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Low-Reynolds-number stirring in simple devices

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Abstract

We examine two models for stirring devices that operate at low Reynolds number. In each, elliptical paddles are used to stir a vat of fluid. In the first model, a single paddle stirs an infinite expanse of inviscid fluid; in the second, three paddles stir a highly viscous fluid. Such models are clearly a caricature of any real mixing device, but they do allow accurate simulation in a genuinely time-dependent geometry, appropriate for impeller-driven mixers. The first model is simple enough to yield an exact expression for the velocity field and so allow numerical particle tracking to be carried out to high precision. The choice of a suitable mode of operation of the device is essentially a matter of optimising the system parameters. In our second model, we show how, by the use of more than one stirring element, a high quality of stirring can be *built in*, giving a design that performs well, regardless of the exact system parameters, such as paddle design or fluid rheology.

Introduction

Many modern applications of fluid mixing pose a particular challenge because the associated flows are laminar, with low Reynolds number. (The Reynolds number $\mathrm{Re} = UL/\nu$, where U, L and ν are, respectively, a typical velocity scale, a typical length scale and the kinematic viscosity of the fluid.) An example is the mixing in microfluidic devices such as used in the biotechnology industry. Fortunately for such applications, it is now well established [2] that good mixing can be achieved in slow laminar flows, provided that fluid particles undergo *chaotic* motions. The challenge is thus to design devices and corresponding modes of operation that achieve this end, of the *chaotic advection* of fluid particles [1].

The stirring effectiveness of chaotic advection was first shown in rather artificial 'devices' [1, 2], chosen because an exact mathematical expression is available for the velocity field, and hence numerical simulation of extreme accuracy is possible; these simple models were entirely adequate for the pedagogical purpose at hand. Over the past twenty years or so, a wide variety of increasingly sophisticated mathematical models have been developed for simple mixing devices [2]. Most rely on a tuning of the system parameters to optimise the mixing quality that is achieved.

A recent significant theoretical advance in the design of laminar mixers is the work of Boyland, Aref and Stremler [3], which concerns stirring achieved by topologically nontrivial motions of three or more stirring elements (e.g., rods used to stir a fluid in a vat). Given only the topology of the motions of the stirring elements, it is possible to compute a rate of stretch of material lines. The fluid rheology, e.g., whether Newtonian or otherwise, is unimportant. Of course, given such moderate input information, the theory does not specify the size of the chaotic region generated by the boundary motions, nor does it specify exactly which material lines enjoy (at least) the predicted rate of stretch. However, in both experiments [3] and numerical simulations [6] the associated designs seem to work remarkably well.

This paper begins by introducing a model for a simple stirring 'device', comprising a single elliptical paddle in an infinite vat of fluid. This model is clearly unrealistic in assuming an infinite expanse of fluid, but it possesses an important feature of all batch mixers, that the geometry of the device changes with time as the stirring element sweeps through the fluid. By contrast, many of the first experimental and numerical studies of chaotic advection were carried out in the *eccentric annular mixer* (see [2] for an account of the history), whose geometry is fixed. As with all other simple models, the elliptic paddle requires careful tuning of its mode of operation to stir the fluid effectively.

We then discuss how this design can be made somewhat more realistic, by adopting a finite geometry and employing more than one stirring element (and a viscous fluid model). In this second model, while different degrees of effectiveness are still possible by varying the system parameters, we shall see that a certain quality of mixing is built in once a topologically nontrivial motion of the stirring elements is specified.

Stirring with a single paddle

One of the simplest stirring devices is a paddle. Consider the flow in two dimensions generated by the motion of an elliptical paddle. For simplicity, we take the fluid to be inviscid, and occupying the entire infinite region exterior to the paddle. This is clearly not intended as a practical model for reality, but it has enough complication to generate chaotic advection yet enough simplicity to permit an exact (classical) mathematical solution for the velocity field.

