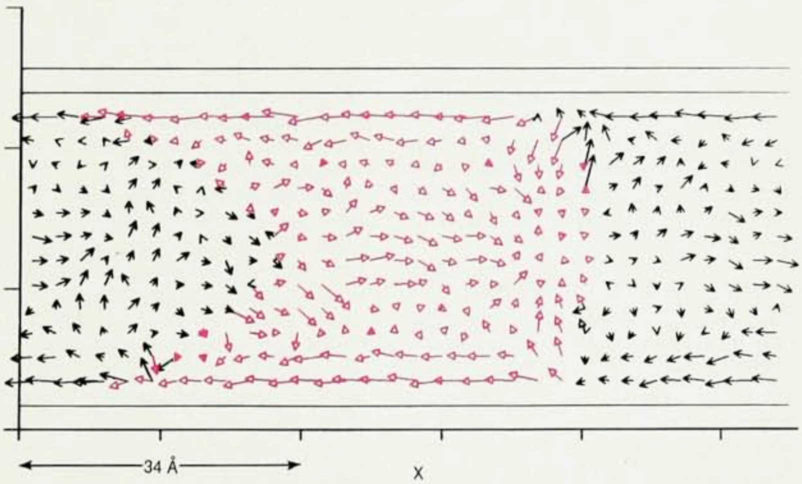
NUMERICAL SIMULATIONS REVEAL FLUID FLOWS NEAR SOLID BOUNDARIES

A thin layer of dust is not blown off the blades of a fan when the fan is turned on; only large dust particles are. Nor can one remove the fine layer of dust from a tabletop by blowing parallel to the table's surface. Richard Feynman, in his famous lectures on physics, used these examples to illustrate that in the relative motion of a viscous fluid past a solid, the component of the fluid velocity along the solid surface vanishes at the solid–fluid interface. Recent molecular dynamics simulations by a group at Schlumberger–Doll Research (Ridgefield, Connecticut) elucidate the nature of fluid flows near a solid boundary, and especially near the line where the meniscus (or interface) between two fluids meets the solid boundary.[1]

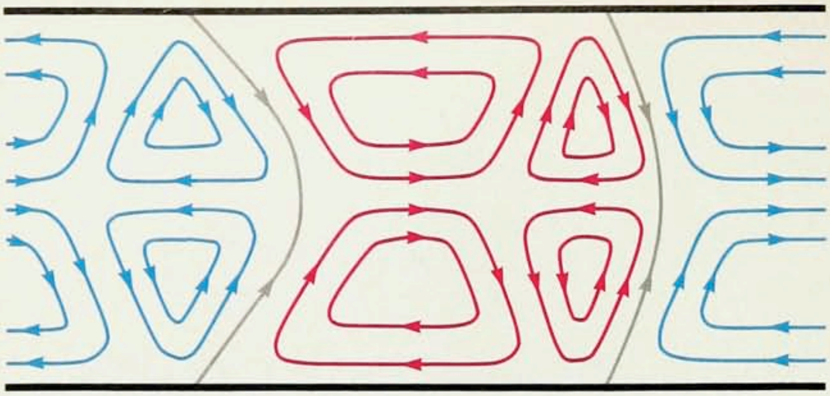


Simulated velocity field of a two-fluid system confined between parallel walls, when each molecule is subjected to a uniform acceleration to the right. The molecular properties of the fluids are defined in such a way that one fluid (red) "wets" the solid walls preferentially. The velocity vectors are shown in a reference frame in which the mean velocity of the interface between the two fluids is zero. The velocity field is consistent with the flow pattern shown on page 18. By symmetry, the velocity field is invariant in the y direction. The Lennard-Jones distance parameter, which is 3.4 Å for liquid argon, sets the length scale in the simulation. (Adapted from a figure provided by the Schlumberger group.)

A viscous fluid flows when it is sheared—by confining it between two parallel plates and moving one with respect to the other, for example—unlike an ideal fluid, which has no viscosity to transfer momentum from the moving plate to the fluid. The condition of zero slip between a flowing viscous fluid and a stationary solid boundary may therefore seem intuitively obvious, because the internal drag, or shear stress, due to viscosity slows down the fluid layers near the boundary. But there has been no microscopic justification for the condition, although it has been used for over a century in solving equations of hydrodynamics.

