Ordering of Small Particles in One-Dimensional Coherent Structures by Time-Periodic Flows

D. O. Pushkin, D. E. Melnikov, and V. M. Shevtsova

Ordering and transport of small particles suspended in an incompressible fluid medium do not necessarily have to follow the flow. We show that for a wide class of time-periodic incompressible flows inertial particles have a tendency to spontaneously align in one-dimensional dynamic coherent structures. This effect may take place for particles so small that often they would be expected to behave as passive tracers and be used in PIV measurement technique. We link the particle tendency to form one-dimensional structures to the nonlinear phenomenon of phase locking. We propose that this general mechanism is, in particular, responsible for the enigmatic formation of the “particle accumulation structures” discovered experimentally in thermocapillary flows more than a decade ago and unexplained until now.

DOI: 10.1103/PhysRevLett.106.234501 PACS numbers: 47.52.+j, 47.55.Kf

Small particles transported by a fluid medium do not necessarily have to follow the flow. We show that for a wide class of time-periodic incompressible flows inertial particles have a tendency to spontaneously align in one-dimensional dynamic coherent structures. This effect may take place for particles so small that often they would be expected to behave as passive tracers and be used in PIV measurement technique. We link the particle tendency to form one-dimensional structures to the nonlinear phenomenon of phase locking. We propose that this general mechanism is, in particular, responsible for the enigmatic formation of the “particle accumulation structures” discovered experimentally in thermocapillary flows more than a decade ago and unexplained until now.

DOI: 10.1103/PhysRevLett.106.234501 PACS numbers: 47.52.+j, 47.55.Kf

Small particles transported by a fluid medium do not necessarily have to follow the flow. We show that for a wide class of time-periodic incompressible flows inertial particles have a tendency to spontaneously align in one-dimensional dynamic coherent structures. This effect may take place for particles so small that often they would be expected to behave as passive tracers and be used in PIV measurement technique. We link the particle tendency to form one-dimensional structures to the nonlinear phenomenon of phase locking. We propose that this general mechanism is, in particular, responsible for the enigmatic formation of the “particle accumulation structures” discovered experimentally in thermocapillary flows more than a decade ago and unexplained until now.

DOI: 10.1103/PhysRevLett.106.234501 PACS numbers: 47.52.+j, 47.55.Kf

In this Letter we report a new type of ordering of inertial particles that results in formation of one-dimensional dynamical particulate coherent structures. It is rather surprising that while this effect is generic for a class of widely encountered time-periodic flows, it has apparently not been analyzed previously. It is even more surprising that the inertia-driven self-assembly of particles into one-dimensional continuous lines was actually observed in experiments on thermocapillary flows more than a decade ago by Schwabe et al. [8] but despite extensive experimental studies [9] has remained unexplained.

The fluid flows we consider occur in the cylindrical geometry. They can be represented as superpositions of a steady toroidal vortex $u^0(r, z)$ and an oscillatory wave traveling azimuthally $u^1(\phi - \Omega t, r, z)$; see Fig. 1. Here $(\phi, r, z)$ are the cylindrical coordinates, $t$ is time, and $\Omega$ is the wave angular velocity. Such flows often emerge as a result of an instability [10,11].

In the experiments of Schwabe the instability was of thermocapillary origin [12]: it develops when a drop of liquid is placed between two cylindrical rods, with the top rod heated. The flow, driven at the cylindrical liquid-gas interface by the Marangoni force [13], undergoes a bifurcation from a steady axially-symmetric vortex to an oscillatory regime with a traveling wave when the temperature difference between the rods is large enough. That particles will self-assemble in this flow was discovered when the experimentalists admixed particles, having sizes of tens of microns, in order to study the flow. To much surprise, they
discovered that under certain conditions such small particles defied the fate of passive tracers and aligned themselves in an ordered spiral structure [see Fig. 2(a) and supplementary movie 1 [14]]. The spiral was closed, rather symmetric and rotated around the axis with no change of shape. It was dubbed “PAS” for “particle accumulation structure” [8]. Notably, the angular frequency of rotation of the spiral was found equal to that of the wave. In other experiments particulate spirals of various shapes were observed both on the ground and in microgravity for small particles of different sizes, shapes, and densities [9,10]. However, the coherent structures were observed only for certain parameter ranges.

