Bounds on Multiscale Mixing Efficiencies

Tiffany A. Shaw

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1 Introduction

We are motivated by the following problem: given the heat sources and sinks on the Earth and a stirring field with certain statistical properties what are the maximum and minimum possible degrees of temperature variance that must be present? The flow in the Earth's atmosphere is an example of a stirring field which acts to redistribute heat. Here we are interested in the optimal solution to this redistribution problem. We expect any stirring would suppress fluctuations in the temperature field and lead to a more uniform distribution, but what kind of stirring minimizes the variance? Can we, given some bulk statistical properties of the stirring field, derive bounds on the variance? What are the characteristics of a good stirring field and how do they depend on the source distribution? Can we define and estimate the eddy diffusivity and mixing efficiency of a stirrer on different length scales? Here we work toward answering these questions by computing rigorous bounds on multiscale mixing efficiencies.

Bounds on mixing have important implications in both physics and engineering. Thiffeault, Doering, and Gibbon [5], hereafter TDG, have shown how techniques used to bound bulk dissipation quantities in the Navier-Stokes equation [2] can be applied to the advection-diffusion of a passive scalar maintained by a steady source. They derived rigorous bounds on the scalar variance and defined an *equivalent diffusivity*, the diffusivity required to produce the same amount of mixing in the absence of stirring. Plasting and Young [4], hereafter PY, enhanced that analysis by including the variance dissipation as a constraint.

Here we construct bounds on the multiscale mixing efficiency of a sitrring field for a passive scalar maintained by a time independent but spatially inhomogeneous source. We focus on the mixing efficiency of a stirring field on different scales by considering the fluctuations of the variance, gradient variance, and inverse gradient variance. Comparing the three measures (the variance, gradient variance, and inverse gradient variance) gives a range of information about the stirring properties of a flow. It has been recognized that L^p norms of the passive scalar fail to quantify the *stirring efficiency* of a mixing process because they are insensitive to small scale structures [1]. We gauge the effectiveness of a stirring field based on its ability to suppress variance relative to the variance in the absence of stirring. On all scales, a smaller variance implies the velocity field is a better stirrer. Thus, a velocity field that gives a larger mixing efficiency than another will be considered more efficient with respect to a particular measure.

Our approach for bounding the multiscale mixing efficiencies follows that of TDG. The bounds are derived in section 3. In section 4 we show that the bounds for a monochromatic source on the torus can be saturated. In an effort to distinguish the three measures more convincingly, in section 5 we investigate the efficiency of a steady shearing flow for a monochromatic source using boundary layer asymptotics. Finally, in section 6, we find bounds on the multiscale mixing efficiencies for a decaying passive scalar maintained by a spatially inhomogeneous source.

2 Advection-diffusion in a space of d-dimensions

The advection-diffusion equation of a passive scalar with a body source $s(\mathbf{x})$ in a d-dimensional domain ($d = 2, 3, ...$) is:

$$\frac{\partial\theta}{\partial t} + \mathbf{u}\cdot\nabla\theta = \kappa\Delta\theta + s(\mathbf{x}) \tag{2.1}$$

where $s(\mathbf{x})$ is a source with spatial mean zero without loss of generality and κ is the molecular diffusivity. Since the body source has spatial mean zero the passive scalar will also have zero spatial mean. The velocity field here is a given steady or time-dependent L^2 divergence-free vector field. The velocity field could be a solution of the Navier-Stokes equation or a specified stochastic process. We will focus on a particular class of stirring fields that are steady, statistically homogeneous, and isotropic with single point statistical properties characteristic of Homogeneous Isotropic Turbulence (HIT):

$$\overline{u_i(\mathbf{x},\cdot)} = 0, \qquad \overline{u_i(\mathbf{x},\cdot)u_j(\mathbf{x},\cdot)} = \frac{U^2}{d}\delta_{ij} \tag{2.2}$$

and

$$\overline{u_i(\mathbf{x},\cdot)\frac{\partial u_j(\mathbf{x},\cdot)}{\partial x_k}} = 0, \qquad \overline{\frac{\partial u_i(\mathbf{x},\cdot)}{\partial x_k}\frac{\partial u_j(\mathbf{x},\cdot)}{\partial x_k}} = \frac{\Gamma^2}{d}\delta_{ij} \tag{2.3}$$

where where $U^2 := \langle|\mathbf{u}|^2\rangle$ is the kinetic energy density, $\lambda = U/\Gamma$ is the so-called Taylor microscale for HIT, and the overbar denotes the steady average defined below. Let us define the advection-diffusion operator and its formal adjoint:

$$\mathcal{L} := \partial_t + \mathbf{u}\cdot\nabla - \kappa\Delta, \qquad \mathcal{L}^\dagger := -\partial_t - \mathbf{u}\cdot\nabla - \kappa\Delta. \tag{2.4}$$

We also define the steady average (assuming it exists),

$$\overline{F}(\mathbf{x}) := \lim_{t\to\infty}\frac{1}{t}\int_0^t F(\mathbf{x},t')dt', \tag{2.5}$$

and the space time average,

$$\langle F\rangle := \frac{1}{V}\int \overline{F}(\mathbf{x})d^d\mathbf{x}. \tag{2.6}$$

From here on our domain will be a periodic box of size L, i.e. $x \in \mathbb{T}^d$, the d-dimensional torus. The Fourier decomposition of the spatially dependent variables are written conventionally as

$$F(\mathbf{x},t) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\hat{F}(\mathbf{k}) \quad \text{where} \quad \hat{F}(\mathbf{k}) = \frac{1}{L^d}\int_{\mathbb{T}^d} e^{-i\mathbf{k}\cdot\mathbf{x}}F(\mathbf{x},t)\; d^d\mathbf{x} \tag{2.7}$$

and $\mathbf{k} = (2\pi/L)\mathbf{n}$ for $\mathbf{n} = (n_1, ..., n_d)$. The L^2 norms of derivatives of the passive scalar will be denoted, for example,

$$\langle|\nabla^p\theta|^2\rangle = \sum_{\mathbf{k}} k^{2p}|\hat{\theta}(\mathbf{k})|^2. \tag{2.8}$$

The conventional non-dimensional number measuring the relative importance of advection to diffusion is the Péclet number

$$Pe := \frac{UL}{\kappa}. \tag{2.9}$$

A standard measure of the well-mixedness of a scalar field is its variance (presuming spatial mean zero) [1]. Weighting the variances at different length scales introduces a family of variances that are sensitive to mixing on different scales. The variances $\langle|\nabla^p\theta|^2\rangle$ for $p = 1, 0, -1$ measure mixing on small, intermediate, and large scales respectively. To gauge the effect of stirring, the variances are compared with variances in the absence of stirring $\langle|\nabla^p\theta_0|^2\rangle = \kappa^{-2}\langle|\nabla^p\Delta^{-1}s|^2\rangle$ for $p = 1, 0, -1$.

We define a non-dimensional *mixing efficiency* for each scale p

$$M_p := \frac{\langle|\nabla^p\theta_0|^2\rangle}{\langle|\nabla^p\theta|^2\rangle} \quad \text{for} \quad p = 1, 0, -1 \tag{2.10}$$

which increases as stirring increases. The mixing efficiency has the advantage of depending only on the structure of the stirring and source and not on their scales.

The *equivalent diffusivity* is the equivalent amount of diffusivity required to achieve the same degree of mixing in the absence of stirring (i.e. a corresponding diffusivity for the diffusion equation) and is defined as

$$\kappa_{\mathrm{eq},p} := \kappa\frac{\langle|\nabla^p\theta_0|^2\rangle^{1/2}}{\langle|\nabla^p\theta|^2\rangle^{1/2}}. \tag{2.11}$$

Equivalent diffusivity should not be confused with effective diffusivity defined in homogenization theory. The effective diffusivity is defined in terms of large-scale transport, i.e. in the presence of large scale gradients of the concentration (G. Papanicolaou lectures) [6]. The equivalent diffusivity is specific to the source and stirring. Lower bounds on the variances provide upper bounds on the mixing efficiencies. These bounds depend on details of the source and stirring as shown in the next section.

3 Bounds on the multiscale mixing efficiencies

Following the method developed by TDG we derive bounds on the multiscale mixing efficiencies.

3.1 Bounds on variance

Multiplying (1) by a smooth, time independent, spatially periodic projector function $\varphi(\mathbf{x})$, taking the space-time average and integrating by parts we obtain

$$\langle\theta(\mathbf{u}\cdot\nabla + \kappa\Delta)\varphi\rangle = -\langle\varphi s\rangle. \tag{3.1}$$

A lower bound on the variance is achieved via the variational principle

$$\langle\theta^2\rangle \geq \max_{\varphi}\min_{\tilde\theta} \ \{\langle\tilde\theta^2\rangle \mid \langle\tilde\theta(\mathbf{u}\cdot\nabla\varphi + \kappa\Delta\varphi)\rangle = -\langle\varphi s\rangle\}. \tag{3.2}$$

We note that TDG derived bounds on the mixing efficiency without optimizing over φ. The optimization over $\tilde\theta$ is equivalent to applying the Cauchy-Schwarz inequality

$$\langle\theta^2\rangle \geq \max_{\varphi}\frac{\langle\varphi s\rangle^2}{\langle(\mathbf{u}\cdot\nabla\varphi + \kappa\Delta\varphi)^2\rangle} = \frac{\langle\varphi s\rangle^2}{\langle\varphi\overline{\mathcal{L}\mathcal{L}^\dagger}\varphi\rangle}. \tag{3.3}$$

Maximizing over φ is equivalent to minimizing the denominator over φ. We constrain φ to have a unit projection onto the source. The corresponding variational problem is:

$$\frac{1}{\langle\theta^2\rangle} \leq \min_{\varphi} \; \{\langle\varphi\overline{\mathcal{L}\mathcal{L}^\dagger}\varphi\rangle \mid \langle\varphi s\rangle = 1\}. \tag{3.4}$$

Thus we must minimize the functional $\mathcal{F} := \left\langle \frac{1}{2}\varphi\overline{\mathcal{L}\mathcal{L}^\dagger}\varphi - \mu(\varphi s - 1)\right\rangle$, whose Euler-Lagrange equation is

$$\frac{\delta\mathcal{F}}{\delta\varphi} = \overline{\mathcal{L}\mathcal{L}^\dagger}\varphi - \mu s = 0 \tag{3.5}$$

where μ is a Lagrange multiplier to enforce the constraint. The minimizer is (after some algebra)

$$\varphi = \frac{\mathcal{M}_0 s}{\langle s\mathcal{M}_0 s\rangle} \tag{3.6}$$

where $\mathcal{M}_0 := (\overline{\mathcal{L}\mathcal{L}^\dagger})^{-1}$ and

$$\langle s\mathcal{M}_0 s\rangle = \langle s\{\kappa^2\Delta^2 - \nabla\cdot(\overline{\mathbf{u}\mathbf{u}}) + \kappa(2\nabla\overline{\mathbf{u}} : \nabla\nabla + \Delta\overline{\mathbf{u}}\cdot\nabla)\}^{-1}s\rangle. \tag{3.7}$$

Thus we obtain the lower bound

$$\langle\theta^2\rangle \geq \langle s\mathcal{M}_0 s\rangle \tag{3.8}$$

which depends only on the mean and quadratic correlations of the stirring field. For flows satisfying HIT this simplifies to the quadratic form

$$\langle s\mathcal{M}_0 s\rangle = \langle s\{\kappa^2\Delta^2 - (U^2/d)\Delta\}^{-1}s\rangle. \tag{3.9}$$

This lower bound on the variance depends on the source function and on the stirring. In Fourier space it is expressed as

$$\langle\theta^2\rangle \geq \sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{\kappa k^4 + U^2k^2/d}. \tag{3.10}$$

An upper bound on the variance may be obtained from simple application of the Cauchy-Schwarz and Poincaré inequalities to the bulk variance dissipation constraint:

$$\langle\theta^2\rangle \leq \frac{L^2}{4\pi^2}\frac{\langle|\nabla^{-1}s|^2\rangle}{\kappa^2}. \tag{3.11}$$

