PHYSICAL REVIEW E VOLUME 61, NUMBER 1 JANUARY 2000

Growth of Taylor vortices: A molecular dynamics study

D. Hirshfeld and D. C. Rapaport
Physics Department, Bar-Ilan University, Ramat-Gan 52900, Israel
(Received 5 May 1999)

Molecular dynamics methods have been used in a quantitative study of the growth and decay of Taylor vortices in a fluid confined between concentric cylinders when the rotation of the inner cylinder is instantaneously started or stopped. Analysis of the temporal evolution of the vortex flow fields shows that the behavior of this microscopic system agrees with experiment. In order to make the analysis entirely self-contained, torque measurements have been used to determine the effective viscosity of the fluid.

PACS number(s): 47.32.Cc, 02.70.Ns, 47.15.−x, 47.20.−k

The traditional approach to fluid mechanics has, in general, managed to avoid addressing the true atomistic nature of matter. Except in cases where the underlying assumptions are clearly violated, this approximation has not affected the predictive capability of a theory whose key premise is that the fluid medium is a continuum. The means of bridging the gap between this representation and the actual atomistic nature of matter is by computer modeling of (classical) discrete-particle systems; of the techniques available, the molecular dynamics (MD) approach provides the greatest flexibility for simulations of this kind.

The computational effort required for MD simulation imposes a severe size limitation, thus presently tractable systems are microscopic in the extreme. While the ability of MD to reproduce relatively complex hydrodynamic behavior, both in and out of equilibrium, is now well-established, the degree to which its quantitative predictions of nonequilibrium flow resemble macroscopic reality has yet to be determined. Self-organized structured flows such as vortex shedding [1], Rayleigh-Bénard convection cells [2], and Taylor-Couette vortices [3], have all been reproduced by MD techniques, but most quantitative aspects, beyond the overall pattern shapes themselves, remain unexplored.

In this Rapid Communication we describe an attempt to use MD in measuring the detailed time-dependence of the Taylor-Couette flow instability [4–6]. This particular flow problem, in which toroidal vortices form spontaneously in a sheared fluid confined to the annular region between rotating cylinders, has been extensively studied both theoretically and experimentally, and there is a substantial amount of data available for comparison. From the MD point of view, the only disadvantage in choosing to study this particular centrifugal flow problem is that unlike vortex shedding and thermal convection where two-dimensional versions of the problem can be modeled, in this case the flow is inherently three dimensional, leading to increased computational requirements.

Taylor-Couette flow has long been recognized as the prototypical system for studying the nature of the onset of flow instability in which simple laminar flow is replaced by more complex (but nonturbulent) structured flow patterns. If the angular velocity of the inner cylinder is ω, and the outer cylinder is at rest, then the overall nature of the flow depends on the Taylor number

$$T=4[(1-\eta)/(1+\eta)]R^2, \tag{1}$$

where

$$R=dr_i\omega/\nu \tag{2}$$

is the dimensionless Reynolds number, r_i and r_o are the inner and outer cylinder radii, $\eta=r_i/r_o$, $d=r_o-r_i$ is the annulus width, and ν the kinematic viscosity. The flow is purely azimuthal at low ω, but at sufficiently high ω corresponding to a critical Reynolds number R_c, or Taylor number T_c, secondary flow appears in the form of a uniformly spaced set of axisymmetric toroidal vortices.

The theoretical analysis of the Taylor instability is based on a perturbation treatment of the Navier-Stokes equations [6,7] that involves a Fourier expansion of each component of the velocity field; for example, the radial component at some fixed distance from the axis, as a function of axial position z, can be expressed as

$$v_r(z,\epsilon)=\sum_{n\geqslant 1} A_{rn}(\epsilon)\cos(nqz), \tag{3}$$

where q is the wave number of the fundamental mode and $\epsilon=T/T_c-1$. The coefficients A_{rn} are then expanded in terms of the small parameter ϵ,

$$A_{rn}(\epsilon)=a_n\epsilon^{n/2}(1+a_{n1}\epsilon+a_{n2}\epsilon^2+\cdots); \tag{4}$$

although ϵ is supposedly a small quantity, the experimental results are found to satisfy Eq. (4) over a much larger range. Corresponding results hold for the azimuthal and axial flow components. At larger R, beyond the values considered in this work, traveling azimuthal waves appear, and at even higher R the flow eventually becomes turbulent.

