Nonlocal viscous transport and the effect on fluid stress

B. D. Todd[*] and J. S. Hansen

Centre for Molecular Simulation, Swinburne University of Technology, P.O. Box 218, Hawthorn, Victoria 3122, Australia

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We demonstrate that, in general, only for fluid flows in which the gradient of the strain rate is constant or zero can the classical Navier-Stokes equations with constant transport coefficients be considered exact. This is typical of two of the most common types of flow: Couette and Poiseuille. For more complicated flow fields in which the streaming velocity involves higher order nonlinear terms, the use of nonlocal constitutive equations gives an exact description of the flow. These constitutive equations involve nonlocal transport kernels. For momentum transport we demonstrate that nonlocality will be significant for any particular flow field if the even moments of the nonlocal viscosity kernel are non-negligible. This corresponds to the condition that the strain rate varies appreciably over the width of the kernel in real space. Such conditions are likely to be dominant for nanofluidic flows.

I. INTRODUCTION

For over 150 years classical Navier-Stokes hydrodynamics [1] has been an enormously successful theoretical tool for predicting the properties of fluids under a huge variety of flow conditions. Its success extends from describing the dynamics of galactic motion [2], the aerodynamics of flight [3], the hydrodynamics of substances from liquid water to dense polymer melts [4], and right down to the flows of fluids on the microscale [5,6]. It has even been demonstrated to remain remarkably accurate down to nanoscale dimensions [7] as long as certain conditions are maintained. In a numerical study on the Lennard-Jones fluid, Travis *et al.* [7,8] demonstrated that for an atomic fluid confined by atomistic walls the Navier-Stokes equations were valid down to confinement spaces as low as 10 atomic diameters. Below this spacing the fluid becomes highly inhomogeneous in space so the assumptions of constant density, constant viscosity, etc. break down, as do the Navier-Stokes equations.

At such small length scales another significant problem arises: the transport properties of fluids become nonlocal in nature. Although this effect has been implicitly built into the theory of generalized hydrodynamics [9] it has only very recently been convincingly demonstrated to be true when the spatial extent of variations in the velocity gradient of the fluid are of the order of the width of the viscosity kernel [10]. The kernel itself is a nonlocal material property of the system with both wave-vector and frequency dependence [9,11] and has recently been accurately computed and parameterized for the Lennard-Jones fluid [12]. Alley and Alder [9] have also computed the kernel for hard sphere fluids at three deferent state points.

The most significant conclusion to follow from Ref. [10] is that accurate predictions of the shear stress profile for a fluid under time-independent flow (or equivalently, the velocity profile of a shearing fluid) is that the full nonlocal viscosity kernel must be used in such circumstances, rather than the local Navier-Stokes (infinite wavelength) viscosity.

This then raises an interesting and, as far as we are aware, unexplored question: *to what extent does curvature in the velocity gradient of fluids affect the Navier-Stokes predictions of the shear stress?* To answer this question, we proceed as follows: In Sec. II A we examine the familiar case of a local kernel with a constant velocity gradient (strain rate), and then consider the effect of introducing a nonlocal kernel and what effect that has on the predicted shear stress profile. In Sec. II B we consider both cases again, but this time with a linear strain rate profile. We note that the cases in Secs. II A and II B are typical of two of the most common types of flows, planar Couette and planar Poiseuille flow, respectively, and the investigations are somewhat illuminating. Then, in Sec. II C we consider the more general case of predictions of the shear stress profile for fluids with nonlinear strain rate profiles. In Sec. III we compare our local and nonlocal predictions with some actual molecular dynamics results and finally offer some conclusions in Sec. IV.

