Influence of vorticity alignment upon scalar gradient production in three-dimensional, isotropic turbulence

M Gonzalez and P Paranthoen
CNRS, UMR 6614/CORIA
Site universitaire du Madrillet
76801 Saint-Etienne du Rouvray, France
E-mail: Michel.Gonzalez@coria.fr, Pierre.Paranthoen@coria.fr

Abstract. We use a stochastic Lagrangian model to investigate how the mechanisms of scalar gradient production may be affected by alignments of vorticity with respect to strain principal axes. The most intense scalar gradient production occurs when vorticity aligns with the ‘intermediate’ strain eigenvector. Mean production conditioned on vorticity aligning with the extensional eigenvector is closer to mean production in the total flow. These differences are explained by the special statistics of both strain eigenvalues and scalar gradient alignment when vorticity aligns with a strain eigenvector.

1. Introduction

The current picture of the overall mixing mechanism in fluid flows is based on the production of small scales of the scalar field that are smoothed down by molecular diffusion. In the view of the scalar gradient approach (Lapeyre et al., 1999; Brethouwer et al., 2003; Gonzalez & Paranthoen, 2010) mixing of scalar patches within the fluid finds expression in enhancement of the local gradient due to stretching followed by diffusive damping.

More specifically, the efficiency of micromixing is revealed by the level of the mean dissipation rate of the energy of scalar fluctuations, a quantity proportional to the variance of the fluctuating scalar gradient. In isotropic turbulence it is only strain, through stretching, that promotes scalar dissipation and hence micromixing. Both strain intensity and scalar gradient alignment with respect to strain principal axes are thus essential to the mixing process. The orientation of the scalar gradient in the strain basis, however, results from the interplay of strain, vorticity, strain basis rotation and molecular diffusion (Lapeyre et al., 1999; Brethouwer et al., 2003). Strain eigenvalues depend on strain, vorticity, pressure and viscous mechanisms. Strain and vorticity interact, making this picture even more complex.

Investigating the very mechanisms of small-scale mixing thus needs models reproducing the detailed behaviour of the scalar gradient. A stochastic Lagrangian model for the scalar gradient derived from the approach of Chevillard & Meneveau (2006) for the velocity gradient has been shown to reliably represent the main features of scalar gradient kinematics (Gonzalez, 2009) and is used in the present study. The main concern is in the connection of scalar gradient production with the ‘geometry’ of vorticity, namely the alignment of vorticity with the strain principal axes. This work thus refers to the question of the way in which the micromixing properties of flows depend on the local features of the velocity field, a problem that has given rise to a number...
of studies (Ruetsch & Maxey, 1991; Pumir, 1994; Warhaft, 2000; Brethouwer et al., 2003). To a certain extent, it is also relevant to the mechanisms and modelling of mixing by vortical structures (Pullin & Lundgren, 2001; Goto & Kida, 2003; Kadoch et al., 2011).

2. Stochastic Lagrangian model for velocity and scalar gradients

2.1. Modelled equations

The model for the velocity gradient tensor has been derived by Chevillard & Meneveau (2006) and has been shown to predict the essential geometric properties and anomalous scalings of incompressible, isotropic turbulence (Chevillard & Meneveau, 2006; Chevillard et al., 2008). Starting from an Eulerian-Lagrangian change of variables and using the Recent Fluid Deformation Approximation the modelled equation for the velocity gradient tensor, $A$, is derived as

$$dA = \left(-A^2 + \frac{Tr(A^2)}{Tr(C^{-1})}C^{-1} - \frac{Tr(C^{-1})}{3T}A\right) dt + \left(\frac{2 \sqrt{T}}{T}\right)^{1/2} dW$$

in which $T$ is the integral time scale and $C_{\tau_0}$ is a model for the Cauchy-Green tensor, $C_{\tau_0} = \exp(\tau_0 A) \exp(\tau_0 A^T)$, where $\tau_0$ is the Kolmogorov time scale. Forcing is ensured by the increment of a tensorial Wiener process, $dW = dt^{1/2} \xi$, where $\xi$ is a tensorial, Gaussian delta-correlated noise with $\langle \xi_{ij} \rangle = 0$ and $\langle \xi_{ij} \xi_{kl} \rangle = 2 \delta_{ik} \delta_{jl} - 1/2 \delta_{ij} \delta_{kl} - 1/2 \delta_{il} \delta_{jk}$.

