GEOMETRIC FEATURES OF HIGH-SCHMIDT NUMBER SCALAR MIXING

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Summary The mixing of passive scalars of decreasing diffusivity, advected in each case by the same three-dimensional Navier-Stokes turbulence, is studied. It becomes more isotropic with decreasing diffusivity. The local flow in the vicinity of steepest negative and positive scalar gradients are in general different, and its behavior is studied for various values of the scalar diffusivity. Mixing approaches monofractal properties with diminishing diffusivity.

MOTIVATION AND NUMERICAL MODEL

Turbulent mixing of dyes or macromolecular substances can be understood by analyzing how these scalar substances are advected and diffused in a fluid medium. For small concentrations, the admixture, or scalar, is passive, or has no dynamic feedback on the flow—which is therefore determined independent of the scalar. Often, the scalar diffusivity is small compared with the viscosity of the fluid, so that their ratio, the so-called Schmidt number, $Sc = \nu/\kappa$, is large. Our interest here lies in the advection and diffusion of passive scalars for large values of Sc. In particular, we wish to understand the recent result from numerical simulations that turbulent mixing becomes more isotropic when Sc is increased [1]. This approach to isotropic state is evident from the fact that deviations from it, as quantified by odd moments of the scalar derivative along a mean scalar gradient, $\partial_{\|}\theta$, decrease as Sc increases from 1 to 64 for a fixed Reynolds number of the turbulent flow [1].

The reason for the anisotropy for $Sc = O(1)$ has long been known to be the presence of ramp-cliff structures in the signature of the scalar field whenever there is a mean gradient in the scalar alone or in both scalar and velocity. These cliff structures of the scalar field are related to sharp fronts of the scalar gradient distribution in three-dimensional space and can be found in the positive far tail of the probability density function (PDF) of the scalar gradient fields.

Analytical approaches to understanding the features are difficult. Significant progress has been made for the so-called Kraichnan model of passive scalars in which the advecting velocity field is assumed to be Gaussian and to vary infinitely rapidly in time; for a review see [2]. However, even for the synthetic Kraichnan velocity field, a systematic study of anisotropy with Sc has not been made. Another approach [3], which follows Batchelor's original model of quasistatic straining motion, provides upper bounds for scalar derivative moments as functions of Sc. However, the problem still contains numerous open questions. For instance, it is unclear as to what changes occur in and around the ramp-cliff structures as $Sc \to \infty$.

Some of these changes were quantified via high-resolution numerical simulations of turbulent mixing [4]. We particularly considered level sets of the steep gradients and related them to the local structure of the advecting flow. Furthermore, the multifractal approach is known to sample efficiently the "singular" structures at small scales [5]. Therefore, we also studied the scalar dissipation field in high-Sc cases.

Our numerical results were obtained in a homogeneously sheared flow [6] with $\langle u_x \rangle = Cy$, where C is a constant, at a Taylor-microscale Reynolds number R_λ of 87 in which the scalar field of constant mean gradient was allowed to evolve according to the advection-diffusion equation. The Schmidt number was varied from 1 to 64. The pseudospectral simulations were done with resolutions of $512 \times 257 \times 512$ grid points for a box of size $2\pi : \pi : 2\pi$. We ensure that the scalar fluctuations are properly resolved by requiring that $k_{max}\eta_B \geq 1.3$ with $k_{max} = \sqrt{2}N_{max}/3$, where $N_{max} = 512$; the Batchelor scale $\eta_B \equiv \eta/\sqrt{Sc}$ and the Kolmogorov scale $\eta \equiv (\nu^3/\epsilon)^{1/4}$. The scalar gradient $\mathbf{G} = \mathbf{e}_y/\pi$ for all runs.

RESULTS

To shed some on the return to isotropic mixing, we show in Figure 1 three slices of the scalar field at the same moment of evolution, each slice corresponding to a different value of Sc. It is clear that the large structure, and the front associated with it, do not change with Sc but internal striations of finer scale accompany larger Sc. These striations increase the relative population of negative gradients. This is what causes the tail of the PDF for the positive gradient values to be effectively unchanged, whereas the events with negative gradients, shows higher probability as Sc increases, thus rendering the PDFs increasingly symmetric.