As the convective time-based Stokes number $St = \frac{2}{9} (a/L)^2 Re \sim 10^{-4} - 10^{-3} \ll 1$, the particle dynamics is dominated by the viscous drag force. Here $a$ is the particle size, $L$ is the characteristic flow length scale, $Re = UL/\nu$ is the Reynolds number, $U$ is the characteristic flow speed, and $\nu$ is the fluid kinematic viscosity. In previous experimental studies of the particle self-ordering researchers looked for additional forces and accounted for flow features specific to thermocapillary and free-surface flows [10]. However, we claim that this phenomenon is generic for the class of volume-preserving flows defined above, and that an interplay of the particle inertia and the viscous drag force alone may cause the ordering. Therefore, we anticipate this effect in such periodic flows, which abound in nature. Their further examples include flows in laminar stirred tanks [15], pyroclastic surges, and microfluidic flows [16]. The arising singular spatial distributions of particles may have profound consequences for particle aggregation and transport; understanding and control of the arising structures may be important as a technological tool.

The starting point of our analysis is the reduced version of the Maxey-Riley equation of particle motion [17], which can be written as

$$\left( \rho + \frac{1}{2} \right) \frac{d\mathbf{v}}{dt} = \frac{3}{2} \frac{D\mathbf{u}}{Dt} + \frac{1}{\tau} (\mathbf{u} - \mathbf{v}) + (\rho - 1) g. \quad (1)$$

Here $t$ is time, $\mathbf{v}$ is the particle velocity, $\mathbf{u}$ is the fluid velocity, $\rho$ is the ratio of the particle to the fluid density, $\tau$ is the particle relaxation time, and $g$ is gravity. The material derivative $\frac{D}{Dt}$ is taken moving with the fluid velocity at the current location of the particle. By the Stokes law, $\tau = (2/9) a^2 / \nu$. This equation describes the Newtonian dynamics of small particles dominated by the inertia (including the added mass effect) and viscous drag forces. It neglects a reverse influence of particles on the flow and particle-particle interactions and is valid when $a/L \ll 1$ and $Ua/\nu \ll 1$. (While in an actual physical system particles may experience other types of hydrodynamic forces, our goal is to demonstrate that even the current “minimal” model can produce the effect.)

We performed numerical simulations, in which the particle dynamics governed by (1) was coupled to the full system of the Navier-Stokes equations describing the thermocapillary fluid flow [18,19]. We find, in physically realistic regimes, that particles assemble in dynamic spirals that closely resemble the experimental results [Fig. 2(b) and supplementary movie 2 [14]]. Besides, we observed formation of particulate spirals that have the number of turns $m$ different from the wave mode $m$ (also integer due to the cylindrical geometry). Similar to experimental findings, each coherent structure is robust in a limited range of governing parameters. As soon as a parameter leaves the range, the coherent structure will disperse. We will come back to these features below. The major lesson learned from the simulations is the basic fact that a mere interplay of the inertia and viscous forces acting on individual particles can lead to the particle ordering.

At this point one could suppose that the effect is specific to the thermocapillary flow. In order to demonstrate that this is not the case, we study particle ordering in a generic analytical model of a flow with a rotating wave. For a cylinder of unit radius we assume,

$$u(t, \phi, r, z) = u^{(0)}(r, z) + bu^{(1)}(\phi - \Omega t, r, z), \quad (2a)$$