The equation governing the growth of the leading-order amplitude A_{r1} in response to a small axisymmetric perturbation (this holds for each of the velocity components) is of the form [6,7]

$$dA_{r1}/dt=\sigma A_{r1}-bA_{r1}^3 \tag{5}$$

where σ is the growth rate and $b>0$; in the $t\to\infty$ limit the amplitude is $A_e=\sqrt{\sigma/b}$. In terms of a normalized amplitude, $A=A_{r1}/A_e$, Eq. (5) becomes

$$dA/dt=\sigma(A-A^3), \tag{6}$$

with solution

$$A(t)=(1+3\exp[-2\sigma(t-t_0)])^{-1/2}, \tag{7}$$

where $A(t_0)=1/2$. Theory predicts that for small ϵ, $\sigma\propto\epsilon$.

Among the experiments that have measured the ϵ-dependence of the flow, some [8,9] have also examined the approach to a steady state following a sudden increase in rotation rate, as well as the decay of the vortex structure following an abrupt decrease. In cases where both initial and final rotation rates correspond to $R>R_c$, the growth and decay processes are symmetric, and the time dependence obeys Eq. (7), but where the transition is between rates corresponding to R values below and above R_c decay is much faster than growth, and only the growth phase follows Eq. (7).

The MD simulations are based on a soft-sphere model, and the details are as described in [3]; general aspects of MD methodology are to be found in [10]. The cylindrical container walls act as nonslip boundaries and dissipate heat generated by the sheared flow. Special periodic boundaries are used in the azimuthal direction; these reduce the computational effort, since only one quadrant of the annulus is represented explicitly. The cylinder radii are $r_i=50$ and $r_o=75$, with distances expressed in MD units so that the unit of length is approximately one atomic diameter; the value $d=25$ is practically the smallest annulus width for which stable vortex development occurs. Since the vortices have an almost square cross section the cylinder length is set to $h=100$ to accommodate the development of four vortices. The overall number density is 0.5, so that approximately 1.2×10^5 atoms are required in the simulation. The outer cylinder is fixed and the inner one rotates with constant angular velocity ω following the instantaneous start; the range of ω considered, 0.01–0.1, includes values both below and above R_c.

Each run begins with the atoms arranged on a grid filling the annulus and assigned random initial velocities. Inner cylinder rotation is then suddenly started and the flow is followed for a total time interval of $10^6\delta t$, where $\delta t=0.005$ is the integration time step (in MD units); this interval is sufficiently long for the system to reach a steady state over the entire range of ω considered. Cylinder rotation is then halted and the simulation continued until azimuthal flow ceases, requiring an interval of $10^5\delta t$ or less. Flow fields are evaluated over a grid having approximately unit spacing in the radial and axial directions, and are averaged both in the azimuthal direction, where no systematic variations occur, and temporally over intervals appropriate for revealing the details of the evolving flow patterns (typically $5000\delta t$ during growth and for steady flow, and $1000\delta t$ during the more rapid decay phase).

A consequence of the sudden start, unlike the gradual ramping used previously [3], is that a significant proportion of the runs that eventually achieved the desired final state evolved along pathways involving changing numbers of vortices. Although four vortices are expected for $h=4d$, in many cases five or six vortices developed initially; in some instances, later in the run (after a delay that might be as long as $2\times10^5\delta t$) these merged into four vortices, but on other occasions the larger number appeared to have stabilized. The measurements described below cannot be carried out when either of these events occurs, since only those growth scenarios in which the desired number of vortices are nucleated directly can be used for the analysis; thus, a substantial proportion of the runs (that differ merely in the choice of initial random velocities) had to be discarded. Anomalous behavior is more likely at higher ω; for $\omega=0.06$ four vortices always formed directly, whereas at $\omega=0.08$ only 30% of the attempts were successful, and at $\omega=0.1$ the success rate fell to below 20%. These anomalous modes, and the different kinds of behavior encountered in gradual and sudden starts, are not artifacts of the simulations but reproduce what is also seen in experiment [11].