The variance in the absence of stirring is

$$\langle\theta_0^2\rangle = \frac{1}{\kappa^2}\langle(\Delta^{-1}s)^2\rangle \tag{3.12}$$

and thus we obtain bounds on the mixing efficiency from bounds on the variance

$$\frac{4\pi^2}{L^2}\frac{\langle|\Delta^{-1}s|^2\rangle}{\langle|\nabla^{-1}s|^2\rangle} \leq M_0^2 \leq \left(\sum_{\mathbf{k}}\frac{|\hat{s}(\mathbf{k})|^2}{k^4}\right)\left(\sum_{\mathbf{k}}\frac{|\hat{s}(\mathbf{k})|^2}{k^4 + Pe^2k^2/d}\right)^{-1}. \tag{3.13}$$

One might expect the variance efficiency to have a lower bound of 1, implying that stirring *always* decreases the variance. We can search for a sharper lower bound by actually optimizing the variance subject to the variance dissipation constraint

$$\langle \theta^2 \rangle \geq \min_{\tilde{\theta}} \ \{ \langle \tilde{\theta}^2 \rangle \mid \kappa \langle |\nabla \tilde{\theta}|^2 \rangle = \langle s \tilde{\theta} \rangle \}. \tag{3.14}$$

That is, we can seek the minimum possible variance subject only to the entropy production balance. The solution of the optimization problem in Fourier space is

$$\hat{\theta}(\mathbf{k}) = \frac{1}{2} \frac{\hat{s}(\mathbf{k})}{\kappa k^2 + \lambda} \tag{3.15}$$

where $\lambda = -1/2\mu$ and μ is the Lagrange multiplier. Enforcing the constraint,

$$\kappa \sum_{\mathbf{k}} k^2 |\hat{\theta}(\mathbf{k})|^2 = \sum_{\mathbf{k}} \hat{\theta}(\mathbf{k}) \hat{s}^*(\mathbf{k}) \quad \Rightarrow \quad \kappa \sum_{\mathbf{k}} \frac{k^2 |\hat{s}(\mathbf{k})|^2}{(\kappa k^2 + \lambda)^2} = 2 \sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{\kappa k^2 + \lambda}. \tag{3.16}$$

where $*$ denotes the complex conjugate.

In the case of a monochromatic source this simplifies to

$$\kappa \frac{k^2}{(\kappa k^2 + \lambda)^2} = 2 \frac{1}{\kappa k^2 + \lambda} \quad \Rightarrow \quad \kappa k^2 = 2(\kappa k^2 + \lambda) \quad \Rightarrow \quad \lambda = -\frac{\kappa k^2}{2} \tag{3.17}$$

and hence

$$\hat{\theta}(\mathbf{k}) = \frac{\hat{s}}{\kappa k^2} = \hat{\theta}_0(\mathbf{k}) \tag{3.18}$$

which implies $M_0 \geq 1$.

In the case of a dichromatic source (k_1 with amplitude s_1, k_2 with amplitude s_2), the constraint requires one to solve a cubic equation for $\xi = \lambda / k_1$

$$(1+\alpha)\xi^3 + \frac{1}{2}(1 + \alpha\beta + 4\beta + 4\alpha)\xi^2 + (\beta + \alpha\beta + \beta^2 + \alpha)\xi + \frac{1}{2}(\beta^2 + \alpha\beta) = 0 \tag{3.19}$$

where $\alpha = c_1/c_2$, $\beta = \mu_1/\mu_2$, $c_1 = s_1^2$, $c_2 = s_2^2$, $\mu_1 = \kappa k_1^2$, and $\mu_2 = \kappa k_2^2$. Then the mixing efficiency is

$$\frac{|\hat{\theta}_0(\mathbf{k})|^2}{|\hat{\theta}(\mathbf{k})|^2} = \frac{4(1 + \frac{\alpha}{\beta^2})}{\frac{1}{(1+\xi)^2} + \frac{\alpha}{(\beta+\xi)^2}}. \tag{3.20}$$

The efficiency goes to 1 in the monochromatic limit $\alpha \to 0$ ($\xi \to -1/2$) as expected. But the minimum value the efficiency bound is less than 1 for $\forall\ \xi$ implying that the variance dissipation constraint is not sufficient to guarantee that there are no stirring flows that could possibly increase the scalar variance. So this analysis does not rule out the existence of *ineffective* stirring fields.

3.1.1 Delta function source

Here we consider a δ-function point source (measure valued) with Fourier coefficients $|\hat{s}(\mathbf{k})| = 1$ as $|\mathbf{k}| \to \infty$. We note this includes white noise sources. As we are interested in the high-Pe

limit we approximate the sums in (3.16) by integrals. The asymptotic form of the upper bound is

$$M_0^2 \lesssim \left(\int_{2\pi/L}^{\infty} \frac{k^{d-1}dk}{k^4}\right)\left(\int_{2\pi/L}^{\infty} \frac{k^{d-1}dk}{k^4 + \frac{U^2}{d\kappa^2}k^2}\right)^{-1}. \tag{3.21}$$

Letting $\xi = kL : 2\pi \to \infty$ we obtain

$$M_0^2 \lesssim \left(\int_{2\pi}^{\infty} \xi^{d-5} d^d \xi\right)\left(\int_{2\pi}^{\infty} \frac{\xi^{d-1}d\xi}{\xi^4 + Pe^2\xi^2/d}\right)^{-1}. \tag{3.22}$$

For $d = 2$ the integrals become

$$\int_{2\pi}^{\infty} \xi^{-3} d\xi = \frac{1}{8\pi^2}, \qquad \int_{2\pi}^{\infty} \frac{\xi d\xi}{\xi^4 + Pe^2\xi^2/2} \sim \frac{\log Pe}{Pe^2} \tag{3.23}$$

resulting in the asymptotic bound

$$M_0 \lesssim \frac{Pe}{\sqrt{\log Pe}}. \tag{3.24}$$

In d=3

$$\int_{2\pi}^{\infty} \xi^{-2} d\xi = \frac{1}{2\pi}, \qquad \int_{2\pi}^{\infty} \frac{d\xi}{\xi^4 + Pe^2\xi^2/2} \sim \frac{1}{Pe} \tag{3.25}$$

resulting in the asymptotic bound

$$M_0 \lesssim \sqrt{Pe}. \tag{3.26}$$

An efficiency scaling of Pe leads to an eddy diffusivity proportional to UL from (3.2). For $d = 3$ there is a dramatic modification to the scaling that implies the eddy diffusivity is proportional to $\sqrt{\kappa}$.

3.2 Bounds on the gradient variance

Beginning with the first step in the TDG procedure

$$\langle \theta(\mathbf{u} \cdot \nabla + \kappa \Delta)\varphi \rangle = -\langle \varphi s \rangle \tag{3.27}$$

we integrate by parts and apply the Cauchy-Schwarz inequality to obtain

$$\langle \varphi s \rangle^2 = \langle (\mathbf{u}\varphi + \kappa \nabla \varphi) \cdot \nabla \theta \rangle^2 \leq \langle |\mathbf{u}\varphi + \kappa \nabla \varphi|^2 \rangle \langle |\nabla \theta|^2 \rangle. \tag{3.28}$$

The sharpness of this bound is discussed at the end of this section. Continuing as usual, we construct a variational principle to obtain a lower bound on the gradient variance

$$\langle |\nabla \theta|^2 \rangle \geq \max_{\varphi} \frac{\langle \varphi s \rangle^2}{\langle |\mathbf{u}\varphi + \kappa \nabla \varphi|^2 \rangle}. \tag{3.29}$$

Thus we minimize the denominator subject to the constraint of φ having a unit projection on the source. Under the homogeneity and isotropy assumptions of HIT the variational problem becomes one of evaluating

$$\min_{\varphi} \; \{\langle \kappa |\nabla \varphi|^2 + U^2 \varphi^2 \rangle \mid \langle \varphi s \rangle = 1\}. \tag{3.30}$$

We want to minimize the functional $\mathcal{F} := \left\langle \frac{1}{2}(\kappa|\nabla\varphi|^2 + U^2\varphi^2) - \mu(s\varphi - 1)\right\rangle$. The solution of the optimization problem is (after some algebra)

$$\langle|\nabla\theta|^2\rangle \geq \langle s\mathcal{M}_1 s\rangle \tag{3.31}$$

where $\mathcal{M}_1 = (-\kappa^2\Delta + U^2)^{-1}$.

A sharp lower bound on the gradient variance is easily proven. Upon taking the inner product of θ with the advection-diffusion equation we obtain the variance dissipation constraint

$$\kappa\langle|\nabla\theta|^2\rangle = \langle s\theta\rangle. \tag{3.32}$$

Inserting $\nabla^{-1}\nabla = 1$ on the right hand side, integrating by parts and applying the Cauchy-Schwarz inequality, we deduce

$$\kappa^2\langle|\nabla\theta|^2\rangle \leq \langle|\nabla^{-1}s|^2\rangle = \kappa^2\langle|\nabla\theta_0|^2\rangle \quad \Rightarrow \quad M_1 \geq 1. \tag{3.33}$$

Hence stirring *always* reduces the gradient variance which was *not* proven for the variance (previous section).

Given the upper and lower bounds on the gradient variance we can bound the small scale mixing efficiency according to

$$1 \leq M_1^2 \leq \frac{1}{\kappa^2}\frac{\langle|\nabla^{-1}s|^2\rangle}{\langle s\mathcal{M}_1 s\rangle}. \tag{3.34}$$

In Fourier space this is

$$1 \leq M_1^2 \leq \left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{k^2}\right)\left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{k^2 + \frac{U^2}{\kappa^2}}\right)^{-1}. \tag{3.35}$$

These bounds only make sense when the sums on the right hand side converge.

Note that if $\kappa \to 0$ and if $s(\mathbf{x}) \in L^2$ then

$$M_1^2 \to \frac{U^2}{\kappa^2}\left(\sum_{k} \frac{|\hat{s}(\mathbf{k})|^2}{k^2}\right)\left(\sum_{k} |\hat{s}(\mathbf{k})|^2\right)^{-1} = \frac{\langle|\nabla^{-1}s|^2\rangle}{\langle s^2\rangle}\frac{U^2}{\kappa^2} = \frac{U^2\ell_s^2}{\kappa^2}. \tag{3.36}$$

where $\ell_s = \langle|\nabla^{-1}s|^2\rangle^{1/2}/\langle s^2\rangle^{1/2}$. So if $s \in L^2$ then $M_1 \leq Pe_s$, but if $s \notin L^2$ then $M_1 = 1$ i.e. there is only suppression of gradient variance if $U\langle|\nabla^{-1}s|^2\rangle^{1/2}/\kappa\langle s^2\rangle^{1/2} \gg 1$.

