Microscopic model for viscous flow in two dimensions

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We report a computer simulation of simple shear flow in order to investigate the transport properties of a two-dimensional microscopic model of a fluid. The numerical results exhibit nonlinear profiles for the fluid velocity, and the viscous resistance depends linearly on the shear rate. These experiments confirm that, in two-dimensional fluids, the Navier-Stokes equations do not exist in their usual form. We propose a phenomenological expression for the viscous part of the pressure.

I. INTRODUCTION

The Boltzmann kinetic theory allows one to derive the fluid equations from microscopic dynamics. This is done by the well-known Chapman-Enskog method[1] where any thermodynamic flux, say Y (which could be, for instance, the nondiagonal part of the pressure tensor), may be expanded in terms of the gradients of the thermodynamic quantities (the fluid velocity is one of these variables):

$$Y = k_1 \nabla X + k_2 \nabla^2 X + k_3 \nabla^3 X + \cdots . \tag{1.1}$$

The symbol X represents the set of the independent equilibrium parameters.

We have omitted any vector sign in this equation; in order to write it in detail, one should account for the various space symmetries and for the positiveness of the entropy production. The quantities such as k_1 (i.e., the coefficient in front of the first spatial derivative of the equilibrium parameters) are the transport coefficients of the Navier-Stokes order. In an isotropic monatomic fluid, they are three independent Navier-Stokes transport coefficients: the shear viscosity, the bulk viscosity, and the heat conductivity. The quantities such as k_2 are the Burnett order transport coefficients.

For dense fluids, the coefficients k_i are given by time integrals of equilibrium autocorrelation functions. It is now well known that, in three-dimensional fluids, the integrals giving the coefficients as k_2 are divergent, although in two-dimensional fluids the transport coefficients are already divergent at the Navier-Stokes order. This divergence is due to the slow decrease of the time correlations which arises itself from hydrodynamical phenomena.[2]

In this paper we investigate the "viscosity" effects in a two-dimensional classical lattice fluid. As the standard shear viscosity coefficient diverges, the Newton relation between the viscous stress and the gradients of the velocity field no longer holds, and our knowledge about the relations replacing the Newton and Fourier relations is rather poor. Therefore we have simulated a stationary microscopic Couette flow to investigate the transport phenomena in this lattice model. In a sense this is a viscosimetry experiment carried out with a computer.

In Sec. II, a definition of the model and the boundary conditions of the Couette flow are given. Section III is devoted to an exposition of the "experimental" results and Sec. IV to their interpretation: some results can be predicted theoretically. Further a few indications are given about the form of the new transport equations replacing the Navier-Stokes equations for this model.

II. DEFINITION

The model which we shall describe has been designed to simulate "realistic" motion of a classical fluid, but with a microscopic evolution law adapted to numerical work. As in digital computers any continuous motion of particles is simulated by discrete jumps, we choose a model where the time, the positions, and the velocities are discrete variables. Since the detailed description of the model was given in a preceding paper,[3] we shall only describe it quite briefly.

The particles are identical and, at time $t=0$, lie on the vertices of a two-dimensional square lattice. The mass of each particle is unity, their kinetic energy $\frac{1}{2}$, and their velocities point toward one of the four directions of the lattice (see Fig. 1). Two particles can lie at the same vertex, provided they have different velocities. The density (i.e., the mean number of particles per vertex) is then smaller than or equal to 4 and the momentum density is smaller than or equal to $\sqrt{2}$.

The time evolution process occurs step by step and each step is the result of two successive operations acting separately on velocity space and po-

sition space, namely collision and translation. As shown in Fig. 1, the collision process changes the situation when there are two particles at a vertex with opposite velocities: in any other case, the situation remains unchanged. This process is carried out simultaneously at each vertex of the lattice.

After that, the translation steps forward all particles in the direction of their velocities. This integer time-evolution process seems to be the simplest one which satisfies the usual microscopic conservation laws.

Let us remark that, due to its anisotropy, this model implies a special form for the Navier-Stokes equations (by supposing that they exist, which is not the case), and the Green-Kubo formula giving the transport coefficient exhibits the same divergence as in any two-dimensional fluid.[3] The energy and number density being connected to each other in a simple way, there exists only one transport coefficient, quite similar to a shear viscosity. In order to investigate the effects of an anomalous viscosity, we studied a stationary Couette flow; external boundary conditions maintain a velocity gradient in the fluid.

