J. Fluid Mech. (2011), *vol.* 675, *pp.* 465–476. © Cambridge University Press 2011
doi:10.1017/S0022112011000292

Optimal stirring strategies for passive scalar mixing

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(Received 4 September 2010; revised 30 October 2010; accepted 12 January 2011; first published online 10 March 2011)

We address the challenge of optimal incompressible stirring to mix an initially inhomogeneous distribution of passive tracers. As a quantitative measure of mixing we adopt the H^{-1} norm of the scalar fluctuation field, equivalent to the (square root of the) variance of a low-pass filtered image of the tracer concentration field. First we establish that this is a useful gauge even in the absence of molecular diffusion: its vanishing as $t \to \infty$ is evidence of the stirring flow's mixing properties in the sense of ergodic theory. Then we derive absolute limits on the total amount of mixing, as a function of time, on a periodic spatial domain with a prescribed instantaneous stirring energy or stirring power budget. We subsequently determine the flow field that instantaneously maximizes the decay of this mixing measure – when such a flow exists. When no such 'steepest descent' flow exists (a possible but non-generic situation), we determine the flow that maximizes the growth rate of the H^{-1} norm's decay rate. This local-in-time optimal stirring strategy is implemented numerically on a benchmark problem and compared to an optimal control approach using a restricted set of flows. Some significant challenges for analysis are outlined.

Key words: mathematical foundations, mixing, nonlinear dynamical systems

1. Introduction

The enhancement of mixing by stirring in incompressible flows is an important phenomenon in a wide variety of applications in sciences and engineering. A natural question is: how efficient a mixer can an incompressible flow be? This fundamental question, more precisely posed, is the subject of this paper.

In principle, given an appropriate quantitative measure of mixing along with suitable constraints on the accessible class of flow fields, the most efficient mixing strategy may be determined by solving an optimal control problem. In practice this may be difficult, so it is useful to consider other approaches that might more easily be implemented, at least theoretically or computationally. Moreover, it is always useful to know absolute limits on how fast mixing could ever be achieved subject to the relevant constraints. Such bounds provide a scale upon which particular strategies may be evaluated to gauge their effectiveness. Here we propose and analyse a theoretical scenario with a

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https://doi.org/10.1017/S0022112011000292 Published online by Cambridge University Press

specific mixing measure subject to particular constraints where these issues can be investigated analytically and via direct numerical simulation. As will be seen, there is an interesting gap between the best available *a priori* analysis and some of the simulation results.

The rest of the paper is organized as follows. In the next section we introduce the basic notions and define the specific problems to be studied. Rigorous bounds on the rate at which mixing measures can decay for constrained stirring flows are derived in § 3, and an optimal mixing strategy is described in § 4. In § 5, we report computational implementations of the optimal strategy and discuss open challenges suggested by the results.

2. Problem description

Consider the advection of a passive scalar field $\theta(\boldsymbol{x}, t)$ by a smooth incompressible flow field $\boldsymbol{u}(\boldsymbol{x}, t)$ described by the partial differential equation

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = 0 \tag{2.1}$$

along with the initial condition $\theta(\boldsymbol{x}, 0) = \theta_0(\boldsymbol{x})$. The stirring field $\boldsymbol{u}$ and the initial distribution θ_0 are periodic in the d-dimensional domain $[0, L]^d$ so the subsequent solution θ is as well. Without loss of generality, θ_0 and θ are spatially mean-zero:

$$\langle \theta(\cdot, t) \rangle \equiv \frac{1}{L^d} \int_{[0,L]^d} \theta(\boldsymbol{x}, t) \, \mathrm{d}\boldsymbol{x} = 0. \tag{2.2}$$

We also restrict attention to spatially mean-zero flows, i.e. $\langle u_i(\cdot, t) \rangle = 0$ for $i = 1, \ldots, d$.

The goal of effective stirring is to redistribute the passive tracer density to achieve a maximal rate of mixing as quantified by the relevant mixing measure. To gauge the effectiveness of the stirring, we adopt as a mixing measure the H^{-1} norm on mean-zero functions where, for any real parameter a, the H^{-a} norm is a weighted sum of the Fourier coefficients of the scalar field:

$$\|\theta(\cdot, t)\|_{H^{-a}}^2 \equiv \||\nabla|^{-a} \theta(\cdot, t)\|_{L^2}^2 = \sum_{\boldsymbol{k} \neq 0} k^{-2a} |\hat{\theta}_{\boldsymbol{k}}(t)|^2 \tag{2.3}$$

with $k = |\boldsymbol{k}|$ and

$$\hat{\theta}_{\boldsymbol{k}}(t) = \frac{1}{L^{d/2}} \int_{[0,L]^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \theta(\boldsymbol{x}, t) \, \mathrm{d}\boldsymbol{x}. \tag{2.4}$$

The operator $|\nabla|^{-a}$ generally acts in Fourier space as multiplication by k^{-a} although when a is an odd integer ∇^{-a} is naturally defined as multiplication by $-\mathrm{i}\boldsymbol{k}/k^{(a+1)}$.

