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Jie Chen and Mark A. Stremler

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Topological chaos and mixing in a three-dimensional channel flow

Jie Chen and Mark A. Stremmer

Department of Engineering Science and Mechanics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA

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Passive mixing is investigated in a mathematical model of steady, three-dimensional, laminar flow through a rectangular channel. Efficient stirring is achieved by imposing spatially periodic transverse boundary velocities that generate asymmetric, counter-rotating rolls aligned with the channel axis. The flow is designed and analyzed using the concept of topological chaos, in which complexity is embedded in the flow through the motion of periodic orbits. A lid-driven flow producing topological chaos is found to stir better than a related flow with solid inserts considered previously [M. D. Finn, S. M. Cox, and H. M. Byrne, Phys. Fluids **15**, L77 (2003)]. The results demonstrate that topological chaos and the Thurston–Nielsen classification theorem can provide insight into mixing enhancement in steady, three-dimensional flows. © 2009 American Institute of Physics. [DOI: [10.1063/1.3076247](http://dx.doi.org/10.1063/1.3076247)]

While the question of how to mix fluids thoroughly and efficiently is far from new (see, e.g., Ref. 1), the complexities often inherent in this question require further advances in our understanding and predictive capabilities. A recent development in the analysis of stirring and mixing² in a laminar flow is based on the existence of periodic orbits in the flow and the complexity of the entanglement, or braiding, of these orbits.³ These periodic orbits can be associated with either the motion of solid objects or the trajectories of fluid particles. The mathematical foundation of this approach, the Thurston–Nielsen (TN) classification theorem,⁴ establishes that certain orbit braidings *guarantee* the occurrence of exponential stretching in the surrounding fluid (as long as that fluid behaves as a continuum). Furthermore, the TN theorem predicts a *quantitative* lower bound on the exponential stretching rate. The guarantee of chaos is based on the topology of the braid formed by the orbits, not the detailed dynamics of the system. The complexity will persist under perturbations in the system dynamics that preserve the braid topology, and often this braid topology is robust to quite substantial perturbations. Exponential stretching is a characteristic of efficient stirring and is typically associated with rapid mixing.^{2,5,6} Thus, this topological approach allows one to make quantitative predictions of mixing effectiveness based on models that only approximate the dynamics of the real system of interest. The mathematical framework has been established for (2+1)-dimensional space-time systems and has been successfully applied to the analysis of several time-dependent, two-dimensional flows; see Ref. 7 for a recent review. In this letter, we demonstrate that this approach can be applied to the analysis of a steady, three-dimensional flow.

Consider briefly the two-dimensional, time-dependent example from Ref. 3, in which three solid rods generate periodic orbits as they stir a viscous fluid at low Reynolds number in a repeated two-step process. In the first step, the right and center rods exchange position by simultaneously moving clockwise along a circular path, as illustrated in Fig.

1(a). In the second step, the left and center rods exchange position by simultaneously moving along a circular path. These steps are repeated to produce a time-periodic motion. If the second exchange is always counterclockwise, as illustrated in Fig. 1(b), the fluid is wrapped between the rods as in Fig. 1(d) and exponential stretching is “built in” to at least some of the surrounding fluid. In the TN theorem this motion is classified as *pseudo-Anosov* (pA). Numerical experiments confirm that the theoretical stretching rate does indeed provide a reasonable estimate of the fluid behavior.⁸ If instead this second step is always clockwise, as illustrated in Fig. 1(c), then the fluid is merely twisted around the rods. This motion of the boundaries is topologically trivial and is classified as *finite order* (FO), which is *isotopic* (i.e., topologically equivalent) to a system with three rods that do not move but may rotate. In this case, the TN theorem establishes a lower bound of zero on the exponential stretching rate. The flow can still exhibit chaotic advection due to the dynamics of the fluid, but the presence of exponential stretching must be determined through further analysis. In particular, the flow may contain fluid particles that move on periodic orbits of pA type.⁹

Many mixing systems involve inherently three-dimensional flows, to which the TN theorem does not formally apply. In Ref. 3 it was suggested that an analogous result might be achieved in a steady, three-dimensional duct flow by inserting a set of solid, braided tubes into the duct, as illustrated in Fig. 1(e). In this way, the axial direction plays the role of time in the topological analysis. Unfortunately, Finn *et al.*¹⁰ found that this approach led to very little of the fluid experiencing the exponential stretching predicted by the TN theorem. Furthermore, they found that a FO braid insert mixed the fluid better than did a pA braid insert. Hence one might conclude that the analogy between an unsteady two-dimensional system and a steady three-dimensional system is not complete enough for the powerful results of the TN theorem to be applicable. However, we show here that it is possible to generate topological chaos in a steady, three-