The velocity gradient is produced by adsorption on parallel boundaries (straight lines) moving with opposite equal velocities. The particles colliding at some time with these boundaries are reintroduced at the next time step in the fluid according to the following laws: (i) the velocity component normal to the boundary is reversed; (ii) the component parallel to the boundary is replaced by a random velocity whose mean value is equal to the boundary velocity (i.e., the boundary is perfectly rough).

We choose to place the boundaries parallel to one of the two bisectors of the directions of the lattice, so that intersections with it occur on the vertices only, as shown on Fig. 2. The adsorption process does not conserve the component of momentum parallel to the boundary; the difference represents the contribution of the colliding particle to the viscous force applied to the boundary. The velocity and the viscous force per unit length cannot exceed $\pm\sqrt{2}$ and $\pm n\sqrt{2}$, respectively (n is

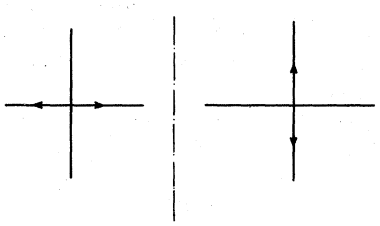

FIG. 1. Collisions at a vertex.

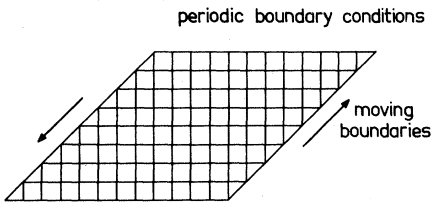

FIG. 2. Boundary conditions of the viscosimeter experiment.

the number density, $0 \leq n \leq 4$), the modulus of the particle velocities being unity. In the computational simulation we must use a lattice of finite length in the direction parallel to the boundaries, and we take in this direction periodic boundary conditions, by inserting at the same distance from the moving boundaries, but below (for example), a particle which has gone away above at the preceding time.

At time $t = 0$ the system is completely filled, with no macroscopic current; because of the boundary conditions, it reaches a new equilibrium after a brief lapse of time. The simplicity of the model allows one to explore the dependence of the Couette flow with respect to parameters such as the boundary tangential velocity V_0 and the distance d between the moving parallel boundaries; in continuous models this requires a larger amount of computational time.

Recently, Cabannes[4] studied a Couette flow in a three-dimensional model with discrete velocities, but which can have different moduli. A conservation equation for energy is obtained which differs from the continuity equation. As expected in a three-dimensional model, the velocity profile is close to being linear. We shall see in Sec. III that the two-dimensional models present very special features and the Navier-Stokes equations do not hold in their usual form.

III. THE NUMERICAL RESULTS

In this section we shall first present the numerical results and then discuss some particular features.

A first unexpected result is that, although the standard viscosity does not exist, the "viscous" force remains proportional to the velocity V_0 of the moving walls, as in the numerical experiment done by Hoover *et al.*[5] This is a little surprising as it could be conjectured that the viscous resistance in a two-dimensional fluid is a nonanalytic function of the thermodynamic force V_0/d at $V_0/d = 0$; recall, for instance, the nonanalytical dependence on the Reynolds number of the viscous drag encountered by a cylinder in a direction perpendicular to its axis at low velocity.[6] This linearity remains exact, at least at the accuracy of our computation,

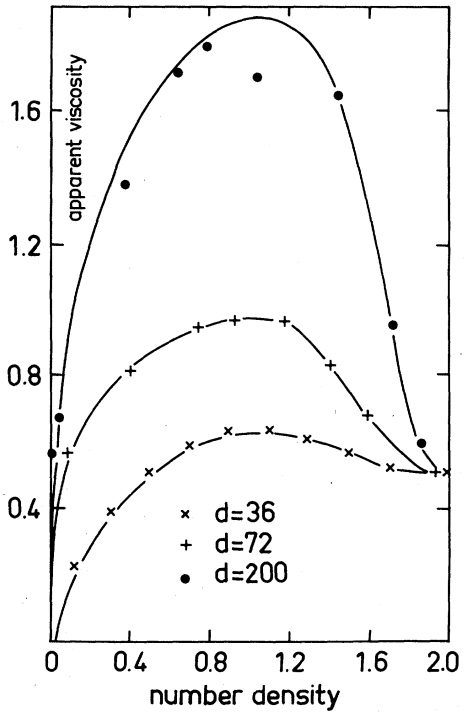

FIG. 3. The apparent viscosity as a function of number density and of the distance between the moving boundaries.

