MODELS & MEASURES OF MIXING & EFFECTIVE DIFFUSION

Zhi Lin
Institute for Mathematics & Its Applications
University of Minnesota, Minneapolis, MN 55455, USA

Katarína Boďová
Department of Applied Mathematics & Statistics
Faculty of Mathematics, Physics and Informatics
Comenius University, 84248 Bratislava, Slovakia

Charles R. Doering
Department of Mathematics, University of Michigan
Ann Arbor, MI 48109-1043, USA
and
Department of Physics and Michigan Center for Theoretical Physics
University of Michigan, Ann Arbor, MI 48109-1040, USA
and
Center for the Study of Complex System, University of Michigan
Ann Arbor, MI 48109-1107, USA

Abstract. Mixing a passive scalar field by stirring can be measured in a variety of ways including tracer particle dispersion, via the flux-gradient relationship, or by suppression of scalar concentration variations in the presence of inhomogeneous sources and sinks. The mixing efficiency or efficacy of a particular 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 steady sinusoidal shear flow mixing gas scalars 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 heatosphere 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 understanding 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...
**Big questions:**

How can we gauge the effectiveness of a stirrer as a mixer?

How might we parameterize stirring as diffusion?

**Outline:**

- Models
- Conflicts
- Resolution
- More models
- Reconciliation
Mathematical models of mixing

Given flow field $\vec{u}(\vec{x},t)$ with $\nabla \cdot \vec{u} = 0$, consider

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

- $\vec{X}(t)$ is passive tracer particle position
- $\kappa$ is the molecular diffusion coefficient

Advection - Diffusion Eq: $\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + s$

- $\theta(\vec{x},t)$ is passive scalar density, concentration
- $s(\vec{x},t)$ is passive scalar source-sink distribution
- plus appropriate initial and boundary conditions
Mathematical measures of mixing

Temptation & tradition suggest characterizing stirring as an "effective" diffusion

\[ \bar{u} \cdot \nabla - \kappa \Delta \rightarrow - \partial_i K_{ij}^\text{eff} \partial_j \]

**Three questions:**

- Which aspects of mixing should be encoded in \( K^{\text{eff}} \)?
- Do different criteria produce different \( K^{\text{eff}} \)?
- Transferable among applications?
Mathematical measures of mixing

Measure 1:  \( K^{PD} = K_{ij}^{\text{eff}} \)

Measure 2:  \( K^{FG} = K_{11}^{\text{eff}} \)

Measure 3:  \( \kappa_p^{VR} = \kappa_p^{\text{eff}} \) for  \( p = +1, 0, -1 \)

\( p = +1, 0, -1 \sim \) “small”, “intermediate”, or “large” scale variance reduction
Mathematical measures of mixing

Measure 1: \( K^{PD} = K_{ij}^{\text{eff}} \)

via tracer particle dispersion

\[
\mathbb{E}\left\{(X_i(t) - X_i(0))(X_j(t) - X_j(0))\right\} \sim 2K_{ij}^{\text{eff}} t
\]

as \( t \to \infty \).
Mathematical measures of mixing

Measure 2: \( K^{FG} = K^{\text{eff}}_{11} \)

via flux - gradient relation, \( T = -Gx + \theta \Rightarrow \)

\[
\partial_t \theta + \bar{u} \cdot \nabla \theta = \kappa \Delta \theta + G \left( \hat{i} \cdot \bar{u} \right)
\]

everything mean zero & periodic on a cell \( \Rightarrow \)

\[
K^{\text{eff}}_{11} = \kappa + \frac{\langle u_1 \theta \rangle}{G} = \kappa \left( 1 + \frac{\langle |\nabla \theta|^2 \rangle}{G^2} \right)
\]
Mathematical measures of mixing

Measure 3: $\kappa_0^{VR} = \kappa^{\text{eff}}$

via concentration variance reduction

For $s(\bar{x})$ mean 0 and $\partial_t \theta + \bar{u} \cdot \nabla \theta = \kappa \Delta \theta + s(\bar{x})$

$$\kappa^{\text{eff}} = \sqrt{\frac{\langle (\Delta^{-1} s)^2 \rangle}{\langle \theta^2 \rangle}}$$
Mathematical measures of mixing