Here we re-examine our application of the Cauchy-Schwarz inequality which was the first step when deriving an upper bound on the gradient variance. In fact the analysis can be improved a bit. We expect the bound to involve only the curl-free part of the field $\mathbf{u}\varphi + \kappa\nabla\varphi$. This can be seen by first evaluating

$$\min_{\tilde{\theta}} \ \{\langle|\nabla\tilde{\theta}|^2\rangle \mid \langle\varphi s\rangle = \langle(\mathbf{u}\varphi + \kappa\nabla\varphi)\cdot\nabla\tilde{\theta}\rangle\} \tag{3.37}$$

with functional $\mathcal{F} := \langle\frac{1}{2}|\nabla\tilde{\theta}|^2 + \lambda(\mathbf{v}\cdot\nabla\tilde{\theta} - \varphi s)\rangle$ where $\mathbf{v} = \mathbf{u}\varphi + \kappa\nabla\varphi$. The solution to the variational problem is (after some algebra):

$$\langle|\nabla\theta|^2\rangle = \frac{\langle\varphi s\rangle^2}{\langle(\nabla\cdot\mathbf{v})(-\Delta^{-1})\nabla\cdot\mathbf{v}\rangle} \geq \frac{\langle\varphi s\rangle^2}{\langle|\mathbf{v}|^2\rangle}. \tag{3.38}$$

The inequality follows immediately from examining the Fourier representation of the denominator. Note that we can decompose $\mathbf{v}$ as follows

$$\mathbf{v} = \underbrace{\mathbf{v} - \nabla\Delta^{-1}\nabla\cdot\mathbf{v}}_{\text{divergence}-\text{free}} + \underbrace{\nabla\Delta^{-1}\nabla\cdot\mathbf{v}}_{\text{curl}-\text{free}}. \tag{3.39}$$

The denominator above is

$$\begin{aligned}\langle(\nabla\cdot\mathbf{v}(-\Delta^{-1})(\nabla\cdot\mathbf{v})\rangle &= \langle[\Delta\Delta^{-1}(\nabla\cdot\mathbf{v})](-\Delta^{-1})(\nabla\cdot\mathbf{v})\rangle \\ &= \langle\nabla(\Delta^{-1}(\nabla\cdot\mathbf{v})\cdot\nabla(\Delta^{-1}(\nabla\cdot\mathbf{v})\rangle \\ &= \langle|\nabla\Delta^{-1}\nabla\cdot\mathbf{v}|^2\rangle.\end{aligned} \tag{3.40}$$

From this it is clear that the explicit optimization over $\tilde{\theta}$ yields a sharper bound by picking out the component of $\mathbf{v}$ which is curl-free.

Interestingly, this new bound depends on the two point correlation and involves a non-local integral operator i.e. for $d = 2$

$$\langle(\nabla\cdot\mathbf{v})(-\Delta^{-1})\nabla\cdot\mathbf{v}\rangle = \frac{1}{L^d}\int d\mathbf{x}\int d\mathbf{y}\nabla_x\cdot\mathbf{v}(\mathbf{x})G(\mathbf{x}-\mathbf{y})\nabla_y\cdot\mathbf{v}(\mathbf{y}) \tag{3.41}$$

where $G(\mathbf{x}-\mathbf{y})$ is the Green's function of $-\Delta$. After integrating by parts

$$\langle(\nabla\cdot\mathbf{v})(-\Delta^{-1})\nabla\cdot\mathbf{v}\rangle = \frac{1}{L^d}\int d\mathbf{x}\int d\mathbf{y}(-\nabla\nabla G) : \overline{\mathbf{v}\mathbf{v}} \tag{3.42}$$

where under the homogeneity assumption,

$$\overline{\mathbf{v}\mathbf{v}} = \varphi(\mathbf{x})\varphi(\mathbf{y})\overline{\mathbf{u}(\mathbf{x})\mathbf{u}(\mathbf{y})} + \kappa^2\nabla\varphi(\mathbf{x})\nabla\varphi(\mathbf{y}). \tag{3.43}$$

It is the first term that prevents the expression from collapsing to $|\mathbf{v}|^2$ (the second term becomes $\kappa^2(\Delta\varphi)^2$ after integrating by parts). The first term depends on the two-point correlation of the velocity field. Under the assumptions of HIT, the velocity field has single-point statistical properties and hence the first term collapses to $U^2\varphi^2/d$ which implies that for HIT a strict application of Cauchy-Schwarz (without minimizing over $\tilde{\theta}$) yields a sharp bound. In turbulence theory, the two-point correlation for Homogeneous Isotropic Turbulence is written as

$$\overline{u_i(\mathbf{x},\cdot)u_j(\mathbf{y},\cdot)} = \delta_{ij}g(|\mathbf{x}-\mathbf{y}|) + \frac{(x_i-y_i)(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^2}(f-g). \tag{3.44}$$

Incompressibility implies that $g(r) = f(r) + rf'(r)/(d-1)$. This new bound introduces dependence on the two-point correlation property of the velocity field. The implication of such two-point statistical properties on the scaling of the bound will be the subject of future investigation. We note that the Cauchy-Schwarz bound cannot be improved for both the variance, because it is a scalar field, and the inverse gradient variance (next section) because it manifestly involves a curl-free field. We will revisit the implications of the two-point statistical properties when we examine the bounds including scalar decay (section 6).

3.2.1 Delta function source

It is clear that a δ-function or white noise source ($|\hat{s}(\mathbf{k})| \sim 1$) will cause the sums in (3.37) to diverge in both $d = 2$ and 3. Thus, in the case of δ-like sources or sinks the mixing efficiency bound is sharp and equal to 1.

3.3 Bounds on the inverse gradient variance

Beginning again with the first step of the TDG procedure

$$\begin{aligned}\langle \varphi s\rangle &= -\langle(\mathbf{u}\cdot\nabla\varphi + \kappa\Delta\varphi)\theta\rangle \\ &= \langle \nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi)\cdot\nabla\Delta^{-1}\theta\rangle \\ &\le \langle|\nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi)|^2\rangle^{\frac{1}{2}}\langle|\nabla^{-1}\theta|^2\rangle^{\frac{1}{2}}.\end{aligned} \tag{3.45}$$

Continuing as usual, we construct a variational principle to obtain a lower bound on the inverse gradient variance

$$\langle|\nabla^{-1}\theta|^2\rangle \ge \max_{\varphi} \frac{\langle\varphi s\rangle^2}{\langle|\nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi|^2\rangle} \tag{3.46}$$

Thus we minimize the denominator subject to the constraint of φ having a unit projection on the source, i.e. we evaluate

$$\min_{\varphi}\ \{\langle|(\nabla\mathbf{u})\cdot\nabla\varphi+\mathbf{u}\cdot\nabla\nabla\varphi+\kappa\nabla\Delta\varphi|^2\rangle \mid \langle\varphi s\rangle = 1\}. \tag{3.47}$$

The assumptions of HIT simplify the problem:

$$\begin{aligned}|(\nabla\mathbf{u})\cdot\nabla\varphi+\mathbf{u}\cdot\nabla\nabla\varphi+\kappa\nabla\Delta\varphi|^2 &= (\nabla\varphi_{,i})\cdot\overline{\mathbf{u}\mathbf{u}}\cdot(\nabla\varphi_{,i}) + \nabla\varphi\cdot\overline{[(\nabla\mathbf{u})^{\mathrm{tr}}(\nabla\mathbf{u})]}\cdot\nabla\varphi+\kappa^2|\Delta\nabla\varphi|^2 \\ &= \kappa^2|\Delta\nabla\varphi|^2 + (\Gamma^2/d)|\nabla\varphi|^2 + (U^2/d)(\Delta\varphi)^2.\end{aligned} \tag{3.48}$$

Thus the variational problem reduces to evaluating

$$\min_{\varphi}\ \left\{\langle\kappa^2|\nabla\Delta\varphi|^2 + (\Gamma^2/d)|\nabla\varphi|^2 + (U^2/d)(\Delta\varphi)^2\rangle \mid \langle\varphi s\rangle = 1\right\}. \tag{3.49}$$

The solution of the variational problem is (after some algebra)

$$\langle|\nabla^{-1}\theta|^2\rangle = \langle s\mathcal{M}_{-1}s\rangle \tag{3.50}$$

$\mathcal{M}_{-1} := (\kappa^2\Delta^3 - (\Gamma^2/d)\Delta + (U^2/d)\Delta^2)^{-1}$. A lower bound on the inverse gradient variance is obtained from simple application of the Cauchy-Schwarz and Poincaré inequalities to the bulk variance dissipation constraint:

$$\langle|\nabla^{-1}\theta|^2\rangle \le \frac{L^8}{256\pi^8\kappa^2}\langle|\nabla s|^2\rangle. \tag{3.51}$$

Because it uses the Poincaré inequality the lower bound is only sharp if the source is monochromatic at the lowest wavenumber, $2\pi/L$.

Given the upper and lower bound on the inverse gradient variance and the value in the absence of stirring, $\langle|\nabla^{-1}\Delta^{-1}s|^2\rangle$, we obtain bounds on the mixing efficiency on large scales

$$\frac{256\pi^8}{L^8}\frac{\langle\nabla^{-1}\Delta^{-1}s|^2\rangle}{\langle|\nabla s|^2\rangle} \le M_{-1} \le \frac{\langle|\nabla^{-1}\Delta^{-1}s|^2\rangle}{\langle s\mathcal{M}_{-1}s\rangle}. \tag{3.52}$$

In Fourier space,

$$\frac{256\pi^8}{L^8}\left(\sum_{\mathbf{k}}\frac{|\hat{s}(\mathbf{k})|^2}{k^6}\right)\left(\sum_{k}k^2|\hat{s}(\mathbf{k})|^2\right)^{-1} \le M_{-1}^2 \le \left(\sum_{k}\frac{|\hat{s}(\mathbf{k})|^2}{k^6}\right)\left(\sum_{\mathbf{k}}\frac{|\hat{s}(\mathbf{k})|^2}{k^6+\frac{U^2}{d\kappa^2}k^4+\frac{\Gamma^2}{d\kappa^2}k^2}\right)^{-1} \tag{3.53}$$

For a monochromatic source the upper bound is

$$M_{-1}^2 \leq 1 + \frac{U^2}{d\kappa^2 k^2} + \frac{\Gamma^2}{d\kappa^2 k^4} = 1 + \frac{U^2}{d\kappa^2 k^2}\left(1 + \frac{\Gamma^2}{U^2 k^2}\right) = 1 + \frac{\mathcal{P}e^2}{d}\left(1 + \frac{1}{\lambda^2 k^2}\right) \tag{3.54}$$

where we define $\mathcal{P}e = U/\kappa k$. Note that the efficiency depends on the shear in the flow directly through Γ. Interestingly, Γ allows for an increase in the mixing efficiency on large scales via stirring on small scales (coupling the different scales). We investigate this potential effect for a steady shearing wind in section 5.

3.3.1 Delta function source

Consider a δ-function source (measure valued). Suppose $\kappa \to 0$ while U^2 and Γ^2 are fixed then the asymptotic form of the upper bound is

$$M_{-1}^2 \lesssim \left(\int_{2\pi/L}^{\infty} \frac{k^{d-1}dk}{k^6}\right)\left(\int_{2\pi/L}^{\infty} \frac{k^{d-1}dk}{k^6 + \frac{U^2}{d\kappa^2}k^4 + \frac{\Gamma^2}{d\kappa^2}k^2}\right)^{-1}. \tag{3.55}$$

Letting $\xi = kL/2\pi : 1 \to \infty$ we obtain

$$M_{-1} \lesssim \left(\int_{1}^{\infty} \xi^{d-7} d\xi\right)\left(\int_{1}^{\infty} \frac{\xi^{d-3}d\xi}{\xi^4 + \frac{U^2L^2}{4\pi^2 d\kappa^2}\xi^2 + \frac{\Gamma^2 L^4}{16\pi^4 d\kappa^2}}\right)^{-1} \tag{3.56}$$

In d=2, letting $\eta = \xi^2$

$$\int_1^\infty \xi^{-5} d\xi = \frac{1}{4}, \qquad \int_1^\infty \frac{\xi^{-1}d\xi}{\xi^4 + \frac{Pe^2}{d}\xi^2 + \frac{L^2}{\lambda^2}\frac{Pe^2}{d}} = \frac{1}{2}\int_1^\infty \frac{d\eta}{\eta(\eta^2 + \alpha\eta + \beta)}, \tag{3.57}$$

where $\alpha = Pe^2/d$ and $\beta = L^2 Pe^2/\lambda^2 d$. In the limit $Pe \to \infty$

$$\int_1^\infty \frac{\xi^{-1}d\xi}{\xi^4 + \frac{Pe^2}{d}\xi^2 + \frac{L^2}{\lambda^2}\frac{Pe^2}{d}} = \frac{1}{2}\int_1^\infty \frac{d\eta}{\eta(\alpha\eta + \beta)}. \tag{3.58}$$

After some algebra we find

$$\int_1^\infty \frac{\xi^{-1}d\xi}{\xi^4 + \frac{Pe^2}{d}\xi^2 + \frac{L^2}{\lambda^2}\frac{Pe^2}{d}} \cong \frac{1}{2\beta}\ln\left(1 + \frac{\beta}{\alpha}\right) \tag{3.59}$$

note that $\beta/\alpha = L^2/\lambda^2$. The efficiency bound becomes (as $Pe \to \infty$)

$$M_{-1}^2 \lesssim \frac{\beta}{2}\frac{1}{\ln\left(1 + \frac{\beta}{\alpha}\right)} = Pe^2\frac{L^2}{\lambda^2}\frac{1}{\ln\left(1 + \frac{L^2}{\lambda^2}\right)} \tag{3.60}$$

Interestingly, the prefactor can be larger for smaller scale flow.

