Abstract. Mixing a passive scalar field by stirring can be measured in a
diverse variety of ways including tracer particle dispersion, via the flux-gradient rela-
tionship, or by suppression of scalar concentration variations in the presence of
inhomogeneous sources and sinks. The mixing efficiency or efficacy of a partic-
ular flow is often expressed in terms of enhanced diffusivity and quantified as
an effective diffusion coefficient. In this work we compare and contrast several
notions of effective diffusivity. We thoroughly examine the fundamental case of
a steady sinusoidal shear flow mixing a scalar sustained by a steady sinusoidal
source-sink distribution to explore apparent quantitative inconsistencies among
the measures. Ultimately the conflicts are attributed to the noncommutative
asymptotic limits of large Péclet number and large length-scale separation. We
then propose another approach, a generalization of Batchelor’s 1949 theory of
diffusion in homogeneous turbulence, that helps unify the particle dispersion
and concentration variance suppression measures.

1. Introduction. Flow-enhanced mixing is an important phenomenon in natural
systems varying in size from as small as human cells to as large as the atmosphere
and the ocean and beyond [5, 6, 15]. The enhancement of molecular mixing by
stirring can be observed even for simple laminar flows, and a quantitative under-
standing of fundamental mechanisms and properties of mixing processes is key to
accurate modeling of these systems.

Passive scalars are mathematically idealized entities that serve as proxies to
formulate and investigate this problem. Given its initial location, the trajectory

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of a passive tracer in $\mathbb{R}^d$ advected by a prescribed flow field $\vec{u}(\vec{x}, t)$ is described by the stochastic differential equation

$$d\vec{X}(t) = \vec{u}(\vec{X}(t), t)dt + \sqrt{2\kappa} d\vec{W}(t),$$

where $\kappa$ is the molecular diffusivity and $\vec{W}$ is canonical $d$-dimensional Brownian motion. Equivalently, the Fokker-Planck equation that governs the evolution of the scalar concentration field $T(\vec{x}, t)$ stirred by an incompressible ($\nabla \cdot \vec{u} = 0$) flow is the advection-diffusion equation

$$\partial_t T + \vec{u} \cdot \nabla T = \kappa \Delta T$$

supplemented with initial concentration $T(\vec{x}, 0)$ and appropriate boundary conditions. In many applications, the scalar field is constantly replenished and depleted by sources and sinks. Consequently, the homogeneous partial differential equation (2) would be appended with an inhomogeneous term corresponding to the source-sink distribution whose relationship with the stirring further adds to the mathematical complexity of the problem.

In this work we first review several different measures established in the literature to characterize the effects of stirring on enhanced mixing. Each measure is associated with a specific physical setting and is amenable to different mathematical analysis and/or approximation. Approximations adopting distinct noncommutative limiting procedures for control parameters may yield conflicting predictions. We then thoroughly investigate a fundamental example of this problem, that of a simple steady shear flow stirring a scalar sustained by a monochromatic source-sink distribution, to expose an apparent contradiction between the mixing measures when the high-Péclet and large length-scale-separation limits are exchanged. Finally, we propose a mathematical framework that utilizes information about single particle dispersion, a generalization of Batchelor’s 1949 theory [1] of diffusion in a field of homogeneous isotropic turbulence, to accurately predict scalar concentration variance reduction by the (in this case, inhomogeneous and anisotropic) flow. This new approach produces a uniformly valid dependence of the effective diffusion on the control parameters, reconciling the apparent inconsistencies.

2. Mixing measures. A conventional modeling approach, and the one we will focus on here, is to describe the flow-enhanced mixing by replacing the advection-diffusion operator with an effective diffusive operator, i.e.,

$$\kappa \Delta T - \vec{u} \cdot \nabla T \rightarrow \nabla \cdot (\mathbf{K}^{\text{eff}} \cdot \nabla T)$$

where $\mathbf{K}^{\text{eff}}$ is an effective diffusivity tensor designed to capture some specific feature(s) of the mixing process.