We consider irrotational flow, in which case the streamfunction $\psi(x,y,t)$ satisfies Laplace's equation

$$\nabla^2\psi = 0.$$

In order to stir the fluid, the paddle must execute some motion: the 'stirring protocol'. It is necessary to select an appropriate protocol that stirs the fluid effectively. Our goal will be to generate a significant region in which fluid particles undergo chaotic motion, characterised by exponential-in-time separation of neighbouring particles. By contrast, stirring is less effective in regular regions, with algebraic-in-time separation of fluid particles. In two dimensions, time dependence of the streamfunction is necessary for chaos. Some immediate candidates for stirring protocols are readily seen to generate exclusively regular particle motions, since they correspond to steady streamlines in an appropriate frame of reference. Examples are: (i) a paddle whose axis is fixed, and which rotates about this axis (i.e., an 'impeller'), because the streamfunction is steady in a frame corotating with the paddle; and (ii) a paddle that sweeps around in a large circle, one 'nose' always pointing towards the centre of the circle, for a similar reason.

The streamfunction ψ is most readily constructed in elliptical coordinates (ξ,η), given by

$$x = c\cosh\xi\cos\eta, \qquad y = c\sinh\xi\sin\eta,$$

for an ellipse centred at the origin, with major axis of length $2a$ along the x-axis, and minor axis of length $2b$ along the y-axis. The constant $c = \sqrt{a^2+b^2}$. If the ellipse is translating

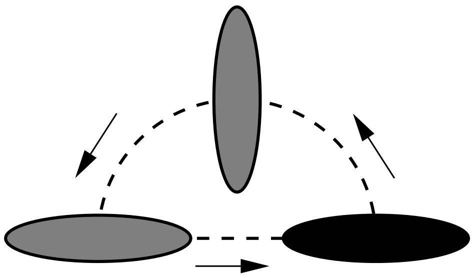

Figure 1: A semi-circular stirring protocol for an elliptical paddle. The ellipse starts at right, moves counterclockwise around the semicircular path, then straight along the x-axis. One loop around the circuit defines a single period of the stirring protocol.

with velocity (U,V) and is rotating about its axis with angular velocity ω, then the appropriate solution to Laplace's equation that satisfies the no-penetration condition on the perimeter of the ellipse is [7, 9]

$$\psi = A\mathrm{e}^{-\xi}(Ub\sin\eta - Va\cos\eta) + \tfrac{1}{4}\omega(a+b)^2\mathrm{e}^{-2\xi}\cos 2\eta,$$

where $A = [(a+b)/(a-b)]^{1/2}$. Corresponding formulae hold for an ellipse centred elsewhere or in a different orientation, but they are easily obtained by appropriate rotation or translation of the axes, and are not given here.

Given the streamfunction, we track fluid particles by solving for each particle the Lagrangian equations of motion, i.e., the coupled ODEs

$$\dot{x} = u(x,y,t), \quad \dot{y} = v(x,y,t), \tag{1}$$

where $u = \psi_y$ and $v = -\psi_x$, subject to an appropriate initial condition for each particle.

A simple stirring protocol that cannot essentially be reduced to steady flow through a change of frame of reference is illustrated in Figure 1. Here the ellipse moves along a semicircular path. On the curved part of the path, the ellipse rotates about its axis so as to point one nose towards the centre of the arc; on the straight part of the path, the ellipse does not rotate about its axis ($\omega = 0$). In this example, the circle has diameter 3, while $a = 2$ and $b = 1$. This is clearly only one possible stirring protocol; its key feature from the point of view of successfully generating chaotic fluid particle trajectories is that the paddle cannot be brought to rest by moving to a new frame of reference, unless the change of frame is itself time dependent.

One simple, mostly qualitative, diagnostic of the stirring quality is the Poincaré map. Here the positions of a few fluid particles are followed by integrating (1) in time. The positions of the particles are then plotted stroboscopically, after $1, 2, \ldots$ periods of the stirring protocol: where the eye sees closed curves in the Poincaré map, there is *regular* motion of fluid particles; where the eye sees a random collection of dots, there is *chaotic* motion.