II. SHEAR STRESS WITH DIFFERENT STRAIN RATES

A. Local and nonlocal viscosity kernel with constant strain rate

We first consider the trivial yet subtle case of a homogeneous fluid with a linear time-independent velocity profile (i.e., constant strain rate). In the most general case, the shear stress is computed from the generalized hydrodynamic expression [9,13]

$$\sigma_{xy}(\mathbf{r}) = \int_{-\infty}^{\infty} d\mathbf{r}' \, \eta(\mathbf{r} - \mathbf{r}') \, \dot{\gamma}(\mathbf{r}'). \tag{1}$$

Microscopically, we traditionally write the infinite wavelength transport properties as delta functions in space, since the material properties of the fluid are constant in all directions. In this case, the local (or Navier-Stokes) viscosity kernel can be expressed as [13]

$$\eta(\mathbf{r} - \mathbf{r}') = \eta_0 \delta(\mathbf{r} - \mathbf{r}'), \tag{2}$$

where $\eta(\mathbf{r} - \mathbf{r}')$ is the viscosity kernel and η_0 is a constant and equals the zero wave vector viscosity. Substitution of Eq. (2) into Eq. (1) gives

*btodd@swin.edu.au

$$\sigma_{xy}(\mathbf{r}) = \eta_0 \int_{-\infty}^{\infty} d\mathbf{r}' \, \delta(\mathbf{r} - \mathbf{r}') \dot{\gamma}(\mathbf{r}') = \eta_0 \dot{\gamma}(\mathbf{r}). \qquad (3)$$

Equation (3) is of course just the standard Navier-Stokes (Newtonian) expression that relates the shear stress σ_{xy} at some point $\mathbf{r}$ to the strain rate $\dot{\gamma}$ at that point via a constant viscosity η_0. For constant strain rate $\dot{\gamma}(\mathbf{r}) = \dot{\gamma} \, \forall \mathbf{r}$ we just have a constant shear stress, $\sigma_{xy} = \eta_0 \dot{\gamma}$, the standard planar Couette flow result.

It is taken for granted that the viscosity kernel for a homogeneous fluid can be written in the form given by Eq. (2), in which the kernel width is infinitesimal (i.e., the viscosity is a local material property of the fluid). However, this is *never* actually true. The viscosity kernels for a variety of fluids, such as hard spheres [9], Lennard-Jones fluids [12], and even water [14] have been computed from molecular dynamics simulations. The fact that the k-space dependence of this kernel is not a simple constant, but is rather distributed in a Lorentzian or Gaussian-like manner [12], signifies that the kernel is not a delta function in space for *any* fluid, no matter how simple. In fact, in Ref. [12] both the k-space and real-space kernels were computed for a simple shifted and truncated Lennard-Jones fluid [the Weeks-Chandler-Anderson (WCA) fluid [15]]. The real-space kernel was found to have a width of roughly three atomic diameters and could be adequately parametrized by either a sum of two Gaussians or a Lorentzian-type function. Strictly speaking then, Eq. (2) is not correct and should be replaced by a more general form:

$$\eta(\mathbf{r} - \mathbf{r}') = \eta_0 f(\mathbf{r} - \mathbf{r}'), \qquad (4)$$

where f is some general normalized and even function with nonzero finite width such that

$$\int_{-\infty}^{\infty} d\mathbf{r} \, f(\mathbf{r}) = 1. \qquad (5)$$

Substituting Eq. (4) into Eq. (1) gives us

$$\sigma_{xy}(\mathbf{r}) = \eta_0 \int_{-\infty}^{\infty} d\mathbf{r}' f(\mathbf{r} - \mathbf{r}') \dot{\gamma}(\mathbf{r}'). \qquad (6)$$

For constant strain rate we find $\sigma_{xy} = \eta_0 \dot{\gamma}$, which is *exactly* the same expression as that obtained when assuming a delta function form of the kernel. Thus we see that for a homogeneous fluid with constant strain rate, the fluid behaves as if it had a local viscosity kernel, η_0. It does this *precisely* because there is no variation in strain rate over the width of the kernel, which allows us to take the strain rate outside of the integral in Eq. (6). This then is the reason why we are justifiably allowed to represent the true, finite-width viscosity kernel as a delta function, or equivalently, as a constant transport coefficient.

