Optimizing the Source Distribution in Fluid Mixing

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The Mixing Enhancement Factor

- The steady advection-diffusion equation

$$\mathbf{u}(\mathbf{x}) \cdot \nabla\theta - \kappa\Delta\theta = s(\mathbf{x}), \qquad \nabla \cdot \mathbf{u} = 0,$$

  describes how a spatial source of passive scalar $s(\mathbf{x})$ is stirred by a velocity field $\mathbf{u}(\mathbf{x})$.
- How well is the source spread out by the stirring? One traditional measure is the variance $\|\theta\|_2^2$ of the concentration (assuming a zero mean concentration).
- A related measure is the enhancement factor

$$\mathcal{E} := \|\widetilde{\theta}\|_2 / \|\theta\|_2 \geq 1\,, \quad \text{(hopefully!)}$$

  which compares the variance to that in the absence of stirring, $\|\widetilde{\theta}\|_2$. Larger $\mathcal{E}$ implies more effective stirring.

Two Optimization Problems

- A natural question is then:

  For a fixed source distribution, which velocity field maximizes the enhancement factor?

- This is a hard question. Let's instead ask an easier, but still relevant one:

  For a fixed velocity field, which source distribution maximizes the enhancement factor?

- The attractive aspect of the source optimization problem is that it has a simple mathematical answer, and the structure of the solution sheds light on the velocity optimization problem.

Source Optimization

Define the linear operators

$$\mathcal{L} := \mathbf{u}(\mathbf{x}) \cdot \nabla - \kappa\Delta \qquad \text{and} \qquad \widetilde{\mathcal{L}} := -\kappa\Delta,$$

from which we can write the solution to advection-diffusion and diffusion equation

$$\theta = \mathcal{L}^{-1}s \qquad \text{and} \qquad \widetilde{\theta} = \widetilde{\mathcal{L}}^{-1}s\,.$$

The enhancement factor is then

$$\mathcal{E}^2 = \langle s\,\widetilde{\mathcal{A}}^{-1}s\rangle / \langle s\,\mathcal{A}^{-1}s\rangle\,,$$

where the self-adjoint operators $\mathcal{A}$ and $\widetilde{\mathcal{A}}$ are

$$\mathcal{A} := \mathcal{L}\mathcal{L}^*\,, \qquad \widetilde{\mathcal{A}} := \widetilde{\mathcal{L}}\widetilde{\mathcal{L}}^* = \kappa^2(-\Delta)^2$$

and we have used the notation $\langle\cdot\rangle$ to denote spatial integration.

The Variational Problem

Maximizing $\mathcal{E}$ is now a simple problem in variational calculus,

$$\delta\mathcal{E}^2 = \frac{2}{\langle s\,\mathcal{A}^{-1}s\rangle}\left\langle\left(\widetilde{\mathcal{A}}^{-1}s - \mathcal{E}^2\,\mathcal{A}^{-1}s\right)\delta s\right\rangle = 0,$$

with solution

$$\mathcal{A}\widetilde{\mathcal{A}}^{-1}s = \mathcal{E}^2\,s.$$

This is an eigenvalue problem for the operator $\mathcal{A}\widetilde{\mathcal{A}}^{-1}$. The optimal enhancement factor is given by its largest eigenvalue, and the corresponding optimal source by the eigenfunction.

It is simple to show that this solution is a global maximum.

For numerical implementation, it is preferable to solve the equivalent self-adjoint eigenvalue problem

$$(\widetilde{\mathcal{A}}^{-1/2}\mathcal{A}\widetilde{\mathcal{A}}^{-1/2})\,r = \mathcal{E}^2\,r\,, \qquad s = \widetilde{\mathcal{A}}^{1/2}\,r\,.$$

A Uniform Flow

As a simple example, consider a spatially-uniform flow $\mathbf{u}(\mathbf{x}) = U\,\hat{\mathbf{e}}_x$ along the x direction, in a periodic domain of size L.

The optimal enhancement factor is then

$$\mathcal{E} = \sqrt{1 + \frac{U^2 L^2}{4\pi^2\kappa^2}} =: \sqrt{1 + \mathrm{Pe}^2}$$

with optimal source

$$s(\mathbf{x}) = A\cos(2\pi x/L) + B\sin(2\pi x/L)$$

where we have defined the Péclet number $\mathrm{Pe} := UL/2\pi\kappa$.