FIG. 1. Stirring of a viscous fluid with solid rods, from Ref. 3, using three different rod interchanges (a)–(c). (d) Stretching and folding of dye lines in a pA case. (e) Braid representation of rod motions in $(2+1)$ -dimensional space time, with time increasing to the right, or in three-dimensional space.

dimensional flow and have the bulk of the fluid experience the exponential stretching predicted by the TN theorem. We accomplish this by using a lid-driven channel flow to produce braiding periodic orbits in the fluid without the use of internal solid rods. We also show that, for this flow, a pA braid produces better mixing than a related FO braid.

The mathematical model we use here is essentially that used in Ref. 11 to analyze pressure-driven flow in a rectangular channel with oblique surface grooves;¹² a similar model has also been used to analyze stirring in an electro-osmotic flow.¹³ We assume steady, laminar flow with Cartesian components (u, v, w) in a channel having a cross section in the (x, y) -plane, as shown in Fig. 2(a), and an axis in the z -direction. The side and bottom walls of the channel are fixed, and thus, by the no-slip condition, the fluid velocity is zero along the boundaries $x = \pm a$ and $y = -b$. On the top wall of the channel, i.e., at $y = b$, we impose a piecewise uniform transverse boundary velocity according to

$$u(x, y = b, z) = \begin{cases} U_L(z) & \text{for } -a \leq x < -c \\ U_C(z) & \text{for } -c \leq x \leq c \\ U_R(z) & \text{for } c < x \leq a, \end{cases} \quad (1)$$

where each of the U_L, U_C, U_R is taken to be piecewise constant in z , with values changing every $z = n\ell$ (for n an integer). The values of U_L, U_C, U_R are chosen to produce braiding fluid trajectories in the channel, as described below.

In order to simplify the analysis of this three-dimensional system, we assume (as in Ref. 11) that the flow at any given cross section is fully developed so that the transverse (u, v) and axial (w) components of velocity are decoupled. For the transverse velocity field we assume Stokes flow, which requires that the streamfunction for the transverse flow satisfies, for any given z , the two-dimensional biharmonic equation

$$\nabla^4 \psi_z(x, y) = \left(\frac{\partial^4}{\partial x^4} + 2 \frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial y^4} \right) \psi_z(x, y) = 0 \quad (2a)$$

subject to the boundary conditions

$$y = b: \quad \psi_z = 0, \quad \partial \psi_z / \partial y = u(x, y = b, z),$$

$$y = -b: \quad \psi_z = 0, \quad \partial \psi_z / \partial y = 0, \quad (2b)$$

$$\text{and } x = \pm a: \quad \psi_z = 0, \quad \partial \psi_z / \partial x = 0,$$

where $u(x, y = b, z)$ is given by Eq. (1). We solve for ψ_z using the numerical method discussed in Refs. 15 and 16. Note that imposing the piecewise constant boundary condition (1) requires an infinite driving force due to the discontinuities, and smoothly varying boundary conditions are more realistic.¹⁷ However, Ref. 11 shows that this model is able to capture the essential features of a corresponding experimental system.¹²

FIG. 2. (Color online) (a) Dimensions and boundary conditions in a cross section of the lid-driven channel. (b) Visualization of the braid $(\sigma_2 \sigma_1^{-1})^3$ generated by the periodic trajectories. Flow is from left to right, arrows indicated directions of boundary velocities, and representative streamlines for the transverse flow are shown in the cross sections. (c) Representative streamlines for the transverse flow (solid light lines) and periodic points (open circles) for the σ_2 stirring protocol. The initial non-trivial material lines (Ref. 14) connecting the periodic points at $z=0$ are shown with the heavy solid and dotted lines. Stretching of these non-trivial material lines at the cross sections (d) $z = \ell$, (e) $z = 2\ell = \ell_f$, and (f) $z = 3\ell_f$.