B. Nonlocal viscosity kernel with linear strain rate

Consider now the case of a nonlocal viscosity kernel and a linear strain rate. We again consider a three-dimensional fluid and assume that flow is in the x direction, with gradient αy in the y direction. Thus

$$\nabla \mathbf{u}(\mathbf{r}) = \begin{pmatrix} 0 & 0 & 0 \\ \alpha y & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad (7)$$

where $\mathbf{u}(\mathbf{r})$ is the streaming velocity of the fluid. This of course is just the geometry associated with planar Poiseuille flow with quadratic velocity profile. For this geometry all nonconstant material properties will be functions only of the y-spatial coordinate. From Eq. (6) we have

$$\sigma_{xy}(y) = \eta_0 \alpha \int_{-\infty}^{\infty} dy' f(y - y') y'. \qquad (8)$$

We now make the substitution $u = y - y' \Rightarrow du = -dy'$, so the integral becomes

$$\int_{-\infty}^{\infty} dy' f(y - y') y' = y \int_{-\infty}^{\infty} du \, f(u) - \int_{-\infty}^{\infty} du \, f(u) u. \quad (9)$$

The first integral on the right-hand side (rhs) of Eq. (9) is just one from the normalization condition, Eq. (5). The second integral on the rhs is zero since the integrand is an odd function of u. Thus Eq. (9) becomes

$$\int_{-\infty}^{\infty} dy' f(y - y') y' = y, \qquad (10)$$

and so from Eq. (8) we have the result

$$\sigma_{xy}(y) = \eta_0 \alpha y \qquad (11)$$

for any choice of $f(y)$. This is a remarkable result because it is equivalent to what one obtains assuming that Newton's law of viscosity is valid, i.e., classical Navier-Stokes hydrodynamics, $\sigma_{xy}(y) = \eta_0 \dot{\gamma}(y)$. It says that even in the case of a quadratic streaming velocity profile we can always expect a linear shear stress profile, no matter what the precise mathematical form of the true viscosity kernel is, as long as the kernel is an even function in space, which physically it must be for a homogeneous fluid. Thus in the case of the two most common simple flow types—planar Couette and Poiseuille flow—the inclusion of a nonlocal viscosity kernel will give *exactly* the same predictions of classical hydrodynamics that assumes a constant local viscosity. This is true no matter how wide the true kernel actually is. Once again, this is a result of the fact that *only* for linear or quadratic velocity profiles, the strain rate (velocity gradient) does not vary over *any* length scale. Mathematically, this is equivalent to saying that Newton's law of viscosity is always exact as long as $d\dot{\gamma}(y)/dy = c$, where c is a constant or zero. In fact, this is a suitable condition for determining the validity of the Navier-Stokes treatment for viscous transport no matter how nanoscale the flow is. In more general cases where this condition is not met, the use of a nonlocal constitutive equation, such as Eq. (6), will be required when variations in the strain rate occur over molecular length scales. This is now further examined in what follows.

C. Nonlocal viscosity kernel with nonlinear strain rate

As any analytic function can be expanded into a polynomial series via Taylor expansion, to simplify the mathematics

we consider first the simple case of a strain rate with form

$$\dot{\gamma}(y) = \alpha y^n, \quad n = 0, 1, 2, \ldots . \tag{12}$$

The result obtained for this single nonlinear polynomial term can be generalized to that of any functional form for the strain rate by taking the infinite series sum of the result. This represents the Taylor series expansion of some general analytic function $\dot{\gamma}(y)$ around $y=0$, as will be demonstrated later. Note also that we will work in the general case where n can be either odd (symmetric velocity profile) or even (asymmetric velocity profile) about $y=0$. Once again, from Eq. (6) we have

$$\sigma_{xy}(y) = \eta_0 \alpha \int_{-\infty}^{\infty} dy' f(y-y') y'^n. \tag{13}$$

Making the substitution $u=y-y'$ gives

$$\sigma_{xy}(y) = \eta_0 \alpha \int_{-\infty}^{\infty} du\, f(u)(y-u)^n. \tag{14}$$