This model, extended to the gradient of a passive scalar, retrieves the main features of the scalar gradient statistics and kinematics (Gonzalez, 2009). The modelled equation for the scalar gradient, $G$, is written

$$dG = - \left(A^T G + \frac{Tr(C^{-1})}{3T_\theta} G\right) dt + \left(\frac{2 \sqrt{T_\theta}}{T_\theta}\right)^{1/2} dW_G$$

where $T_\theta$ is the scalar integral time scale and $dW_G = dt^{1/2} \xi$ is the increment of a Wiener process where $\xi$ is a vectorial, Gaussian noise such that $\langle \xi_i \rangle = 0$ and $\langle \xi_i \xi_j \rangle = \delta_{ij}$.

In the model represented by Eqs. (1) and (2) stretching is exactly accounted for, while models are devised for the pressure Hessian – second term of Eq. (1) –, viscous effects – third term of Eq. (1) – and molecular diffusion – second term of Eq. (2) –. A detailed review on this class of stochastic Lagrangian models has been given by Meneveau (2011).

2.2. Numerical solution

Time scales are normalised by the integral time scale ($T = 1$). The scalar integral time scale and the Kolmogorov time scale are respectively prescribed as $T_\theta = 0.4$ and $\tau_0 = 0.1$ – corresponding to a Taylor microscale Reynolds number close to 150 (Chevillard & Meneveau, 2006).

Equations (1) and (2) are solved using a second-order predictor-corrector scheme (Welton & Pope, 1997). The calculation is run for $2 \times 10^7 T$ with time step $10^{-2}$ and the statistics of the velocity and scalar gradients are derived from their respective stationary time signals.

3. Analysis of scalar gradient production conditional on vorticity alignments

We focus on production mechanisms of scalar gradient in the case of significant alignment of vorticity, $\omega$, with strain principal axes. Alignment of vorticity with a strain eigenvector, $e_1$, defined by $|\cos(\omega, e_1)| \geq c$ where $c$ is a given threshold is denoted by $\omega//e_1$. Vectors $e_1$, $e_2$ and $e_3$ are, respectively, the extensional, ‘intermediate’ and compressional strain eigenvectors with corresponding eigenvalues $\lambda_1$, $\lambda_2$ and $\lambda_3$ such that $\lambda_1 + \lambda_2 + \lambda_3 = 0$ and $\lambda_1 > \lambda_2 > \lambda_3$.
The dependence of scalar gradient production on vorticity alignments is clear in Figs. 1 and 2. Both the mean square of scalar gradient norm, $|G|^2$, and the mean production term of $|G|^2$ conditioned on $|\cos(\omega, e_i)| \geq c$ with $c$ spanning the range 0.7 to 0.99 display similar trends: their largest values are found when alignment of vorticity with $e_2$ prevails, while for vorticity aligning with $e_1$ both the square of the gradient norm and its production term are closer to their respective mean values in the total flow. Incidentally, these results suggest that the most intense scalar dissipation occurs when $\omega//e_2$. Alignment of vorticity with $e_3$ corresponds to the smallest production which, because the scalar gradient tends to align normally to vorticity (Brethouwer et al., 2003; Gulitski et al., 2007), can be explained by a weaker alignment of the scalar gradient with the compressional direction. The discussion is focused on cases $\omega//e_1$ and $\omega//e_2$ in which the production mechanism mostly takes place.

**Figure 1.** Mean square of scalar gradient norm conditioned on vorticity alignments.

**Figure 2.** Mean production of $|G|^2$ conditioned on vorticity alignments.

Although production is promoted by alignment of the scalar gradient with the compressional direction, it cannot be understood in terms of alignment properties alone. In particular, the difference in gradient production between cases $\omega//e_1$ and $\omega//e_2$ is not explained by statistical alignment of the scalar gradient with the compressional direction. As shown in Fig. 3, alignment with the compressional direction is even slightly better for $\omega//e_1$ than for $\omega//e_2$ – with condition $|\cos(\omega, e_i)| \geq 0.8$ –. The picture obtained with $|\cos(\omega, e_i)| \geq 0.99$ is almost the same. The conditioned p.d.f’s of strain eigenvalues (Fig. 4), however, show that extreme values of the compressional strain eigenvalue, $\lambda_3$, are more probable when $\omega//e_2$ than when $\omega//e_1$. Conditional mean eigenvalues are given in Table 1. Larger absolute values of $(\lambda_i)$’s for $\omega//e_2$ are consistent with the fact that the largest production of strain occurs when alignment of vorticity with the ‘intermediate’ strain eigenvector is strong (Tsinober, 2000). Since the alignment of scalar gradient with the compressional direction is not much different when vorticity aligns with either $e_1$ or $e_2$ – and is even better for $\omega//e_1$ –, it is most likely the difference in the statistics of $\lambda_3$ that results in a larger mean production by compressional strain, $\langle -\lambda_3 |G|^2 \cos^2(G, e_3) \rangle$, when $\omega//e_2$ (Table 2).

