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Abstract

Studies in two dimensions have been made of the evolution of an initially linear interface between two liquid areas by both continuum hydrodynamics and molecular dynamics. It was found that at both levels the interface evolves into a fractal curve. While the limiting fractal dimensionalities (D) of the continuum and molecular interfaces differ, this difference is no greater than that that can be induced in the hydrodynamic results by marked changes in the initial conditions and/or fluid parameters. There is, however, a marked qualitative difference in the initial values of D. This is discussed and shown to be a natural consequence of the molecular discreteness of the real liquids.

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Studies in two dimensions have been made of the evolution of an initially linear interface between two liquid areas by both continuum hydrodynamics and molecular dynamics. It was found that at both levels the interface evolves into a fractal curve. While the limiting fractal dimensionalities (D) of the continuum and molecular interfaces differ, this difference is no greater than that that can be induced in the hydrodynamic results by marked changes in the initial conditions and/or fluid parameters. There is, however, a marked qualitative difference in the initial values of D. This is discussed and shown to be a natural consequence of the molecular discreteness of the real liquids.

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Since its introduction by Mandelbrot [1], the concept of "fractal dimension" has been found to be applicable to an extraordinary diversity of systems whose studies appear to span from geological [2] to biological [3] sciences through physics, chemistry, and engineering, with no discrimination between "basic" and "applied" problems. However, there appears to be one important limitation inherent in the fractal concept, and that concerns the physical scale over which it is operative. Specifically, the need to define a surface at all length scales appears to preclude its application down to the level of interatomic distances, since at and below that level such a *unique* interface ceases to be defined. However, there is increasing evidence that the structures predicted from continuum mechanics (e.g., the Navier-Stokes equations) can also be found to emerge from atomistic simulations (molecular dynamics) using variously realistic interatomic potentials. As examples recent work has found this to be the case for vortex formation in turbulent flow [4,5], while work by Koplik, Banavar, and Willemsen [6,7] has demonstrated the atomistic modeling of boundary layers. However, key to the observation of macroscopic fractal surfaces is strong nonlinearity in the continuum equation, a feature shared with the atomistic equations used in the microscopic simulations [4–7], since the interatomic force laws are highly nonlinear. This raises the interesting possibility that fractal behavior can be observed in *microscopic* simulations of motion in situations when the analogous *macroscopic* interfaces are known to be fractal. The object of this article is to demonstrate that this is indeed the case; specifically that at both the continuum (macroscopic) and atomic (microscopic) levels the evolution of a fluid interface show closely similar behavior and specifically fractal character.

Currently two of us (R.W.D. and S.R.D.) are involved

in extensive studies on two-fluid mixing in two dimensions. In these studies, we chose to examine what occurs when the two fluids are identical, inviscid, and gravity is absent. It transpired that the surface [8], on being subjected to small perturbations, somewhat to our surprise, developed a fractal character. This is illustrated in Figs. 1(a)–1(c), which show, respectively, (a) a typical profile of the interface; (b) a plot from which D, the fractal dimension, is determined; and (c) a plot of D against time.

In order to study the same situations by molecular dynamics, we used a two-dimensional lattice of atoms interacting by a 6-12 Lennard-Jones potential, which approximated the Ar-Ar potential. In order to accelerate the simulation, we used an atomic mass of 16 a.u.

Initially, the lattice was separated into two halves, the atoms in each initially being given a suitably chosen set of random velocities, and then allowed to thermalize, during which process both melted. The simulation was then halted and the two liquid halves were joined. The simulation was restarted and the interface evolution was monitored as a function of time. In Figs. 2(a)–2(c), we show the lattice analogs of the continuum result in Fig. 1. Since the temperatures used were ∼300 K, we were in effect dealing with superheated liquids. In order to prevent spontaneous disintegration, we held the boundary atoms fixed throughout.