We can write the power function inside the integral as

$$(y-u)^n = y^n \left[1 - \frac{u}{y} \right]^n, \tag{15}$$

which we can expand to give

$$(y-u)^n = y^n \left[1 - a_1 \frac{u}{y} + a_2 \left(\frac{u}{y} \right)^2 - a_3 \left(\frac{u}{y} \right)^3 + \cdots \pm a_n \left(\frac{u}{y} \right)^n \right], \tag{16}$$

where a_n are coefficients of the expansion and we note that the last term is $+a_n$ if n is even and $-a_n$ if n is odd. Substitution of Eq. (16) into Eq. (14) gives

$$\sigma_{xy}(y) = \eta_0 \alpha y^n \int_{-\infty}^{\infty} du\, f(u) \left[1 - a_1 \frac{u}{y} + a_2 \left(\frac{u}{y} \right)^2 - a_3 \left(\frac{u}{y} \right)^3 \right.$$
$$\left. + \cdots \pm a_n \left(\frac{u}{y} \right)^n \right]$$
$$= \eta_0 \alpha y^n \left[\int_{-\infty}^{\infty} du\, f(u) - \frac{a_1}{y} \int_{-\infty}^{\infty} du\, u f(u) \right.$$
$$\left. + \frac{a_2}{y^2} \int_{-\infty}^{\infty} du\, u^2 f(u) + \cdots \pm \frac{a_n}{y^n} \int_{-\infty}^{\infty} du\, u^n f(u) \right]. \tag{17}$$

From the symmetry of the kernel f, we note that for all odd powers of u we have

$$\int_{-\infty}^{\infty} du\, f(u) u^m = 0, \quad m \text{ odd}. \tag{18}$$

Therefore

$$\int_{-\infty}^{\infty} du\, f(u)(y-u)^n = y^n \left[1 + \frac{a_2}{y^2} \int_{-\infty}^{\infty} du\, f(u) u^2 \right.$$
$$+ \frac{a_4}{y^4} \int_{-\infty}^{\infty} du\, f(u) u^4 + \cdots$$
$$\left. + \frac{a_n}{y^n} \int_{-\infty}^{\infty} du\, f(u) u^n \right] \tag{19}$$

for n even, or

$$\int_{-\infty}^{\infty} du\, f(u)(y-u)^n = y^n \left[1 + \frac{a_2}{y^2} \int_{-\infty}^{\infty} du\, f(u) u^2 \right.$$
$$+ \frac{a_4}{y^4} \int_{-\infty}^{\infty} du\, f(u) u^4 + \cdots$$
$$\left. + \frac{a_{n-1}}{y^{n-1}} \int_{-\infty}^{\infty} du\, f(u) u^{n-1} \right] \tag{20}$$

for n odd. So finally we have for n even

$$\sigma_{xy}(y) = \eta_0 \alpha y^n \left[1 + \frac{a_2}{y^2} \int_{-\infty}^{\infty} du\, f(u) u^2 + \frac{a_4}{y^4} \int_{-\infty}^{\infty} du\, f(u) u^4 \right.$$
$$\left. + \cdots + \frac{a_n}{y^n} \int_{-\infty}^{\infty} du\, f(u) u^n \right]$$
$$= \eta_0 \alpha y^n \left[1 + \frac{b_2}{y^2} + \frac{b_4}{y^4} + \cdots \frac{b_n}{y^n} \right]$$
$$= \eta_0 \alpha [b_n + b_{n-2} y^2 + b_{n-4} y^4 + \cdots + y^n], \tag{21}$$

where the coefficients b_k are given by the even moments of the kernel,

$$b_k \equiv a_k \int_{-\infty}^{\infty} du\, f(u) u^k. \tag{22}$$

Similarly, for n odd we have

$$\sigma_{xy}(y) = \eta_0 \alpha [b_{n-1} y + b_{n-3} y^3 + b_{n-5} y^5 + \cdots + y^n]. \tag{23}$$

The equivalent local (Newtonian) shear stress is given as

$$\sigma_{xy}^L(y) = \eta_0 \alpha y^n. \tag{24}$$

We can see now that the local and nonlocal shear stresses are not in general the same for flows where the curvature of the strain rate is nonzero. The degree of nonlocality depends on the relative contribution of the different moments to the total stress given by Eqs. (21) and (23), which in turn depends on how much variation in strain rate takes place over the width of the kernel (i.e., the degree of curvature of the strain rate profile with respect to the kernel width). While Eqs. (21) and (23) above are just the simplified expressions for a strain rate that is either an odd or even power of y, as previously stated the general case for some arbitrary function can be obtained by summing over an infinite series of terms given in Eqs. (21) and (23), as long as the strain rate function is analytic. Thus a full Taylor series expansion of a more

complicated strain rate function will still result in a polynomial series such as given by Eqs. (21) and (23), and hence the conclusion remains the same.