*Multiscale* Measure 3(a): $\kappa_p^{VR} = \kappa_p^{\text{eff}}$

via concentration (*inverse*) gradient variance reduction

For $s(\bar{x})$ mean 0 and $\partial_t \theta + \bar{u} \cdot \nabla \theta = \kappa \Delta \theta + s(\bar{x})$

$$
\kappa_{\pm 1}^{\text{eff}} = \sqrt{\frac{\left\langle \left| \nabla^{\pm 1} \Delta^{-1} s \right|^2 \right\rangle}{\left\langle \left| \nabla^{\pm 1} \theta \right|^2 \right\rangle}}
$$
Mathematical measures of mixing

Measure 1: $K^{PD} = K_{ij}^{\text{eff}} \sim \frac{1}{2t} \mathbb{E}\left\{ (X_i(t) - X_i(0))(X_j(t) - X_j(0)) \right\}$

Measure 2: $K^{FG} = K_{11}^{\text{eff}} = \kappa \left( 1 + \frac{\left| \nabla \theta \right|^2}{G^2} \right)$

Measure 3: $\kappa_p^{VR} = \kappa_p^{\text{eff}} = \sqrt{\frac{\left| \nabla^p \Delta^{-1} s \right|^2}{\left| \nabla^p \theta \right|^2}}$ for $p = +1, 0, -1$
Strength of stirring

Dimensionless \textit{Péclet} number: \( \text{Pe} \equiv \frac{U\ell}{\kappa} \)

\( U \sim \) velocity scale \quad \ldots \quad \ell \sim \) length scale

Dimensionless \textit{Enhancement} or \textit{Efficacy} factor:

\[
E(\text{Pe}) \equiv \frac{\kappa^\text{VR}_p}{\kappa} \quad \text{or} \quad \frac{\kappa^\text{PD,FG}}{\kappa}
\]
Fact:

In terms of tracer dispersion or flux-gradient relation, there are flows for which the enhancement may be as large as

\[ E(\text{Pe}) = \frac{K^{FG}}{\kappa} \sim \text{Pe}^2 \text{ as } \text{Pe} \to \infty. \]

Fact:

In terms of concentration variance reduction in presence of steady sources & sinks the enhancement cannot be that big.

**Theorem:** \( E(\text{Pe}) = \frac{K^{VR}}{\kappa} \leq \text{Pe}^1 \text{ as } \text{Pe} \to \infty. \)
Resolution

• What length scale $l$ is used in $\text{Pe} = \frac{Ul}{\kappa}$?

In examples where $\frac{K_{FG}^{p}}{\kappa} \sim \text{Pe}^2$ as $\text{Pe} \to \infty$,

$$\text{Pe} \equiv \frac{U l_{\text{flow}}}{\kappa}.$$ 

In theorem where $E(\text{Pe}) = \frac{K_{VR}^{p}}{\kappa} \leq \text{Pe}^1$ as $\text{Pe} \to \infty$,

$$\text{Pe} \equiv \frac{U l_{\text{source}}}{\kappa} = \left(\frac{l_{\text{source}}}{l_{\text{flow}}}\right) \times \frac{U l_{\text{flow}}}{\kappa}.$$
Example: Basic Two-scale Model

A single-scale flow stirring a single-scale source-sink distribution

\[ \tilde{u}(\tilde{x}) = \hat{i} \sqrt{2} U \sin k_u y \]

\[ s(\tilde{x}) = \sqrt{2} S \sin k_s x \]

Two parameters:

\[ \text{Pe} \equiv \frac{U}{\kappa k_u} \quad \text{and} \quad r = \frac{\ell_{\text{source}}}{\ell_{\text{flow}}} = \frac{k_u}{k_s} \]
Dispersion/Flux-gradient mixing measure

- a.k.a. **Homogenization Theory** (HT) …
- … presumably good for \( r = k_u/k_s \gg 1 \):

\[
\frac{K_{FG}}{\kappa} = 1 + \text{Pe}^2 \quad \Rightarrow \quad \text{HT approximation is}
\]

\[
0 = K_{FG} \frac{d^2 \theta_{HT}(x)}{dx^2} + s(x) \quad \Rightarrow \quad \theta_{HT}(x) = \frac{\sqrt{2} \sin k_s x}{\kappa k_u^2 (1 + \text{Pe}^2)}
\]