The mechanism is simple: the optimal source is such that 'hot' is swept onto 'cold' and vice versa. We will see that this is a general feature of optimal sources.

A Perturbed Flow

Consider now a two-dimensional uniform flow along the x–axis perturbed by a weak flow,

$$\mathbf{u}(x,y) = U\,\hat{\mathbf{e}}_x + \varepsilon\,\mathbf{u}_1(x,y)$$

where

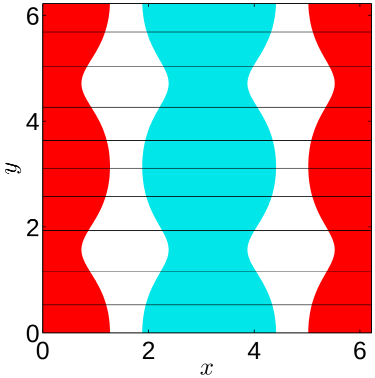
$$\mathbf{u}_1(x,y) = u_{1x}(y)\,\hat{\mathbf{e}}_x + u_{1y}(x)\,\hat{\mathbf{e}}_y\,,$$

Because the base flow is in the $\hat{\mathbf{e}}_x$ direction, the $u_{1x}(y)\hat{\mathbf{e}}_x$ term is a shear flow perturbation, and the $u_{1y}(x)\hat{\mathbf{e}}_y$ term is a wavy flow perturbation.

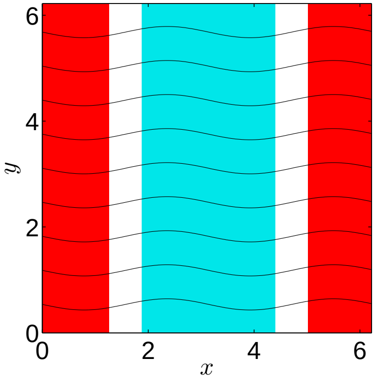
The modification to the enhancement factor can be computed easily using perturbation theory.

Shear vs Wavy Flow

Red = 'hot', Blue = 'cold', $(L = 2\pi,\ \kappa = 0.01)$



Shear: the optimal source is localized in regions of faster flow.



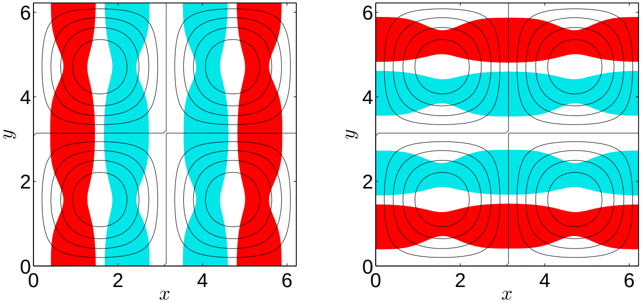
Wavy: no change to the optimal source.

Cellular Flow

Consider now a cellular flow with streamfunction ($L = 2\pi$, $\kappa = 0.01$)

$$\psi(x, y) = \sin x \, \sin y + \delta_1 \, \sin 2x + \delta_2 \, \sin 2x \, \sin 2y$$

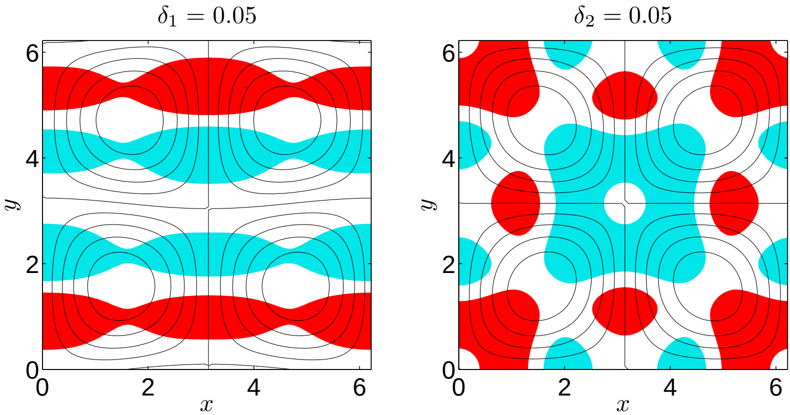
For $\delta_1 = \delta_2 = 0$, we find numerically the doubly-degenerate optimal sources:



The optimal source avoids stagnation points. We still see the tendency of hot to be swept onto cold.