To demonstrate this explicitly, we repeat the above derivation, only this time assuming a general arbitrary form for the strain rate, $\dot{\gamma}$. We also assume that $\dot{\gamma}(y)$ is analytic about the midpoint of the flow $y=0$, so it can be Taylor expanded. We can therefore express $\dot{\gamma}(y)$ as

$$\dot{\gamma}(y) = \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} y^n, \tag{25}$$

where $\dot{\gamma}^n$ is the nth derivative of $\dot{\gamma}$ with respect to y. Thus the nonlocal shear stress can be expressed as

$$
\begin{aligned}
\sigma_{xy}(y) &= \eta_0 \int_{-\infty}^{\infty} dy' f(y-y') \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} y'^n \\
&= \eta_0 \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} \int_{-\infty}^{\infty} dy' f(y-y') y'^n.
\end{aligned}
\tag{26}
$$

The integrand in Eq. (26) can be expanded in the same manner as was done from Eqs. (13)–(23), which will give

$$\sigma_{xy}(y) = \eta_0 \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} [b_n^n + b_{n-1}^n y + b_{n-2}^n y^2 + b_{n-3}^n y^3 + \cdots + y^n] \tag{27}$$

$$= \eta_0 \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} \left[\sum_{i=0}^{n} b_{n-i}^n y^i \right], \tag{28}$$

where $b_0^n = a_0 \int_{-\infty}^{\infty} du\, f(u) = a_0 \equiv 1$. Here we also note that the coefficients b_k^n are analogous to those defined in Eq. (22) except that now an entire set of coefficients b_k exists for each value of n in the Taylor expansion (hence the notation b_k^n). Equation (27) could be further simplified by collecting all coefficients of terms y^n together (in effect removing the term in square brackets and simply having a sum over n with new coefficients c_n). However, we keep it in this form so that we can compare it directly with the expression for the local shear stress, which is simply

$$\sigma_{xy}^L(y) = \eta_0 \sum_{n=0}^{\infty} \frac{\dot{\gamma}^n(0)}{n!} y^n. \tag{29}$$

Clearly, Eqs. (27) and (29) are not the same. Thus for any general strain rate in which the curvature is nonzero, nonlocality will become important when the contributions of the moments of the kernel become non-negligible in Eq. (27). Our approach here gives greater insight into the effect of nonzero strain rate curvature on the fluid stress than traditional gradient expansion treatments [10].

III. COMPARISON WITH MOLECULAR DYNAMICS

Using nonequilibrium molecular dynamics (NEMD) it is possible to demonstrate the effect of the nonlinear strain rate. Initially, however, it would be insightful to show that for a
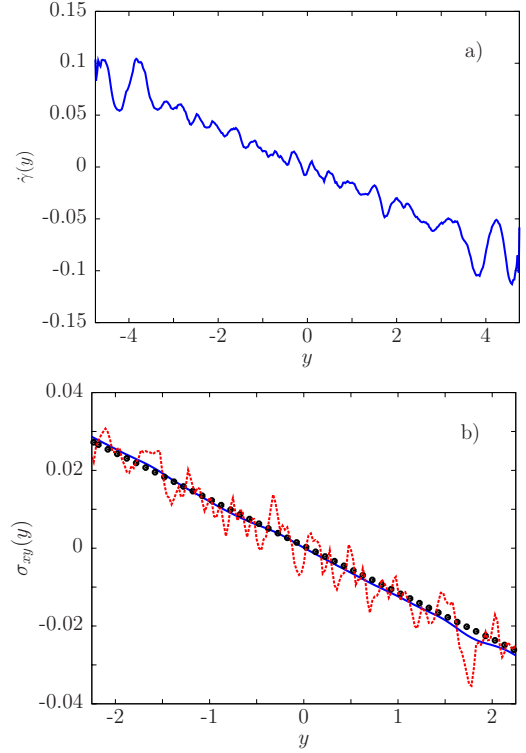