We focus on the H^{-1} norm which is the large-scale mixing measure previously studied by a subset of the authors (Doering & Thiffeault 2006; Shaw, Thiffeault & Doering 2007). It measures the variance of a low-pass-filtered image of the concentration field: the smaller the H^{-1} norm, the more homogeneous is the scalar field on large spatial scales. It also has the appealing property that a doubling of spatial gradients of the scalar field leads to a halving of the norm. In many applications molecular diffusion, implemented mathematically by an additional $\kappa \Delta \theta$ term on the right-hand side of (2.1), dissipates the variance, i.e. the H^0 norm, of the scalar field. But even in the absence of molecular diffusion when the H^0 norm is conserved, or when the diffusion is ineffective on the length and time scales of interest, the relatively large-scale structures in the scalar field may nevertheless decay when

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a 'mix norm' like the H^{-1} norm is employed. This idea was introduced by Mathew, Mezić & Petzold (2005) for the $H^{-1/2}$ norm and is extended to other norms here.

For $a > 0$ the norms H^{-a} provide a quantitative measure of mixing in the sense of ergodic theory. To see this consider Lagrangian particle trajectories $\boldsymbol{X}(t)$ defined by

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{u}(\boldsymbol{X}(t), t) \tag{2.5}$$

with random initial condition $\boldsymbol{X}(0)$ distributed according to the bounded density $\rho_0(\boldsymbol{x})$. Then the tracer particle positions are distributed according to the solution $\rho(\boldsymbol{x}, t)$ of

$$\partial_t \rho + \boldsymbol{u} \cdot \nabla \rho = 0 \tag{2.6}$$

with initial condition $\rho_0(\boldsymbol{x})$. Incompressible advection conserves the variance of $\rho(\boldsymbol{x}, t)$: the mean-zero field $\theta = \rho - L^{-d}$ also satisfies the advection equation, and multiplying (2.1) by θ, integrating over the domain and integrating by parts yields $\mathrm{d}\|\theta\|_{L^2}/\mathrm{d}t = 0$. Hence the variance of the density does not measure mixing. Rather, the stirring field $\boldsymbol{u}(\boldsymbol{x}, t)$ is called *mixing* if for every periodic square-integrable function $g(\boldsymbol{x})$ on $[0, L]^d$,

$$\lim_{t\to\infty} \int_{[0,L]^d} g(\boldsymbol{x})\rho(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} = \langle g \rangle. \tag{2.7}$$

See, for example, Lasota & Mackey (1994). The utility of the H^{-a} norms (2.3) is indicated by the following theorem, an extension of Mathew *et al.* (2005).

THEOREM. *Suppose the spatially mean-zero function $\theta(\boldsymbol{x}, t)$ is bounded uniformly in $L^2([0, L]^d)$ for all $t > 0$. Then*

$$\lim_{t\to\infty} \int_{[0,L]^d} g(\boldsymbol{x})\,\theta(\boldsymbol{x}, t)\,d\boldsymbol{x} = 0 \quad \forall g \in L^2 \quad \Longleftrightarrow \quad \lim_{t\to\infty} \|\theta(\cdot, t)\|_{H^{-a}} = 0, \tag{2.8}$$

for any $a > 0$. See the appendix for an elementary proof that also applies to many other measures which could serve just as effectively as a mix norm in this regard.

The upshot is that more rapid self-averaging characteristic of the intuitive notion of mixing is indicated by more rapid decay of the H^{-a} norm. Alternative measures have also been used to characterize mixing and the associated control problem (see, for example, Sharma & Gupte 1997; D'Alessandro, Dahleh & Mezić 1999; Vikhansky 2002; Schumacher & Sreenivasan 2003; Balogh, Aamo & Krstic 2005; Mathew *et al.* 2005; Thiffeault & Finn 2006; Mathew *et al.* 2007; Constantin *et al.* 2008; Cortelezzi, Adrover & Giona 2008; Thiffeault & Pavliotis 2008; Gubanov & Cortelezzi 2010). The H^{-1} norm adopted here, however, allows for the development of a particularly straightforward and operational stirring strategy.

Constraints must be imposed upon the available flow fields in order to formulate an optimization problem. We focus on the constraints of bounded instantaneous kinetic energy, proportional to the L^2 norm of the velocity $\|\boldsymbol{u}(\cdot, t)\|_{L^2}^2$, or bounded instantaneous power dissipation in the flow, which for Newtonian fluids with periodic boundary conditions is proportional to the H^1 norm of the velocity $\|\nabla \boldsymbol{u}(\cdot, t)\|_{L^2}^2 = \sum_{i,j=1}^{d} \|\partial_i u_j(\cdot, t)\|_{L^2}^2$. That is, we consider flow fields $\boldsymbol{u}$ satisfying either

$$\int_{[0,L]^d} |\boldsymbol{u}(\boldsymbol{x}, t)|^2 \mathrm{d}\boldsymbol{x} = U^2 L^d \tag{2.9}$$

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or

$$\int_{[0,L]^d} |\nabla \boldsymbol{u}(\boldsymbol{x},t)|^2 \mathrm{d}\boldsymbol{x} = \int_{[0,L]^d} \frac{1}{4}\sum_{i,j=1}^{d} (\partial_i u_j + \partial_j u_i)^2 \mathrm{d}\boldsymbol{x} = \frac{L^d}{\tau^2} \tag{2.10}$$

defining, respectively, the root-mean-square velocity $U = \langle |\boldsymbol{u}|^2 \rangle^{1/2}$ or the rate of strain $\tau^{-1} = \langle |\nabla \boldsymbol{u}|^2 \rangle^{1/2}$ of the stirring.

The fixed-power constraint is natural for engineering applications where the focus is on overcoming viscous dissipation to maintain the stirring. The fixed-energy constraint is certainly natural from a mathematical point of view, but it is also relevant in applications where the stirring strength is characterized by the kinetic energy density in the flow rather than by the effort expended by the agent sustaining the stirring.