In $d = 3$

$$\int_1^\infty \xi^{-4}d\xi = \frac{1}{4}, \qquad \int_1^\infty \frac{d\xi}{\xi^4 + \frac{Pe^2}{d}\xi^2 + (\frac{pL}{2\pi})^2\frac{Pe^2}{d}} \to \int_1^\infty \frac{d\xi}{Pe(\xi^2 + \frac{L^2}{\lambda^2})} \tag{3.61}$$

after a change of variables $\eta = \frac{\lambda}{L}\xi : \frac{\lambda}{L} \to \infty$

$$\int_1^\infty \frac{d\xi}{\xi^4 + \frac{Pe^2}{d}\xi^2 + (\frac{pL}{2\pi})^2\frac{Pe^2}{d}} \cong \frac{1}{Pe}\frac{\lambda}{L}\int_{\frac{\lambda}{L}}^\infty \frac{d\eta}{\eta^2+1} = \frac{1}{Pe}\frac{\lambda}{L}\left(\frac{\pi}{2} - \arctan\frac{\lambda}{L}\right) \tag{3.62}$$

hence

$$M_{-1}^2 \lesssim \frac{L}{\lambda}Pe^2\frac{1}{\left(\frac{\pi}{2} - \arctan\frac{\lambda}{L}\right)}. \tag{3.63}$$

4 Saturating the multiscale mixing efficiency bounds

The HIT bounds on the multiscale mixing efficiencies derived in the previous section simplify in the case of a monochromatic source

$$M_1 \leq \sqrt{1 + Pe^2/k_s^2}, \tag{4.1a}$$
$$M_0 \leq \sqrt{1 + Pe^2/k_s^2 d}, \tag{4.1b}$$
$$M_{-1} \leq \sqrt{1 + Pe^2/k_s^2 d + L^2 Pe^2/\lambda^2 k_s^4 d} \tag{4.1c}$$

where we have rescaled $[0, L]^d$ to $[0, 1]^d$ so that k_s is a multiple of 2π. We note that each efficiency scales as Pe which corresponds to replacing the molecular diffusivity by an eddy diffusivity proportional to UL. An anomalous scaling results if the efficiencies are not linear in Pe. Figure 2 from TDG showed the mixing efficiency M_0 versus Péclet number from direct numerical simulations (DNS) of the advection-diffusion equation for a monochromatic source $\sin k_s x$ and the Zeldovich sine flow [3]. TDG discussed the possibility of saturating the upper bound for the $\sin k_s x$ source; however it was clear from the DNS calculations that the sine flow was not the optimal stirrer and no other stirring field was put forth.

Here we show that the TDG upper bound on the variance for $s(\mathbf{x}) = \sin k_s x_1$ and $\mathbf{x} \in \mathbb{T}^d$ i.e., $\mathbf{x} \in [0, L]^d$, is saturated by the sweeping flow suggested by W. R. Young. Consider the steady advection-diffusion equation with source $s(\mathbf{x}) = \sqrt{2} S \sin k_s x_1$ and uniform stirring field $\mathbf{u}(\mathbf{x}) = (U/\sqrt{d}) \sum_{n=1}^d \hat{\mathbf{i}}_n$:

$$\frac{U}{\sqrt{d}} \sum_{n=1}^{d} \frac{\partial \theta}{\partial x_n} = \kappa \sum_{n=1}^{d} \frac{\partial^2 \theta}{\partial x_n^2} + \sqrt{2} S \sin(k_s x_1). \tag{4.2}$$

We sweep on an angle for a long time (to kill the transients) and then switch the sweeping by an appropriate angle (repeating appropriately) as to satisfy the HIT assumptions.

Letting $\theta(\mathbf{x}) = \sum_{n=1}^d F_n(x_n)$, we end up with a system of constant coefficient ODEs

$$\frac{d^2 F_1}{dx_1^2} - \frac{U}{\sqrt{d}\kappa} \frac{dF_1}{dx_1} + \frac{\sqrt{2} S}{\kappa} \sin(k_s x_1) = 0 \tag{4.3a}$$
$$\frac{d^2 F_n}{dx_n^2} - \frac{U}{\sqrt{d}\kappa} \frac{dF_n}{dx_n} = 0 \qquad \text{for} \quad 2 \leq n \leq d \tag{4.3b}$$

with periodic boundary conditions $F_n(0) = F_n(L)$ whose solution is

$$F_1 = \frac{\sqrt{2} S L^2}{(4\pi^2 \kappa^2 + \frac{U^2}{d} L^2)} \left[\kappa \sin(k_s x_1) - \frac{UL}{2\sqrt{d}\pi} \cos(k_s x_1) \right] \tag{4.4a}$$
$$F_n = 0 \qquad \text{for} \quad 2 \leq n \leq d. \tag{4.4b}$$

The variance is

$$\langle \theta^2 \rangle = \frac{S^2 L^4}{(4\pi^2 \kappa^2 + \frac{U^2}{d} L^2)^2} \left[\kappa^2 + \frac{U^2 L^2}{4\pi^2 d} \right] \tag{4.5}$$

and since $\langle \theta_0^2 \rangle = S^2 L^4 / 16\pi^4 \kappa^2$ the mixing efficiency is

$$M_0 = \sqrt{1 + \frac{U^2 L^2}{4\pi^2 d \kappa^2}} = \sqrt{1 + \frac{Pe^2}{4\pi^2 d}} \tag{4.6}$$

which is the bound derived by TDG. Given the steady solution we can compute the other two mixing efficiencies. After some straight-forward algebra we find

$$M_1 = M_{-1} = \sqrt{1 + \frac{Pe^2}{4\pi^2 d}} = M_0. \tag{4.7}$$

Interestingly, M_0 and M_{-1} are precisely saturated but M_1 is off by a d factor. Since the uniform flow lacks shear the large scale mixing efficiency, M_{-1}, is identical to the others.

The result is fairly intuitive: to reduce the variance (on any length scale) one should simply blow the source onto the sink and vice versa — if one can do this simply. We note that this type of sweeping flow is somewhat pathological in the sense that it simply transports the source onto the sink which can be done simply on the torus. There is no dependence on diffusion. However, such sweeping flows are not allowed on the sphere or in bounded domains. Furthermore, the sweeping flow is not optimal for non-1D sources. This makes it clear that the optimal stirrer is a function of both the source shape and the domain. Formulating the optimization problem for the optimal stirring field is a subject of current and future investigation. It is a nasty non-linear problem.

To emphasize the relationship between the source and the stirring field which saturates the bound we perform an analogous calculation to the previous one (for $d = 2, 3$) however we impose a δ-function source distribution. Taking the Fourier transform of the steady advection-diffusion equation with $s = \delta(\mathbf{x})$ we obtain

$$\sum_k \hat{\theta}(\mathbf{k}) = \sum_k \frac{\hat{s}(\mathbf{k})}{\kappa k^2 + iUk_d} \tag{4.8}$$

where k_d is the dth component of the horizontal wavenumber. Approximating the integrals by sums (we are only interested in the asymptotic behaviour)

$$d = 2: \qquad \langle|\nabla^p\theta|^2\rangle = \int_0^{2\pi} d\phi \int_{2\pi/L}^{\infty} \frac{k^{2p+1}dk}{\kappa^2 k^4 + U^2k^2\cos^2\theta} \tag{4.9a}$$

$$d = 3: \qquad \langle|\nabla^p\theta|^2\rangle = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_{2\pi/L}^{\infty} \frac{k^{2(p+1)}dk}{\kappa^2 k^4 + U^2k^2\cos^2\theta}. \tag{4.9b}$$

The variances in the absence of stirring are found by calculating the above integrals with $U = 0$. Straight-forward evaluation of the integrals yields

$$d = 2: \qquad M_1 = 1, \quad M_0 \sim \frac{\sqrt{Pe}}{4\pi}, \quad M_{-1} \sim \frac{3\sqrt{Pe}}{8\pi} \tag{4.10}$$

$$d = 3: \qquad M_1 = 1, \quad M_0 \sim \frac{\sqrt{Pe}}{\sqrt{2}\pi}\frac{1}{\sqrt{\log(Pe/2)}}, \quad M_{-1} \sim \frac{2\sqrt{Pe}}{\sqrt{3}\pi}. \tag{4.11}$$

The anomalous scaling in Pe suggests that the uniform flow is far from the optimal allowed by the bound for the δ-function source in both $d = 2$ and 3. This emphasizes the source-dependent nature of the optimal stirrer.

Given that the the optimal HIT stirrer for $s = \sin k_s x$ was at an angle, the calculations from TDG were repeated for a tilted source and the Zeldovich sine flow to see if we could get closer to the bound. Tilting the source is equivalent to tilting the stirring. Figure 1 shows the results of the DNS calculation for $p = 1, 0, -1$. The plot of M_0 includes the PY bound. What is clear from this figure is that for a non-optimal flow the three bounds scale differently in Pe. In the next section we investigate the bounds for a simple steady shear flow in an effort to understand the scaling in Pe as well as to explore the dependence of M_{-1} on the Taylor microscale.

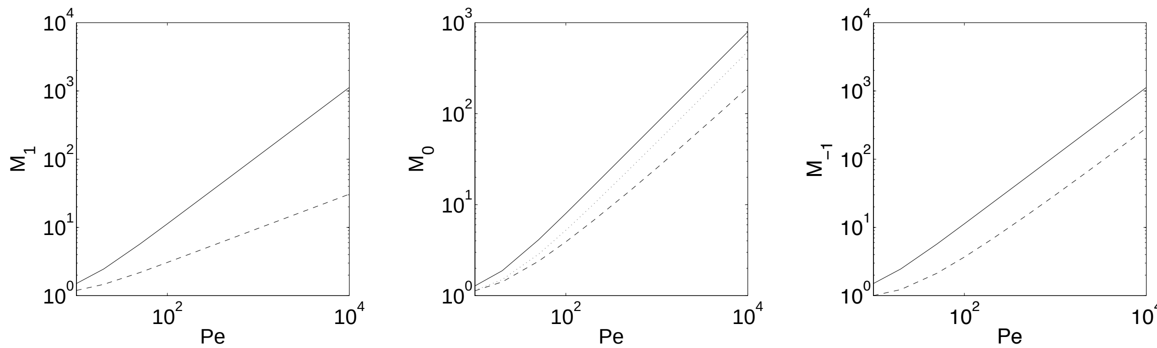

Figure 1: From left to right, mixing efficiencies M_p $p = 1, 0, -1$ for the Zeldovich sine flow with source $\sin k(x + y)$. The solid lines are the respective upper bounds from section 3. The dotted line is the PY variance bound and the dashed lines are the result of direct numerical simulations with U fixed.