One such feature is transient passive particle dispersion with $\mathbf{K}^{\text{eff}}$ defined by

$$K^{\text{eff}}_{ij} = \frac{1}{2} \lim_{t \to \infty} \frac{d}{dt} \mathbb{E}[(X_i(t) - X_i(0))(X_j(t) - X_j(0))], \quad i, j = 1, \ldots, d$$

where $\vec{X}(t) = (X_1(t), \ldots, X_d(t))^T$ is the trajectory described by (1) and the statistical average $\mathbb{E}[:]$ is taken over all Brownian paths $\vec{W}(t)$. The effective diffusion tensor $K_{ij}$ is often defined as $\lim_{t \to \infty} \frac{1}{2t} \mathbb{E}[(X_i(t) - X_i(0))(X_j(t) - X_j(0))]$, but these are equivalent when the covariance elements converge no more than linearly with time.
The steady sinusoidal shear $\vec{u} = \hat{i} \sqrt{2} U \sin(k_u y)$, where $\hat{i}$ is the unit vector in the $x$–direction, is a case in point. The effective diffusivity tensor defined by the long-time dispersive behavior of particles is the Taylor dispersion result [16]

$$K^{\text{eff}} = \begin{pmatrix} \kappa(1 + Pe^2) & 0 \\ 0 & \kappa \end{pmatrix}$$

where the strength of the advection is gauged by the non-dimensional Péclet number $Pe = Ul_u/\kappa$ with the flow-characteristic length-scale $l_u = k_u^{-1}$.

In the absence of steady sources and sinks, and when the separation between the characteristic length-scale of the scalar density distribution, call it $l_d$, and that of the flow, $l_u$, is very large, homogenization theory [5, 8, 9] asserts that the scalar concentration evolves according to a diffusion equation with effective diffusion tensor $K^{\text{eff}}$ for a broad collection of deterministic and stochastic flows. The normalized tensor $\kappa^{-1}K^{\text{eff}}$ emerges naturally as a dimensionless measure of the mixing efficacy of the stirring, and previous analysis for the $l_d/l_u \to \infty$ homogenization limit has shown that each component in the normalized tensor is bounded above in terms of the Péclet number according to

$$E_{HT}^{ij} := \frac{K^{\text{eff}}_{ij}}{\kappa} \leq 1 + Pe^2.$$  

Taylor dispersion, and in particular the steady sinusoidal shear flow, saturates the bound for $K_{11}^{\text{eff}}$.

Homogenization theory explicitly assumes the large length-scale separation between the flow and the scalar field. In one incarnation a steady large-scale gradient is imposed in one spatial direction to formulate the so-called “cell problem” [6]. This is implemented theoretically by writing $T = -G_x + \theta$ so the advection-diffusion equation (2) becomes the evolution equation for the concentration fluctuation field $\theta$:

$$\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + G (\hat{i} \cdot \vec{u}).$$

The flow and fluctuation fields are then assumed to be periodic and mean-zero on a cell of size $l_u$ across which the “mean” scalar gradient $G$ is held constant. This model serves as the starting point for many studies of turbulent mixing [13].

The solution of (7) provides another, potentially distinct, measure of mixing enhancement in terms of the scalar flux-gradient relationship. If the effective diffusion coefficient $K_{11}^{\text{eff}}$ is defined as the ratio of the mean scalar flux in the $x$–direction to the mean scalar gradient in the $x$–direction, then

$$E_{FG}^{11} := \frac{K_{11}^{\text{eff}}}{\kappa} = \frac{\langle \hat{i} \cdot (\vec{u} T - \kappa \nabla T) \rangle}{\kappa G} = 1 + \frac{\langle |\nabla \theta|^2 \rangle}{G^2} \leq 1 + Pe^2$$

where $\langle \cdot \rangle$ denotes the long time and spatial average within a periodic cell. The second expression for $E_{FG}^{11}$ in terms of $\theta$ follows from the time-cell average of $\theta$ times (7) which implies that $\kappa \langle |\nabla \theta|^2 \rangle = G \langle \hat{i} \cdot \vec{u} \rangle$, and the upper bound follows from

$$\frac{\langle |\nabla \theta|^2 \rangle}{G} \leq \frac{\langle \theta (\vec{u} \cdot \hat{i}) \rangle}{\kappa} = \frac{\langle \nabla \theta \cdot \nabla^{-1} (\hat{i} \cdot \vec{u}) \rangle}{\kappa} \leq \frac{\langle |\nabla \theta|^2 \rangle + \langle |\nabla^{-1} \vec{u}|^2 \rangle}{\kappa} = Pe \langle |\nabla \theta|^2 \rangle$$

(9)
where the Péclet number is defined in terms of the rms velocity $U$ and the characteristic length-scale of the flow $l_u$ as

$$U^2 := \langle |\vec{u}|^2 \rangle, \quad l_u^2 := \langle |\nabla^{-1} \vec{u}|^2 \rangle / \langle |\vec{u}|^2 \rangle. \quad (10)$$

Here the inverse gradient operator $\nabla^{-1}$ has the Fourier symbol $-i|\vec{k}|^{-2} \vec{k}$ operating on mean-zero functions. The same shear flow $\vec{u} = i\sqrt{2} U \sin(k_u y)$ that saturates the bound in (6) also saturates the bound in (8) because the steady-state solution to (7) is $\theta(y) = \sqrt{2} G U \sin(k_u y) / \kappa k_u^2$. In homogenization theory, the effective diffusivity defined in (4) is often computed by solving (7).