FIG. 1. (Color online) (a) Piecewise polynomial fit of NEMD data of the strain rate profile in a Poiseuille flow. Data at the far end points are not included in order to highlight the profile in the channel interior. The fluid is a Weeks-Chandler-Andersen (WCA) fluid [15], with density $\rho=0.6$, temperature $T=0.726$, and viscosity $\eta_0=0.679$. The width of the channel is $L_y=10.2$ and the external force field is $F_e=0.02$. All quantities are given in usual reduced molecular dynamics units; see, for example, Ref. [30]. (b) Resulting shear stress profiles in the midchannel as predicted by the local description (dotted line) and the nonlocal description (full line). Exact molecular dynamics data (circles) are also shown for comparison.

fluid flow with linear strain rate the local treatment indeed suffices.

Consider an atomic fluid confined between two parallel atomistic walls located at positions $-L_y/2$ and $L_y/2$, where L_y is the width of the channel, such that the y direction is the direction of confinement. In the x and z directions the system is periodic (or infinite in extent). A constant external force field, F_e (or equivalently a constant pressure gradient), acts on the fluid in the x direction, such that a flow is generated in this direction. This, of course, results in the classical Poiseuille flow. As mentioned above, this system has previously been studied intensively using NEMD and we will not go into details about the simulation technique, but refer to Ref. [7] and references therein. Figure 1(a) shows NEMD data of the strain rate profile for such a Poiseuille flow. Simulation details can be found in the figure caption. It is seen that near the wall-fluid boundary the profile is not linear which is due to the large density variation in this region [16]. However, in the interior of the channel the system is homogeneous which is also manifested in the linear strain rate profile. According to Sec. II this means that the local Newtonian expression for the shear stress is valid. This can readily be tested by comparing the predicted stress with the stress computed in the

NEMD simulations. To this end we note that the stress can be evaluated via the density profile, $\rho(y)$, by [17]

$$\sigma_{xy}(y) = - \int_{-L_y/2}^{y} dy' F_e(y') \rho(y') = -F_e \int_{-L_y/2}^{y} dy' \rho(y'),$$
(30)

where $\rho(y)$ is easily obtained in the simulation. In Fig. 1(b) the predicted local stress profile calculated using Eq. (3) and the strain rate profile in Fig. 1(a) is plotted (dotted line) together with the NEMD data (circles). The zero wavevector viscosity is extrapolated from data given in Hansen *et al.* [12]. Only the profiles in the interior of the channel are included. It is seen that the local prediction is in excellent agreement with the molecular dynamics results, which is also expected from the fact that the strain rate is linear. The results can furthermore be compared with the nonlocal constitutive model, Eq. (6), where

$$\eta_0 f(y) = \frac{\eta_0}{2\sqrt{2\pi}} [\sigma_1 e^{-(\sigma_1 y)^2/2} + \sigma_2 e^{-(\sigma_2 y)^2/2}],$$
(31)

where $\sigma_1 = 1.812$ and $\sigma_2 = 4.670$ as given in Ref. [12]. It should also here be mentioned that this functional form is not the only satisfactory expression for the kernel, but it is the most convenient form [10,12]. The full line in Fig. 1 represents the convolution of the strain rate profile in Fig. 1(a) with the kernel given in Eq. (31). It is clearly seen that the local and nonlocal models predict the same shear stress as expected; however, there is an advantage using the nonlocal approach in that it smoothens the profile eliminating the statistical noise considerably.