It can be seen from Figs. 1(a) and 2(a) that there is qualitatively a very close similarity between the two interfaces, while Figs. 1(b) and 2(b) and 1(c) and 2(c) first show that there is *quantitative* similarity in the actual values of D, and second show that their temporal evolutions are also closely similar. There is, however, a clear difference between the behavior at early times, which has to be addressed. To do so, we return to Fig. 2(a), which shows the atomistic interface. In order to make a fractal
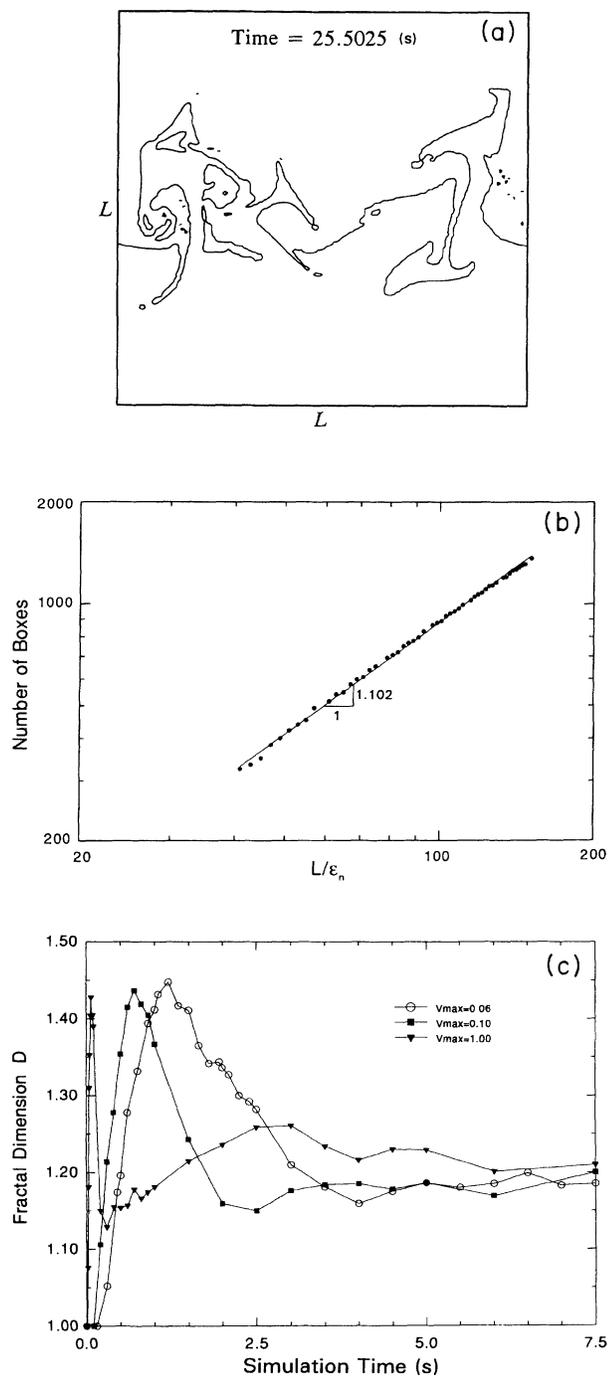
Time = 25.5025 (s) (a)

(b)

analysis, one needs a continuous curve: the curve shown was obtained by smoothly joining the midpoints of two adjacent atoms from different sides to the initial interface.

Clearly this is a somewhat arbitrary procedure. However, for that particular interface, it is unimportant since D turns out to be insensitive to how the surface is defined. The reason is simple, the uncertainty in surface location is $\sim \pm 1$ interatomic spacing, while the scale of surface fluctuations in Fig. 2(a) is ~ 5–10 interatomic spacings. At earlier times, this is not the case. This can be seen from Figs. 3(a) and 3(b) where continuum and atomic interfaces are shown for $t \simeq 0$. In the continuum case D has changed abruptly from 1 to ~ 2 simply because the mo-

(a)

(c)