Given either of these flow constraints two obvious questions are:

(i) What flow *minimizes* the mixing measure evaluated at a final time $t_{fin} > 0$?

(ii) What flow *maximizes* the instantaneous decay rate of the mixing measure?

These questions have different answers implying different 'optimal' stirring strategies. Mathew *et al.* (2007) studied problem (i) and solved it numerically for a limited set of flow-field configurations using the $H^{-1/2}$ norm as the mixing measure. They computed the controls in the form of a time-varying linear combination of two simple cellular flows. That approach is global in time since it requires keeping track of the complete evolutionary history of the system within the interval $[0, t_{fin}]$.

In this paper, we address question (ii) and consider flows that produce the steepest descent of the H^{-1} mixing measure at each instant in time. This local-in-time strategy identifies an optimal mixing flow $\boldsymbol{u}(\boldsymbol{x},t)$ at time t using only a snapshot of the scalar field $\theta(\boldsymbol{x},t)$ at that instant. It should be noted that for the optimization problem (i) seeking to minimize the mixing measure at a final time, natural constraints might also be the total action (the integral of $\|\boldsymbol{u}(\cdot,t)\|_2^2$ from $t=0$ to t_{fin}) or the total energy (proportional to the time integral of $\|\nabla \boldsymbol{u}(\cdot,t)\|_2^2$ from $t=0$ to t_{fin}).

3. Absolute bounds on mixing rates

As a starting point, it is useful to identify absolute limits on the rate at which scalar fields might be mixed by fluids satisfying the instantaneous energy or power constraints. Towards this end we note that incompressible advection conserves not only the variance of θ but also that the (weak) maximum principle ensures that the L^∞ norm (the supremum of $|\theta|$ over the spatial domain) is conserved as well, i.e. $\|\theta(\cdot,t)\|_{L^\infty} = \|\theta_0\|_{L^\infty}$ at every time $t > 0$.

First consider the fixed-energy constraint (2.9). Multiplying (2.1) by $-\Delta^{-1}\theta$, integrating over the spatial domain, and integrating by parts implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla^{-1}\theta\|_{L^2}^2 = \frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}}^2 = -2\int \theta\, \boldsymbol{u}\cdot\nabla(\Delta^{-1}\theta)\,\mathrm{d}\boldsymbol{x}. \tag{3.1}$$

The Hölder and Cauchy–Schwarz inequalities then give

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}}^2 \geqslant -2\,\|\boldsymbol{u}\|_{L^2}\,\|\theta\|_{L^\infty}\,\|\theta\|_{H^{-1}} = -2UL^{d/2}\,\|\theta_0\|_{L^\infty}\,\|\theta\|_{H^{-1}}, \tag{3.2}$$

and dividing both sides by $2\,\|\theta\|_{H^{-1}}$ and integrating in time yields

$$\|\theta(\cdot,t)\|_{H^{-1}} \geqslant \|\theta_0\|_{H^{-1}} - UL^{d/2}\,\|\theta_0\|_{L^\infty} t. \tag{3.3}$$

This rigorous estimate does not rule out perfect mixing as measured by the H^{-1} norm after a finite time, but it does bound the absolute minimum mixing time from below

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by

$$t_{mix} = \frac{1}{UL^{d/2}} \frac{\|\theta_0\|_{H^{-1}}}{\|\theta_0\|_{L^\infty}} = \frac{l_0}{2\pi U}, \tag{3.4}$$

singling out a length scale

$$l_0 = 2\pi \frac{\langle |\nabla^{-1}\theta_0|^2 \rangle^{1/2}}{\|\theta_0\|_{L^\infty}} \quad (\leqslant L \text{ due to the Poincaré and Hölder inequalities}) \tag{3.5}$$

characterizing the spatial extent or 'size' of initial inhomogeneities in the scalar field. The lower bound in (3.3) simply states that under the constant energy constraint, the time it takes to achieve complete mixing is at least as long as the time it takes to transport scalar inhomogeneities across the characteristic distance $\sim l_0$ at the r.m.s. speed U of the flow. Whether or not this limiting mixing rate can actually be achieved, or even approached, by any suitably constrained stirring flow remains to be seen.

The analysis is rather different for flows subject to the fixed-power constraint (2.10). For convenience we define the filtered scalar field

$$\varphi(\boldsymbol{x}, t) = \left(\Delta^{-1}\theta\right)(\boldsymbol{x}, t) = -\sum_{\boldsymbol{k}\neq 0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\theta}} k^{-2} \hat{\theta}_{\boldsymbol{k}}(t). \tag{3.6}$$

Then starting from (3.1) more integrations by parts yield

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}}^2 = \frac{\mathrm{d}}{\mathrm{d}t}\|\nabla\varphi\|_{L^2}^2 = -2\sum_{i,j=1}^{d} \int \varphi \, \frac{\partial u_i}{\partial x_j} \, \frac{\partial^2 \varphi}{\partial x_i \partial x_j} \, \mathrm{d}\boldsymbol{x} \tag{3.7}$$

and the Hölder and Cauchy–Schwarz inequalities imply

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}}^2 \geqslant -2\,\|\varphi\|_{L^\infty}\,\|\nabla \boldsymbol{u}\|_{L^2}\,\|\Delta\varphi\|_{L^2} = -2\,\|\varphi\|_{L^\infty}\,\frac{L^{d/2}}{\tau}\,\|\theta_0\|_{L^2}. \tag{3.8}$$

In order to close the differential inequality, it is necessary to bound the sup-norm $\|\varphi\|_{L^\infty}$ in terms of the H^{+1} norm of φ, i.e. $\|\nabla\varphi\|_{L^2} = \|\nabla^{-1}\theta\|_{L^2} = \|\theta\|_{H^{-1}}$, and some conserved (or otherwise *a priori* bounded) quantities. This is possible in two and three spatial dimensions.