James Clerk Maxwell, in 1879, discussed a model in which fluid molecules were reflected by solid walls. Maxwell considered two kinds of reflections: Either the angle of reflection was the same as the angle of incidence, as in specular reflection, or the angle of reflection was random and the kinetic energy of the reflected molecules depended on the temperature of the walls, which were treated as a structureless heat bath. By a simple calculation assuming that the fluid molecules obeyed the laws of the kinetic theory of gases, Maxwell showed that the tangential component of the fluid velocity at the walls was proportional to the shear stress times a factor called the slip length, which in turn was proportional to the mean free path for the fluid molecules. Because the mean free path in a dense liquid is on the order of the intermolecular distance, and therefore microscopically small, Maxwell argued that the no-slip condition must be valid for hydrodynamic equations, which describe macroscopic behavior.

Although Maxwell did not treat realistic liquids and solids, his seems to be the only sensible and theoretically interesting treatment that addresses the origin of the no-slip condition, according to Joel Koplik (Schlumberger–Doll). "But," Koplik adds, "Maxwell's treatment does not shed any light on the nature of the fluid flows near the boundary. For example, it does not tell us whether molecules within a mean free path of the wall are stuck to it or whether they execute a rolling motion, similar to that of a rigid ball rolling on a surface, so that the instantaneous tangential velocity at the wall is zero." The simulations the Schlumberger group reports show that fluid molecules neither stick to nor roll



Flow pattern for a two-fluid system confined between parallel walls and accelerated to the right. In this pattern, suggested by an experiment by Elizabeth B. Dussan V., a jet flows back into the fluid, in the eddies to the left of the menisci (gray lines). (Adapted from a figure provided by the Schlumberger group.)

near the walls. Each molecule executes a Brownian motion on which are superposed a uniform drift reflecting the average flow of the fluid and a temporary localization near the walls due to the attraction to the wall molecules.

Wetting and contact angles

The need to understand fluid flows that give rise to the no-slip boundary condition becomes especially critical when one asks what the appropriate boundary condition is at the line where the meniscus between two fluids meets the solid boundary. Analytical studies of hydrodynamic equations break down when the no-slip boundary condition is straightforwardly applied to each fluid: In the standard treatment of the flow of one fluid with respect to the other, which is due to Chun Huh and L. E. Scriven (University of Minnesota, Minneapolis), the energy dissipated into heat due to viscous drag diverges for any volume element that contains the contact line. Furthermore, as Roger Dashen (University of California, San Diego) pointed out to us, straightforward application of the no-slip boundary condition to a two-fluid system leads to a contradiction if one assumes that the condition arises because the fluid layers adjacent to the walls are stationary. It implies that the contact line does not move! "Understanding fluid flows near the contact line is therefore one of the classic unsolved problems in fluid dynamics," Dashen said.

Questions about the dynamics of menisci and their contact lines are intimately related to issues of great technical significance. The shape of the meniscus separating two fluids confined by solid walls depends on which of the fluids "wets" the solid preferentially. The angle the meniscus makes with the solid surface is not uniquely determined, however, by the chemical compositions of the fluids and the solid, but depends, among other things, on surface roughness and chemical contaminants. If the angle is zero, one says that one of the fluids wets the solid completely. A fluid that wets a porous rock completely will not be extracted when the rock is penetrated with a fluid that does not wet it. Studies of contact angles and of the factors on which they depend, especially when one fluid is forced to displace another, are therefore of considerable technical importance in improving methods for flotation of molten ores and extraction of oil from porous rock.

Molecular dynamics

The Schlumberger group—Jayanth R. Banavar, Jorge F. Willemsen and Koplik—simulated numerically fluid flows between two parallel solid walls. Both the walls and the fluid were assumed to be made of inert molecules interacting via the Lennard–Jones potential. (The Lennard–Jones potential has an attractive part that varies inversely as the 6th power of the distance between the molecules and a repulsive part that varies as the 12th power of the inverse of the distance.) But the molecules constituting the walls were assumed to be 10^{10} times heavier than those in the fluid: A layer of the heavier molecules was almost stationary on the time scale of the simulation and so acted like a wall. The behavior of this collection of molecules was studied by the molecular dynamics technique, in which Newton's equations of motion are integrated numerically.

