Nonuniform mixing

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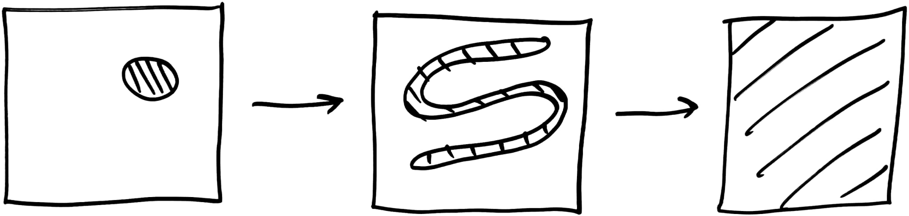
Uniform mixing

The usual scenario in mixing is that we want to homogenize some initial distribution of particles or dye.



This will happen naturally via molecular diffusion, but is greatly accelerated by stirring.

See for instance Welander, P. (1955). *Tellus,* **7** (2), 141–156.

Mathematical description

The advection-diffusion equation governs the evolution of a passive scalar concentration $\theta(\boldsymbol{x}, t)$:

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = D \, \nabla^2 \theta, \qquad \nabla \cdot \boldsymbol{u} = 0,$$

where $\boldsymbol{u}(\boldsymbol{x}, t)$ is a divergence-free velocity field, and D is the diffusivity.

With no-flux boundary conditions

$$(\boldsymbol{u} \, \theta - D \nabla \theta) \cdot \hat{\boldsymbol{n}} = 0$$

at the boundary $\partial\Omega$ of the domain Ω, the integral $\int_\Omega \theta \, \mathrm{d}V$ is conserved.

Eventually everything is mixed

How do we know that the concentration will eventually mix? A few integration by parts and use of boundary conditions give

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \theta^2\,\mathrm{d}V = -2D\int_\Omega |\nabla\theta|^2\,\mathrm{d}V \le 0.$$

The decay of variance (L^2 norm) is monotonic: it can never increase. It can only stop decreasing if θ is uniform in space ($\nabla\theta \equiv 0$).

This bound underpins the usefulness of variance as a measure of mixing.

Nonuniform mixing

The relaxation to a uniform state requires this uniform state to be a steady solution of the advection–diffusion equation.

Perhaps surprisingly, this is not always the case!

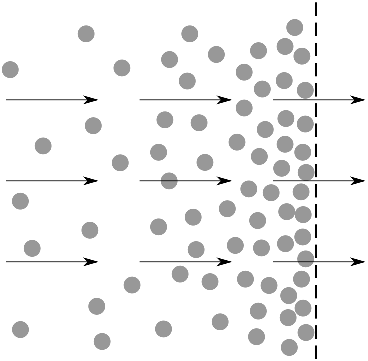
A uniform state is a steady solution of the advection-diffusion equation only if $\nabla \cdot \boldsymbol{u} = 0$ (which we take as given), as well as

$$\boldsymbol{u} \cdot \hat{\boldsymbol{n}} = 0 \quad \text{on the boundary } \partial\Omega.$$

For $\boldsymbol{u} \cdot \hat{\boldsymbol{n}} \neq 0$, the uniform state $\theta =$ const. solves the advection–diffusion equation, but does not satisfy the boundary conditions. The equilibrium state is nonuniform.

An example: particle filter

The simplest example of this is a filter: $\boldsymbol{u} \cdot \hat{\boldsymbol{n}} \neq 0$ at the boundary, since fluid can cross the filter, but the particles cannot.



The equilibrium state is then nonuniform: particles tend to accumulate at suction regions on the boundary.

Relaxation to equilibrium

With $\boldsymbol{u} \cdot \hat{\boldsymbol{n}} \neq 0$ on the boundary, the evolution of variance is now given by

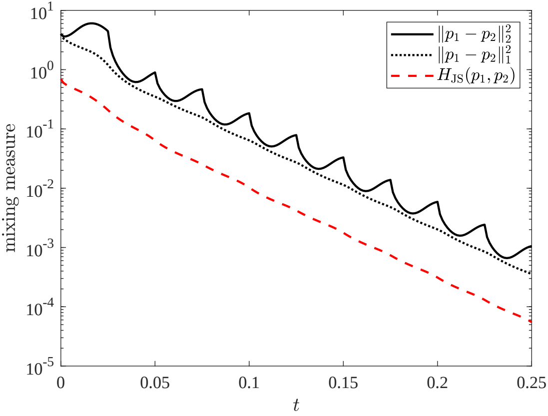
$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \theta^2 \, \mathrm{d}V = \int_{\partial\Omega} \theta^2 \boldsymbol{u} \cdot \hat{\boldsymbol{n}} \, \mathrm{d}S - 2D \int_{\Omega} |\nabla\theta|^2 \, \mathrm{d}V.$$

Note the boundary term on the right is not sign-definite. Hence variance no longer has to decrease monotonically. It can exhibit transient growth.