Another mixing measure was recently introduced motivated by problems with spatially inhomogeneous scalar sources and sinks [3, 11, 14, 17]. Transporting particles from sources to sinks by advection may help to suppress the inevitable inhomogeneities in the scalar field beyond that which molecular diffusion can accomplish alone. Inhomogeneities in the scalar concentration may be measured by its space-time averaged variance, and stirring efficacies can be defined in terms of the suppression of scalar variance on various spatial length-scales. In particular, in the presence of a given source-sink distribution $s(\vec{x}, t)$, Thiffeault et al. introduced the notion of scale dependent equivalent diffusivities [3, 17]

$$\kappa_{eq}^p = \sqrt{\langle |\nabla p \Delta^{-1} s|^2 \rangle} / \kappa \sqrt{\langle |\nabla p \theta_0|^2 \rangle} = \kappa \sqrt{\langle |\nabla p \theta|^2 \rangle}$$

(11)

where the unstirred “reference” scalar field $\theta_0$ satisfies

$$\partial_t \theta_0 = \kappa \Delta \theta_0 + s$$

(12)

while the stirred scalar field $\theta$ satisfies

$$\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + s.$$  

(13)

The associated mixing efficacies

$$\mathcal{E}_p := \frac{\kappa_{eq}^p}{\kappa}$$

(14)

are measures of the statistical steady-state flow-enhanced concentration variance reduction field on small ($p = 1$), intermediate ($p = 0$), and large ($p = -1$) spatial scales. Here the source-sink distribution $s(\vec{x}, t)$ is, without loss of generality, spatially mean 0. This notion parametrizes the flow-enhanced mixing by the effective or “equivalent” molecular diffusion coefficient that achieves the same level of scalar concentration variance suppression that the stirring supplies.

Rigorous analysis shows that given a stationary source-sink distribution $s(\vec{x}, t)$, the efficacies and equivalent diffusivities are bounded by

$$\mathcal{E}_p \leq \tilde{C} \ Pe$$

(15)

as $Pe \to \infty$ for a wide class of deterministic and stochastic flows with a prefactor $\tilde{C}$ depending on $l_s/l_u$, where $l_s$ is a length-scale characterizing the source-sink distribution. This linear-in-$Pe$ bound can be saturated for some source-sink and flow combinations, as shown by Plasting and Young [11]. Moreover, for time-dependent flows with statistical homogeneity and isotropy properties often associated with fully developed turbulence, even smaller estimates for $\mathcal{E}_p$, i.e., asymptotic upper bounds $\lesssim Pe^\alpha$ with $\alpha < 1$, hold for certain classes of source-sink distributions and depend on the spatial dimension [3]. These estimates have also been shown to be sharp [10].
The discrepancy between the $Pe^2$ scaling (6) and the $Pe^1$ scaling (15) of the diffusion enhancement factors casts doubt on the universal applicability of the approaches and their associated mixing measures, and raises questions about modeling mixing by (7) when $Pe$ is large. This discrepancy may to some extent be attributed to the necessity of a scale separation between the tracer concentration and flow fields in the basic particle dispersion analysis, and its inevitable implication in flux-gradient models. Equivalently, maximally enhanced diffusion in these approaches requires time to develop, time which may be as large as $O(l_u^2/\kappa)$, the effective “mean free time” for a typical tracer from the initial distribution to move by molecular diffusion onto a streamline in another direction. Said differently, Taylor dispersion may require a long time to emerge [18].

In the presence of sustained scalar sources and sinks this separation of time scales may never effectively be achieved: a relevant time scale in the sourced problem is the lesser of $l_u^2/\kappa$, the time for enhanced Taylor-like dispersion to appear, and $l_s/U$, the time it takes for a particle to be advected by the flow from a source to a sink. If $l_s/U < l_u^2/\kappa$, the bulk of the scalar variance may be dominated by particles that are most recently replenished and depleted rather than by particles that have been in the system for a long time, and are thus relatively well mixed. Transient features of particle dispersion cannot be neglected and the simple parameterization of the advection-diffusion operator with a stationary tensor may not be valid. As a result, mixing efficacies for source-sink problems may differ from those deduced from transient mixing problems when $Pe > l_s/l_u$. The specific example analyzed in detail in the next section precisely illustrates this noncommutativity of the large length-scale-separation limit and the large Péclet number limit. These two distinct asymptotic limits can produce different predictions for the effective diffusion scaling.