In Ref. 18 it was shown that a two-dimensional, time-dependent flow governed by the equivalent of Eq. (2) can generate braiding fluid trajectories analogous to those of the solid rods in Fig. 1(c). If we assume the axial flow in the present system is uniform, the results in Ref. 18 can be applied directly to steady channel flow by identifying time with axial position. However, the appropriate assumption is to satisfy the no-slip condition on the channel walls. We thus take the axial component of velocity to be given by the solution for Poiseuille flow in a rectangular duct, namely,¹⁹

$$\frac{w(x,y)}{W} = 1 - \left(\frac{y}{b}\right)^2 + 4 \sum_{n=1}^{\infty} \frac{(-1)^n \cosh(\alpha_n x/b)}{\alpha_n^3 \cosh(\alpha_n a/b)} \cos\left[\frac{\alpha_n y}{b}\right], \quad (3)$$

where $W = (-dp/dz)(b^2/2\mu)$ is a velocity scale and $\alpha_n = (2n-1)\pi/2$. Adding an appropriate axial boundary velocity on $y=b$ due to the surface grooves is a straightforward extension of the work presented here.

We choose U_L, U_C, U_R as follows to produce three periodic fluid particle trajectories that form a three-dimensional braid analogous to the (2+1)-dimensional pA braid in Fig. 1(c) and Ref. 18. We take the flow to be spatially periodic in the axial direction with period $\ell_f = 2\ell$. For the first half of the period, $0 \leq z < \ell$, we take $U_L < 0$ and $U_C = U_R > 0$ so that the transverse flow consists of two counter-rotating rolls of unequal size. The relative size of these rolls is set such that (i) there exists two points $(0, y_C, 0)$ and $(x_R, y_R, 0)$ that lie on the same stream surface and exactly exchange position in the (x, y) -plane by the time they reach $z = \ell$, and (ii) the point $(x_L, y_L, 0) = (-x_R, y_R, 0)$ is a fixed point in the transverse flow, as shown in Fig. 2(c). For the channel geometry $a/2 = b = c = d$, these two conditions can be met by taking $U_L \approx -1.231U$ and $U_C = U_R = U$. If we choose U to also be the average axial velocity, namely, $U = \int w(x, y) dA / 4ab \approx 0.457W$, the necessary channel length is $\ell \approx 10.701b$. When viewed as shown in Fig. 2(c), with the axial flow coming toward the reader, the left periodic point is stationary while the right two periodic points exchange position in the clockwise direction. We refer to this three-stranded braid operation, or stirring protocol, as σ_2 . For the second half of the period, we take the transverse flow to be a reflection about the y -axis of the above flow; that is, for $\ell \leq z < 2\ell$ we take $U_L = U_C = -U$ and $U_R \approx 1.231U$. Now the right periodic point is stationary while the left two periodic points exchange positions in the counter-clockwise direction. We refer to this stirring protocol as σ_1^{-1} . Periodically alternating the transverse velocity field between these two counter-rotating flows produces the periodic orbits shown in Fig. 2(b), which has the representation²⁰ $(\sigma_2 \sigma_1^{-1})^3$; that is, the braid $\sigma_2 \sigma_1^{-1}$ is repeated three times. Each “strand” in the braid returns to its initial position in the (x, y) -plane after three periods of the flow. The similarity between the trajectories in Fig. 2(b) and the braid in Fig. 1(e) is clear, and they are, in fact, topologically equivalent.

One limitation of the simplified mathematical model is apparent in Fig. 2(b): the periodic axial discontinuity in the transverse velocity field leads to nonsmooth particle trajectories. In reality the system will have smooth transitions between channel sections that will certainly affect the specific

parameters considered here, but it is expected that a properly tuned experimental implementation will contain periodic orbits that form a topologically equivalent pA braid.

According to the TN theorem, a collection of fluid trajectories that are equivalent to a pA braid will cause two-dimensional, nontrivial material lines¹⁴ to grow as $\lambda^n \geq \lambda_{TN}^n$, where n is the period of the braid and λ_{TN} is the predicted lower bound from the TN theorem. For this steady, three-dimensional channel flow, we consider the stretching and folding of a material surface that begins as a nontrivial material line in an initial channel cross section. The TN theorem is applied to the downstream growth of the lines generated by the intersections of this surface with the spatially periodic channel cross sections at $z = n\ell_f$. Note that since the axial flow is nonuniform, different portions of a material surface can take significantly different amounts of time to reach a given cross section; we discuss this “exit time” variation below. For the braid we have here, $\sigma_2 \sigma_1^{-1}$, the predicted lower bound on the growth of the cross-sectional surface length is³ $\lambda_{TN} = (3 + \sqrt{5})/2 \approx 2.618$.