Several novel techniques for simulating hydrodynamic behavior have been discussed in the past few years. One such technique, known for both its novelty and its computational ease, replaces the continuum velocity and pressure fields of hydrodynamics by cellular automata, and the differential equations of hydrodynamics by rules for the automata. The rules satisfy conservation laws, such as those for mass and momentum, that also motivated the hydrodynamic equations. (See the column by Leo Kadanoff in PHYSICS TODAY, July 1986, page 7.) Dashen told us, however, that questions regarding the no-slip boundary condition and the dynamics of menisci involved details of the interaction between the fluid and solid molecules and therefore could be addressed only in a molecular dynamics simulation.

The molecular dynamics technique has been used extensively over the past 30 years to study the equilibrium properties of solids, liquids and other condensed systems; its use for hydrodynamical studies is a relatively recent development (see, for example, the article by William G. Hoover in PHYSICS TODAY, January 1984, page 44). In 1986, Dennis C. Rapaport (Bar-Ilan University) and Enrico Clementi (IBM, Kingston, New York) used molecular dynamics to simulate the flow of a two-dimensional fluid past a circular obstacle.[2] The simulation at large Reynolds number (that is, for small values of the coefficient of viscosity or for large fluid velocities) demonstrated the appearance of eddies and their periodic shedding into the wake behind the obstacle. Last year Michele Mareschal and Ed Kestemont (Université Libre de Bruxelles) used molecular dynamics to simulate convection rolls in a Rayleigh–Benard system, in which a fluid in a gravitational field is subjected to a thermal gradient.[3]

A molecular dynamics simulation produces snapshots of the molecular configurations in the system being simulated. In a fluid, this means attaching a position coordinate and a velocity vector to each molecule at each time step in the integration of the equations of motion. To study hydrodynamic behavior, which is a macroscopic property of the fluid and not a microscopic property of individual molecules, the Schlumberger group had to average molecular positions and velocities over finite bins and time steps to obtain positions and velocities representative not of the molecules but of finite elements of the fluid. The simulation used only 1536 molecules (per fluid) confined to a cell of linear dimension up to 100 Å. (By contrast, the simulations reported by the IBM Kingston group had used up to 2×10^5 molecules.) The equations of motion were integrated for intervals of up to 10^{-9} seconds using a time step of about 10^{-14} sec. Each bin contained about 10 molecules and the averaging procedure used up to 5000 steps. If the bin size for averaging had been too large, there would not have been enough fluid velocity vectors to reveal the spatial patterns in the flow; if too many time steps had been used for averaging, the dynamical features of the flows would have been lost. On the other hand, small bins and too few time steps in the averaging would not have revealed smooth and steady hydrodynamic flows but would have shown the disorder characteristic of molecular motion. The success of the Schlumberger simulation therefore rested on the judicious choice of the bin size and the time steps in the averaging procedure.

Poiseuille flow

When a viscous and incompressible fluid is forced to flow between two walls, by the application of pressure at one end, for example, not all points on the fluid front move with the same velocity. The tangential component of the fluid velocity is a quadratic function of the distance from the walls, vanishing at the walls and having its maximum value in the middle. This parabolic velocity profile defines a flow pattern called Poiseuille flow, which has been well characterized by analytical studies of the equations of hydrodynamics. But one must impose the no-slip boundary condition on the hydrodynamic equations to obtain analytical solutions corresponding to Poiseuille flow.