First consider $d = 3$. For mean-zero functions on the 3-torus, there exists an $\mathcal{O}(1)$ pure number C_3 so that

$$\|\varphi\|_{L^\infty} \leqslant C_3\,\|\nabla\varphi\|_{L^2}^{1/2}\,\|\Delta\varphi\|_{L^2}^{1/2} = C_3\,\|\theta\|_{H^{-1}}^{1/2}\,\|\theta_0\|_{L^2}^{1/2}. \tag{3.9}$$

For an elementary proof of the inequality, see Doering & Gibbon (1995). Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}} \geqslant -\frac{C_3 L^{3/2}}{\tau}\,\|\theta_0\|_{L^2}^{3/2}\,\|\theta\|_{H^{-1}}^{-1/2} \tag{3.10}$$

and

$$\|\theta(\cdot, t)\|_{H^{-1}} \geqslant \|\theta_0\|_{H^{-1}} \left[1 - \frac{3C_3}{2\tau}\left(\frac{L\,\|\theta_0\|_{L^\infty}}{\|\theta_0\|_{H^{-1}}}\right)^{3/2} \times t\right]^{2/3} \tag{3.11}$$

as long as the term in brackets is non-negative. Again the rigorous analysis does not rule out perfect mixing in a finite time but bounds the minimal mixing time from below by

$$t_{mix} = \tau \times \frac{2}{3\,C_3}\left(\frac{\ell_0}{2\pi L}\right)^{3/2}, \tag{3.12}$$

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where

$$\ell_0 = 2\pi \frac{\|\theta_0\|_{H^{-1}}}{\|\theta_0\|_{L^2}} \quad (\leqslant L \text{ by Poincaré's inequality}) \tag{3.13}$$

is another length scale characterizing the size of inhomogeneities in the initial distribution. We note that for the same initial distribution, $\ell_0 \geqslant l_0$ defined for the fixed-energy optimal stirring in (3.5).

The linear dependence of t_{mix} on τ is not surprising. This rigorous estimate is, however, more than naïve-dimensional analysis because the lower bound on the mixing time allows for a nontrivial L-dependence. The minimal mixing time estimate in (3.12) suggests that the availability of larger *domain* length scales L for the flow to access may in fact facilitate mixing, perhaps by allowing for more effective 'folding' to accompany judiciously localized 'stretching'. The suggestion (which remains a conjecture at this point) is that if N^3 copies of the same initial distribution with basic scale ℓ_0 are assembled into a larger periodic domain $[0, N \times L]^3$, the scalar might possibly be mixed faster by a flow with the same r.m.s. rate of strain than on the elementary cell $[0, L]^3$.

A similar sort of system size dependence is suggested in two dimensions. The $d = 2$ analogue of (3.9) is (again, see Doering & Gibbon 1995 for an elementary derivation)

$$\|\varphi\|_{L^\infty} \leqslant C_2 \|\nabla\varphi\|_{L^2} \sqrt{1 + \log\left[\frac{L\,\|\Delta\varphi\|_{L^2}}{2\pi\|\nabla\varphi\|_{L^2}}\right]} = C_2 \|\theta\|_{H^{-1}} \sqrt{1 + \log\left[\frac{L\,\|\theta_0\|_{L^2}}{2\pi\|\theta\|_{H^{-1}}}\right]} \tag{3.14}$$

for an $\mathcal{O}(1)$ constant C_2. Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}} \geqslant -\frac{C_2 L}{\tau}\,\|\theta_0\|_{L^2} \sqrt{1 + \log\left[\frac{L\,\|\theta_0\|_{L^2}}{2\pi\|\theta\|_{H^{-1}}}\right]}. \tag{3.15}$$

This differential inequality also does not prevent $\|\theta\|_{H^{-1}}$ from vanishing in finite time, but it guarantees that $\|\theta\|_{H^{-1}}$ cannot vanish before the absolute minimum mixing time

$$t_{mix} = \tau\,\frac{e}{2\pi C_2} \int_{\log L/\ell_0}^{\infty} \frac{\mathrm{e}^{-\zeta}}{\sqrt{\zeta}}\,\mathrm{d}\zeta, \tag{3.16}$$

where ℓ_0 is defined in (3.13). For $L \gg \ell_0$ the minimum mixing time is

$$t_{mix} \sim \tau \times \frac{\ell_0}{L} \times \left(\log\frac{L}{\ell_0}\right)^{-1/2}, \tag{3.17}$$

again allowing for the possibility that it may take less time to mix within a larger volume.

In contrast to these potentially finite-time mixing scenarios, if the flow field is constrained to have a *uniformly* bounded (in space and time) rate of strain, then it can decay at most exponentially. In any spatial dimension if $\|(\boldsymbol{\nabla u})_{sym}\|_{L^\infty} \leqslant \gamma < \infty$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\theta\|_{H^{-1}}^2 = 2\int \nabla^{-1}\theta \cdot (\boldsymbol{\nabla u}) \cdot \nabla^{-1}\theta\,\mathrm{d}\boldsymbol{x} \geqslant -2\gamma\,\|\theta\|_{H^{-1}}^2 \tag{3.18}$$

and Grönwall's inequality implies an exponential lower bound on the mixing measure:

$$\|\theta(\cdot, t)\|_{H^{-1}} \geqslant \|\theta_0\|_{H^{-1}}\,\mathrm{e}^{-\gamma t}. \tag{3.19}$$

Thus if the rate of strain is bounded, then the mixing rate cannot be increased by increasing the domain scale (holding all other constraints fixed). Therefore, if there

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is any real precision regarding the L-dependence in estimate (3.12) or (3.17), then it depends crucially on a fixed-power flow's freedom to locally intensify the strain.