Quantitative analysis of vortex structure and development depends on a knowledge of ν. The Taylor-Couette flow apparatus originated as a device for measuring viscosity [12] and the MD version will be used here in a similar fashion (in contrast, the analysis of [3] was based on an assumed value of ν). If ω is small enough for the flow to be purely azimuthal, then the total torque acting on either of the cylinders, G_l, can be derived from the theoretical shear rates at the boundaries [7],

$$G_l=4\pi\rho\nu h r_i^2\omega/(1-\eta^2). \tag{8}$$

Above R_c, a perturbation expansion for the torque can be developed in terms of ϵ [13],

$$G=G_l[1+g_1(\eta)\epsilon+g_2(\eta)\epsilon^2+\cdots]; \tag{9}$$

note that this result differs from the original in that the expansion parameter has been rescaled and there is a factor of 2 difference in the definition of T. An earlier theoretical derivation [7] led to an expression involving ω and ω^{-1}, which does not convey the fact that the vortices produce a perturbing torque superimposed on Eq. (8); experimental data have been fit to other powers of ω [14], as well as to Eq. (9).

The torque is obtained directly during the simulation from measurements of the momentum changes experienced by the atoms as they collide with the cylinder walls; the results, after the system reaches a steady state, are shown in Fig. 1. The fit included in the figure consist of two parts. Below R_c the fit is to Eq. (8), where ν is the only unknown; this yields a constant viscosity value $\nu=0.809$ (the assumed value used in [3] was $\nu=1$). Above R_c the fit is to Eq. (9), using a value of T_c derived below; the resulting coefficients (for $\eta=2/3$) are $g_1=0.485, g_2=-0.089$. Allowing for the fact that the perturbation result [13] is actually for $\eta=1/2$ and that g_2 cannot be determined very accurately, these estimates are in satisfactory agreement with the theoretically computed values $g_1=0.425$ and $g_2=-0.313$.

The final flow profiles in the axial direction (not shown) are very similar to the previous gradually ramped results [3], differing by less than the scatter in the measurements; the quality of the amplitude fit to Eq. (4) is the same as in Fig. 3 of [3] (the change in ν merely alters the scale of the horizontal axis). The revised Reynolds number estimate from this fit is $R_c=86.5$ (corresponding to $T_c=5985, \omega_c=0.056$), which marks the location of the break in the torque curve (Fig. 1). Theory predicts $R_c=76.6$ for cylinders of infinite length [6]; experiment shows this value to be independent of

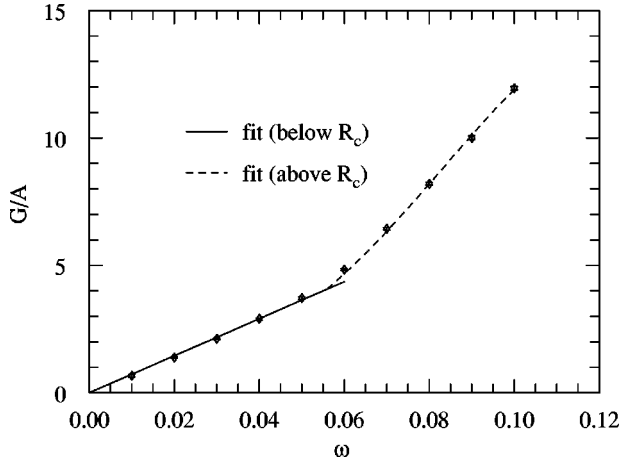

FIG. 1. Torque per unit area (G/A) as a function of angular velocity (ω) with fits based on azimuthal and vortex flows (MD units are used throughout).

cylinder length [15], although there is a certain dependence on the ramping rate [16]. The conclusion is that not only can the analysis of the MD results be carried out in a completely self-contained fashion free of any assumptions about the fluid properties, but the measured R_c is actually surprisingly close to the theoretical prediction.