5 Steady Shear Flows

From the previous section it is clear that the most efficient stirring for monochromatic sources on the torus is the sweeping flow. Here we investigate the effect of shear on the mixing efficiency on different scales to understand the scaling behaviour at large Pe (i.e. the scaling when we do not saturate the bound). The results would directly apply to HIT stirring analogous to blowing for a very long time (the sine flow having a long period). From the analysis of section 3 we would expect to see a large difference between the three norms for such sheared stirring. We treat the simplest problem by considering the long time behaviour of a passive tracer goverened by the advection-diffusion equation

$$\mathbf{u} \cdot \nabla\theta = \kappa\Delta\theta + s(\mathbf{x}) \tag{5.1}$$

with a stirring field $\mathbf{u} = \sqrt{2}U \sin k_u y\hat{\mathbf{i}}$ and source $s(\mathbf{x}) = \sqrt{2}S \sin k_s x$ ($\sqrt{2}$ for normalization). Here the domain is the 2-dimensional torus $x \in \mathbb{T}^2$. The non-dimensional number governing the amount of shear is $r = k_u/k_s$. We are particularily interested in the limits $Pe \gg 1$ with r fixed and $r \gg 1$ with Pe fixed. The solution takes the form

$$\theta(\mathbf{x}) = f(y)\sin(k_s x) + g(y)\cos(k_s x) \tag{5.2}$$

which results in a system of ODEs:

$$-\sqrt{2}Uk_s \sin(k_u y)g(y) = \kappa \left[-k_s^2 + \frac{d^2}{dy^2}\right] f(y) + \sqrt{2}S \tag{5.3a}$$

$$\sqrt{2}Uk_s \sin(k_u y)f(y) = \kappa \left[-k_s^2 + \frac{d^2}{dy^2}\right] g(y). \tag{5.3b}$$

The stirring field is an odd function of y and hence from (5.4a) we deduce that $g(y)$ is also odd in y and hence that $f(y)$ is even in y. This can also be seen by integrating (5.4a) over a period. Since the functions $f(y)$ and $g(y)$ are periodic we consider the domain $y \in [0, l/2]$ where $l = 2\pi/p$. We infer boundary conditions given the even-oddness of the functions f and g:

$$g(0) = g(l/2) = 0, \quad f'(0) = f'(l/2) = 0. \tag{5.4}$$

Upon setting $\tilde{y} = k_s y$, $\hat{f} = fUk_s/S$, $\hat{g} = gUk_s/S$, $r = k_u/k_s$, and $\mathcal{P}e = \sqrt{2}U/\kappa k_s$ we obtain the non-dimensional ODEs

$$\frac{1}{\mathcal{P}e}\left[-1+\frac{d^2}{d\tilde{y}^2}\right]\hat{f}(\tilde{y}) + 1 = -\sin(r\tilde{y})\hat{g}(\tilde{y}) \tag{5.5a}$$

$$\frac{1}{\mathcal{P}e}\left[-1+\frac{d^2}{d\tilde{y}^2}\right]\hat{g}(\tilde{y}) = \sin(r\tilde{y})\hat{f}(\tilde{y}). \tag{5.5b}$$

The next sections outline the boundary layer analysis (since the solution is slowly varying except in isolated boundary layers) and regular perturbation theory which were used to investigate the limits mentioned above.

5.1 Boundary layer solution

This is the limit $\mathcal{P}e \gg 1$ and r fixed. Proceeding as usual, we construct an inner and outer solution. The outer solution is obtained by expanding in powers of $\mathcal{P}e^{-1}$:

$$\hat{f}_{out} = \sum_{n=0}^{\infty} \mathcal{P}e^{-n}\hat{f}_n, \qquad \hat{g}_{out} = \sum_{n=0}^{\infty} \mathcal{P}e^{-n}\hat{g}_n. \tag{5.6}$$

Thus, in the outer region the solution is approximated to leading order by

$$\hat{f}_{out} = 0, \qquad \hat{g}_{out} = -\frac{1}{\sin(k_u y)}. \tag{5.7}$$

The boundary layer scaling was determined from a dominant balance argument. The left hand side of (5.6a) is $\mathcal{O}(1)$, $\forall\ \epsilon$ thus we choose $\epsilon = \mathcal{P}e^{-1/3}$ and rescale y: $\eta = \tilde{y}/\epsilon$ to achieve a self-consistent scaling of the leading order terms. Expanding in ϵ according to

$$\hat{f}_{in} = \sum_{n=-1}^{\infty} \epsilon^n \hat{f}_n, \qquad \hat{g}_{in} = \sum_{n=-1}^{\infty} \epsilon^n \hat{g}_n \tag{5.8}$$

(note that the leading term is $\mathcal{O}(1/\epsilon)$) yields at order $\mathcal{O}(1/\epsilon)$:

$$\frac{d^2\hat{f}_{-1}}{d\eta^2} + r\eta\hat{g}_{-1} + 1 = 0, \qquad \frac{d^2\hat{g}_{-1}}{d\eta^2} - r\eta\hat{g}_{-1} = 0. \tag{5.9}$$

Letting $\xi = r^{1/3}\eta$, $F = r^{2/3}\hat{f}_{-1}$, and $G = r^{2/3}\hat{g}_{-1}$ this simplifies the system of ODEs to

$$F'' + \xi G + 1 = 0, \qquad G'' - \xi F = 0. \tag{5.10}$$

with boundary conditions

$$F'(0) = 0, \qquad G(0) = 0. \tag{5.11}$$

The other boundary conditions come from the requirement of matching to the outer solution: $F(\xi) \to 0$ and $G(\xi) \to -1/\xi$ as $\xi \to \infty$.

We note that this system of ODEs can be cast into the Airy equation with a complex argument $\phi(z) = F + iG$ but we resorted instead to shooting to get the solution numerically. The solution was obtained by shooting backward (which was the more stable direction) from the $\xi \to \infty$ solution whose asymptotic behavior may be deduced from (5.10)

$$F \approx -\frac{2}{\xi^4} + \frac{\beta}{\xi^{10}}, \qquad G \approx -\frac{1}{\xi} + \frac{\alpha}{\xi^7} \tag{5.12}$$

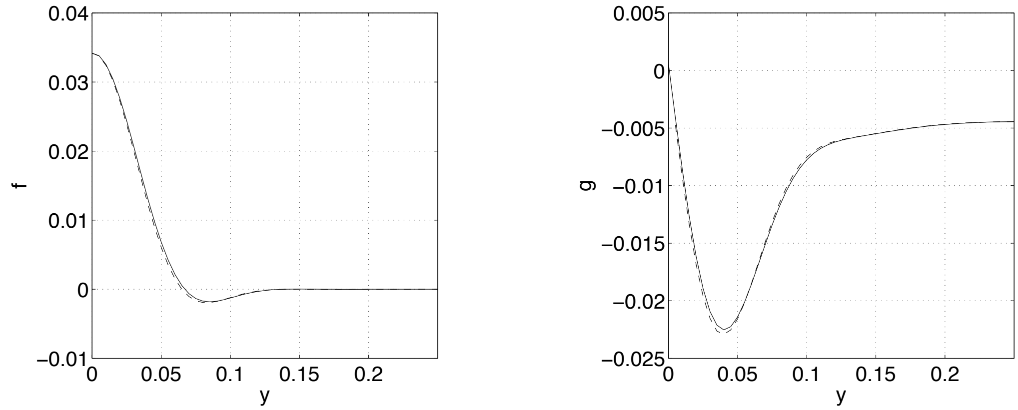

Figure 2: Comparison of the direct numerical solution (solid) and the boundary layer solution (dashed) for $Pe = 1000$.

where α and β were adjusted numerically to obtain a solution which satisfied the boundary conditions at $\xi = 0$. Before calculating higher order terms, we compared the boundary layer solution against the solution from a direct numerical simulation of the advection-diffusion equation. Figure 2 shows a plot of the two solutions for $Pe = 1000$. The agreement suggests that leading terms do indeed capture the asymptotic behaviour. The inner solution is thus well described by

$$\hat{f}_{in} = \frac{r^{-2/3}}{\epsilon}F(\xi), \qquad \hat{g}_{in} = \frac{r^{-2/3}}{\epsilon}G(\xi). \tag{5.13}$$

The final approximate solution to the coupled ODEs to leading order is the composite of the inner and outer solutions (recovering all the scalings and letting $\delta = \epsilon / r^{1/3} k_s$)

$$f(y) = \frac{S}{Uk_s}\hat{f}_{in} = \frac{S}{Uk_s}\frac{r^{-2/3}}{\epsilon}F\left(\frac{r^{1/3}k_s}{\epsilon}y\right) = \frac{S}{Uk_s}\frac{1}{k_u\delta}F\left(\frac{y}{\delta}\right) \tag{5.14a}$$

$$\begin{aligned} g(y) = \frac{S}{Uk_s}k_u y\ \hat{g}_{in}\ \hat{g}_{out} &= \frac{S}{Uk_s}\frac{r^{-2/3}}{\epsilon}G\left(\frac{r^{1/3}k_s}{\epsilon}y\right)\frac{k_u y}{\sin(k_u y)} \\ &= \frac{S}{Uk_s}\frac{1}{k_u\delta}G\left(\frac{y}{\delta}\right)\frac{k_u y}{\sin(k_u y)}. \end{aligned} \tag{5.14b}$$

Armed with this we can compute the multiscale mixing measures $\langle|\nabla^p\theta|^2\rangle$ for $p = 0, 1, -1$.

5.1.1 Variance

The variance is (N.B. only computing over 1/4 period)

$$\langle\theta^2\rangle = \frac{1}{2}\left(\langle f^2\rangle + \langle g^2\rangle\right) = \frac{1}{2}\frac{4}{l}\left(\int_0^{l/4} f^2(y)dy + \int_0^{l/4} g^2(y)dy\right) \tag{5.15}$$

letting $\eta = y/\delta : 0 \to \pi/2k_u\delta$

$$\langle\theta^2\rangle = \frac{1}{\pi}\frac{S^2}{U^2k_s^2}\frac{1}{k_u\delta}\left(\int_0^{\frac{\pi}{2k_u\delta}} F^2(\eta)d\eta + \int_0^{\frac{\pi}{2k_u\delta}} G^2(\eta)\frac{k_u^2\eta^2\delta^2}{\sin^2(k_u\eta\delta)}d\eta\right). \tag{5.16}$$

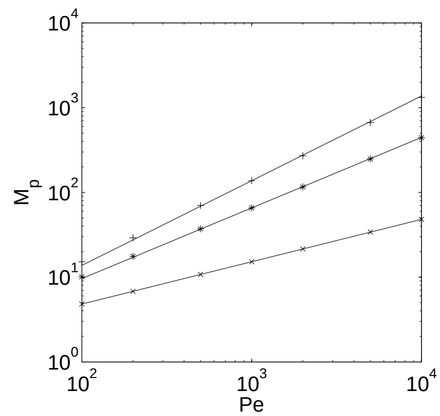

Figure 3: Mixing efficiencies for $p = 1$ denoted by x, $p = 0$ denoted by *, and $p = -1$ denoted by + for the steady shearing flow with $r = 1$ from direct numerical simulations with U fixed. The solid lines are the asymptotic scalings.

Here we are interested in the scaling as $\delta \to 0$. In that case we are justified in replacing the upper limit of the integral of $F^2(\eta)$ by infinity since the outer solution is zero. More care must be taken with the integral involving $G^2(\eta)$. We note that $k_u^2\eta^2\delta^2/\sin^2(k_u\eta\delta)$ is bounded by 0 and $\pi/2$ and hence we can apply Lebesgue's dominated convergence theorem to obtain

$$\langle\theta^2\rangle \approx \frac{1}{\pi}\frac{S^2}{U^2k_s^2}\frac{1}{k_u\delta}\left(\int_0^\infty F^2(\eta)d\eta + \int_0^\infty G^2(\eta)d\eta\right). \tag{5.17}$$

Recall from section 2 that $\langle\theta_0^2\rangle = S^2/\kappa^2k_s^4$ and hence the mixing efficiency is

$$M_0 \sim Cr^{1/3}\mathcal{P}e^{5/6}, \qquad C = \sqrt{\frac{\pi}{2}}\frac{1}{\sqrt{\int_0^\infty F^2(\eta)d\eta + \int_0^\infty G^2(\eta)d\eta}}. \tag{5.18}$$

Figure 3 shows M_0 as a function of Pe from direct numerical simulations. The scaling fits $Pe^{5/6}$. There is only a 5% difference between the prefactor calculated from the boundary layer solution and that calculated from the direct numerical simulation for $Pe = 1000$ (after rescaling Pe to $\mathcal{P}e$). Remarkably, the $Pe^{5/6}$ scaling is also observed for the HIT stirring (figure 1). The scaling in r was also confirmed. The $Pe^{5/6}$ scaling would hold for different values of r with a corresponding change in the value of the prefactor.