HT appx of \( \kappa_{VR}^p = \sqrt{\frac{\langle (\Delta^{-1} S)^2 \rangle}{\langle \theta_{HT}^2 \rangle}} = \sqrt{\frac{\langle \nabla^{\pm 1} \Delta^{-1} S \|^2 \rangle}{\langle |\nabla^{\pm 1} \theta_{HT}|^2 \rangle}} = \kappa(1 + \text{Pe}^2) \)
Exact solution (for $r = 1$)

High-Pe (fixed $r$) asymptotic analysis: *Internal-layer theory* (ILT)

\[
E_0 = \kappa_0^{VR}/\kappa \sim r^{7/6} \ Pe^{5/6}
\]

\[
E_{+1} = \kappa_{+1}^{VR}/\kappa \sim r^{1/2} \ Pe^{1/2}
\]

\[
E_{-1} = \kappa_{-1}^{VR}/\kappa \sim r \ Pe
\]
\[ E_{+1} = \frac{\| \nabla \theta_0 \|^2}{\sqrt{\langle |\nabla \theta|^2 \rangle}} \]

The graph shows a plot of \( E_{+1} \) vs. \( Pe = \frac{U}{kk_u} \). The lines represent different values of \( r \) as indicated by the legend:

- \( r = 10^6 \)
- \( r = 10^5 \)
- \( r = 10^4 \)
- \( r = 10^3 \)
- \( r = 10^2 \)
- \( r = 10^1 \)
- \( r = 10^0 \)
- \( r = 10^{-1} \)

Legend:
- Exact
- HT: 1 + Pe^2
- ILT: C \sqrt{rPe}
Stirring strength–scale separation phase diagram
Stirring strength–scale separation phase diagram

**HT:**
- $r \gg 1$
- $r \geq Pe$

- $r \ll 1$
- $Pe \ll 1$
- $1$
- $Pe \gg 1$
Stirring strength–scale separation phase diagram

HT:
$r \gg 1$
$r \geq Pe$

ILT:
$Pe \gg 1$
$r \leq Pe$
Outline

• Models
• Conflicts
• Resolution
• More models
• Reconciliation
Questions:

• HT fails to predict the scalar variance sustained by steady sources & sinks when $Pe > r >> 1$. Why?

• Can information about particle dispersion predict variance suppression at high Péclet numbers?
Particle dispersion is time and initial-location dependent …

\[ \mathbb{E}\left\{ (X_i(t) - X_i(0))(X_j(t) - X_j(0)) \right\} \sim 2K_{i,j}^{PD}t \]

\[ K_{i,j}^{PD}(t; \tilde{X}(0)) \equiv \frac{d}{dt}\frac{1}{2} \mathbb{E}\left\{ (X_i(t) - X_i(0))(X_j(t) - X_j(0)) \right\} \]

- \( K^{PD} \sim \kappa \text{Pe}^2 = \mathcal{O}(\kappa^{-1}) \) takes \( \mathcal{O}(\ell_{\text{flow}}^2/\kappa) \) time to develop

... but \( K_{i,j}^{PD}(t; \tilde{X}(0)) \sim \kappa + U^2t \) (at most) for \( t \ll \frac{\ell_{\text{flow}}^2}{\kappa} \).
Effective diffusion $K_{11}^{PD}(t,y_0)$ vs. time

\[ \mathbf{u}(x) = \hat{i} \sqrt{2} U \sin k_x y \]

\[ K(t, Y_0) = \frac{1}{2} \frac{d}{dt} \left( \mathbf{E}[\mathbf{r}(t)^2] - \mathbf{E}[\mathbf{r}(t) \cdot \mathbf{r}(t) + \mathbf{r}(t) \cdot \mathbf{r}(t)] - \mathbf{E}[\mathbf{r}(t) \cdot \mathbf{r}(t) + \mathbf{r}(t) \cdot \mathbf{r}(t)] \right) \]

\[ = \kappa + \frac{U^2}{k_x^4} \left[ 1 - e^{-k_x^2 \kappa t} \cos(2k_x Y_0) \frac{3}{2} e^{-k_x^2 \kappa t} - e^{-k_x^2 \kappa t} \right] \frac{U \kappa k_x \cos(k_x Y_0)}{\sqrt{2}} \sqrt{2} \kappa e^{-k_x^2 \kappa t} \]
More modeling

• Concentration variance for stirred scalars sustained by inhomogeneous sources and sinks is dominated by the “latest” stuff introduced or deleted from the system.