4. Optimal stirring

Recalling (3.1) we write

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla^{-1}\theta\|_2^2 = -2\int \boldsymbol{u}\cdot(\theta\nabla\varphi)\,\mathrm{d}\boldsymbol{x} = -2\int \boldsymbol{u}\cdot\mathbb{P}(\theta\nabla\varphi)\,\mathrm{d}\boldsymbol{x}, \tag{4.1}$$

where $\mathbb{P}(\cdot)$ is the projector onto divergence-free fields defined by

$$\mathbb{P}(\boldsymbol{v}) = \boldsymbol{v} - \nabla\Delta^{-1}(\nabla\cdot\boldsymbol{v}). \tag{4.2}$$

Then with either the fixed-energy (2.9) or fixed-power (2.10) constraints, it is easy to see that the optimal stirring field maximizing the rate of decay of the mix-norm H^{-1} is

$$\boldsymbol{u}_e = U\,\frac{\mathbb{P}(\theta\nabla\varphi)}{\langle|\mathbb{P}(\theta\nabla\varphi)|^2\rangle^{1/2}} \tag{4.3}$$

or

$$\boldsymbol{u}_p = \frac{1}{\tau}\,\frac{-\Delta^{-1}\mathbb{P}(\theta\nabla\varphi)}{\langle|\nabla^{-1}\mathbb{P}(\theta\nabla\varphi)|^2\rangle^{1/2}} \tag{4.4}$$

if the norm in the denominator does not vanish. So long as the relevant optimal stirring exists, the ideal instantaneous stirring strategy is to implement it at each instant of time. But if either of the norms in the denominators vanishes, then $\mathbb{P}(\theta\nabla\varphi)=0$ throughout the domain and *no* incompressible flow can instantaneously decrease the mix-norm H^{-1}.

A sufficient (but not to our knowledge necessary) condition for such degeneracies is that the scalar field θ satisfies

$$\Delta\theta = F(\theta), \tag{4.5}$$

which includes cases where θ is an eigenfunction of the Laplacian. Such situations arise naturally as convenient initial conditions, but we suspect that they are non-generic distributions among solutions of the advection equation. Nevertheless, when and if this situation develops, some other strategy must be adopted to stir the fluid.

The natural thing to do when $\mathbb{P}(\theta\nabla\varphi)=0$ is to find the flow that maximizes the rate of increase of the rate of decrease of the norm. That is, seek the flow that minimizes

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\|\theta\|_{H^{-1}}^2 = 2\int[\boldsymbol{u}\cdot\nabla\varphi\,\nabla\theta\cdot\boldsymbol{u} - (\boldsymbol{u}\cdot\nabla\theta)\Delta^{-1}(\boldsymbol{u}\cdot\nabla\theta)]\,\mathrm{d}\boldsymbol{x}. \tag{4.6}$$

Then the optimal incompressible flow $\boldsymbol{u}$ solves the eigenvalue problem

$$\lambda\boldsymbol{u} = \mathbb{P}((\boldsymbol{u}\cdot\nabla\theta)\nabla\varphi + (\boldsymbol{u}\cdot\nabla\varphi)\nabla\theta - 2[\Delta^{-1}(\boldsymbol{u}\cdot\nabla\theta)]\nabla\theta) \tag{4.7}$$

for the fixed-energy constraint or

$$\lambda\boldsymbol{u} = -\Delta^{-1}\mathbb{P}((\boldsymbol{u}\cdot\nabla\theta)\nabla\varphi + (\boldsymbol{u}\cdot\nabla\varphi)\nabla\theta - 2[\Delta^{-1}(\boldsymbol{u}\cdot\nabla\theta)]\nabla\theta) \tag{4.8}$$

for the fixed-power constraint. In either case we seek the eigenvector (field) corresponding to the minimum eigenvalue $\lambda_- < 0$ to use as the stirring field momentarily until $\mathbb{P}(\theta\nabla\varphi)\neq 0$.

This local-in-time optimal stirring strategy is a limiting case of the short-horizon optimization studied by Cortelezzi *et al.* (2008) when the horizon becomes infinitesimal, albeit with a much broader class of available flows. In order to implement

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it in practice the full scalar field must be monitored so that the optimal flow field can be computed at each instant. This is not impractical for theoretical and computational studies, but of course globally monitoring a scalar distribution in the laboratory or in nature and subsequently physically imposing a favoured flow field can be quite challenging. Nevertheless insights gained from mathematical implementations may be helpful for some applications.