5.1.2 Gradient variance

The gradient is

$$\langle|\nabla\theta|^2\rangle = \frac{k^2}{2}\left[\langle f^2\rangle + \langle g^2\rangle\right] + \frac{1}{2}\left[\langle (f')^2\rangle + \langle (g')^2\rangle\right] \tag{5.19}$$

noting that the first term was computed in the previous section we focus attention on the second term. Computing the gradient we obtain

$$\frac{1}{2}\left[\langle (f')^2\rangle + \langle (g')^2\rangle\right] = \left\langle\left(\frac{S}{Uk_s}\frac{1}{k_u\delta^2}F'(y/\delta)\right)^2\right\rangle +$$
$$\left\langle\left(\frac{S}{Uk_s}\frac{1}{k_u\delta^2}G'(y/\delta)\frac{k_uy}{\sin(py)} + \frac{S}{Uk_s}\frac{1}{k_u\delta}G(y/\delta)\left[\frac{k_uy}{\sin(k_uy)}\right]'\right)^2\right\rangle. \tag{5.20}$$

The leading order contribution to the integral is the square of the first term ($1/\delta^2$ versus $1/\delta$). Hence

$$\frac{1}{2}\left[\langle (f')^2\rangle + \langle (g')^2\rangle\right] \approx \frac{1}{\pi}\frac{S^2}{U^2k_s^2}\frac{1}{k_u\delta^3}\left[\int_0^{\frac{\pi}{2k_u\delta}}(F')^2(\eta)d\eta + \int_0^{\frac{\pi}{2k_u\delta}}(G')^2(\eta)\frac{k_u^2\eta^2\delta^2}{\sin^2(k_u\eta\delta)}d\eta\right] \quad (5.21)$$

and by the same arguments as the previous section (DCT etc.) we obtain

$$\langle|\nabla\theta|^2\rangle \approx \frac{1}{\pi}\left(\int_0^\infty (F')^2(\eta)d\eta + \int_0^\infty (G')^2(\eta)d\eta\right)\frac{S^2}{U^2k_s^2}\frac{1}{p\delta^3}. \quad (5.22)$$

Recall from section 2 that $\langle|\nabla\theta_0|^2\rangle = S^2/\kappa^2k_s^2$ and hence the mixing efficiency is

$$M_1 \approx C\mathcal{P}e^{1/2}, \quad C = \sqrt{\frac{\pi}{2}}\frac{1}{\sqrt{\int_0^\infty (F')^2(\eta)d\eta + \int_0^\infty (G')^2(\eta)d\eta}}. \quad (5.23)$$

The boundary layer and direct numerical solution prefactors differ by approximately 1% for $Pe = 1000$. Figure 3 shows the scaling of M_1 from the direct numerical solution that confirms the $Pe^{1/2}$ scaling. The scaling in r was also confirmed. Interestingly, stirring at small scales does not enhance the mixing efficiency on small scales. This is because the decrease in gradient variance due to stirring on small scales is compensated by the increase in gradient variance in the boundary layer.

5.1.3 Inverse gradient variance

The inverse gradient variance is

$$\langle|\nabla^{-1}\theta|^2\rangle = \langle|\nabla^{-1}(f(y)\sin(k_sx) + g(y)\cos(k_sx))|^2\rangle \quad (5.24)$$

This is the trickiest of the three multiscale mixing measures. We can simplify the integral by noting that the leading Fourier component of $g(y)$ is zero. Expanding $f(y)$ in a Fourier series

$$f(y) = \sum_{n=0}^\infty f_n\cos(nk_uy) \quad (5.25)$$

we obtain

$$\nabla^{-1}(f(y)\sin(k_sx)) = \sum_{n=0}^\infty \frac{k_s}{k_s^2+n^2k_u^2}f_n\sin(nk_uy)\sin(k_sx)\hat{\mathbf{i}} + \frac{nk_u}{k_s^2+n^2k_u^2}f_n\sin(nk_uy)\cos(k_sx)\hat{\mathbf{j}} \quad (5.26)$$

and

$$\langle|\nabla^{-1}(f(y)\sin(k_sx))|^2\rangle = \sum_{n=0}^\infty\frac{|f_n|^2}{k_s^2+n^2k_u^2} = \frac{1}{k_s^2}|f_0|^2 + \frac{1}{k_u^2}\sum_{n=1}^\infty\frac{|f_n|^2}{n^2+r^2}$$
$$\leq \frac{1}{k_s^2}|f_0|^2 + \frac{1}{k_u^2}\sum_{n=1}^\infty\frac{|f_n|^2}{n^2} \leq \frac{1}{k_s^2}|f_0|^2 + \frac{1}{k_u^2}\frac{\pi}{6}\sup_n|f_n|^2. \quad (5.27)$$

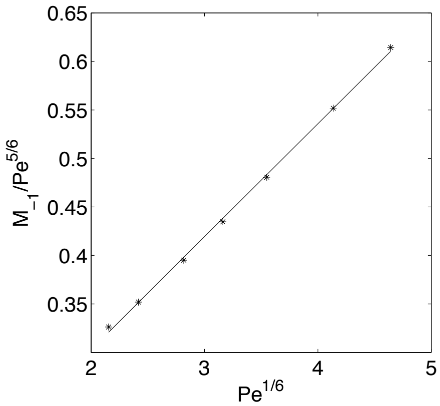

Figure 4: $M_{-1}/Pe^{5/6}$ versus $Pe^{1/6}$ from direct numerical simulations (*). The solid line is the asymptotic scaling.

Computing the first Fourier coefficient

$$|f_0| = \frac{1}{\pi}\int_0^{l/4} f(y)dy = \frac{1}{\pi}\frac{S}{Uk_s}\int_0^{\infty} F(\eta)d\eta \tag{5.28}$$

and recalling from section 2 that $\langle|\nabla^{-1}\theta_0|^2\rangle = S^2/\kappa^2 k_s^6$ we obtain the large scale mixing efficiency scaling

$$M_{-1} \sim C\mathcal{P}e \tag{5.29}$$

where C is a prefactor depending on the integral of F (square of the mean versus the mean of the square). Figure 3 of the direct numerical solution confirms the Pe scaling. The boundary layer and direct numerical solution prefactors differ by 15%.

We note two interesting things; first to leading order there is no dependence on r even though we might have expected that increased shear would increase mixing on large scales (see section 3). Second we expect that the next order term would be proportional to M_0 i.e. that

$$M_{-1} \sim Pe + r^{1/3}Pe^{5/6}. \tag{5.30}$$

Figure 4 shows a plot of $M_{-1}/Pe^{5/6}$ versus $Pe^{1/6}$ from direct numerical simulations. A very non-rigorous check of the scaling involves comparing the slope of the line in figure 4 to the prefactor above. The slopes differ by 20%. Note in that plot the current limit of large Péclet and fixed r requires $r < 0.1\sqrt{Pe}$ i.e. $r < 3$ ($\delta < 1$).

There are still some things we do not understand. Are there universal scalings in Pe? Namely for the steady flow and the Zeldovich sine flow we get the same scalings. Do these scalings appear for other flows with this source?

5.2 Regular perturbation expansion

We now seek the behaviour of the multiscale mixing efficiencies for $r \gg 1$, $\mathcal{P}e$ fixed. Going back to our system of ODEs and setting $\tilde{y} = k_u y$ we obtain

$$\frac{\mathcal{P}e}{r^2}\sin(\tilde{y})f = \left[-\frac{1}{r^2} + \frac{d^2}{d\tilde{y}^2}\right]g \tag{5.31a}$$

$$-\frac{\mathcal{P}e}{r^2}\sin(\tilde{y})g = \left[-\frac{1}{r^2} + \frac{d^2}{d\tilde{y}^2}\right]f + \frac{\sqrt{2}S}{\kappa k_s^2}\frac{1}{r^2}. \tag{5.31b}$$

Now we perform a regular perturbation expansion in powers of r^{-2}:

$$f = \sum_{n=0}^{\infty} f_n r^{-2n}, \qquad g = \sum_{n=0}^{\infty} g_n r^{-2n} \tag{5.32}$$

At $\mathcal{O}(1)$ we obtain

$$f_0'' = 0 \rightarrow f_0 = \text{const}, \qquad g_0'' = 0 \rightarrow g_0 = \text{const} \tag{5.33}$$

continuing as usual we obtain at $\mathcal{O}(r^{-2})$

$$\mathcal{P}e \sin(\tilde{y}) f_0 = -g_0 + g_1'', \qquad -\mathcal{P}e \sin(\tilde{y}) g_0 = -f_0 + f_1'' + \frac{\sqrt{2}S}{\kappa k_s^2}. \tag{5.34}$$

The average over a period of the first and second equations implies $g_0 = 0$ and $f_0 = \sqrt{2}S/\kappa k_s^2$. Thus, $f_1 = \text{const}$, and $g_1 = -(\sqrt{2}S/\kappa k_s^2)\mathcal{P}e \sin(\tilde{y}) + \text{const}$. Continuing, we obtain at $\mathcal{O}(r^{-4})$:

$$\mathcal{P}e \sin(\tilde{y}) f_1 = -g_1 + g_2'', \qquad -\mathcal{P}e \sin(\tilde{y}) g_1 = -f_1 + f_2''. \tag{5.35}$$

The average over a period of the first and second equations imply

$$f_1 = -\frac{\sqrt{2}}{2\pi} \frac{S}{\kappa k_s^2} \mathcal{P}e^2, \qquad g_1 = -\frac{\sqrt{2}S}{\kappa k_s^2} \mathcal{P}e \sin(\tilde{y}). \tag{5.36}$$

Hence to leading order the solution is

$$\theta \approx \frac{\sqrt{2}S}{\kappa k_s^2} \left[\left(1 - \frac{\mathcal{P}e^2}{2\pi r^2} \right) \sin(k_s x) - \frac{\mathcal{P}e}{r^2} \sin(\tilde{y}) \cos(k_s x) \right]. \tag{5.37}$$

Given the asymptotic solution for $r \gg 1$ at fixed $\mathcal{P}e$ we compute the variance as (keeping only the leading order term and the $\mathcal{O}(r^{-2})$ term)

$$\langle \theta^2 \rangle \approx \frac{S^2}{\kappa^2 k_s^4} \left(1 - \frac{1}{\pi} \frac{\mathcal{P}e^2}{r^2} \right) \tag{5.38}$$

which implies

$$M_0 \sim 1 + \frac{1}{\pi} \frac{\mathcal{P}e^2}{r^2}. \tag{5.39}$$

It is clear from this result that stirring on ever small scales (increased shear) ceases to suppress the variance. This is because in the limit $r \gg 1$ the flow is diffusion dominated hence the mixing efficiency goes to one.

The gradient to leading order is

$$\nabla\theta \approx \frac{\sqrt{2}S}{\kappa k_s^2} \left[\left(1 - \frac{1}{\pi} \frac{\mathcal{P}e^2}{r^2} \right) k_s \cos(k_s x) + \frac{\mathcal{P}e}{r^2} \sin(\tilde{y}) k \sin(k_s x) \right] \hat{\mathbf{i}} + \left[-\frac{\mathcal{P}e}{r^2} \cos(\tilde{y}) \cos(k_s x) \right] \hat{\mathbf{j}} \tag{5.40}$$

and so the gradient variance is

$$\langle |\nabla\theta|^2 \rangle \approx \frac{S}{\kappa k_s^2} \left(1 - \frac{1}{\pi} \frac{\mathcal{P}e^2}{r^2} \right) \tag{5.41}$$

which implies the mixing efficiency is identical on small and intermediate scales $M_1 = M_0$.