Figure 2 shows the Poincaré map associated with the protocol in Figure 1. There are two large regular regions visible, and a significant *chaotic sea*; indeed the bulk of the fluid, sufficiently far from the ellipse, undergoes regular particle motion. One may attempt to devise a better stirring protocol, in the sense of one that increases the size of the chaotic region, or one that increases the stretch rate experienced by fluid elements (this latter, *quantitative* diagnostic of the stirring clearly requires a more sophisticated measure than the 'by-eye' examination of the Poincaré map). One might choose a less symmetrical path for the paddle, or a different paddle aspect ratio; one might adopt a more

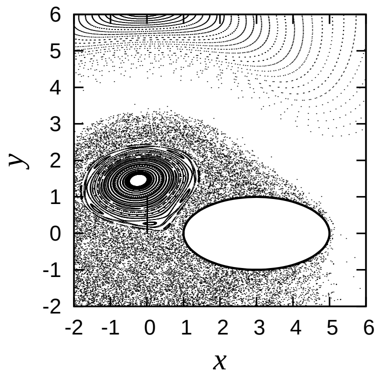

Figure 2: Poincare map for the stirring protocol in Figure 1, with parameter values as indicated in the text.

sophisticated model for the fluid than the simple inviscid, irrotational one used here; one might confine the fluid in a finite vat. But with a single paddle, the only option is to tune the stirring protocol and the other parameters of the system to obtain the desired end of improved stirring performance. It is in the nature of chaotic flows that the resulting, tuned stirring protocol has an unfortunate susceptibility to further parametric perturbations; this is an undesirable feature of any real mixer, since one would like the design to be largely insensitive to the precise details of the underlying design.

The next section indicates how this parametric fussiness can be avoided, and high quality stirring can be 'built in' by the simple device of using multiple stirring elements.

Stirring with a multiple paddles

There does not appear to be a simple analytical expression available for the flow driven by n elliptical paddles, when $n > 1$. In computing such a flow, we must therefore resort to a numerical evaluation of the velocity field. Since numerical errors grow geometrically in the simulation of chaotic particle motions, it is highly desirable to have a means of computing the velocity field with a truncation error smaller than that introduced by the time integration routine for the fluid particles. Such a method has been described elsewhere [6, 10] when the stirring elements have circular cross-section; the method allows simulation in finite or infinite domains, and of either inviscid, irrotational flow or highly viscous (Stokes) flow. The method uses a complex-variable formulation of the problem: the complex potential $w(z, z^*, t)$ is subject to either Laplace's equation

$$\frac{\partial^2 w}{\partial z \partial z^*} = 0 \tag{2}$$

or the biharmonic equation

$$\frac{\partial^4 w}{\partial^2 z \partial^2 z^*} = 0 \tag{3}$$

in a time-dependent multiply connected geometry (here z^* is the complex conjugate of z).

The corresponding streamfunction takes the form

$$\psi = f(z) + f^*(z^*)$$

or

$$\psi = z^* f(z) + z f^*(z^*) + g(z) + g^*(z^*),$$

respectively, in the models (2) or (3), for some analytic functions f and g. The solution for f (or for f and g, as appropriate)

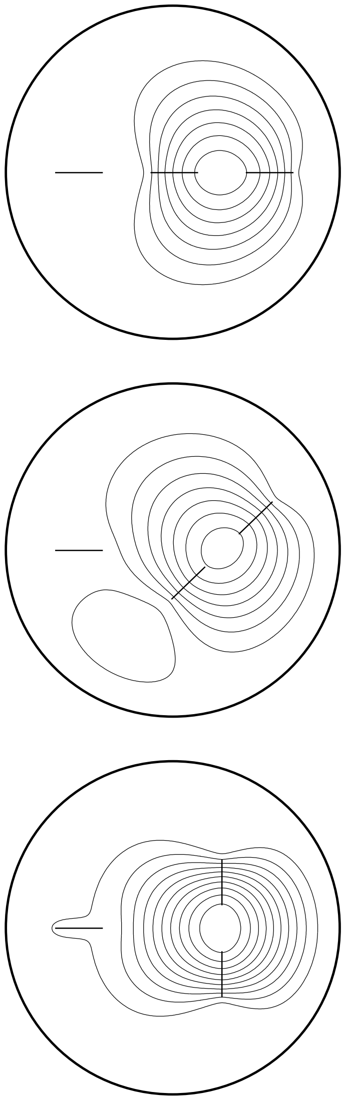

Figure 3: Instantaneous streamlines at three instants during an exchange of the rightmost pair of stirring elements.