• “Old” particles are relatively well mixed and so don’t contribute substantially to the observed variance.

• Variance supression is controlled by particle dispersion rate on relatively short, rather than long, time scales at high Pe.

• In the presence of sustained sources & sinks, even as $t \to \infty$ we cannot neglect transient behavior of $K^{PD}$ …
Dispersion-diffusion theory (DDT)

Given a stirring flow \( u(x,t) \) and its associated \( K_{ij}^{PD} (t-t_0 \mid x_0, t_0) \), density due to stuff injected at \( x_0, t_0 \) may best be described by

\[
\partial_t \rho(\vec{x}, t \mid \vec{x}_0, t_0) = \partial_i K_{ij}^{PD} (t - t_0 \mid \vec{x}_0, t_0) \partial_j \rho
\]

\[
\lim_{t \downarrow t_0} \rho(\vec{x}, t \mid \vec{x}_0, t_0) = \delta(\vec{x}, t \mid \vec{x}_0)
\]

Then the total density in presence of sources and sinks is at best described by

\[
\theta_{DDT} (\vec{x}, t) = \int_{-\infty}^{t} dt_0 \int d\vec{x}_0 \rho(\vec{x}, t \mid \vec{x}_0, t_0) s(\vec{x}_0, t_0)
\]

… which does not satisfy an inhomogeneous diffusion equation!

On a periodic domain $[0,L]^d$

$$
\rho(\vec{x},t \mid \vec{x}_0,t_0) = \frac{1}{L^d} \sum_k \exp\left\{ i \vec{k} \cdot (\vec{x} - \vec{x}_0) - k_i k_j \int_{t_0}^t K^{PD}_{ij} (t' - t_0 \mid \vec{x}_0,t_0) dt' \right\}
$$

Note: if $K^{PD}_{ij} \sim [\kappa + U^2 (t - t_0)] \delta_{ij}$ as $t - t_0 \to 0$, then

$$
\theta_{DDT} (\vec{x},t) = \int_{-\infty}^t dt_0 \int d\vec{x}_0 \rho(\vec{x},t \mid \vec{x}_0,t_0) s(\vec{x}_0)
$$

\[\downarrow\]

$$
\hat{\theta}_{DDT} (\vec{k}) \sim \hat{s}(\vec{k}) \int_0^\infty e^{-\kappa k^2 \tau - \frac{1}{2} k^2 U^2 \tau^2} d\tau
$$

\[\Rightarrow\] as Pe $\to \infty$, $\hat{\theta}_{DDT} (\vec{k}) \sim \frac{\hat{s}(\vec{k})}{kU}$ so $\kappa_0^{VR} = \sqrt{\frac{\langle (\Delta^{-1}s)^2 \rangle}{\langle \theta_{DDT}^2 \rangle}} \sim U\ell_{\text{source}}$
Reconciliation

• $64$ question: Is DDT quantitatively accurate?

• For single-scale flow stirring single-scale source …
More reconciliation

- DDT respects the rigorous bounds on $\kappa_0^{\text{VR}}$.

- For the single-scale source, the rigorous bound is

$$E(\text{Pe}) = \frac{\kappa_0^{\text{VR}}}{\kappa} \leq [1 + r^2 \text{Pe}^2]^{1/2} \sim r \text{Pe} \ldots$$

… for large $r$ or for large $\text{Pe}$!