The eigenvalue problems in (4.7) and (4.8) are generally difficult. To make some analytical progress, consider the special case $\theta_0(\boldsymbol{x}) = \sin(kx)$ that we will use as an initial condition in the computational test reported in the next section in spatial dimension $d = 2$. Introducing the stream function so that $u = \partial\psi/\partial y$ and $v = -\partial\psi/\partial x$ and taking the curl of (4.7),

$$-\lambda\Delta\psi = -2\nabla\times\mathbb{P}\boldsymbol{v} = -2\nabla\times(\boldsymbol{v} - \nabla\Delta^{-1}(\nabla\cdot\boldsymbol{v})) = -2\nabla\times\boldsymbol{v} = 2\frac{\partial v_x}{\partial y}, \tag{4.9}$$

where $\boldsymbol{v}(\boldsymbol{x}, t) = (\boldsymbol{u}\cdot\nabla\theta)\nabla\varphi + (\boldsymbol{u}\cdot\nabla\varphi)\nabla\theta - 2[\Delta^{-1}(\boldsymbol{u}\cdot\nabla\theta)]\nabla\theta$. Writing $\psi(x, y) = \sum_{m,n}\hat{\psi}_{mn}\exp\{2\pi\mathrm{i}(mx + ny)/L\}$ produces a matrix equation for the Fourier coefficients $\hat{\psi}_{mn}$. With the fixed-energy constraint (2.9), finite-resolution ($n, m \leqslant N$) numerical solutions to this matrix equation show that the minimum eigenvalue is always associated with the Nth harmonic, suggesting that the optimal flow depends on the imposed Fourier cutoff. Focusing instead on the fixed-power constraint (2.10), it is readily shown that to leading order in the initial data wavenumber k the minimum eigenvalue we seek is

$$\min_{m,n}\lambda_{mn}(k) = \lambda_{m^*,1}(k) \sim -\frac{1}{k^2}\left[1 + \mathcal{O}\left((kL)^{-4}\right)\right] \tag{4.10}$$

and the associated eigenfunction, modulo an arbitrary phase shift in y, is approximately proportional to the first harmonic, i.e. $u \propto \sin(2\pi y/L)$ and $v = 0$.

Two final remarks: first, note that unless the scalar field is a superposition of the lowest available modes, it can be *unmixed*. Indeed, simply reversing the optimal flow momentarily unmixes the scalar as defined by the H^{-1} norm. Second, note that any of these stirring fields can be regarded as solutions of the incompressible Euler, Navier–Stokes, or other equations of motion with an appropriate body force.

5. Computational tests and discussion

The first test of the optimal stirring strategy uses the initial scalar distribution $\theta_0(x) = \sin x$ (with $\ell_0/L = 1$) in a domain of size $L = 2\pi$ in $d = 2$ spatial dimensions. We implemented the fixed-power constraint with $\tau^{-1} = 6.25\times(2\pi)^2$, equivalent to the amplitude of the bi-component control utilized by Mathew *et al.* (2007). Figure 1(*a*) shows the evolution of the scalar mix norms. It is interesting to note that, at least for this particular initial distribution, the result of the instantaneous H^{-1} optimization follows the optimal control result with the limited set of stirring fields – as measured by the $H^{-1/2}$ mix norm – up to time $T \approx 0.2$ with an initial flow closely related to the simple sine shear flow. After the initial transient where the flow is chosen to maximize $(\mathrm{d}^2/\mathrm{d}t^2)\|\theta\|^2_{H^{-1}}$, a robust exponential decay of the H^{-1} norms emerges. In order to compare with the two-component flow optimal control results of Mathew *et al.* (2007), we also computed the $H^{-1/2}$ norm that they utilized and reported. Not unexpectedly, expanding the set of available flows from two possibilities to everything within the constant power constraint allows for faster mixing. Nevertheless the

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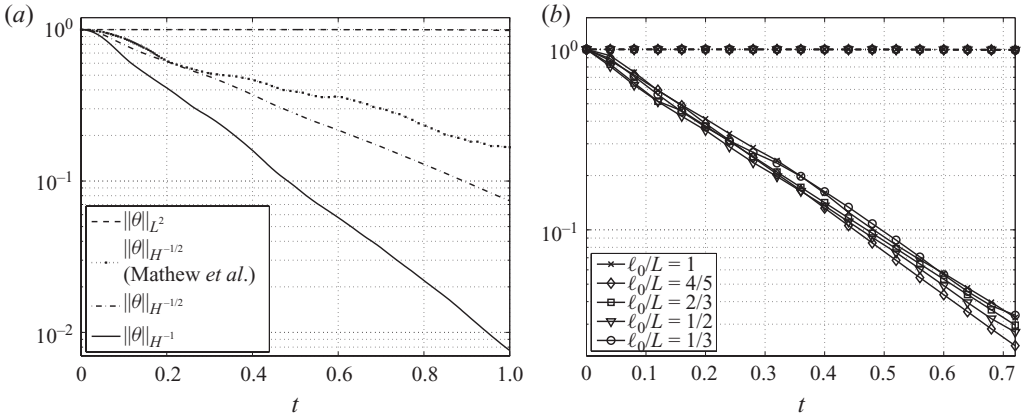


FIGURE 1. (*a*) Evolution of mixing measures with the fixed-power constraint for $\theta_0(\boldsymbol{x}) = \sin(x)$. A standard pseudo-spectral scheme with 512^2 resolution was utilized and the conserved L^2 norm was monitored as a numerical check. All norms are rescaled by their initial values. (*b*) Decay of H^{-1} for different values of ℓ_0/L (solid lines). The $\ell_0/L = 1$ case uses $\theta_0 = \sin x$, while the $\ell_0/L = 4/5$ initial distribution is a sum of five low-wavenumber harmonics, $\theta_0 = \sin x + 1.92(-0.542\cos 2x + 0.8267\sin y - 0.6592\cos 2y + 0.3998\sin x\cos y + 0.6516\cos x\sin y)$. The $\ell_0/L = 2/3$ data are $\theta_0(x) = \sin x + \sqrt{5/3}\sin 3y$. The $\ell_0/L = 1/2$ case uses discontinuous (non-periodic) initial data, $\theta_0 = \sin[2(1 + 0.5\sin y)x]$, and the $\ell_0/L = 1/3$ initial data are $\sin 3x$. The dot-dashed lines illustrate conservation of L^2 norms with different data in the simulations.

local-in-time optimization strategy employed here leaves room for further improvement via more global-in-time control.