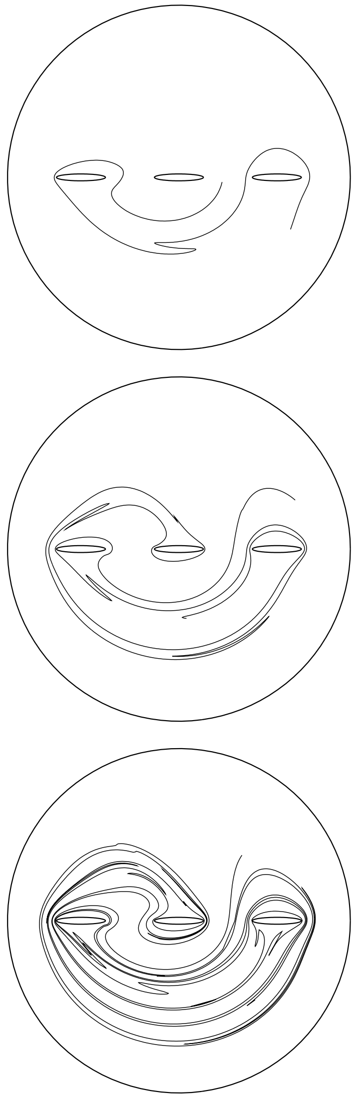

Figure 4: The stretching of a line element, initially of unit length and located between the points $(2/7, \pm 1/2)$ under the stirring protocol described in the text. The vat is a unit circle, centred at the origin.

is sought in the form of a finite system of singularities (located inside the stirring elements, and hence not in the physical fluid domain) together with Laurent series centred in each stirring element. The coefficients of the singularities and the terms in the Laurent series are determined numerically by minimising the squared error in the boundary conditions; the series coefficients decay geometrically and so only a few terms (around 10 to 20) need be kept in order to generate a highly accurate velocity field.

If the same expansions are used for elliptical paddles, they do not converge so rapidly and they struggle to provide an acceptable level of accuracy when the paddles depart from circular symmetry. However, if the component of the solution associated with each paddle is modified, by making a suitable conformal mapping of the ellipse, parametrised by $z = z(\theta)$, say, to a circle, parametrised by $Z = \exp i\theta$, say, and the complex potential is written in terms of Z rather than z, then the series become spectrally convergent once more, and the velocity field can readily be computed, almost down to machine precision. The extraordinary accuracy is maintained even down to elliptical paddles of extreme aspect ratio (we have computed flows down to $b/a = O(10^{-7})$). In fact, by an appropriate conformal mapping, exactly flat paddles, of zero mathematical width, can be simulated by this method, with no numerical difficulties.

The numerical method allows an arbitrary number of stirring elements, of different sizes and aspect ratios, translating and rotating in arbitrary fashion. We illustrate in Figure 3 Stokes flow with $n = 3$ stirring rods, in a circular vat. Each elliptical paddle has aspect ratio $b/a = 10^{-3}$ and length $2a = 2/7$; the radius of the vat is scaled to unity. The three paddles initially lie equispaced along the real (horizontal) axis. The figure illustrates the instantaneous flow pattern as the positions of the rightmost pair are exchanged; the exchange is accomplished by rotating the centres c_1 and c_2 of the two paddles about the point c_3 mid-way between c_1 and c_2. As the paddles are moved, they are rotated about their axes so as always to 'point towards' c_3. Note that the flow at any instant is smooth and laminar.