3. Explicit example: Sinusoidal source-sink and shearing. Consider the simplest nontrivial case where the steady single length-scale flow

$$\bar{u}(\bar{x}, t) = i\sqrt{2} U \sin(k_u y)$$

is stirring the steady single-scale source

$$s(\bar{x}, t) = \sqrt{2} S \sin(k_s x)$$

as depicted in Figure 1. The non-dimensional control parameters are the Péclet number $Pe$ and the length-scale separation ratio $r$, which we define as

$$Pe = \frac{U}{\kappa k_u}, \quad r = \frac{k_u}{k_s} = \frac{l_u}{l_s}.$$ (18)

The reference, unstirred, steady scalar concentration is $\theta_0(x) = \sqrt{2} S \sin(k_s x)$ while the exact steady ($t \to \infty$) stirred solution $\theta_\infty(x, y)$ solving

$$\sqrt{2} U \sin(k_u y) \partial_x \theta_\infty = \kappa \Delta \theta_\infty + \sqrt{2} S \sin(k_s x)$$

has the form

$$\theta_\infty(x, y) = f(y) \sin(k_s x) + g(y) \cos(k_s x)$$

where $f$ and $g$ are $2\pi/k_u$-periodic functions that can be computed via numerical or asymptotic methods.

Different dependencies of the different mixing enhancement measures at large Péclet numbers are by now well documented [9, 14, 16, 18]. In the limit $r \to \infty$ the
Figure 1. The sinusoidal shear $\bar{u} = i\sqrt{2} U \sin(k_y y)$ with source distribution $s(\bar{x}, t) = \sqrt{2} S \sin(k_x x)$ in the shaded background.

Figure 2. $\frac{K_{11} \kappa}{Pe^2 \kappa}$ vs $k_u^2 \kappa t$ for $k_u y_0 = 0, \frac{\pi}{2}, \frac{\pi}{4}$. 
direct approximate solution obtained by homogenization theory, i.e., the solution of the steady inhomogeneous diffusion equations effective diffusivity given by the particle dispersion or flux-gradient definition, is simply

$$\theta_{HT}(x) = \frac{\sqrt{2} S \sin(k_s x)}{k_s^2 (1 + Pe^2)} \theta_0(x).$$

(21)

This suggests that the homogenization theory approximation is

$$E_p^{HT} = \sqrt{\frac{\langle |\nabla \theta_0|^2 \rangle}{\langle |\nabla \theta_{HT}|^2 \rangle}} = 1 + Pe^2$$

(22)

for all $p$, although careful application of homogenization arguments to the gradient of the scalar field reduces the homogenization theory prediction for $E_1$ to $O(Pe)$ as $Pe \to \infty$.

To see (22) we derive the explicit formula for tracer particle position covariance from the solutions of the stochastic differential equations written as

$$X(t) = x_0 + \sqrt{2U} \int_0^t \sin(k_u Y(s)) ds + \sqrt{2\kappa} W_1(t),$$

$$Y(t) = y_0 + \sqrt{2\kappa} W_2(t)$$

(23)

where $\vec{X}(t=0) = (x_0, y_0)^T$ and $W_1$ and $W_2$ are two independent Brownian motions. The entries in the 2-by-2 covariance tensor $C(y_0, t)$ are computed as

$$C_{11}(y_0, t) = E[(X(t) - x_0)^2]$$

$$= 2\kappa t + 2U^2 \int_{[0,t]^2} E[\sin(k_u Y(s)) \sin(k_u Y(\tau))] ds d\tau$$

$$= 2\kappa t + \frac{2U^2}{\kappa k_u^4} \left[ k_u^2 \kappa t - 1 + e^{-k_u^2 \kappa t} - \frac{3 - 4e^{-k_u^2 \kappa t} + e^{-4k_u^2 \kappa t}}{12} \cos(2k_u y_0) \right],$$

$$\sim 2(\kappa + \frac{U^2}{\kappa k_u^2}) t, \quad \text{as} \quad t \to \infty,$$

(24)

$$C_{12}(y_0, t) = E[(X(t) - x_0)(Y(t) - y_0)]$$

$$= 2U \sqrt{\kappa} \int_0^t E[W_2(t) \sin(k_u Y(s))] ds$$

$$= \frac{2\sqrt{2} U \cos(k_u y_0) t}{k_u} \left( 1 - e^{-k_u^2 \kappa t} - e^{-k_u^2 \kappa t} \frac{k_u^2 \kappa t}{k_u^2 \kappa t} \right) \to 0, \quad t \to \infty,$$

(25)

$$C_{22}(y_0, t) = E[(Y(t) - y_0)^2] = 2\kappa t.$$

(26)

The homogenization theory approximation (5), i.e., classical Taylor dispersion, follows from the long time limits of these quantities. Figure 2 shows the temporal evolution of $K_{11}$ for different values of $y_0$. Note that it takes time $\approx 100/k_u^2 \kappa$ for the full $Pe^2$ enhancement to emerge.