The question that immediately arises is what type of flow causes the steepest negative scalar gradients, and their increase with increasing Sc? To answer these questions, we have performed an eigenvalue analysis of the local velocity gradients in the vicinity of the largest scalar gradients. Here, pure straining motion corresponds with three real eigenvalues and local vortical motion with a conjugate complex pair and a real third eigenvalue. We performed this analysis in the vicinity of the steepest positive and negative scalar gradients only. For positive gradients, i.e. for the cliffs, local straining becomes somewhat more dominant with growing Sc, while, for the negative tails, the swirling and straining motion contribute in almost equal parts for large Sc. This is consistent with the view that the cliffs are associated with the front stagnation point of a moving fluid parcel, where the velocity field is predominantly straining, while the negative slopes come from

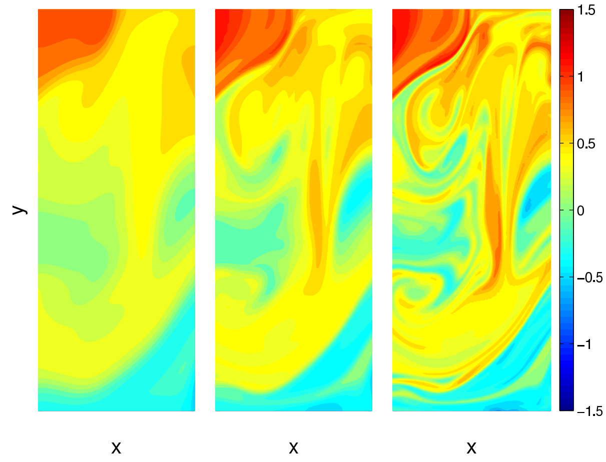

Figure 1. Slices of the total scalar field (mean plus fluctuation) for $Sc = 1$ (left), 8 (middle), and 64 (right), all of which are advected by the same flow. Only a fraction of the simulation domain is shown.

the wake region behind such parcels where the fluid motion is both vortical and straining.

The geometric properties of the scalar gradient level sets were also studied by means of box-counting analysis. The box counting dimension D_0 of a level set F, embedded in the three-dimensional space, is defined as the scaling exponent of $N_\delta(F) = N_0\delta^{-D_0}$ where $N_\delta(F)$ is the number of cubes of size δ that are needed to cover F. While for lower Sc differences between the positive level set and its negative counterpart were detected, they disappear more and more with increasing Schmidt number.

The variation of the level set threshold at fixed Schmidt numbers clearly indicates the multifractal character of the gradient fields. For operational purposes, it is more convenient to consider the scalar dissipation field, $\epsilon_\theta(\mathbf{x}, t) = \kappa \sum_{j=1}^{3} (\partial_j \theta)^2$. We define the measure

$$\mu_r^{(i)} = \frac{X_r^{(i)}}{X_L} = \frac{\int_{V_r^{(i)}} \epsilon_\theta(\mathbf{x} + \mathbf{x}_i, t) \mathrm{d}^3\mathbf{x}}{\int_V \epsilon_\theta(\mathbf{x}, t) \mathrm{d}^3\mathbf{x}} \tag{1}$$

where $V_r^{(i)}$ is the ith cube with length r. The spectrum of generalized dimensions [5], $D_q(q)$, obeys the following scaling relation

$$\sum_i \left(\mu_r^{(i)}\right)^q \sim r^{(q-1)D_q} \,. \tag{2}$$

It was found that the spectrum of generalized dimensions gets flatter with increasing Sc means that in the limit of very large Sc the scalar dissipation rate becomes a monofractal, i.e. $D_q = D_0$ for all q. The physical picture is as follows: large "singular" spikes of the scalar dissipation rate fill out the whole space more and more, so that the "quiet" regions in-between become less prevalent. The degree of spatial and temporal intermittency decreases, which is just the property to which the spectrum is sensitive. We can quantify this result also by fitting a bimodal multifractal cascade model to the data. For $Sc = 8$ we obtain $p = 0.86$, for $Sc = 64$ a value of $p = 0.81$, decreasing to 0.58 for experimental data at $Sc = 1900$. The model would yield a monofractal dissipation field for equidistributed energy flux, i.e. $p = 0.5$.

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