FIG. 1. Simulation [9] of interfacial [8] dynamics for an inviscid fluid (density of 1000 kg/m^3) contained with two horizontal solid planes a distance $L = 1$ m apart. The vertical walls (separated by L) impose a periodic boundary condition. The finite-difference mesh consisted of a uniform grid of cells of size $L/150$. The fluid velocity components (u,v) within each cell were initially assigned random magnitudes whose absolute value was $V_{max} \leq 1$ m/s. (a) A typical interface after a rather long period of evolution. (b) Computation of fractal dimension D (at 25.5025 s) by covering the simulation domain with a collection of squares (boxes) of side length ϵ_n. (c) Evolution of D showing the initial jump due to the initial perturbation and its subsequent stabilization.
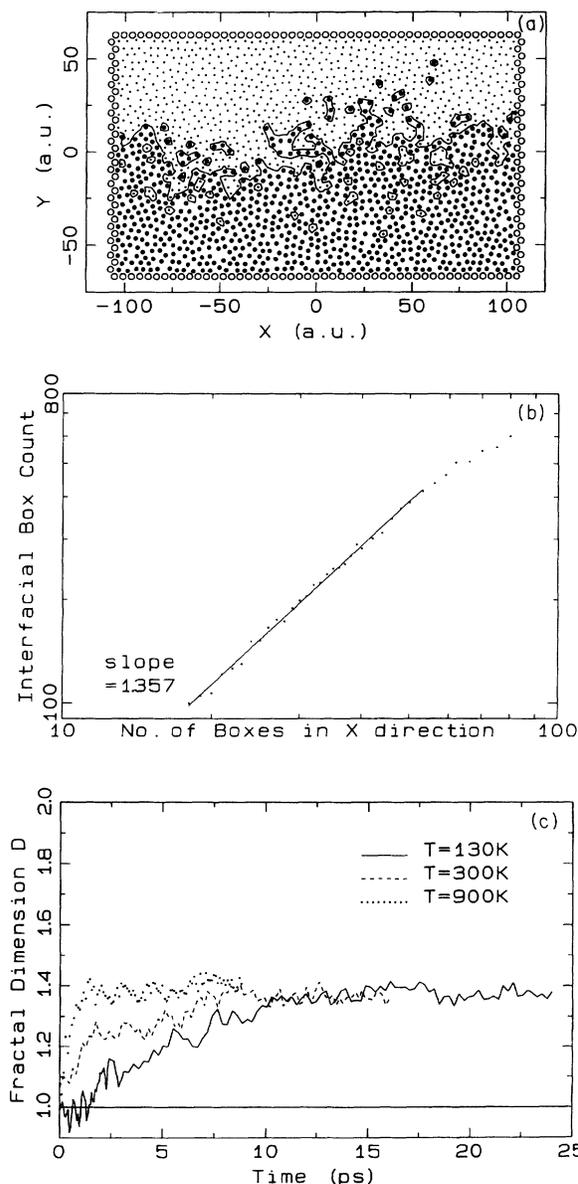

(b)

(c)

FIG. 2. Results for the molecular-dynamics (MD) simulations. (a) Typical interface, well on into the simulation (at 16 ps, 300 K). (b) Computations of the fractal dimension D for the MD interface [see caption Fig. 1(b) for procedure]. (c) Plot of D as a function of time—note absence of an initial jump (see text).
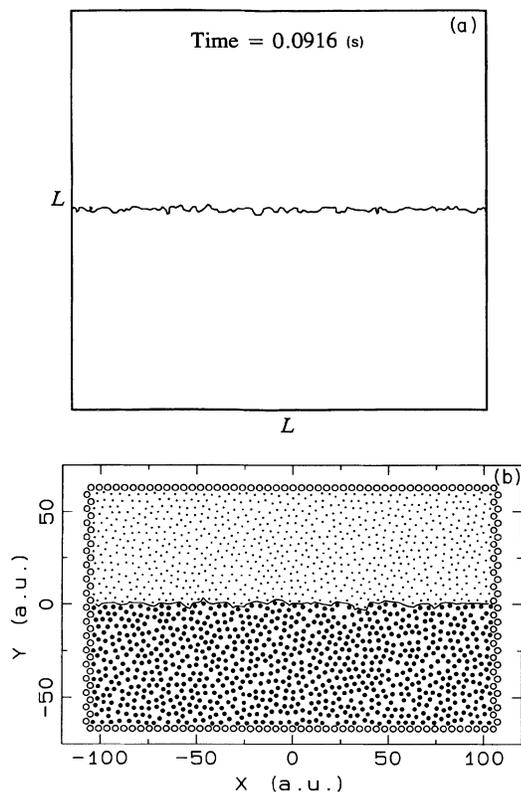
FIG. 3. Interfaces at very short time showing the initial response to the initial perturbation: (a) for the continuum case, and (b) for the MD simulation (at 0.1 ps, 300 K).