In contrast, it has been shown [17] that the efficacy $E_0$ of any flow on the torus, steady or time-dependent, stirring the simple monochromatic source-sink distribution is bounded according to

$$E_0 \leq \sqrt{1 + \tau^2 Pe^2}.$$

(27)
Because \( rPe = U/κk_s \), this upper bound does not depend on any length-scales in the flow. In fact, for this source-sink distribution this bound is saturated by a steady, spatially uniform wind directly blowing source to sink and sink to source.

For the sinusoidal shear flow \( \mathbf{u}(x, t) = \hat{i} \sqrt{2} U \sin(k_y y) \), a detailed high-\( Pe \) asymptotic analysis for the exact steady-state solution \( \theta_{\infty} \) [14], what we will refer to here as Internal Layer Theory (ILT), shows

\[
E_0 \sim r^{7/6} Pe^{5/6}, \quad E_{-1} \sim r Pe, \quad E_{+1} \sim r^{1/2} Pe^{1/2}
\]

as \( Pe \to \infty \) at fixed \( r \). Comparing the asymptotic bounds (22) and (28), it is clear that with two control parameters, \( Pe \) and \( r \), the large-\( Pe \) asymptotics does not commute with large-\( r \) asymptotics. As a result, the dependence of \( E_0 \) on large Péclet numbers has two distinguished regimes that cross over near \( r = Pe \).

Figure 3 illustrates the accuracy of different theoretical estimates for \( E_0 \) by comparison with the exact value for \( 10^{-1} \leq Pe \leq 10^6 \) and \( r = 10^m, m = -1, 0, \ldots, 6 \). The exact behavior of \( E_0 \) shows that the two limits, \( Pe \to \infty \) and \( r \to \infty \), do not generally commute and thus lead to two distinct asymptotic regimes of the \( Pe \) dependence: the \( 1 + Pe^2 \) regime for \( Pe \lesssim r \) and the \( r^{7/6} Pe^{5/6} \) regime for \( Pe \gtrsim r \). The question we now turn to is whether transient particle dispersion information can be utilized to correctly predict steady-state concentration variance suppression in the presence of steady sources and sinks.

4. Dispersion-diffusion theory. In order to reconcile the notions of effective diffusion in terms of particle dispersion, on the one hand, and source-sink sustained scalar variance suppression, on the other hand, we propose what we call Dispersion-Diffusion Theory (DDT). Specifically, we retain the dependence of the effective
diffusivity tensor on time [1] and initial location [18] by defining
\[
K(\vec{x}_0, t) := \frac{1}{2} \frac{d}{dt} C(\vec{x}_0, t) = \frac{1}{2} \frac{d}{dt} E[(X_i(t) - X_i(0))(X_j(t) - X_j(0))].
\] (29)

Then without sources and sinks, it is hypothesized that the probability density of a single passive particle may be approximated by the diffusion equation
\[
\frac{\partial}{\partial t} \rho(\vec{x}, t; \vec{x}_0, t_0) = \frac{\partial}{\partial \vec{x}_i} K_{ij}(\vec{x}_0, t - t_0) \frac{\partial}{\partial \vec{x}_j} \rho(\vec{x}, t; \vec{x}_0, t_0)
\] (30)

with initial distribution \( \rho(x, t_0; \vec{x}_0, t_0) = \delta(\vec{x} - \vec{x}_0) \). For spatially periodic problems with period \( L \), this fundamental solution is
\[
\rho(\vec{x}, t; \vec{x}_0, t_0) = \frac{1}{L^d} \sum_{\frac{\vec{x}_0}{L} \in \mathbb{Z}^d} e^{\vec{k} \cdot (\vec{x} - \vec{x}_0) - \frac{1}{2} \vec{k} \cdot K(\vec{x}_0, t - t_0) \cdot \vec{k}}.
\] (31)

Now we propose to approximate the solution to (13) with a source-sink distribution \( s(\vec{x}, t) \) by the integral
\[
\theta_{\text{DDT}}(\vec{x}, t) = \int_0^t dt_0 \int_{[0, L]^d} d\vec{x}_0 \rho(\vec{x}, t; \vec{x}_0, t_0)s(\vec{x}_0, t_0).
\] (32)

That is, we simply apply the principle of linear superposition to the particle density introduced (or depleted) at all positions \( \vec{x}_0 \) at all past times \( t_0 \). Note: it is straightforward to show that \( \theta_{\text{DDT}} \) does not satisfy an “effective” advection-diffusion equation, even if \( s(\vec{x}) \) is steady.