if the other main parameters (i.e., number density and size of the system) are modified. In addition to the velocities $\pm V_0$ of the moving walls, the viscous force depends on the distance d between them and on the number density n. In the case where the Navier-Stokes equations exist, the viscous force per length unit can be expressed by

$$f = \theta V_0/d\,, \tag{3.1}$$

where θ stands for viscosity. This formula is not exact in our case; however, we shall define an apparent viscosity θ by (3.1), θ being then dependent (as usual) on the number density n, and (less usually) on the distance d. The results obtained are summarized in Fig. 3. One observes that the viscosity exists in the usual sense (i.e., θ becomes d independent at large d) near $n = 2$ only. The viscous force is a function of the distance d between the moving boundaries which vanishes more slowly than $1/d$ when d increases. At $n = 0$, the viscous force no longer depends on d; the fluid at $n \to 0$ behaves like an ideal Knudsen gas without collision. By comparing Fig. 3 and Fig. 4, one may understand the difference between the actual results and the ones which were found in the case of a normal viscosity.

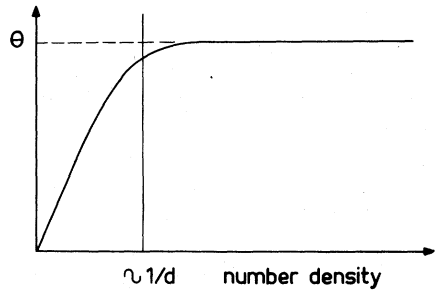

FIG. 4. Apparent viscosity in a Couette flow for a usual gas near $N = 0$ (Maxwell paradox).

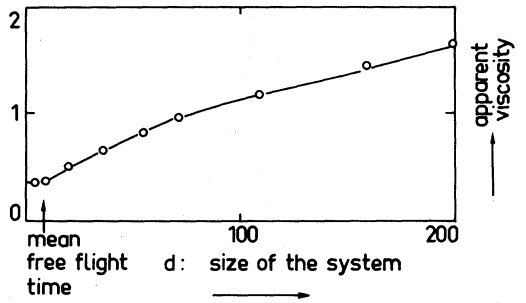

FIG. 5. Apparent viscosity as a function of the distance between the moving boundaries at $n = 1.08$.

To show more explicitly the connection between the viscous force and the size of the system, we plotted in Fig. 5 $\theta(d)$ at a given density ($n = 1.08$) chosen arbitrarily in an intermediate region. To complete our study of the model we give in Fig. 6 the velocity profiles for different densities. Because of the symmetry of the profiles (which is verified in the experiment), Fig. 6 represents a half-system only. The velocity is measured by averaging the microscopic current along lines parallel to the moving boundaries as shown in Fig. 7.

We observe that the velocity v of the fluid is given in any case by

$$v(x) = V_0 \nu(x/d, n)\,, \tag{3.2}$$

$\pm V_0$ being the velocities of the moving boundaries

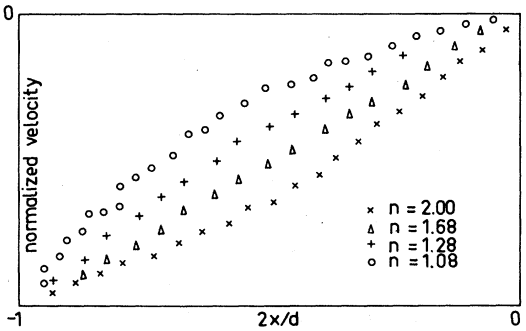

FIG. 6. Velocity profile for different number densities.

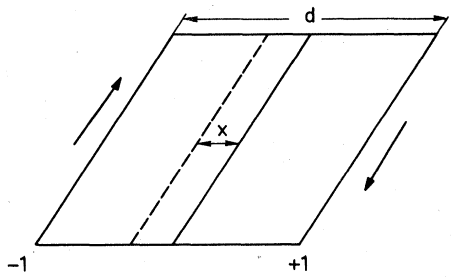

FIG. 7. The position parameter x in the velocity profiles.

and n the mean density. Equation (3.2) means that there is universal law (independent of the choice of the unit length) describing the velocity profiles, at least if d is not too small (i.e., in the fluid regime, as opposed to the free molecular regime). As appears in Fig. 6, the velocity profiles are not linear. Thus one can infer that the Navier-Stokes equations do not take their usual form for this model. Furthermore, one observes that, at low number density (typically less than 1.2), the velocity profiles seem to have an infinite gradient near the moving walls. In Sec. IV, we shall try to explain these peculiar features.