To check for a possible dependence of the mixing rate on ℓ_0/L, we also considered different initial data, and the results are displayed in figure 1(*b*). As is evident, the mixing scheme implemented here generates robust exponential decay of the H^{-1} mix norm. Exponential decay at a rate independent of the initial data is the sort of behaviour that might be expected for a uniform-boundedness constraint on the rate of strain, rather than finite-time mixing that the best available analysis allows for when only the root-mean-square rate of strain is bounded *a priori*. In fact, we observed that the sup-norm of the rate of strain of the optimal stirring generally increases with time so it is not at all obvious (from the point of view of mathematical analysis) how the exponential decay is maintained. It is possible that the rigorous lower bounds on the mix norm may only be saturated by a global-in-time, i.e. optimal control, stirring strategy. On the other hand, it may be that further improvement in the analysis will eventually bring theory and simulations into accord. At this stage, however, the discrepancy between rigorous analysis and computational observations constitutes an important open question.

Figure 2 shows the snapshots of the scalar field evolution with initial distribution $\theta_0(x) = \sin x$ under the local fixed-power optimal mixer. The optimal flow generates a suggestively self-similar cascade of the scalar fluctuations to small scales. Other initial conditions generate similar cascades in the scalar concentration.

The H^{-1} mix norm for the local fixed-energy optimal mixer with initial scalar distribution $\theta_0(x) = \sin x$, initially perturbed according to the fixed-power scheme (4.8), is compared with the fixed-power result in figure 3. The amplitudes U and $1/\tau$ of the constraints are those for the cellular flows in Mathew *et al.* (2007), which

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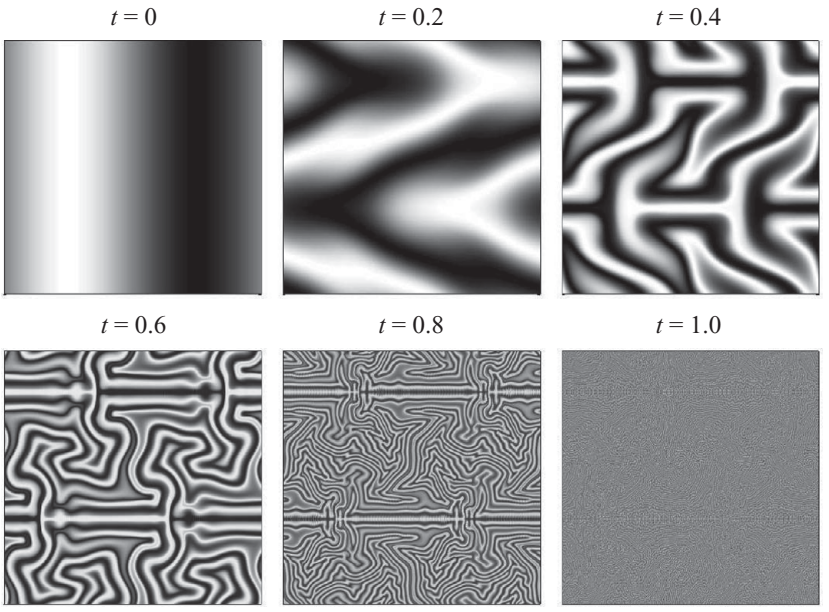


FIGURE 2. Evolution of the scalar field in $[0, 2\pi]^2$ with optimal mixing strategy (4.4) and solution to (4.8) with fixed power and $\theta_0(\boldsymbol{x}) = \sin x$.

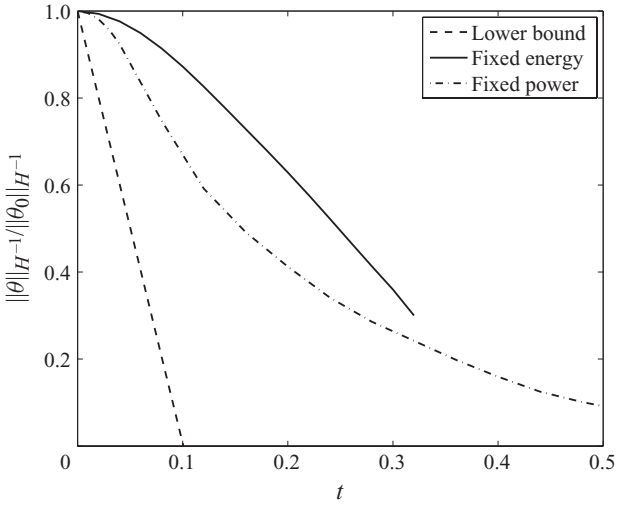


FIGURE 3. H^{-1} mix norm normalized by its initial value using the local optimal mixing strategies (4.3) with fixed energy (solid line) and the local optimal mixing strategy (4.4) with fixed power (dash-dotted line) and initial distribution $\theta_0(\boldsymbol{x}) = \sin x$. The amplitudes U and $1/\tau$ coincide with those in Mathew *et al.* (2007). This degenerate $\sin x$ scalar distribution was initially perturbed according to the fixed-power scheme (4.8) for both subsequent stirring strategies. The lower bound (dashed) from (3.3) is for fixed energy.

means that the simple sine shear flow that emerges near $t = 0$ has larger amplitude for the fixed-power case than for fixed energy, and hence faster initial mixing for fixed power. The rate of change of the mix norm for the fixed-power constraint eventually

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decreases consistent with exponential decay, but the rate of change of the mix norm for the fixed-energy constraint steadily increases. The flow in the fixed-energy case rapidly concentrates on small scales and resolution of the 512^2 computation becomes questionable after time $t \approx 0.32$, so the simulation data are truncated there. These available data are not incompatible with the linear decay of the mix norm and finite-time mixing suggested by (3.3) and (3.4)–(3.5), but higher resolution computations will be necessary for further confirmation.