Perturbed Cellular Flow

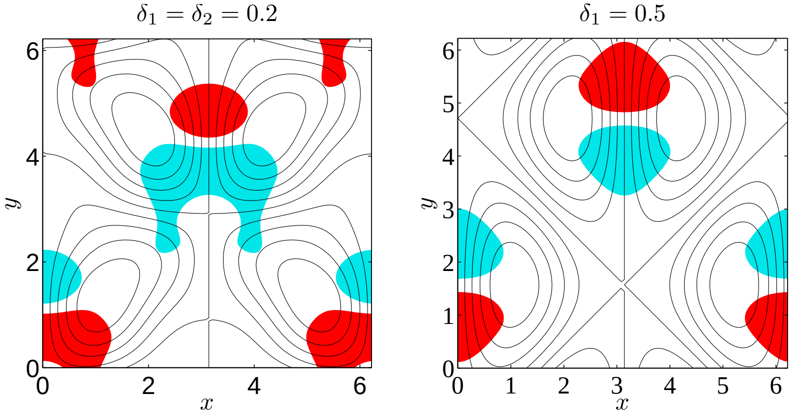
Adding perturbations to the cellular flow breaks the symmetry and thus the degeneracy of the optimal solution.



Yet again the optimal source avoids stagnation points, hot is swept onto cold, and faster regions are favored.

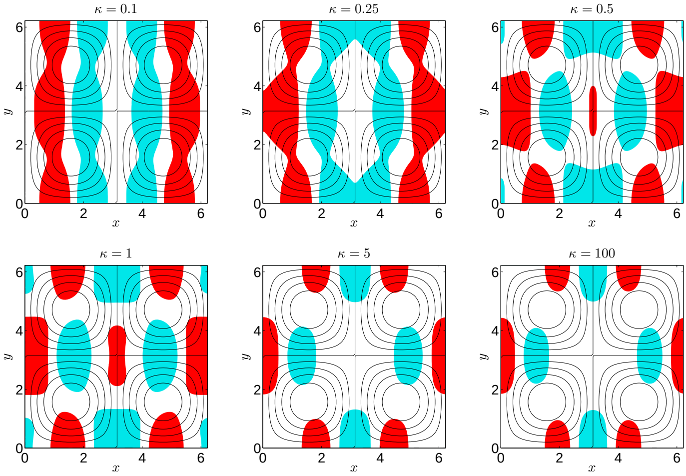
Large Perturbations

Things can get a bit strange...



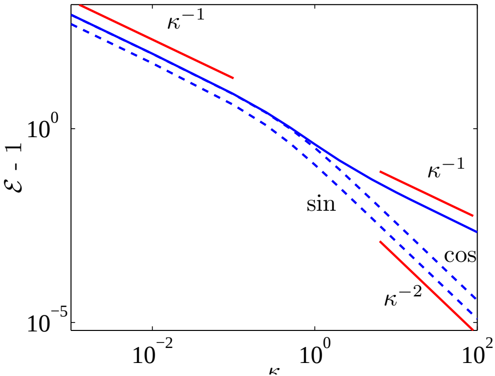
Again the optimal source avoids stagnation points, and hot is swept onto cold.

Dependence on Diffusivity



The optimal source converges to an invariant pattern. For large κ case there are sources and sinks over some hyperbolic points.

Dependence on Diffusivity (cont'd)



Optimal source (solid line), and $\sin x$ and $\cos x$ reference sources (dashed lines). For small κ, the enhancement factor scales like κ^{-1}.

Conclusions (part 1)

- In both the perturbation problem and the numerical examples, the optimal source distributions tend to exhibit the following features:
    1. Avoidance of stagnation points of the flow, especially elliptic;
    2. Localization over regions of rapid flow;
    3. Alignment of the source contours perpendicular to the local velocity, so that hot is swept onto cold and vice versa.
- The optimization procedure is numerically straightforward.
- Also used a more general measure that weighs scalar gradients differently, similar to the mix-norm [Mathew et al., 2005].
- We are also working on optimizing boundary sources (more relevant in industrial problems) with Jai Sukhatme.
- Three-dimensionality (easy) and time-depence (tedious) should be included.
- Velocity optimization is the next stage (hard but fun).

References

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