Using the sinusoidal transverse force (STF) method [18] it is possible to simulate fluid flows with a sinusoidal or cosine strain rate profile, i.e., profiles with a large degree of nonlinearity. As for the direct NEMD method, the STF method is well described in the literature and we will refer the reader to Refs. [12,18,19]. The applied force field used in this present work is

$$F_e(y) = F_0 \cos(k_n y),$$
(32)

where F_0 is the force amplitude and k_n is the wave vector of excitation given as $k_n = 2\pi n/L_y$, n being the wave number. In the limit of small force field amplitude, the stress can be computed directly via [10,12]

$$\sigma_{xy}(y) = -\frac{F_0 \rho}{k_n} \sin(k_n y),$$
(33)

where ρ is the fluid density. In Fig. 2(a) we have plotted the strain rate profile, which is given by $\dot{\gamma}(y) = -\dot{\gamma}_{k_n} \sin(k_n y)$, where $\dot{\gamma}_{k_n}$ is the strain rate Fourier coefficient obtained in the STF simulation [19]. The local stress profile is plotted in Fig. 2(b) (dotted line), together with the nonlocal stress profile (full line) and the simulation data using Eq. (33) (circles). For flows with strong nonlinear strain rate it can be seen that the local Newtonian constitutive equation relating the stress with the strain rate fails. It must here be pointed out that for sufficiently small values of wave number, n, the local prediction agrees quite well with the exact measured stresses [10].
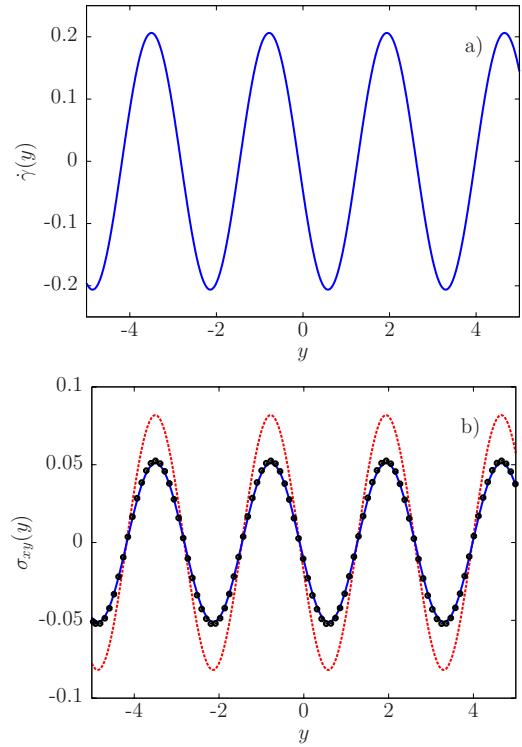

FIG. 2. (Color online) (a) The strain rate profile for a STF flow. The fluid is a Weeks-Chandler-Andersen (WCA) fluid, with density $\rho = 0.485$, temperature $T = 0.726$, and viscosity $\eta_0 = 0.397$. The external force field amplitude is $F_0 = 0.25$ and the wave vector is $k_n = 2.311$. All quantities are given in usual reduced molecular dynamics units; see, for example, Ref. [30]. (b) Resulting shear stress profiles as predicted by the local description (dotted line) and the nonlocal description (full line). Exact molecular dynamics data (circles) are also shown for comparison.

As mentioned earlier, this is because the strain rate does not vary to such a degree that nonlocal effects are important. In principle it is possible to calculate the moments of the general normalized function, $f(y)$, given in Eq. (4), and therefore the effects of the higher order terms in the Taylor expansion of the stress, Eq. (27). However, since the stress is given as a trigonometric function, the expansion converges very slowly and will therefore not provide much useful information in this particular example.

IV. CONCLUSION

We have shown that in all but the simplest flows, nonlocal constitutive equations should be invoked for a complete description of the flow and stress fields. We find that the degree of importance of nonlocal effects can in fact be determined by computing the even moments of the viscosity kernel. This is mathematically equivalent to stating that nonlocality dominates transport phenomena when the variation in the strain rate is of the order of the width of the viscosity kernel, which in turn will be of the order of molecular length scales. While this condition will never dominate for macroscopic flows, it is likely to be fundamentally important for microscopic phenomena such as flows confined to nanometer dimensions.

Other potential applications include shock wave phenomena [9,20–23], shear banding [24], flows of micellar solutions [25], suspensions of rigid fibers [26], jammed glassy systems [27], the influence of boundary conditions [28,29], and possibly even turbulence.