The authors gratefully acknowledge discussions with Igor Mezić and Anna Mazzucato. This work was supported by NSF Awards PHY-0555324 & PHY-0855335 (CRD) and DMS-0806821 (J-LT). This research was initiated at the *Optimal Transport* program at NSF's Institute for Pure and Applied Mathematics and developed further at the *Complex Fluids & Complex Flows* program at NSF's Institute for Mathematics & Its Applications and at the *Geophysical Fluid Dynamics* program at Woods Hole Oceanographic Institution, supported by NSF and ONR.

Appendix. Proof of theorem

We use the norm (2.3) for mean-zero functions, $\|\theta\|_{H^{-a}} = \left(\sum_{\boldsymbol{k}} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}|^2\right)^{1/2}$, although the proof easily generalizes to other norms. Suppose that $\theta(\cdot, t)$ is uniformly bounded in $L^2([0, L]^d)$, so that $\|\theta(\cdot, t)\|_{L^2} \leqslant C$, and $\lim_{t\to\infty} \|\theta(\cdot, t)\|_{H^{-a}} \to 0$ for some $a > 0$. Then for any $g \in L^2([0, L]^d)$,

$$\left|\int_{[0,L]^d} \theta g \,\mathrm{d}\boldsymbol{x}\right| = \left|\sum_{k\leqslant K} k^{-a}\,\hat{\theta}_{\boldsymbol{k}}\, k^a\,\hat{g}^*_{\boldsymbol{k}} + \sum_{k>K} \hat{\theta}_{\boldsymbol{k}}\,\hat{g}^*_{\boldsymbol{k}}\right|$$
$$\leqslant \|\theta\|_{H^{-a}} \left(\sum_{k\leqslant K} k^{2a}|\hat{g}_{\boldsymbol{k}}|^2\right)^{1/2} + \|\theta\|_{L^2}\left(\sum_{k>K}|\hat{g}_{\boldsymbol{k}}|^2\right)^{1/2}. \quad \text{(A 1)}$$

Given $\epsilon > 0$, first choose $K(\epsilon)$ such that $\left(\sum_{k>K(\epsilon)}|\hat{g}_{\boldsymbol{k}}|^2\right)^{1/2} \leqslant \epsilon/2C$, then choose $T(\epsilon)$ such that $\|\theta(\cdot, T(\epsilon))\|_{H^{-a}} \leqslant \frac{\epsilon}{2}\left(\sum_{k\leqslant K(\epsilon)} k^{2a}|\hat{g}_{\boldsymbol{k}}|^2\right)^{-1/2}$, for $t > T(\epsilon)$. Then

$$\left|\int_{[0,L]^d} \theta g \,\mathrm{d}\boldsymbol{x}\right| \leqslant \frac{1}{2}\left(1 + C^{-1}\|\theta\|_{L^2}\right)\epsilon \leqslant \epsilon, \quad t > T(\epsilon), \quad \text{(A 2)}$$

which implies that θ converges weakly to zero as $t \to \infty$. (This is true even for $a = 0$).

Conversely, suppose $\|\theta(\cdot, t)\|_{L^2} \leqslant C$ for all t and $\lim_{t\to\infty}\int_{[0,L]^d} \theta g \,\mathrm{d}\boldsymbol{x} \to 0$ for all $g \in L^2([0, L]^d)$. By choosing $g = \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})$ we see that all the Fourier coefficients $\hat{\theta}_{\boldsymbol{k}}(t) \to 0$ as $t \to \infty$. Also, because $\|\theta(\cdot, t)\|^2_{L^2} = \sum_{\boldsymbol{k}}|\hat{\theta}_{\boldsymbol{k}}(t)|^2 \leqslant C^2$, each $|\hat{\theta}_{\boldsymbol{k}}(t)| \leqslant C$ for all t.

Thus,

$$\|\theta\|^2_{H^{-a}} = \sum_{k\leqslant K} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}|^2 + \sum_{k>K} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}|^2 \leqslant \sum_{k\leqslant K} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}|^2 + K^{-2a}\|\theta\|_{L^2}. \quad \text{(A 3)}$$

For any $\epsilon > 0$, choose $K(\epsilon) \geqslant (2C/\epsilon)^{1/2a}$ so that $k^{-2a}\|\theta\|_{L^2} \leqslant k^{-2a}C \leqslant \epsilon/2$ for $k \geqslant K(\epsilon)$. (This requires $a > 0$). Then because for any finite K, $\sum_{k\leqslant K} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}(t)|^2 \to 0$ as $t \to \infty$, there exists $T(\epsilon) < \infty$ such that $\sum_{k\leqslant K(\epsilon)} k^{-2a}|\hat{\theta}_{\boldsymbol{k}}(t)|^2 < \epsilon/2$ for all $t > T(\epsilon)$. From (A 3) we conclude that $\|\theta\|^2_{H^{-a}} < \epsilon$ for all $t > T(\epsilon)$, which proves the result.

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