In the simulation that the Schlumberger group reports, Poiseuille flow emerges quite naturally when molecules are subjected to a uniform external force in a direction parallel to the walls. Poiseuille flow has been seen earlier in numerical simulations: The IBM Kingston group studied it in molecular dynamics simulations using walls that had physical properties similar to those assumed by Maxwell in his theoretical model, and Kadanoff, Guy McNamara and Gianluigi Zanetti obtained the flow pattern using cellular automata.[4] But confirmation of this well-characterized fluid flow in the Schlumberger simulation showed, first, that simulations of a few thousand molecules using the molecular dynamics technique may be usefully employed to study hydrodynamics and, second, that the no-slip boundary condition is a natural outcome of the interaction between the molecules of the solid and the fluid. Furthermore the simulation showed that the mean fluid flow imposes a uniform drift on the molecular Brownian motion and that attraction between molecules in the walls and those in the fluid localizes the fluid molecules near the walls only temporarily.

Moving contact lines

To study the flow of two immiscible fluids and the dynamics of the meniscus separating them, the Schlumberger group modified the potential between molecules of different species. The interaction between the molecules of the same species was of the standard Lennard-Jones form, but the attractive part (r^{-6}, where r is the intermolecular distance) of the potential between different species was reduced. In the simulations for the velocity field shown in the figure on page 17, the attractive interaction between the two liquids was completely removed, while those between each of the two liquids and the walls were reduced by different amounts. The latter choice led to preferential wetting.

Molecular dynamics simulation of the two-fluid system showed that the contact angle the meniscus makes with the walls changes slowly with time. The fluid that preferentially wets the walls forms a thin film along the walls when it moves or is displaced by the other fluid. Most important, the simulations show that the no-slip condition breaks down at the contact line and that a jet flows back into the fluid (see the figures on pages 17 and 18).

The behavior seen in the simulations is consistent with observations made by Elizabeth B. Dussan V. (now at Schlumberger-Doll Research) in 1977. Dussan used a dye to study qualitatively the motion of the interface between oil and glycerin in a vertical Plexiglas tube when the glycerin was pumped up so that it displaced the oil. "It would be very nice if the simulations could be extended to give a more quantitative handle on the contact angle," Dussan told us. "The angle changes rapidly near the boundary, but it is difficult to determine precisely the shape of the meniscus a few microns away from the boundary." The simulations might also help map out the viscous drag and thereby provide useful insights into the singularities obtained in earlier theoretical treatments of fluid flows near the contact line.

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References

1. J. Koplik, J. R. Banavar, J. F. Willemsen, Phys. Rev. Lett. **60**, 1282 (1988).
2. D. C. Rapaport, E. Clementi, Phys. Rev. Lett. **57**, 695 (1986).
3. M. Mareschal, E. Kestemont, Nature **329**, 427 (1987).
4. L. Hannon, G. C. Lie, E. Clementi, Phys. Lett. A **119**, 174 (1986). L. P. Kadanoff, G. McNamara, G. Zanetti, Comp. Sys. **1**, 791 (1987).

VERY SMALL TUNNEL JUNCTIONS SENSE THE EFFECT OF SINGLE ELECTRONS

In most capacitors the gain or loss of a single electron is hardly noticed. But in the very small tunnel junctions that can now be made, the capacitance is so small—on the order of 10^{-16} farads or less—that the addition of just one electron can change the electric potential across the barrier by several millivolts. In that case, a single electron certainly can make a difference. The change in potential when an electron tunnels across the junction is enough to impede the tunneling of the next electron. The resulting block of current flow—called the Coulomb blockade—should show up in the current-voltage characteristics of small-capacitance tunnel junctions at low temperatures.

Ivar Giaever (General Electric) and Hans-Rudi Zeller (now at Brown Boveri) found such a blockade in 1968 as they were measuring the current-voltage characteristics of tunnel junctions containing isolated metal grains within the insulating barrier. (A tunnel junction consists of an insulator sandwiched between two conductors.) The two experimenters postulated that the observed behavior resulted from the electron charging effects. John Lambe (now at the Jet Propulsion Laboratory) and Robert Jaklevic (Ford Motors Scientific Laboratory) saw similar structure the next year. After a long hiatus, the electron charging effect is now attracting considerable attention because of improved experimental techniques and recent theoretical predictions of related phenomena.

Last year Theodore Fulton (AT&T Bell Labs, Murray Hill) and Gerald