Scalar gradient destruction by extensional strain is also stronger for $\omega//e_2$ than for $\omega//e_1$ (Table 2). This results this time from both scalar gradient alignment and extensional eigenvalue statistics. Because the scalar gradient tends to lie in the plane normal to vorticity, alignment of the scalar gradient with the extensional strain direction, $e_1$, is better when $\omega//e_2$ (Fig. 5) and,
Figure 3. P.d.f of the alignment of scalar gradient with the strain compressional direction conditioned on $|\cos(\omega, e_i)| \geq 0.8$; $i = 1$, extensional direction; $i = 2$, 'intermediate' direction.

Figure 4. P.d.f's of strain eigenvalues conditioned on $|\cos(\omega, e_1)| \geq 0.8$ (left) and $|\cos(\omega, e_2)| \geq 0.8$ (right); $i = 1$, extensional eigenvalue; $i = 2$, 'intermediate' eigenvalue; $i = 3$, compressional eigenvalue.

in addition, the extensional eigenvalue, $\lambda_1$, assumes larger values for $\omega//e_1$ (Fig. 4 and Table 1).

From Fig. 4 and Table 1, it is also clear that differences in the statistics of the ‘intermediate’ strain eigenvalue, $\lambda_2$, between cases $\omega//e_1$ and $\omega//e_2$ are small. The difference in scalar gradient destruction caused by the action of the ‘intermediate’ strain component (Table 2), which is extensional on the mean, thus rather lies in alignment statistics; the alignment of the scalar gradient with $e_2$ is indeed better for $\omega//e_1$ than for $\omega//e_2$ (Fig. 5).
Table 1. Mean strain eigenvalues conditioned on $|\cos(\omega, e_i)| \geq 0.8$ ($i = 1, 2$).

| $|\cos(\omega, e_1)| \geq 0.8$ | $|\cos(\omega, e_2)| \geq 0.8$ |
|-----------------------------|-----------------------------|
| $\langle \lambda_1 \rangle$ | 1.70                        |
| $\langle \lambda_2 \rangle$ | 0.595                       |
| $\langle \lambda_3 \rangle$ | -2.29                       |

Table 2. Contributions of extensional, ‘intermediate’ and compressional strain to the mean production of scalar gradient norm conditioned on $|\cos(\omega, e_i)| \geq 0.8$ ($i = 1, 2$).

| $|\cos(\omega, e_1)| \geq 0.8$ | $|\cos(\omega, e_2)| \geq 0.8$ |
|-----------------------------|-----------------------------|
| $\langle -\lambda_1 | G^2 \cos^2(G, e_1) \rangle$ | -1.22                       |
| $\langle -\lambda_2 | G^2 \cos^2(G, e_2) \rangle$ | -0.653                      |
| $\langle -\lambda_3 | G^2 \cos^2(G, e_3) \rangle$ | 11.5                        |
| total                       | 9.63                        |

Finally, differences in the statistics of both strain eigenvalues and scalar gradient alignment result in the budget of Table 2: destruction of scalar gradient norm by extensional strain is stronger when $\omega//e_2$ than when $\omega//e_1$, but is balanced by the effects of compressional and ‘intermediate’ strain which eventually leads to a larger production rate when $\omega//e_2$. Considering closer alignment of vorticity with strain eigenvectors – up to threshold 0.99 for $|\cos(\omega, e_i)|$ – leads to similar results and the same picture of the production mechanism.