This approximation models each individual tracer particle’s position by a Gaussian probability distribution with the proper variance (and here, with mean zero, although mean displacements could be included as well). Dispersion-Diffusion Theory generalizes Batchelor’s 1949 theory [1] for stirring by homogeneous turbulence by retaining the initial position dependence in the effective diffusivity; this matters for inhomogeneous flows such as the steady sinusoidal shear flow.

The exponential decay in the kernel (31) suggests that the integral (32) may be dominated by the behavior of \( \rho \) for small \( t - t_0 \). This is the mathematical implementation of the physical statement that the bulk features of the scalar field are determined by the particles most recently injected and depleted by \( s \), although this feature is not uniform in the wavenumbers \( \vec{k} \) (i.e., in the relevant length-scales).

To evaluate the DDT approximation we define
\[
\hat{f}(y) + i \hat{g}(y) := \frac{\sqrt{2} k_u S}{2 \pi} \sum_{n \in \mathbb{Z}} \int_0^\infty dt \int_0^{\frac{2 \pi}{k_s}} e^{in k_u (y - y_0) - \frac{1}{2} (k_s nk_u) C(y_0, t) (k_s nk_u)^T} dy_0.
\] (33)

Then from (31), (32) and (24-26) we have
\[
\theta_{\text{DDT}}(x, y) = \hat{f}(y) \sin(k_x x) + \hat{g}(y) \cos(k_x x)
\] (34)

with real functions
\[
\hat{f}(y) = \frac{\sqrt{2} S}{U k_s} \sum_{n = -\infty}^{\infty} \cos(nk_u y) I_n, \quad \hat{g}(y) = \frac{\sqrt{2} S}{U k_s} \sum_{n = -\infty}^{\infty} \sin(nk_u y) I_n
\] (35)

and the dimensionless integrals
\[
I_n = \frac{k_u k_s U}{2 \pi} \int_0^\frac{2 \pi}{k_s} \cos(nk_u y_0) e^{-\frac{1}{2} (k_s nk_u) C(y_0, t) (k_s nk_u)^T} dy_0, \quad n \in \mathbb{Z}.
\] (36)
As an approximation to the exact solution \( \theta_\infty \), we use \( \theta_{\text{DDT}} \) to compute the multiscale mixing measures and to evaluate its ability to recover the parameter dependences of the efficacies for large Péclet number and/or large scale separation. From (33) through (36) and Parseval’s Formula, the approximate multi-scale mixing efficacies are

\[
\begin{align*}
\mathcal{E}_0 &= \sqrt{\frac{\langle \theta_0^2 \rangle}{\langle \theta_{\text{DDT}}^2 \rangle}} = \frac{r^2 Pe}{\sqrt{\sum_n I_n^2}}, \\
\mathcal{E}_{+1} &= \sqrt{\frac{\langle \nabla \theta_0 \nabla \theta_{\text{DDT}} \rangle}{\langle \nabla^2 \theta_{\text{DDT}} \rangle}} = \frac{r Pe}{\sqrt{\sum_n (1 + r^2 n^2) I_n^2}}, \\
\mathcal{E}_{-1} &= \sqrt{\frac{\langle \nabla^{-1} \theta_0 \nabla^{-1} \theta_{\text{DDT}} \rangle}{\langle \nabla^{-2} \theta_{\text{DDT}} \rangle}} = \frac{r Pe}{\sqrt{\sum_n I_n^2 / (1 + r^2 n^2)}}
\end{align*}
\]

where the sums \( \sum_n (\cdot) \) are taken over all integer values of \( n \).

In the limit of large scale separation, \( r = k_u / k_s \to \infty \), a straightforward change of variables to \( z = k_u y_0 \) and \( \tau = \frac{U^2 k_u^2 t}{\kappa k_s^2} \) in (36) using (24-26) suggests

\[
\sum_n I_n^2 \sim I_0^2 = \frac{r^2}{Pe^2}.
\]

Thus, the intermediate and large scale mixing efficacies approximated by \( \theta_{\text{DDT}} \) satisfy

\[
\mathcal{E}_0 \sim \mathcal{E}_{-1} \sim Pe^2
\]

in the limit \( r \to \infty \) for large but finite \( Pe \) in agreement with the homogenization theory prediction 1 + \( Pe^2 \).

