physics* **95**, pp. 2988–3000.
- Bird, R. B., Armstrong, R. C., and Hassager, O., 1987a, *Dynamics of Polymer Liquids: Vol. I Fluid Mechanics (2nd ed.)*, John Wiley and Sons, New York.
- Bird, R. B., Hassager, O., Armstrong, R. C., and Curtiss, C. F., 1987b, *Dynamics of Polymer Liquids: Vol. II Kinetic Theory (2nd ed.)*, John Wiley and Sons, New York.

- Chen, Z., and Clark, T., 1991, "A Comparison of Nonlocal Investigations in Solids and Fluids: An Introduction," ESP2A.91036, Society of Engineering Science Preprint.
- Clark, T., 1991, *Departures from Spectral Equilibrium in Homogeneous Anisotropic Turbulence*, Ph.D. Thesis, University of New Mexico, Albuquerque, New Mexico.
- Crochet, M. J., Davies, A. R., and Walters, K., 1984, *Numerical Solution of Non-Newtonian Flow*, Elsevier, Amsterdam.
- Crochet, M. J., 1989, *Rubber Chemistry and Technology* **62**, pp. 426.
- Curtiss, C. F., Bird, R. B., and Hassager, O., 1976, "Kinetic Theory and Rheology of Macromolecular Solutions," *Advances in Chemical Physics* **35**, pp. 31–117.
- Curtiss, C. F., and Bird, R. B., 1983, *Physica* **118A**, pp. 191-204.
- de Borst, R., 1987, "Computation of Post-Bifurcation and Post-Failure Behavior of Strain Softening Solids," *Computers and Structures* **25**, pp. 211–224.
- Debbaut, B., Marchal, J. M., and Crochet, M. J., 1988, "Numerical Simulation of Highly Viscoelastic Flows Through an Abrupt Contraction," *Journal of Non-Newtonian Fluid Mechanics* **29**, pp. 119–146.
- El-Kareh, A. W., and Leal, L. G., 1989, "Existence of Solutions for all Deborah Number for a Non-Newtonian Model Modified to Include Diffusion," *Journal of Non-Newtonian Fluid Mechanics* **33**, pp. 257–287.
- Keunings, R., 1987, "Simulation of Viscoelastic Fluid Flows," C. L. Tucker III (Eds.), *Fundamentals of Computer Modeling for Polymer Processing*, Verlag.
- Marchal, J. M., and Crochet, M. J., 1987, "A New Mixed Finite Element for Calculating Viscoelastic Flow," *Journal of Non-Newtonian Fluid Mechanics* **26**, pp. 77–114.
- Oldroyd, J. G., 1950, "On the Formation of Rheological Equations of State," *Proceedings of the Royal Society* **A200**, pp. 523–541.
- Ottinger, H. C., 1992, "Incorporation of Polymer Diffusivity and Migration into Constitutive Equations," *Rheologica Acta* **31**, pp. 14–21.
- Phan-Thien, N., Johnson, N. L., Dotson, P. J., and Graham, A. L., 1990, "Constitutive Equations with a Stress Diffusion Term," LA-UR-90-1995, Los Alamos National Laboratory.
- Schreyer, H. L., 1990a, "Analytical Solutions for Non-Linear Strain-Gradient Softening and Localization," *Journal of Applied Mechanics* **53**, pp. 522–528.
- Schreyer, H. L., October 1990b, personal communication.