The time dependence of the velocity components was measured during the vortex growth and decay phases of a series of runs with ω in the range 0.06–0.1; at lower rotation rates no vortices were observed. Analysis was confined to those runs in which the expected four vortices developed directly without transient states involving additional vortices, and each such run was repeated with different initial random velocities to assess the reproducibility of the four-vortex pattern; it turns out that there is very little difference between the separate sets of results (as demonstrated below). The time-dependent Fourier amplitudes, Eq. (3), were determined from these measurements, and the $n=1$ amplitudes of all three velocity components were fit to Eq. (7) by adjusting the growth parameter σ. The radial results are shown in Fig. 2 for a range of ω, together with the fits; the other components

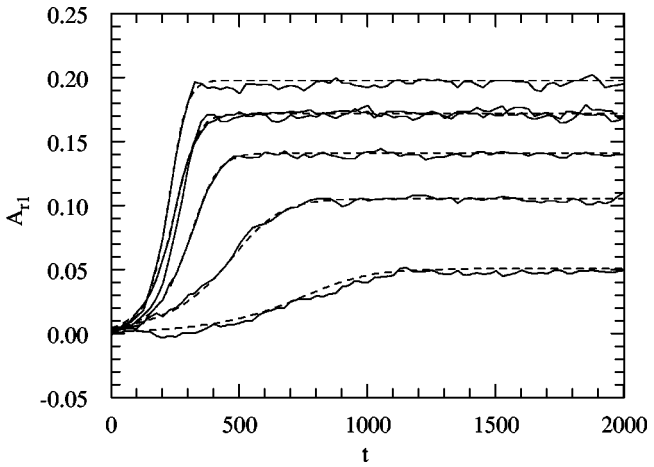

FIG. 2. Growth of the fundamental amplitude A_{r1} of the radial velocity as a function of time (t) together with the theoretical fits (dashed curves) for ω values in the range 0.06–0.1 (the curves become steeper with ω); for $\omega=0.09$ two separate runs are shown.

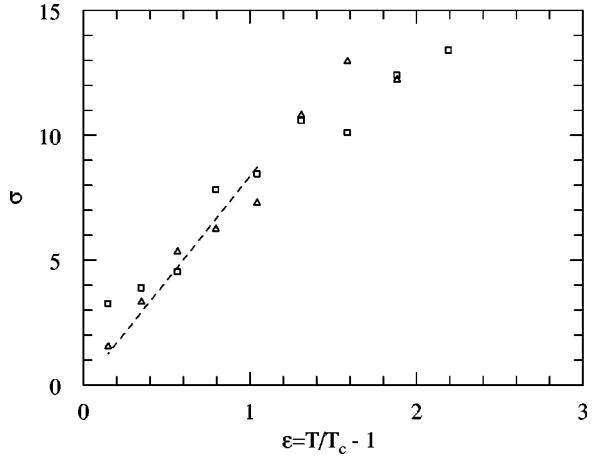

FIG. 3. Dependence of the radial velocity growth parameter σ on Taylor number; the linear fit is for $\epsilon<1$.

behave in an almost identical manner. The theoretical curves are seen to provide an excellent fit to the data. In order to demonstrate the reproducibility of the vortex growth, one example of the results from two runs with different initial conditions is included.

Figure 3 shows the measured dependence of σ on ϵ, which is predicted to be linear at small ϵ. Only the radial component results are shown, but the others are essentially the same. The availability of two distinct runs for each ω provides an indication of the variability of σ. The results are noisy, but a linear fit for $\epsilon\leqslant 1$ ($\omega\leqslant 0.08$) yields $d\sigma/d\epsilon = 8.4$; this compares favorably with the value 13.5 obtained by extrapolating experimental data [8] available over the range $\eta=$ 0.85–0.95 (there expressed in terms of a parameter $p=\sigma\nu/d^2$ that has the dimensions of inverse time) to the present $\eta=2/3$. The relatively high uncertainty in σ exaggerates the difference between runs (see Fig. 2); the functional form is such that a slight alteration in the curve is sufficient to produce a relatively large change in σ (and an even larger change in $d\sigma/d\epsilon$).