We have checked in some particular cases that, after a rather short delay of time, the velocity profiles reach a stationary state. In fact, it could be argued that our "experiment" has shown nonlinear profiles because the usual Couette profile would be reached at very large times only and that these nonlinear profiles do not imply a nonclassical behavior for the fluid. To give an idea of the value of this delay we plotted in Fig. 8 the time dependence of the normalized viscous force on the moving boundaries. As the nonstationary force for a given numerical run fluctuates wildly, we have only given the dependence versus time of a force averaged on various initial conditions. We observed that the normalized viscous force depends

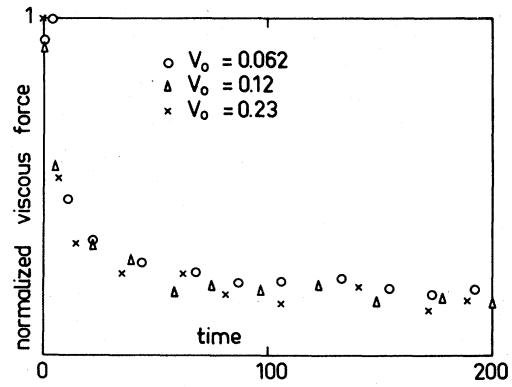

FIG. 8. Time dependence of the normalized viscous force on the moving boundaries.

on the size of the system, on number density (but very slightly), but not on the velocity of the moving boundaries. Figure 8 shows that the delay needed for reaching a time-independent stress on the boundary is approximately 50 for $n=2$ and $d=36$; for larger d this delay increases but remains smaller than 2000 for $d<200$. There is another, but less direct way to show that a stationary state is reached. In fact, let us consider the equations of momentum conservation which are

$$\frac{\partial J_x}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}(n+P) = 0\,; \tag{3.3a}$$

$$\frac{\partial J_y}{\partial t} + \frac{1}{2}\frac{\partial}{\partial y}(n-P) = 0\,. \tag{3.3b}$$

In Eq. (3.3), J_x and J_y are the (x,y) components (the x,y axes are parallel to the directions of the lattice) of the momentum $\vec{J}$, and P represents the viscous "pressure." Owing to the symmetry of the Couette flow, one can guess that the number density remains uniform. Thus, from (3.3), the pressure P is also constant in a steady Couette flow. We verified that the mean number density is constant throughout all the flow with a relative deviation less than 10^{-3}. A microscopic definition of the pressure P can be found by noticing that P changes its sign if the axes (x,y) are rotated by $\frac{1}{2}\pi$. The only combination allowed for P is

$$P(x,y) = E(n)\langle a(x,y) - b(x,y) + c(x,y) - d(x,y)\rangle\,. \tag{3.4}$$

In Eq. (3.4) the quantities (a,b,c,d) are equal to one (or zero) if there is (or is not) a particle at the site (x,y) with a velocity pointing toward (x_+,y_+,x_-,y_-), respectively, as shown in Fig. 9, and if $E(n)$ is a function of density only. In Eq. (3.4), the average is taken on the initial conditions. We find that the viscous pressure P is constant, although there is a slight decrease of the order of 3% near the moving boundaries in a layer of a mean-free-flight length. The value of the mean-free-flight time is given in Fig. 10 and was calculated theoretically.[7] By increasing the size of our system, we can reduce the relative importance of this kinetic boundary layer.

Let us give a last qualitative feature; by removing the collisions, one gets a flow wherein everything can be computed very simply. The corresponding velocity profile is shown in Fig. 11 and, as we shall see in Sec. IV, the viscous force (a misleading expression is this case) can be related in a simple way to the velocity v_0 of the moving boundaries.

After these verifications, there is little doubt that our numerical experiments show actually that the velocity profile in a Couette flow in our model

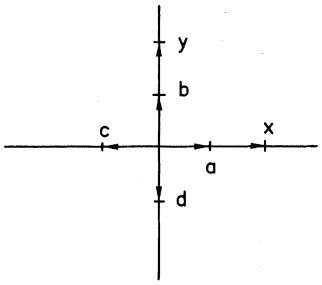

FIG. 9. Four cardinal directions of the lattice.

is not linear, as would be predicted by the Navier-Stokes equations; the question is: what sort of "generalized" Navier-Stokes equation can explain the observed behavior?