Topologically nontrivial motions involving three stirring elements are readily constructed by considering motions that correspond to nontrivial *plaiting* or *braiding* motions [3]. One such motion is achieved by moving the stirring rods according to the following protocol: first the right-hand pair are interchanged, in a counterclockwise motion, then the new left-hand pair are interchanged, but clockwise. This pair of interchanges constitutes a single period of operation of the device (i.e., one application of the stirring protocol); it is akin to the natural plaiting of three strands of hair.

The batch stirring device described above, with multiple stirring elements, serves as a simplified model for commercial planetary mixers. Although it now becoming apparent that topologically nontrivial motions such as described above build in a high mixing quality, standard batch mixers do not at present employ any such stirring protocol (but see [8]). It might superficially appear that a complicated system of gearing is necessary to generate the motions described in the previous paragraph, and that this might be the reason for the commercial vacuum; however, with some ingenuity, topologically equivalent motions are readily accomplished with only simple gearing, such as already used on commercial devices, together with fixed baffles [6].

The evolution of a line element of unit initial length is shown in Figure 4, after one, two and three applications of the stirring protocol. (In this case we have increased the aspect ratio of the paddles so that $a = 1/7$ and $b = 1/50$, so the finite thickness of the paddles can be seen.) The number of points in the line has been dynamically increased where necessary to maintain adequate resolution. The requirement of good resolution effectively constrains accurate calculations of the length of the line element to two or three further periods of the stirring protocol beyond those illustrated in Figure 4. We find that the length of the line after one, two and three periods of the protocol is, respectively, 4.3, 14 and 42. The dramatic rate of line stretch is relatively insensitive to the exact motions of the stirring elements or their exact dimensions. This is the hallmark of a topologically chaotic mixer design.

Conclusions

We have illustrated in this paper a simple model for a stirring 'device' that uses a single elliptical paddle in an infinite expanse of inviscid fluid undergoing irrotational motion. While this is not intended as a true model for any realistic device, it is a good pedagogical tool for illustrating the concept of chaotic advection, using no more than a basic undergraduate knowledge of classical hydrodynamics and the numerical solution of ordinary differential equations. In this respect, it is in the same spirit as Aref's 'blinking vortex flow' [1], although (marginally) more realistic, in possessing no flow singularities (these play havoc with numerical computations of the evolution of material lines). The model allows one to experiment (numerically) to find good stirring protocols by varying the system parameters, including the path taken by the stirring element and its shape and size.

Better than this parametric optimisation is to use topological ideas to build in some degree of mixing quality [3, 6, 8]. Then the stirring device that is so designed operates 'robustly' in the sense that it remains insensitive to the nature of the fluid being mixed and to its exact specifications, provided the topology of the motion of the stirring elements is unaltered.

So far we have, as illustrated here, simulated flows in the two mathematically 'easy' limits (for a Newtonian fluid at zero and infinite Reynolds numbers) and it would be highly desirable to investigate the effectiveness of the topologically designed stirring devices for a Newtonian fluid at finite Reynolds number [5], or for other fluids. Results from the two cases already studied [6] show a promising indication of the robustness of the topological designs, but clearly further research is warranted.

Finally, we note that one important question that needs to be considered with any mathematical model is its degree of applicability. To address this question in the present context, we have performed laboratory experiments on a batch mixer with a single stirring element (of circular cross-section) [4]. Our results indicate that the two-dimensional Stokes flow approximation performs well for genuinely small Reynolds numbers (e.g., $\mathrm{Re} = O(10^{-3})$). However, when the Reynolds number is merely moderate ($\mathrm{Re} = O(1)$), there are significant changes to the streamlines of the flow. Furthermore, the flow is no longer quasi-steady (i.e., it depends on more than just the *instantaneous* motions of the boundaries). However, for *topologically chaotic* flows generated using three or more stirring elements, we expect a much greater degree of robustness of the results to changes in the Reynolds number. Of course, the requisite experiments to demonstrate this have not yet been performed (but see [3]); we hope in the future to carry out such experiments, which may provide strong validation of the topologically chaotic theory.

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