As shown in Figure 4, the dispersion-diffusion approximation to the efficacy (DDT) is visually indistinguishable from the exact value. While the homogenization theory prediction (HT, dot-dashed line) applies up to \( Pe \approx r \) and the internal layer asymptotic approximation (ILT, dotted line) is accurate for \( Pe > \max\{r, 1\} \), the dispersion-diffusion approximation is uniformly accurate.

Note that the dispersion-diffusion approximation (along with the exact results, of course) respect the rigorous efficacy bound (27). The efficacies for a range of \( r \) are plotted vs. \( r Pe \) in Figure 5. It is interesting to observe that the simple sine flow nearly saturates the absolute upper bound, which holds for all possible stirring flows, when \( r \approx Pe \). We expect the dispersion-diffusion approximation to respect the efficacy bound more generally as well. This is because at high \( Pe \) we expect the major contribution to \( \theta_{\text{DDT}}(\vec{x}, t) \) in (32) to come from integration times \( t_0 \) within \( l_s / U \) of \( t \). Tracer particle position variance may reasonably be (upper) estimated by

\[
E[(X_i(t) - X_i(0))(X_j(t) - X_j(0))] \lesssim (2\kappa t + U^2 t^2)
\]

as \( t \to 0 \), so for steady sources and sinks each Fourier mode may be estimated

\[
|\hat{\theta}_{\text{DDT}}(k)| \gtrsim \frac{|\hat{s}(k)|}{k U}
\]

as \( Pe \to \infty \). This implies that

\[
\mathcal{E}_0^{\text{DDT}} \lesssim \frac{Ul_{\text{source}}}{\kappa} = l_{\text{source}} \frac{l_u}{\kappa} = r Pe
\]
Figure 4. $E_0$ vs $Pe$, for $r = 10^m$, $m = -1, 0, \ldots, 6$.

Figure 5. $E_0$ and the rigorous upper bound (solid line) vs $rPe$, for $r = 10^m$, $m = -1, 0, \ldots, 6$. 
where the distinguished length-scale characterizing a general source-sink distribution is

\[ l_2^{source} \approx \frac{\langle (\Delta^{-1}s)^2 \rangle}{\langle |\nabla^{-1}s|^2 \rangle}, \] (43)

as long as it is non-vanishing. Should \( l^{source} \) vanish, i.e., if the source-sink distribution contains too many small length-scale components, we would expect different (sublinear) high-\( Pe \) scaling [3].

To evaluate the potential for the various theories to capture the mixing efficacies at large and small scales, we plot the different \( \mathcal{E}_{-1} \) and \( \mathcal{E}_{+1} \) and their approximations in Figure 6 and 7. For the large-scale mixing efficacy \( \mathcal{E}_{-1} \), the homogenization approximation is accurate up to \( Pe \sim r \) while the dispersion-diffusion approximation appears to capture the correct scaling for any \( Pe \) modulo a constant prefactor error. The direct homogenization approximation fails to capture the correct behavior of the small-scale efficiency \( \mathcal{E}_{+1} \) for any \( Pe > 1 \), which is not unexpected since it explicitly neglects small scale structure in the scalar field. But a careful homogenization analysis focusing on the gradient of the scalar field [7] predicts \( \mathcal{E}_{+1} \sim Pe \) in the \( 1 < Pe < r \) regime and this does correctly capture the intermediate behavior. The DDT approximation, on the other hand, appears to follow the direct (naı́ve) homogenization approximation for \( Pe \lesssim r \) but then adopts the correct scaling when \( Pe \gg r \), albeit with a prefactor error.

To visualize the detailed structures in the scalar field as captured by the various approximations, Figure 8 compares the exact \( \theta_\infty \) and the \( \theta_{DDT} \) and \( \theta_{HT} \) approximations for \( Pe = 10^m, m = 1, \cdots, 5 \) for fixed \( r = 1000 \). The panels in each column (fixed \( Pe \)) are plotted in the same grayscale from \(-1 \) (black) to \( 1 \) (white) where the scalar fields are normalized by the magnitude of the sup-norm of the corresponding exact solution, \( \|\theta_\infty\|_\infty \). As Péclet increases with the intensity of the flow,
internal layers develop in the strongly-sheared regions where the speed is relatively small; in the weakly-sheared regions, however, the speed is large and the scalar field is well mixed and has small variance. It is clear from the figure that although the dispersion-diffusion approximation fails to capture the details of the layers, it does reveal the bulk behavior of the scalar field and more importantly, recovers the correct bulk scalar variance. The homogenization theory approximation greatly overestimates the effect of the stirring when $Pe > r$.