IV. INTERPRETATION

In this section we shall try to relate the results of our "experiments" to existing theories.

We shall first examine in more detail the adsorption process which communicates momentum from the walls to the fluid, and relate the microscopic adsorption law to the apparent velocity of the boundary. Let us denote by $\{n_1, n_2, n_3, n_4\}$ the mean number density of particles on the boundaries with velocities pointing toward the direction (1, 2, 3, 4), respectively, as shown in Fig. 12 and p the probability that, if a particle collides along a moving boundary, the next time it will get a velocity in the direction 3. If two particles (instead of one) are colliding at the same vertex on the boundary (which means they have different velocities), we just reverse the velocities in order to keep constant the number of particles. This arises from the discrete nature of the velocity space; it complicates a little the expression for the velocity

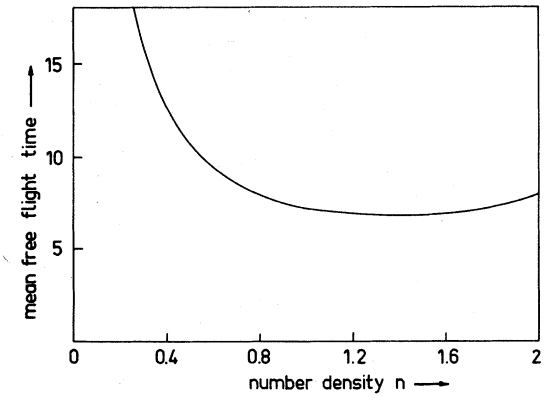

FIG. 10. Mean-free-flight time as a function of the number density.

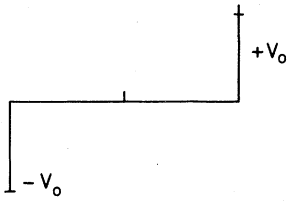

FIG. 11. Velocity profile of the collisionless gas.

of the moving boundaries. Let us assume that, close to the boundary there is no correlation between the particles with different velocities at the same vertex; then, from the definition of the adsorption process,

$$n_4 - n_3 = [n_1(1-n_2) + n_2(1-n_1)](1-2p)\,. \tag{4.1a}$$

At each collision the momentum normal to the boundary changes its sign. Thus,

$$n_1 + n_2 = n_3 + n_4\,. \tag{4.1b}$$

Let V_0 be the fluid velocity close to the boundary. Thus,

$$n_1 - n_3 = (n_1 + n_3)V_0 \times 2^{-1/2}\,; \tag{4.1c}$$

$$n_2 - n_4 = -(n_2 + n_4)V_0 \times 2^{-1/2}\,. \tag{4.1d}$$

Defining n as the mean particle number per site, from (4.1)

$$\tfrac{1}{4}nV^2 - \frac{V}{1-2p} + (1 - \tfrac{1}{4}n) = 0\,, \tag{4.2}$$

where $V = V_0 \times 2^{-1/2}$. This connects the value of the boundary velocity with the number density and the probability P; for a given p this velocity decreases with density, as expected. Figure 13 gives a comparison of the solution of (4.2) and "experimental" observation; the agreement is better than 3%.

Another point can be predicted theoretically: in the collisionless limit (i.e., if the mean free path is much larger than the distance between the walls), the expression for the "viscous" force is

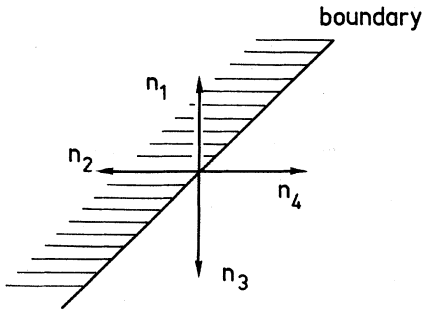

FIG. 12. Geometry of the boundary and of the lattice directions.