$$u^{(0)}_r(r, z) = -\frac{\pi}{2H} (r - r^3) \cos \frac{\pi z}{H},$$

$$u^{(0)}_z(r, z) = -2(r^2 - 1/2) \sin \frac{\pi z}{H}. \quad (2b)$$

$$u^{(1)}(\phi, r, z) = -(3r^2 - 4r^3) \sin(m\phi) \sin \frac{\pi z}{H},$$

$$u^{(1)}_\phi(\phi, r, z) = (r^2 - r^3) m \cos(m\phi) \sin \frac{\pi z}{H}. \quad (2c)$$
Here, \( H \) is the cylinder height, \( m \) is the (integer) wave number, and \( b \) is the wave amplitude. The Eqs. (2b) mimic the Poiseuille flow in a finite cylinder, and the Eqs. (2c)—a rotating wave. The flow is scaled by \( U \), so that the maximum value of \( u_z \) is 1 at \( z = H/2 \) and \( r = 0, \) or \( 1 \). This model is not intended to be a rigorous description of the flow observed in experiments or numerical simulations; rather, it is a phenomenological model that captures the essential features of flows with rotating waves. It satisfies impermeability boundary conditions. A model satisfying no-slip conditions on the solid walls and zero axial vorticity component on the free-surface would be significantly more complicated. Nevertheless, this simplified model successfully reproduces the principle features of the particle ordering, as is showed below.

Instead of solving (1), we deal with the “inertial equation” [5], obtained as the first order approximation of (1) in St:

\[
v(x) = u - \tau (\rho - 1) \left( \frac{D u}{D t} - g \right) + O(St^2). \tag{3}
\]

This equation describes particle motion as advection plus a perturbation due to the inertial effects. Since \( \nabla \cdot u = 0 \), it is the nonzero divergence of the second term that must be responsible for the phase volume changes accompanying formation of the accumulation structures. The chief advantage of using (3) instead of (1) lies in the reduction of the formation of coherent structures from the initially three-dimensional particle distribution to account for the spontaneous formation of one-dimensional structures. The chief advantage of using (3) instead of (1) lies in the reduction of the particle phase space from six to three dimensions (in the frame rotating with the wave).

Then from the viewpoint of dynamical systems the coherent structures are attractors in the three-dimensional space and can be readily studied by means of the Poincare section. We define the latter as the instances when particles cross the equatorial plane \( z = 1/2 \) (in the reference frame rotating with the wave).

The model (2) and (3) contains five parameters \( H, m, a, \) \( \Omega, \) and \( (\rho - 1)\tau \), and can be studied numerically. At this point our goal is twofold: first, to show that the model may account for the spontaneous formation of one-dimensional coherent structures from the initially three-dimensional particle distributions for a realistic choice of parameters. Second, to demonstrate that it requires no fine-tuning of the parameters, i.e., the structures are stable for certain parameter ranges.

We choose \( H = 1, m = 3, \) and \( b = 0.3 \) to account for the flow and the rotating wave characteristics observed in experiments and our numerical simulations, and \( (\rho - 1)\tau = 10^{-3} \) to account for the particle properties. The main tunable parameter is \( \Omega \) and for now we set it to 0.5. Numerical solution of (2) and (3) bears out formation of coherent structures similar to the ones observed in experiments [9] and direct numerical simulations [19].

We clearly observe that particles do not need to touch the fluid-gas interface in order to align. Figure 3 demonstrates that the coherent structures are stable fixed points of the Poincare map. It also shows that the particle ordering proceeds via two distinct steps: first, particles concentrate in the center and near the circumference of the Poincare section. Second, the cylindrical symmetry is broken and the particles are attracted to the stable fixed points. In the physical space these steps correspond to clustering of particles in two-dimensional toroidal coherent structures, and to transformation of the latter into one-dimensional closed spirals. The two processes have different characteristic times but take place simultaneously. (These steps of

![FIG. 4 (color online). Synchronization of a particle and the wave. Here \( m = 3 \). (a) Schematic trajectory of an individual particle in the laboratory frame. (b), (c) The equatorial plane in two instances of time separated by the particle turnover time \( T_p \). The phase locking means the particle phase relative to the wave is the same for the consecutive locations 1 and 2. If the particle gets out of phase, ‘2’, interaction with the flow structure will adjust the particle azimuthal drift (red arrow) to resume the phase.]
Synchronization due to phase locking is ubiquitous in nature. The present modeling suggests that PAS formation in thermocapillary flows is another instance of this general phenomenon and that formation of one-dimensional coherent particulate structures should be encountered in other oscillatory vortical flows when (i) the particle turnover motion is transversal to the direction of wave propagation and (ii) the frequencies of the particle turnover motion are commensurate with the oscillation frequencies.