5. Conclusion. By direct comparison of various mathematical models and measures of mixing we have shown that different definitions of effective diffusion predict distinct large $Pe$ scalings of flow-enhanced diffusion. The discrepancies result from the diverse physical mechanisms motivating the different definitions of the mixing measures. In particular,

- In the transient mixing problem ($s \equiv 0$) the long-time behavior of the well-dispersed scalar density is controlled by the advection and diffusion of tracer particles ignoring scalar density structure on length-scales of the stirring. As a result, the effect of the stirring may be described by a diffusion equation with an effective diffusion tensor enhanced by as much as a factor of $Pe^2$.

- In the presence of sources and sinks, the scalar concentration generally depends on the length-scales of both the flow and the source-sink distribution. We cannot generally use the long-time, large length-scale dispersion results to approximate the system with an effective diffusion equation: homogenization
theory is not applicable without the pristine separation of scales between the stirring and the source-sink distribution. The enhancement of molecular diffusion by stirring generally depends in a nontrivial way on both $Pe$ and the scale separation $r$.

- Dispersion-Diffusion Theory, motivated by the desire to utilize the essential information in the particle dispersion process in the presence of sources and sinks, reconciles the non-commutative limiting procedures adopted in the literature. DDT retains the dynamical and inhomogeneous aspects of the effective diffusivity tensor used in homogenization approach and approximates the scalar concentration with an integral similar to the solution of a diffusion equation with sources and sinks.

- The Dispersion-Diffusion approximation should generally respect the upper bound in (15). Indeed, at high Péclet number the dominant contribution to $\theta_{DDT}$ comes from the most recent times which, due to the gaussian nature of the approximation, leads to variance suppression $\lesssim Pe^1$.

We may thus utilize the classical particle dispersion perspective to accurately predict enhanced mixing via scalar variance suppression, even for highly anisotropic and inhomogeneous flows and without a separation of length-scales. This is crucial for problems where the sources and sinks possess the same range of scales as the stirring. We do not, however, yet see how to uniformly reconcile the predictions of the flux-gradient model in (7). This model is frequently adopted as the defining framework for turbulent stirring and mixing, but it incorporates infinite scale separation from the start so no such reconciliation may be possible. This raises the question of the relevance of the flux-gradient model to applications involving statistically steady state mixing in the presence of sources and sinks.

Dispersion-Diffusion Theory may be applied to more general source-sink distributions [3] and/or more complicated flows like homogeneous and isotropic turbulence where, following Batchelor [1], the dispersive behavior of passive particles is modeled

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**Figure 8.** Scalar fields for $(x, y) \in [0, 2\pi/k_x] \times [0, 2\pi/k_u]$ when $r = 1000$. 

| Pe=10  | Pe=100 | Pe=1000 | Pe=10000 | Pe=100000 |
|--------|--------|----------|-----------|------------|
| Exact  | DDT    | HT       |           |            |

- **Exact** represents the exact solution.
- **DDT** utilizes Dispersion-Diffusion Theory.
- **HT** is a comparison.
MIXING MEASURES AND EFFECTIVE DIFFUSION

by

\[
\mathbb{E}[(X_i(t) - X_i(0))(X_j(t) - X_j(0))] \sim (2\kappa t + U^2 t^2 + \ldots) \delta_{ij}, \tag{44}
\]

at least for displacements within the inertial range. The term in the covariance \( \sim t \) is due to molecular diffusion while the term \( \sim t^2 \) characterizes the short term drift. For source-sink distributions with a well-defined spatial scale falling below some “outer” scale \( l_o \) of the turbulence (i.e., \( r \lesssim 1 \)), a calculation very similar to that in (40) through (43) with the simple dispersion relation (44) yields

\[
\mathcal{E}_p \sim r Pe, \tag{45}
\]

for \( Pe \gg 1 \gtrsim r \), which saturates the scaling of the rigorous upper bounds. This suggests that homogeneous isotropic turbulence may be a nearly optimal mixer in this sense of steady state scalar variance reduction. An important aspect of the future research is to test this conjecture with direct numerical simulations and/or experiments for passive scalars that are sustained by steady sources and sinks while being stirred by turbulent flows.

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