Figure 5. P.d.f’s of $\cos(G, e_1)$ (left) and $\cos(G, e_2)$ (right) conditioned on $|\cos(\omega, e_i)| \geq 0.8$; $i = 1$, extensional direction; $i = 2$, ‘intermediate’ direction.
4. Conclusion

The stochastic Lagrangian model for both the velocity and the scalar gradients predicts a significant influence of vorticity alignment on scalar gradient production. It appears that the most intense production and the largest gradient norm are found when vorticity aligns with the ‘intermediate’ strain eigenvector. Mean production conditioned on vorticity aligning with the extensional strain eigenvector is closer to mean production in the total flow, while mean production is weak in the case of vorticity alignment with the compressional strain eigenvector. These differences – especially those between vorticity alignments with the extensional, $e_1$, or the ‘intermediate’ eigenvector, $e_2$ – are explained by the statistics of both strain eigenvalues and scalar gradient alignment with the strain principal axes. More precisely, when $\omega//e_2$ better alignment of the scalar gradient with the extensional direction and larger extensional strain eigenvalue lead to larger destruction of the scalar gradient norm than when $\omega//e_1$. However, larger compressional eigenvalue makes production higher for $\omega//e_2$. In addition, when $\omega//e_2$ weaker alignment of the scalar gradient with $e_2$ brings about smaller destruction of the scalar gradient. These mechanisms result in a larger mean production of scalar gradient norm for $\omega//e_2$ than for $\omega//e_1$.

References

Brethouwer, G., Hunt, J. C. R. & Nieuwstadt, F. T. M. 2003 Micro-structure and Lagrangian statistics of the scalar field with a mean gradient in isotropic turbulence. J. Fluid Mech. 474, 193–225.

Chevillard, L. & Meneveau, C. 2006 Lagrangian dynamics and statistical geometric structure of turbulence. Phys. Rev. Lett. 97, 174501.

Chevillard, L., Meneveau, C., Biferale, L. & Toschi, F. 2008 Modeling the pressure Hessian and viscous Laplacian in turbulence: comparisons with DNS and implications on velocity gradient dynamics. Phys. Fluids 20, 101504.

Gonzalez, M. 2009 Kinematic properties of passive scalar gradient predicted by a stochastic Lagrangian model. Phys. Fluids 21, 055104.

Gonzalez, M. & Paranthoën, P. 2010 On the role of unsteady forcing of tracer gradient in local stirring. Eur. J. Mech. B/Fluids 27, 143–152.

Goto, S. & Kida, S. 2003 Enhanced stretching of material lines by antiparallel vortex pairs in turbulence. Fluid Dyn. Res. 33, 403–431.

Gulitski, G., Khomymanski, M., Kinzelbach, W., Lüthi, B., Tsinober, A. & Yorish, S. 2007 Velocity and temperature derivatives in high-Reynolds-number turbulent flows in the atmospheric surface layer. Part 3. Temperature and joint statistics of temperature and velocity derivatives. J. Fluid Mech. 589, 103–123.

Kadoch, B., Iyer, K., Donzis, D., Schneider, K., Farge, M. & Yeung, P. K. 2011 On the role of vortical structures for turbulent mixing using direct numerical simulation and wavelet-based coherent vorticity extraction. J. Turbulence 12, N20.

Lapeyre, G., Klein, P. & Hua, B. L. 1999 Does the tracer gradient vector align with the strain eigenvectors in 2D turbulence? Phys. Fluids 11, 3729–3737.

Meneveau, C. 2011 Lagrangian dynamics and models of the velocity gradient tensor in turbulent flows. Annu. Rev. Fluid Mech. 43, 219–245.

Pullin, D. I. & Lundgren, T. S. 2001 Axial motion and scalar transport in stretched spiral vortices. Phys. Fluids 13, 2553–2563.

Pumir, A. 1994 A numerical study of the mixing of a passive scalar in three dimensions in the presence of a mean gradient. Phys. Fluids 6, 2118–2132.
RUETSCH, G. R. & MAXEY, M. R. 1991 Small-scale features of vorticity and passive scalar in homogeneous isotropic turbulence. *Phys. Fluids A* **3**, 1587–1597.

TSINOBER, A. 2000 Vortex stretching versus production of strain/dissipation. In *Turbulence Structure and Vortex Dynamics* (ed. J. C. R. Hunt & J. C. Vassilicos), pp. 164–191. Cambridge University Press.

WARHAFT, Z. 2000 Passive scalars in turbulent flows. *Annu. Rev. Fluid Mech.* **32**, 203–240.

WELTON, W. P. & POPE, S. B. 1997 PDF model calculations of compressible turbulent flows using smoothed particle hydrodynamics. *J. Comput. Phys.* **134**, 150–168.