To evaluate the relevance of this lower bound, we track the evolution of the material surfaces that begin as the two nontrivial material lines shown in Fig. 2(c). The stretching and folding of these surfaces at various cross sections are shown in Figs. 2(d)–2(f). These results demonstrate that the stirring generated by the periodic orbits has a substantial effect on the entire fluid domain. Since the underlying mechanism for this deformation is topological, all nontrivial material lines in this flow will generate material surfaces that rapidly approach the periodic structure emerging in Fig. 2(f). Based on the exponential growth of the surfaces considered here, we estimate that $\lambda \approx 5.47$ for this flow; this estimate converges after roughly three to four periods of the flow. The actual stretching in this flow is well beyond the lower bound predicted by the TN theorem. This additional complexity suggests that this flow contains more periodic orbits than just those of the designed pA braid.

We compare this approach to previous work by using lid-driven motions to generate channel flows analogous to those considered in Ref. 10. The FO mixer A from Ref. 10 is, in our notation, $\sigma_2 \sigma_1 \sigma_1 \sigma_1$, and the pA mixer B is $\sigma_2 \sigma_1^{-1} \sigma_2^{-1} \sigma_1$. We evaluate mixing by tracking 10001 passive tracer particles initially placed uniformly along lines of constant y in the plane $z=0$. Here we choose $y=0.2b$, which initially lies above the center “rod” and below the other two rods and is thus a nontrivial material line, and $y=-0.5b$, which initially lies below all three periodic orbits, or rods. Similar to Ref. 10, we show in Fig. 3 the axial displacement of these tracers after an elapsed time $\Delta t = 10.5\ell/U$. For comparison we include the results for pure Poiseuille flow. Chaotic particle transport is characterized by rapid variation in longitudinal dispersion, while smooth distributions of axial displacement indicate regions of regular (nonchaotic) particle motion.²¹ All three stirred flows show both regular and chaotic motion. The “valleys” in the axial displacement come from particles that are transported close to an outer boundary and spend significant time there due to the no-slip condition.

If the fluid is perfectly mixed, every tracer particle will

FIG. 3. Axial dispersion of 10001 passive particles initially placed at $z=0$ along the straight lines $y=0.2b$ (top) and $y=-0.5b$ (bottom). Normalized axial positions are given as a function of initial x position. Panel columns are labeled according to the corresponding braid representation. Standard deviations, S , are for the corresponding braided lines; the Poiseuille flow values are $S=7.075\ell$ for the line $y=0.2b$ and $S=4.467\ell$ for $y=-0.5b$.

uniformly sample the channel cross section, and the net axial displacement will approach transport by the mean axial velocity, U , with $\Delta z=10.5\ell$. We quantify the mixing in each channel by computing the standard deviation, S , of the axial particle displacement about this mean displacement, with a lower value of S corresponding to better mixing. The worst mixer in this group is clearly the pure Poiseuille flow, followed by the FO protocol A. Both of the pA mixers produce better results than the FO mixer, with the pA braid considered here generating the best results. It is perhaps counterintuitive that chaotic particle transport and the corresponding random variations in longitudinal dispersion are what lead to the net axial displacement approaching that of a uniform flow.

The results of this letter differ significantly from Ref. 10, in which the best mixing was achieved by the FO stirring protocol A. In Ref. 10, fluid trajectories closest to the underlying braid have small axial velocities due to the no-slip condition on the solid rods, while the bulk of the fluid flows around the rods without much transverse motion. Here, in contrast, fluid throughout the channel cross section experiences substantial transverse motion, and the braiding motion of the periodic trajectories, or “ghost rods,”⁹ dominates the system. These results show that topological chaos can be applied to the analysis of stirring in a three-dimensional, lid-driven channel flow. This finding suggests that further research is needed to determine if and when the two-dimensional TN classification theorem can be used to investigate stirring in three-dimensional mixers.

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²In a miscible fluid-fluid system containing distinct regions, such as differently colored dyes, mixing is the process by which the system is

homogenized. Stirring is the part of the process in which interfaces between these regions are stretched and folded, and mixing is completed through molecular diffusion across these interfaces. It is generally expected, although not proven, that efficient stirring leads to rapid mixing. For this letter, we consider mixing in the limit of negligible diffusion.

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