Finally, we make an observation about the role of momentum balance in the shear stress. With appropriately known boundary conditions one can solve the momentum continuity equation directly and obtain the shear stress. For planar Couette flow, this always leads to a constant shear stress, whereas for planar Poiseuille flow it is trivial to show that the shear stress is directly proportional to the integral of the density profile [17], as is done in Eq. (30). It is the momentum balance that governs the stress profile for any particular flow geometry, and it is this property of a system that is fundamental. The use of a correctly formulated nonlocal constitutive equation therefore links the nonlocal nature of atomic correlations to momentum balance and transport. This is an interesting relationship and one that would merit further investigation.

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[1] G. G. Stokes, *Mathematical and Physical Papers, Volume 1* (Cambridge University Press, New York, 1880).
[2] C. Clarke and R. Carswell, *Principles of Astrophysical Fluid Dynamics* (Cambridge University Press, Cambridge, England, 1995).
[3] G. Rubbert and G. Saaris, SAE J., 680304 (1968).
[4] R. B. Bird, R. C. Armstrong, and O. Hassager, *Dynamics of Polymeric Liquids* (Wiley, New York, 1987).
[5] P. Tabeling, *Introduction to Microfluidics* (Oxford University Press, New York, 2005).
[6] H. Bruus, *Theoretical Microfluidics* (Oxford University Press, New York, 2008).
[7] K. P. Travis, B. D. Todd, and D. J. Evans, Phys. Rev. E **55**, 4288 (1997).
[8] K. P. Travis and K. E. Gubbins, J. Chem. Phys. **112**, 1984 (2000).
[9] W. E. Alley and B. J. Alder, Phys. Rev. A **27**, 3158 (1983).
[10] B. D. Todd, J. S. Hansen, and P. J. Daivis, Phys. Rev. Lett. **100**, 195901 (2008).
[11] S. Hess, Phys. Lett. **90A**, 293 (1982).
[12] J. S. Hansen, P. J. Daivis, K. P. Travis, and B. D. Todd, Phys. Rev. E **76**, 041121 (2007).
[13] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, London, 1990).
[14] D. Bertolini and A. Tani, Phys. Rev. E **52**, 1699 (1995).
[15] J. D. Weeks, D. Chandler, and H. C. Andersen, J. Chem. Phys. **54**, 5237 (1971).

[16] S. Toxvaerd, J. Chem. Phys. **74**, 1998 (1981).
[17] B. D. Todd, D. J. Evans, and P. J. Daivis, Phys. Rev. E **52**, 1627 (1995).
[18] E. M. Gosling, I. R. McDonald, and K. Singer, Mol. Phys. **26**, 1475 (1973).
[19] A. Baranyai, D. J. Evans, and P. J. Daivis, Phys. Rev. A **46**, 7593 (1992).
[20] B. L. Holian, W. G. Hoover, B. Moran, and G. K. Straub, Phys. Rev. A **22**, 2798 (1980).
[21] L. Holian and P. S. Lomdahl, Science **280**, 2085 (1998).
[22] E. J. Reed, L. E. Fried, W. D. Henshaw, and C. M. Tarver, Phys. Rev. E **74**, 056706 (2006).
[23] E. J. Reed, L. E. Fried, and J. D. Joannopoulos, Phys. Rev. Lett. **90**, 235503 (2003).
[24] J. K. G. Dhont, Phys. Rev. E **60**, 4534 (1999).
[25] C. Masselon, J.-B. Salmon, and A. Colin, Phys. Rev. Lett. **100**, 038301 (2008).
[26] R. L. Schiek and E. S. G. Shaqfeh, J. Fluid Mech. **296**, 271 (1995).
[27] J. Goyon, A. Colin, G. Ovarlez, A. Ajdari, and L. Bocquet, Nature (London) **454**, 84 (2008).
[28] S. Hess and W. Loose, Physica A **162**, 138 (1989).
[29] S. Heidenreich, P. Ilg, and S. Hess, Phys. Rev. E **75**, 066302 (2007).
[30] D. A. Mcquarrie, *Statistical Mechanics* (Harper and Row, New York, 1976).