The inverse gradient to leading order is

$$\nabla^{-1}\theta \approx \frac{\sqrt{2}S}{\kappa k_s^2}\left[1 - \frac{1}{\pi}\frac{\mathcal{P}e^2}{r^2}\frac{k}{k_s^2}\sin(k_s x) + \frac{\mathcal{P}e}{r^2}\sin(\tilde{y})\frac{k_s}{k_s^2+p^2}\cos(k_s x)\right]\hat{\mathbf{i}} + \left[-\frac{\mathcal{P}e}{r^2}\cos(\tilde{y})\frac{p}{k_s^2+p^2}\cos(k_s x)\right]\hat{\mathbf{j}} \tag{5.42}$$

and hence the inverse gradient variance is

$$\langle|\nabla^{-1}\theta|^2\rangle \approx \frac{S}{\kappa k_s^6}\left(1 - \frac{1}{\pi}\frac{\mathcal{P}e^2}{r^2}\right) \tag{5.43}$$

and hence $M_{-1} = M_0$ (as suspected). Thus in the limit $r \gg 1$ and $\mathcal{P}e$ fixed all of the efficiencies are the same.

Summarizing the different limits, we find that the norms scale differently in Pe for fixed r and the scalings were confirmed with the direct numerical solution. However, the norms behave similarly for fixed Pe and $r \gg 1$ where the flow is diffusion dominated.

6 Bounds on the multiscale mixing efficiencies with scalar decay

Now consider the advection-diffusion equation for the concentration of a passive scalar $\theta(\mathbf{x}, t)$ which has a slow decay rate α maintained by a body source $s(\mathbf{x})$ with spatial mean zero:

$$\frac{\partial\theta}{\partial t} + \mathbf{u}\cdot\nabla\theta = \kappa\Delta\theta + s(\mathbf{x}) - \alpha\theta \tag{6.1}$$

where κ is the molecular diffusivity. The decay rate may have various interpretations such as the decay rate due to chemical kinetics, or radiative relaxation in meteorology (relevant for the sphere). We follow the procedure of TDG which was used to derive upper bounds on mixing efficiency for $\alpha = 0$ to derive upper bounds on $\langle|\nabla^p\theta|^2\rangle$ for $p = 0, 1, -1$ when $\alpha \neq 0$. We re-define the advection-diffusion operator and its formal adjoint to include the slow decay: $\mathcal{L}_\alpha := \partial_t + \mathbf{u}\cdot\nabla - \kappa\Delta - \alpha$ and $\mathcal{L}_\alpha^\dagger := -\partial_t - \mathbf{u}\cdot\nabla + \kappa\Delta - \alpha$. Now we proceed with computing bounds on the multiscale mixing efficiencies.

6.1 Bounds on the variance

Following the TDG procedure, we perform the following optimization:

$$\langle\theta^2\rangle \geq \max_{\varphi}\min_{\tilde{\theta}}\{\langle\tilde{\theta}^2\rangle \mid \langle\tilde{\theta}(\mathbf{u}\cdot\nabla\varphi + \kappa\Delta\varphi - \alpha\varphi)\rangle = -\langle\varphi s\rangle\} \tag{6.2}$$

upon applying the Cauchy-Schwarz inequality and maximizing over φ we obtain

$$\langle\theta^2\rangle \geq \langle s\mathcal{M}_0^\alpha s\rangle \tag{6.3}$$

where $\mathcal{M}_0^\alpha := (\overline{\mathcal{L}_\alpha\mathcal{L}_\alpha^\dagger})^{-1}$. Substituting the definition of $\mathcal{L}_\alpha$ and restricting to HIT

$$\begin{aligned}\langle s\mathcal{M}_0^\alpha s\rangle &= \langle s\{\kappa^2\Delta^2 - \overline{\mathbf{u}\mathbf{u}} : \nabla\nabla + \kappa(2\nabla\overline{\mathbf{u}}\cdot\nabla\nabla + \nabla\overline{\mathbf{u}}\cdot\nabla) - \alpha\overline{\mathbf{u}}\cdot\nabla - 2\alpha\kappa\Delta + \alpha^2\}^{-1}s\rangle \\ &= \langle s\{\kappa^2\Delta^2 - (U^2/d)\Delta - 2\kappa\alpha\Delta + \alpha^2\}^{-1}s\rangle.\end{aligned} \tag{6.4}$$

The variance in the absence of stirring is

$$\langle\theta_0^2\rangle = \langle s\{\kappa^2\Delta^2 - 2\kappa\alpha\Delta + \alpha^2\}^{-1}s\rangle \tag{6.5}$$

and hence an upper bound on the mixing efficiency is

$$(M_0^\alpha)^2 \leq \frac{\langle s\{\kappa^2\Delta^2 - 2\kappa\alpha\Delta + \alpha^2\}^{-1}s\rangle}{\langle s\{\kappa^2\Delta^2 - (U^2/d)\Delta - 2\kappa\alpha\Delta + \alpha^2\}^{-1}s\rangle}. \tag{6.6}$$

In Fourier space this is

$$(M_0^\alpha)^2 \leq \left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{\kappa^2k^4 + 2\kappa\alpha k^2 + \alpha^2}\right)\left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{\kappa^2k^4 + (U^2/d + \kappa\alpha)k^2 + \alpha^2}\right)^{-1}. \tag{6.7}$$

Clearly, the upper bound depends on the Fourier transform of the source function s. In the next section we investigate the high-Pe behaviour of M_0^α for a measure valued source. To determine the high-Pe behaviour we approximate the sums by integrals and take the limit of infinite volume noting that the α term allows the integrals to converge:

$$(M_0^\alpha)^2 \lesssim \left(\int_0^\infty \frac{|\hat{s}(\mathbf{k})|^2 k^{d-1}d^dk}{k^4 + 2\kappa\alpha k^2 + \alpha^2}\right)\left(\int_0^\infty \frac{|\hat{s}(\mathbf{k})|^2 k^{d-1}d^dk}{\kappa^2k^4 + (\frac{U^2}{d} + 2\kappa\alpha)k^2 + \alpha^2}\right)^{-1}. \tag{6.8}$$

Letting $\xi = \mathbf{k}\sqrt{\frac{\kappa}{\alpha}}$ in d-D we obtain:

$$(M_0^\alpha)^2 \lesssim \left(\int_0^\infty \frac{|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2\xi^{d-1}d\xi}{\xi^4 + 2\xi^2 + 1}\right)\left(\int_0^\infty \frac{|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2\xi^{d-1}d\xi}{\xi^4 + (\tilde{\mathcal{P}e}^2 + 2)\xi^2 + 1}\right)^{-1}. \tag{6.9}$$

where $\tilde{\mathcal{P}e} := U\ell/\kappa = U/\sqrt{\kappa\alpha}$ where $\ell = \sqrt{\kappa/\alpha}$ is the diffusive length scale i.e. the distance travelled by diffusion before decay.

6.1.1 Delta function source

Consider a delta function point source so that there is a separation of scales between the source and the stirring field. In $d = 2$ we obtain

$$\int_0^\infty \frac{\xi d\xi}{\xi^4 + 2\xi^2 + 1} = \frac{1}{2}, \qquad \int_0^\infty \frac{\xi d\xi}{\xi^4 + (\tilde{\mathcal{P}e}\tilde{\mathcal{P}e}^2 + 2)\xi^2 + 1} = \frac{1}{2}\frac{\ln\frac{\xi_1}{\xi_2}}{\xi_1 - \xi_2} \tag{6.10}$$

where ξ_1 and ξ_2 are the solutions of the quartic equation:

$$\xi_{1,2} = \frac{\left(\tilde{\mathcal{P}e}^2 + 2\right) \mp \tilde{\mathcal{P}e}^2\sqrt{1 + 4\tilde{\mathcal{P}e}^{-2}}}{2} = \frac{\left(\tilde{\mathcal{P}e}^2 + 2\right) \mp \tilde{\mathcal{P}e}^2\left(1 + 2\tilde{\mathcal{P}e}^{-2} - 2\tilde{\mathcal{P}e}^{-4} + ...\right)}{2}.$$

In the large $\tilde{\mathcal{P}e}$ limit the mixing efficiency is

$$M_0^\alpha \lesssim \frac{\tilde{\mathcal{P}e}}{2\ln\tilde{\mathcal{P}e}}. \tag{6.11}$$

Note this is a distinct scaling as regards κ compared to the problem with $\alpha = 0$. An efficiency scaling of $\sim \tilde{\mathcal{P}e}$ implies the eddy diffusivity would scale as $\sqrt{\kappa}$. For $d = 3$ we have

$$\int_0^\infty \frac{\xi^2 d\xi}{\xi^4 + 2\xi^2 + 1} = \frac{\pi}{4}, \qquad \int_0^\infty \frac{\xi^2 d\xi}{\xi^4 + (\tilde{\mathcal{P}e}^2 + 2)\xi^2 + 1} = \frac{\pi}{2} \frac{\sqrt{\xi_1} - \sqrt{\xi_2}}{\xi_1 - \xi_2}. \tag{6.12}$$

In this limit the mixing efficiency is

$$M_0^\alpha \lesssim \frac{1}{2}\sqrt{\tilde{\mathcal{P}e}}. \tag{6.13}$$

Thus for $d = 3$ we also have an anomalous scaling in $\tilde{\mathcal{P}e}$ with an equivalent diffusivity proportional to $\kappa^{1/4}$.

6.2 Bounds on the gradient variance

For the gradient variance the optimization problem is

$$\langle |\nabla\theta|^2 \rangle \geq \max_{\varphi} \min_{\tilde{\theta}} \{ \langle |\nabla\tilde{\theta}|^2 \rangle \mid \langle \nabla\tilde{\theta} \cdot (\mathbf{u}\varphi + \kappa\nabla\varphi - \alpha(\nabla(\Delta^{-1}\varphi)))|^2 \rangle = -\langle \varphi s \rangle \} \tag{6.14}$$

upon applying the Cauchy-Schwarz inequality (we will revisit this approach at the end of this section) we obtain

$$\langle |\nabla\theta|^2 \rangle \geq \max_{\varphi} \leq \frac{\langle s\varphi \rangle^2}{\langle |\kappa\nabla\varphi + \varphi\mathbf{u} - \alpha(\nabla(\Delta^{-1}\varphi))|^2 \rangle}. \tag{6.15}$$

Under the assumptions of HIT

$$\langle |\kappa\nabla\varphi + \mathbf{u}\varphi - \alpha(\nabla(\Delta^{-1}\varphi))|^2 \rangle = \langle \kappa^2 |\nabla\varphi|^2 + |\bar{\mathbf{u}}|^2 \varphi^2 + \alpha^2 |\nabla(\Delta^{-1}\varphi)|^2 - 2\kappa\alpha\nabla(\Delta^{-1}\varphi) \cdot \nabla\varphi \rangle \tag{6.16}$$

The solution to the optimization problem is (after some algebra)

$$\langle |\nabla\theta|^2 \rangle \geq \langle s \mathcal{M}_1^\alpha s \rangle \tag{6.17}$$

where $\mathcal{M}_1^\alpha := (-\kappa^2\Delta + \frac{U^2}{d} + 2\kappa\alpha + \alpha^2\Delta^{-1})^{-1}$. Given the gradient variance in the absence of stirring we obtain a bound on the small scale mixing effciency

$$(M_1^\alpha)^2 \leq \frac{\langle s\{-\kappa^2\Delta + 2\kappa\alpha + \alpha^2\Delta^{-1}\}^{-1} s \rangle}{\langle s\{-\kappa^2\Delta + \frac{U^2}{d} + 2\kappa\alpha + \alpha^2\Delta^{-1}\}^{-1} s \rangle}. \tag{6.18}$$

In Fourier space the bound is expressed as

$$(M_1^\alpha)^2 \leq \left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{k^2(\kappa + \frac{\alpha}{k^2})^2} \right) \left(\sum_{\mathbf{k}} \frac{|\hat{s}(\mathbf{k})|^2}{k^2(\kappa + \frac{\alpha}{k^2})^2 + \frac{U^2}{d}} \right)^{-1}. \tag{6.19}$$

Once again since we are interested in the high-$\tilde{\mathcal{P}e}$ behaviour we approximate the sums by integrals

$$(M_1^\alpha)^2 \lesssim \left(\int_0^\infty \frac{k^2 |\hat{s}(\mathbf{k})|^2 k^{d-1} d^d k}{\kappa^2 k^4 + 2\kappa\alpha k^2 + \alpha^2} \right) \left(\int_0^\infty \frac{k^2 |\hat{s}(\mathbf{k})|^2 k^{d-1} d^d k}{\kappa^2 k^4 + (\frac{U^2}{d} + 2\kappa\alpha) k^2 + \alpha^2} \right)^{-1}. \tag{6.20}$$

Letting $\xi = \mathbf{k}\sqrt{\frac{\kappa}{\alpha}}$ in d-D we obtain:

$$(M_1^\alpha)^2 \lesssim \left(\int_0^\infty \frac{\xi^2|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2\xi^{d-1}d\xi}{\xi^4+2\xi^2+1}\right)\left(\int_0^\infty \frac{\xi^2|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2\xi^{d-1}d\xi}{\xi^4+(\frac{U^2}{\kappa\alpha}+2)\xi^2+1}\right)^{-1}. \tag{6.21}$$

Clearly the convergence of these integrals depends on the property of the source. We must have for $\alpha \neq 0$, $s \in H^{-1}$.