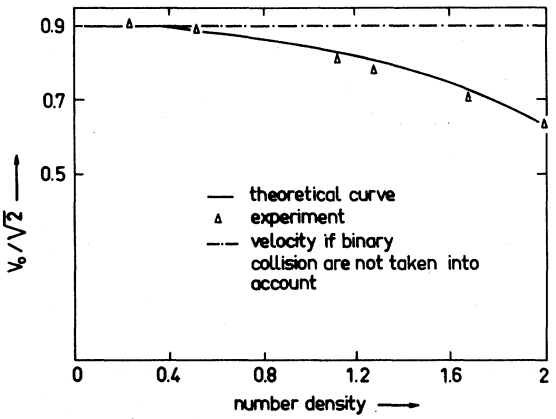

FIG. 13. Influence of number density on the velocity of the fluid near the boundaries for $p = 32/648$.

easy to derive:

$$f = n_2(1-n_1)(1-p) - n_1(1-n_2)p + n_4(1-n_3)(1-p) - n_3(1-n_4)p \,. \tag{4.3}$$

By using Eq. (4.1), one finds

$$f = (\tfrac{1}{2}n)V \,. \tag{4.4}$$

This result is verified with a relative deviation less than 10^{-5}.

It remains to approach the main problem: how does the viscous pressure P depends on the number density and on the momentum. Although we cannot give any quantitative answer, we find some results in this direction. The first point is that the Navier-Stokes expression of P,

$$P = \theta\left(\frac{\partial J_x}{\partial x} - \frac{\partial J_y}{\partial y}\right) , \tag{4.5}$$

[where θ is the viscosity that is assumed to exist, and $\vec{J} = (J_x, J_y)$ is the momentum] gives a linear profile for the fluid velocity, which is in clear contradiction with our observations (Fig. 6).

We tried thus to replace the spatial derivatives of the velocity field in (4.5) by a more general operation giving as a particular case the derivatives. The mathematical devices are used in the theory of noninteger derivatives. Let us define, for any function f vanishing outside of a bounded support:

$$\frac{\partial(F,f)}{\partial x} = C\int_{-\infty}^{+\infty} \frac{f(x-t)}{F(|t|)}\,dt = \lim_{\epsilon\to 0}\left(\int_{-\infty}^{-\epsilon} dt + \int_{\epsilon}^{\infty} dt\right)\frac{f(x-t)}{F(|t|)} \,, \tag{4.6}$$

where C is the Cauchy principal value and F a function to be defined. If the integration from zero to infinity is possible, this C may be omitted. In the particular case of the noninteger derivative of the αth order:

$$F(x) = 2\Gamma(-\alpha)x^{\alpha+1} \,. \tag{4.7}$$

One recovers the usual derivative as the limit of (4.6) with (4.7) $\alpha \to 1$ (integer).

Let us suppose that, the viscous pressure P can be expressed by

$$P = \theta\left(\frac{\partial(F,J_x)}{\partial x} - \frac{\partial(F,J_y)}{\partial y}\right) \tag{4.8}$$

in place of (4.5). With the symmetry of the chosen Couette flow J_x and J_y depend only on one variable, say x. As verified in the numerical simulation, the viscous pressure P does not depend on x and is trivially related to the viscous force by

$$\tfrac{1}{2}P = f = \theta\,\partial(F,J_x)/\partial x \,. \tag{4.9}$$

As the velocity profiles and the (n,d) dependence of f are known, Eq. (4.9) is an integral Volterra equation of the first kind. Inserting (3.2) and (4.6) in (4.9), one finds

$$f = \theta V_0 \times d \times C\int_{-1}^{+1} \frac{\nu(x-t)}{F(td,n)}\,dt \,, \tag{4.10}$$

where ν is the normalized velocity profile.

One recovers here that f is proportional to V_0. The case of the usual Navier-Stokes equations corresponds to $F(xd) = d^2F(x)$ which is consistent with (3.1). In principle the d dependence of the viscous force f make it possible to invert (4.10) to find an expression for $F(x)$; unfortunately, it seems that this problem is not well posed in the Hadamard's sense (i.e., even if f and the velocity profile $\nu(x)$ are known very accurately, one gets very poor information about F). Nevertheless, one can guess that the operation (4.6) has a differential nature and, for this reason, the sign C is needed in it.

To conclude, we see that the numerical experiment carried out with this model of classical fluid exhibits two unexpected properties of transport phenomena in fluids of less than two dimensions: (i) The viscous resistance is proportional to the velocity of the moving walls. (ii) Because of the density dependence of F, one cannot explain our results by means of universal (i.e., depending only on the dimensionality of space and on a few other qualitative properties of the model) and "renormalized" law as the one predicted by current theories.[2,8]

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