ment the interface has width (when $t \simeq 0$ but $\neq 0$), D jumps to $\simeq 2$. The jump is almost instantaneous because the response to the initial perturbation is that rapid. At $t \simeq 0$ a perturbed fluid element is affected only by the perturbation since the time scale of the bulk response is much longer; hence the initial jump in D, which then falls to the value characteristic of the true interface, rather than the perturbation, as this begins to evolve.

On the other hand, it can be seen from Fig. 3(b) that for the lattice the value of D at $t \simeq 0$ is essentially arbitrary since much of the interface "width" at that early time was already present at $t = 0$, because the convention used to define the interface did not produce an exactly straight line. Moreover, the situation can be further complicated by the uncontrollable nature of the initial union of the two lattice segments, which arises from the initial juxtaposition across the interface of atoms whose relative separation is entirely random, as is the resultant impulse profile. Given these uncertainties, intrinsic in the discrete nature of matter at the atomic level, it is entirely reasonable to argue that the concept of fractal interfaces at the atomic level is only valid if the scale of their structure is clearly several interatomic spacings.

One can also express this difference in terms of a Fourier decomposition of the $t \simeq 0$ interfaces. For the continuum there is no lower bound on the wavelength and thus no upper bound on the frequency; hence the

quasi-instantaneous response described above.

For the lattice this is not the case, since allowed wavelengths are bounded from below by the first-neighbor spacing of the atoms. This in turn imposes an upper bound on the response frequency and precludes the quasi-instantaneous response shown by the continuum, and *even at* $t \simeq 0$ it imposes on the response the *natural* time scale of the lattice as a whole. As a consequence, while the perturbation of uniting the two halves of the lattice is a step function in time with no upper bound in its Fourier transform, only those frequency components that lie *below* this cutoff can initiate deformation of the interface. Consequently ultrahigh-frequency components responsible for the width in Fig. 3 for the continuum are disallowed. Hence arises this single qualitative difference between continuum and lattice results.

At longer times, the fractal characteristics of the lattice interface appear to be virtually identical to those of the macroscopic systems. Moreover, when this regime is attained we find very little, if any, dependence of D on the initial conditions, and such dependence as may be is only comparable to that found in continuum simulations initiated by varying initial perturbations. This was also true for simulations run for an atomic array of double the width, and for an array in which the 6-12 potential was reduced by 20% for one of the initial two halves. The first finding indicates insensitivity to boundary conditions, and the second shows a similar lack of great sensitivity to the presence or absence of surface tension between the two fluids.

In summary, we have demonstrated that the fractal character of fluid interfaces, demonstrated by macroscopic hydrocode simulations of fluid mixing, is also displayed at the microscopic level by molecular-dynamics simulations of mixing at the atomic level. This would appear to be yet another demonstration of the remarkable generality of fractal behavior and, perhaps just as significantly, demonstrates that another important qualitative concept of macroscopic hydrodynamics can also be manifested at the microscopic level.

In addition, this would also appear to demonstrate the microscopic onset of turbulence at the interface, since this is certainly present in the hydrocode simulation. While this is incidental to the present work, it would appear to present the possibility of studying turbulent flow under regimes of more specific interest from a purely atomic viewpoint that would be free from the uncertainties regarding boundary conditions inherent in hydrocode simulations.

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