Here we re-examine the application of the Cauchy-Schwarz inequality. The analysis can be improved by evaluating

$$\min_{\tilde{\theta}}\{\langle|\nabla\tilde{\theta}|^2\rangle \mid \langle\nabla\tilde{\theta}\cdot(\mathbf{u}\varphi+\kappa\nabla\varphi-\alpha(\nabla(\Delta^{-1}\varphi)))\rangle = \langle\varphi s\rangle\} \tag{6.22}$$

with functional $\mathcal{F} := \langle\frac{1}{2}|\nabla\tilde{\theta}|^2+\lambda(\mathbf{v}\cdot\nabla\tilde{\theta}-\varphi s)\rangle$ where $\mathbf{v} = \mathbf{u}\varphi+\kappa\nabla\varphi-\alpha(\nabla(\Delta^{-1}\varphi))$. As in section 3 the solution to the optimization problem depends on the two-point correlation statistics of the velocity field

$$\langle|\nabla\theta|^2\rangle = \frac{\langle\varphi s\rangle^2}{\langle(\nabla\cdot\mathbf{v})(-\Delta^{-1})\nabla\cdot\mathbf{v}\rangle} \geq \frac{\langle\varphi s\rangle^2}{\langle|\mathbf{v}|^2\rangle}. \tag{6.23}$$

In the case of HIT a strict application of the Cauchy-Schwarz inequality yields the optimal bound. Again this analysis does not apply to either the variance or inverse gradient variance.

6.2.1 Delta function source

As for the case of $\alpha = 0$, a δ-function or white noise source will cause the integrals in (6.21) to diverge and thus $M_1^\alpha = 1$ for δ-function sources.

6.3 Bounds on the inverse gradient variance

For the inverse gradient variance the variational problem is

$$\langle|\nabla^{-1}\theta|^2\rangle \geq \max_{\varphi}\min_{\tilde{\theta}}\{\langle|\nabla^{-1}\tilde{\theta}|^2\rangle \mid \langle\nabla\Delta^{-1}\tilde{\theta}\cdot\nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi-\alpha\varphi)|^2\rangle = \langle\varphi s\rangle\} \tag{6.24}$$

upon applying the Cauchy-Schwarz inequality

$$\langle|\nabla^{-1}\theta|^2\rangle \geq \max_{\varphi}\frac{\langle s\varphi\rangle^2}{\langle|\nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi-\alpha\varphi)|^2\rangle}. \tag{6.25}$$

Under the HIT assumptions

$$\langle|\nabla(\mathbf{u}\cdot\nabla\varphi+\kappa\Delta\varphi-\alpha\varphi)|^2\rangle = \langle\kappa|\Delta\nabla\varphi|^2+\frac{\Gamma^2}{d}|\nabla\varphi|^2+\frac{U^2}{d}(\Delta\varphi)^2+\alpha^2|\nabla\varphi|^2-2\alpha\kappa\nabla\varphi\cdot\Delta\nabla\varphi\rangle.$$

The solution to the optimization problem is (after some algebra)

$$\langle|\nabla^{-1}\theta|^2\rangle \geq \langle s\mathcal{M}_{-1}^\alpha s\rangle \tag{6.26}$$

where $\mathcal{M}_{-1}^\alpha := (\kappa^2\Delta^3-(\Gamma^2/d)\Delta+(U^2/d)\Delta^2+2\kappa\alpha\Delta^2-\alpha^2\Delta)^{-1}$. Given the inverse gradient variance in the absence of stirring we obtain a bound on the large scale mixing effciency

$$(M_1^\alpha)^2 \leq \frac{\langle s\{\kappa^2\Delta^3+2\kappa\alpha\Delta^2-\alpha^2\Delta\}^{-1}s\rangle}{\langle s\{\kappa^2\Delta^3-\frac{\Gamma^2}{d}\Delta+\frac{U^2}{d}\Delta^2+2\kappa\alpha\Delta^2-\alpha^2\Delta\}^{-1}s\rangle}. \tag{6.27}$$

In Fourier space the bound is expressed as

$$(M_{-1}^{\alpha})^2 \leq \left(\sum_{\mathbf{k}} \frac{|\hat{s}(k)|^2}{\kappa^2 k^6 + 2\kappa\alpha k^4 + \alpha^2 k^2} \right) \left(\sum_{\mathbf{k}} \frac{|\hat{s}(k)|^2}{\kappa^2 k^6 + (\frac{U^2}{d} + 2\kappa\alpha) k^4 + (\alpha^2 + \Gamma^2) k^2} \right)^{-1}. \quad (6.28)$$

Once again since we are interested in the high $\tilde{\mathcal{P}e}$ behaviour we approximate the sums by integrals

$$(M_{-1}^{\alpha})^2 \lesssim \left(\int_0^{\infty} \frac{|\hat{s}(k)|^2 k^{d-1} d^d k}{k^2(\kappa^2 k^4 + 2\kappa\alpha k^2 + \alpha^2)} \right) \left(\int_0^{\infty} \frac{k^2 |\hat{s}(k)|^2 k^{d-1} d^d k}{k^2(\kappa^2 k^4 + (\frac{U^2}{d} + 2\kappa\alpha) k^2 + \alpha^2 + \Gamma^2)} \right)^{-1} (6.29)$$

Letting $\xi = \mathbf{k}\sqrt{\frac{\kappa}{\alpha}}$ in d=D we obtain:

$$(M_{-1}^{\alpha})^2 \lesssim \left(\int_0^{\infty} \frac{|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2 \xi^{d-1} d^d \xi}{\xi^2(\xi^4 + 2\xi^2 + 1)} \right) \left(\int_0^{\infty} \frac{|\hat{s}(\xi\sqrt{\frac{\alpha}{\kappa}})|^2 \xi^{d-1} d^d \xi}{\xi^2(\xi^4 + (\tilde{\mathcal{P}e}^2 + 2)\xi^2 + 1 + \frac{\Gamma^2}{\alpha^2})} \right)^{-1}. \quad (6.30)$$

In d=2 there may be an infra-red divergence problem. The integrals converge if $|\hat{s}(\mathbf{k})|^2 = f(k)$ if $f(k) \approx k^{\beta}$ where $\beta > 0$ (we require mean zero sources as to prevent blow up at 0). This is our only restriction on the source. How the Fourier transform decays as $\mathbf{k} \to 0$ indicates the large scale structure of the source. Exploration of the bound's behavior remains a task for the future.

6.3.1 Delta function sources

In d=3

$$\int_0^{\infty} \frac{d\xi}{\xi^4 + 2\xi^2 + 1} = \frac{\pi}{4}, \qquad \int_0^{\infty} \frac{d\xi}{\xi^4 + (\tilde{\mathcal{P}e}^2 + 2)\xi^2 + 1 + \frac{\Gamma^2}{\alpha^2}} = \frac{\pi}{2} \frac{\sqrt{\xi_1} - \sqrt{\xi_2}}{(\xi_2 - \xi_1)\sqrt{\xi_1 \xi_2}} \quad (6.31)$$

where ξ_1 and ξ_2 are roots of the quadratic equation:

$$\xi_{1,2} = \left(\tilde{\mathcal{P}e}^2 + 2\right) \pm \sqrt{\tilde{\mathcal{P}e}^4 + 4\tilde{\mathcal{P}e}^2 - \frac{4\Gamma^2}{\alpha^2}}. \quad (6.32)$$

In the limit of $\tilde{\mathcal{P}e} \gg 1$ we get to leading order in $\tilde{\mathcal{P}e}$:

$$\xi_1 = \tilde{\mathcal{P}e}^2 - \tilde{\mathcal{P}e}^2 \sqrt{1 - 4\frac{\Gamma^2\kappa^2}{U^4}} \approx \frac{1}{2}\frac{\tilde{\mathcal{P}e}^2}{Pe_{\lambda}^2}, \qquad \xi_2 \approx 2\tilde{\mathcal{P}e}, \qquad \xi_1 - \xi_2 \approx \tilde{\mathcal{P}e}^2 \sqrt{1 - 4\frac{\Gamma^2\kappa^2}{U^4}} \quad (6.33)$$

hence

$$\int_0^{\infty} \frac{d\xi}{\xi^4 + (\frac{U^2}{\kappa\alpha} + 2)\xi^2 + 1 + \frac{\Gamma^2}{\alpha^2}} = \frac{\pi}{2} \frac{\sqrt{2\tilde{\mathcal{P}e}}}{2\tilde{\mathcal{P}e}\sqrt{\frac{\tilde{\mathcal{P}e}^3}{Pe_{\lambda}^2}}} \quad (6.34)$$

where $Pe_{\lambda} = U\lambda/\kappa$ where λ (a Péclet number using a length scale of the velocity field). Hence

$$(M_{-1}^{\alpha})^2 \leq \frac{Pe^2}{Pe_{\lambda}} \quad (6.35)$$

note that the efficiency may be larger when there is stronger shear $\Gamma \gg 1$ as was found in the case of $\alpha = 0$. Table 2 summarizes the high-Pe scaling for HIT in the case of $\alpha = 0$ and $\alpha \neq 0$ for a δ-function source.

$\alpha = 0$	d=2	d=3
M_1	1	1
M_0	$\frac{Pe}{\sqrt{\log Pe}}$	$\sqrt{Pe}$
M_{-1}	$\frac{PeL}{\lambda\sqrt{\log(1+L^2/\lambda^2)}}$	$Pe\sqrt{\frac{L}{\lambda}}$

$\alpha \neq 0$	d=2	d=3
M_1^α	1	1
M_0^α	$\frac{\tilde{Pe}}{\sqrt{\log \tilde{Pe}}}$	$\sqrt{\tilde{Pe}}$
M_{-1}^α	$\star$	$\frac{\tilde{Pe}}{\sqrt{Pe_\lambda}}$

Table 2. High-Pe scalings of the multiscale mixing efficiencies for a δ-function source. The $\star$ indicates that the scaling depends on $|\hat{s}(\mathbf{k})|$ as $k \to 0$ and $\tilde{\mathcal{P}e} := U\ell/\kappa = U/\sqrt{\kappa\alpha}$ where $\ell = \sqrt{\kappa/\alpha}$.

7 Conclusions and future work

Multiscale mixing efficiencies are susceptible to rigorous analysis. Upper (lower) bounds on multiscale mixing efficiencies were obtained from lower (upper) bounds on appropriately weighted variances. Bounds on large-scale mixing are sensitive to small-scale stirring. The bounds can be sharp (sweeping flows on the torus). Furthermore, the efficiency of some complex random flows can be understood via simple steady state scalings. Finally, the inclusion of a decay term in the advection-diffusion equation introduces new features namely new high-Pe dependences of the equivalent diffusivity on the molecular diffusivity.

The current analysis has only answered some of the questions posed in the introduction hence, there are exciting problems that are the subject of current and future investigation. For example, extending the current analysis to bounded domains (sphere etc.) and formulating an appropriately constrained variational problem for the optimal (source specific) stirring field.

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