- Plot $E(\text{Pe})$ as a function of $(r \text{Pe})$: 
Reconciliation, continued

- How does DDT perform for variance suppression at large & small scales, i.e., for $\kappa_{\pm 1}^{VR}$?
$E_{-1} = 10^r$
\[ E_{+1} = \frac{1}{\sqrt{\frac{\langle |\nabla \theta_0|^2 \rangle}{\langle |\nabla \theta|^2 \rangle}}} \]
Density pictures \((r = 562)\)

<table>
<thead>
<tr>
<th>Pe=10</th>
<th>Pe=100</th>
<th>Pe=1000</th>
<th>Pe=10000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DDT</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HT</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Stirring strength–scale separation phase diagram

DDT approximation for $\kappa_0^{VR}$ is uniformly accurate
Conjecture (potential application)

- Single-scale source, sink & stirring is a special scenario …
  … what about real turbulent mixing?

- DDT hints how particle dispersion data may predict steady state source-sink sustained variance suppression.

- Homogeneous isotropic turbulence $\rightarrow$

$$E[(X_i(t) - X_i(0))(X_j(t) - X_j(0))] = (2\kappa t + U^2 t^2 + C_R \epsilon t^3 + \ldots) \delta_{ij}$$

… w/turbulent energy dissipation rate per unit mass $\epsilon \sim U^3/\ell_{flow}$.
On a periodic domain \([0, L]^d\)

\[
\rho(\vec{x}, t \mid \vec{x}_0, t_0) \approx \frac{1}{L^d} \sum_k \exp \left\{ i k \cdot (\vec{x} - \vec{x}_0) - \frac{1}{2} k^2 \left[ 2\kappa (t - t_0) + U^2 (t - t_0)^2 + \cdots \right] \right\}
\]

\[
\theta_{\text{DDT}}(\vec{x}, t) = \int_{-\infty}^{t} dt_0 \int d\vec{x}_0 \rho(\vec{x}, t \mid \vec{x}_0, t_0) s(\vec{x}_0)
\]

\[
\downarrow
\]

\[
\hat{\theta}_{\text{DDT}}(\vec{k}) = \hat{s}(\vec{k}) \int_{0}^{\infty} e^{-\kappa k^2 \tau - \frac{1}{2} k^2 U^2 \tau^2} d\tau
\]

\[
\Rightarrow \text{ as } Pe = \frac{U l_{\text{flow}}}{\kappa} \to \infty \text{ at fixed } r = \frac{l_{\text{source}}}{l_{\text{flow}}},
\]

\[
\hat{\theta}_{\text{DDT}}(\vec{k}) \sim \frac{\hat{s}(\vec{k})}{k U}
\]
Concrete conjecture:

Does Statistically Homogeneous

Isotropic Turbulence saturate

the upper bound on $E(\text{Pe})$?

$$\kappa^{\text{eff}} \approx \kappa_0^\text{VR} = \sqrt{\frac{\langle (\Delta^{-1})^2 \rangle}{\langle \theta_{\text{DDT}}^2 \rangle}} \sim \kappa \, r \, \text{Pe}$$

$$= \left( \frac{\ell_{\text{source}}}{\ell_{\text{flow}}} \right) U \ell_{\text{flow}}$$

with

$$\ell_{\text{source}} = \sqrt{\frac{\langle (\Delta^{-1})^2 \rangle}{\langle \Delta^{-1/2} \rangle^2}}$$

i.e., "mixing length" $\sim \ell_{\text{source}}$
\[ \Rightarrow \text{as } \text{Pe} = \frac{UL_{\text{flow}}}{\kappa} \to \infty \text{ at fixed } r = \frac{l_{\text{source}}}{l_{\text{flow}}}, \]

\[ \hat{\theta}_{\text{DDT}}(\vec{k}) \sim \frac{s(\vec{k})}{kU} \]
Last words

• Different definitions of effective diffusion may indeed yield different effective diffusivities.

• We cannot generally use long-time transient dispersion results for source-sink problems.

• There may not be an effective diffusion equation to describe source-sink stirring.

• Flux-gradient model does not contain all the relevant information for source-sink stirring.

• Transient mixing and source-sink stirring are different phenomena using different features of the flow:
Scalar source-sink stirring is all about *transport*

Transient mixing is all about *shearing, stretching & straining*
THE END