[1] D. Di Carlo, D. Irinia, R.G. Tompkins, and M. Toner, Proc. Natl. Acad. Sci. U.S.A. 104, 18892 (2007); D. Di Carlo, J.F. Edd, K.J. Humphry, H.A. Stone, and M. Toner, Phys. Rev. Lett. 102, 094503 (2009).
[2] J. H. Seinfeld and S. N. Pandis, Atmospheric Chemistry and Physics (Wiley, New York, 1998).
[3] E.g., M. R. Maxey, Phys. Fluids 30, 1915 (1987).
[4] C. Pasquero, A. Provenzale, and E. A. Spiegel, Phys. Rev. Lett. 91, 054502 (2003); C. Escauriuzia and F. Sotiropoulos, J. Fluid Mech. 641, 169 (2009).
[5] T. Sapsis and G. Haller, Atmos. Sci. 66, 2481 (2009); T. Sapsis and G. Haller, Chaos 20, 017515 (2010).
[6] R. D. Vilela and A. E. Motter, Phys. Rev. Lett. 99, 264101 (2007).
[7] I. J. Benczik, T. Toroczkai, and T. Té, Phys. Rev. Lett. 89, 164501 (2002).
[8] D. Schwabe, P. Hintz, and S. Frank, Microgravity Sci. Technol. 9, 163 (1996).
[9] D. Schwabe, A.I. Mizev, M. Udhayasankar, and S. Tanaka, Phys. Fluids 19, 072102 (2007); S. Tanaka, H. Kawamura, I. Ueno, and D. Schwabe, Phys. Fluids 18, 067103 (2006).
[10] R. Hide and P.J. Mason, Adv. Phys. 24, 47 (1975).
[11] J. M. Lopez, F. Marques, A.H. Hirsa, and R. Miraghaie, J. Fluid Mech. 502, 99 (2004).
[12] F. Preisser, D. Schwabe, and A. Scharmann, J. Fluid Mech. 126, 545 (1983).
[13] L. E. Scriven and C. V. Sterling, Nature (London) 187, 186 (1960).
[14] See supplemental material at http://link.aps.org/supplemental/10.1103/PhysRevLett.106.234501 for two movies. Other experimental movies are available free of charge following the links in [9].
[15] M. M. Alvarez, J.M. Zalc, T. Shinbrot, P.E. Arratia, and F.J. Muzzio, AIChE J. 48, 2135 (2002).
[16] A. Burgisser and G.W. Bergantz, Earth Planet. Sci. Lett. 202, 405 (2002); K. Seifjane, J.R. Moffat, O.K. Matar, and R.V. Craster, Appl. Phys. Lett. 93, 074103 (2008).
[17] M. R. Maxey and J.J. Riley, Phys. Fluids 26, 883 (1983); E.E. Michaelides, J. Fluid Eng. 119, 233 (1997); M. R. Maxey, Phys. Fluids 30, 1915 (1987).
[18] V. Shvetsova, D.E. Melnikov, and A. Nepomnyashchy, Phys. Rev. Lett. 102, 134503 (2009).
[19] D. Melnikov, D. Pushkin, and V. Shvetsova, EPJ ST 192, 29 (2011).
[20] D. Schwabe and A.I. Mizev EPJ ST 192, 13 (2011).
[21] E. Ott, Chaos in Dynamical Systems (Cambridge University Press, Cambridge, England, 1993).