Of course variance must ultimately decay, which we know from other considerations. But the above equation does not show that, and suggests that variance can be poorly-behaved if used as a measure of mixing.

Relaxation to equilibrium: Example

A simple example is a constant flow $U\hat{\boldsymbol{x}}$ on the interval $[0, 1]$. We apply no-flux boundary conditions and periodically reverse the direction of the flow ('breathing').



Notice that variance (solid line) shows significant oscillations.

Entropy and f-divergence

A better measure of mixing in the nonuniform case is the f-divergence:

$$H_f[p_1, p_2] := \int_\Omega p_2\, f(p_1/p_2)\, \mathrm{d}V.$$

Here p_1 and p_2 are two normalized probability densities, and f is a convex function with $f(1) = 0$, $f'' \geq 0$.

For example we can choose

$$f(u) = u \log u$$

which gives the Kullback–Leibler divergence or relative entropy.

H_f measures the 'distance' (divergence) between p_1 and p_2. We set $p_1 = \theta(\boldsymbol{x}, t)$, and p_2 to the steady solution.

Relaxation of f-divergence

The reason f-divergence is a nice measure of mixing is that

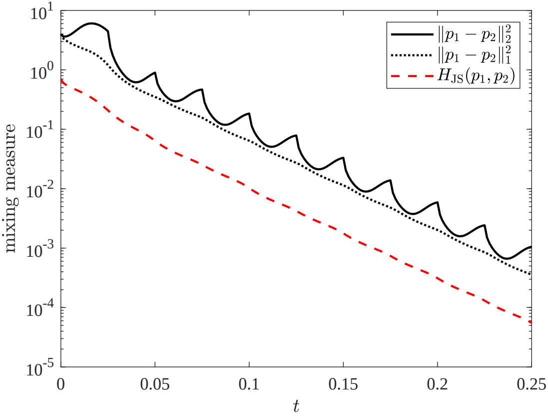
$$\frac{\mathrm{d}}{\mathrm{d}t} H_f[p_1, p_2] = -D \int_\Omega p_2\, f''(p_1/p_2)\, |\nabla(p_1/p_2)|^2 \,\mathrm{d}V \leq 0$$

for general no-flux boundary conditions, that is, even if $\boldsymbol{u} \cdot \hat{\boldsymbol{n}} \neq 0$. The relaxation of f-divergence is thus always monotonic.

This is essentially an H-theorem from statistical physics. The novelty here is that in those applications the boundary conditions are not important, since quantities such as momentum vanish at infinity. In the fluid-dynamical context it is precisely the no-flux boundary conditions that give this monotonic evolution of H_f.

Relaxation of f-divergence: Example

Return to the earlier periodic flow example: the dashed red line is the f-divergence. Notice how nice and monotonic it is compared to variance (solid).



The dotted line is the L^1 norm $\int_\Omega |p_1 - p_2| \, \mathrm{d}V$, and is also monotonic!

L^1 norm

The previous plot suggests that the L^1 norm

$$\int_\Omega |p_1 - p_2| \,\mathrm{d}V = \int_\Omega |\theta| \,\mathrm{d}V$$

is also monotonic in time.

Indeed, this follows from

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega |\theta| \,\mathrm{d}V = -2D \int_{\{\theta=0\}} |\nabla\theta| \,\mathrm{d}S \leq 0$$

where the integral on the right is taken over the zero level set of $\theta(\cdot, t)$.

This again holds even in the nonuniform case, but it is less useful mathematically. In practice, it suggests that L^1 is a more reliable measure of mixing than variance for nonuniform mixing.

Conclusions

- Mixing is usually regarded as the relaxation to a uniform state.
- The concentration variance (L^2 norm) is often taken as a convenient measure, since it relaxes monotonically to a uniform state.
- However, in some cases the ultimate state is not uniform.
- For example: suction boundary conditions, or divergent flows (not discussed).
- In those nonuniform cases variance is less reliable, since it can exhibit oscillations: it is not constrained to decay monotonically.
- Better measures of mixing in the nonuniform case are the entropy-like quantities called f-divergence, or the L^1 norm.
- See Thiffeault, J.-L. (2021). *Physical Review Fluids,* **6** (9), 090501.

References I

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Welander, P. (1955). *Tellus,* **7** (2), 141–156.