Amplitude decay is shown in Fig. 4; the vortex collapse process is considerably more rapid than the growth and begins almost immediately after the inner cylinder rotation is stopped. Clearly the decay curves fail to follow the theoretical prediction, which would amount to the time-reversed

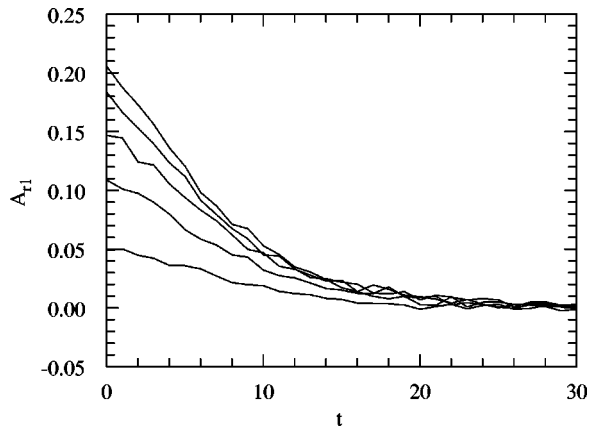

FIG. 4. Amplitude decay of the fundamental mode of the radial velocity for ω values in the range 0.06–0.1.

image of Fig. 2 (nor can the curves be fit to simple exponentials); in this respect simulation resembles experiment [8,9]. In order to make a rough comparison between the growth and decay rates, we estimated each of the rates from a linear fit over the range 0.25–0.75 times the steady-state amplitude; the decay rate is found to vary from about ten times the growth rate at $\omega = 0.06$ to three times at $\omega = 0.1$.

To summarize, we have used MD simulation to reproduce, at a quantitative level, the time-dependent development of the vortices that characterize the Taylor-Couette flow instability. Neither the fact that the width of the annular region is of the order of a mere 25 atomic diameters, nor the extreme conditions arising from the relatively high shear rate, both of which are consequences of the size limitations inherent in the methodology, appear to alter the behavior in any substantial way. A more systematic study of the size dependence of the roll structure and dynamics will be published in the future.

The computations were carried out both on the IBM/SP2 computer at the Inter-University Computation Center and on a computer whose purchase was funded by the Israel Science Foundation.

[1] D. C. Rapaport and E. Clementi, Phys. Rev. Lett. **57**, 695 (1986); D. C. Rapaport, Phys. Rev. A **36**, 3288 (1987).

[2] M. Mareschal and E. Kestemont, J. Stat. Phys. **48**, 1187 (1987); D. C. Rapaport, Phys. Rev. Lett. **60**, 2480 (1988); M. Mareschal *et al.*, *ibid.* **61**, 2550 (1988); A. Puhl, M. M. Mansour, and M. Mareschal, Phys. Rev. A **40**, 1999 (1989); D. C. Rapaport, *ibid.* **46**, 1971 (1992); **46**, R6150 (1992).

[3] D. Hirshfeld and D. C. Rapaport, Phys. Rev. Lett. **80**, 5337 (1998).

[4] G. I. Taylor, Philos. Trans. R. Soc. London, Ser. A **223**, 289 (1923).

[5] S. Chandrasekhar, *Hydrodynamic and Hydromagnetic Stability* (Oxford University Press, Oxford, 1961).

[6] R. C. Di Prima and H. L. Swinney, *Hydrodynamic Instabilities and the Transition to Turbulence*, edited by H. L. Swinney and J. P. Gollub (Springer, Berlin, 1981), p. 139.

[7] A. Davey, J. Fluid Mech. **14**, 336 (1962).

[8] R. J. Donnelly, K. W. Schwarz, and P. H. Roberts, Proc. R. Soc. London, Ser. A **283**, 531 (1965).

[9] J. P. Gollub and M. H. Freilich, Phys. Fluids , **19**, 618 (1976).

[10] D. C. Rapaport, *The Art of Molecular Dynamics Simulation* (Cambridge University Press, Cambridge, England, 1995).

[11] T. B. Benjamin and T. Mullin, J. Fluid Mech. **121**, 219 (1982).

[12] R. J. Donnelly, in *Ordered and Turbulent Patterns in Taylor-Couette Flow*, edited by C. D. Andereck and F. Hayot (Plenum, New York, 1992), p. 1.

[13] R. C. Di Prima and P. M. Eagles, Phys. Fluids **20**, 171 (1977).

[14] R. J. Donnelly and N. J. Simon, J. Fluid Mech. **7**, 401 (1960).

[15] J. A. Cole, J. Fluid Mech. **75**, 1 (1976).

[16] K. Park, G. L. Crawford, and R. J. Donnelly, Phys. Rev. Lett. **47**, 1448 (1981).