An Investigation of the Relationship Between Flow Topology and the Distribution of a Passive Scalar in Isotropic Turbulence

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Abstract
Data obtained from direct numerical simulations of isotropic homogenous turbulence and the distribution of a passive scalar with an applied mean gradient is analysed using the topological techniques developed by Chong, Perry and Cantwell [1]. Several simulations were run at various values of $Re_\lambda$ and Schmidt number ($Sc$). Comparing the numerical results obtained, some relationships between the scalar characteristics and the topological features in the flow have been identified. Results from this work may be useful in the development of improved mixing processes by isolating the effect of the various topological features in the flow on the distribution of a passive scalar.

Introduction
Transport of scalars by turbulent fluid motion is of fundamental importance in processes such as pollutant formation, mass and heat transfer and chemical reactions. In recent years there has been a push for improved combustion efficiency and decreased pollutant emissions from a range of devices from power plants to jet engines. These devices generally use turbulent fluid motion to enhance mixing of the reactants. Particularly in cases of relatively rapid chemical reaction, the mixing rate is the major factor determining the rate of reaction. Improved methods for predicting and controlling turbulent flows may therefore lead to improved efficiencies and reduced emissions in a variety of devices.

In this study the distribution of a scalar with an imposed mean gradient in isotropic, homogenous turbulence is investigated using direct numerical simulation (DNS). DNS of three dimensional turbulence was developed three decades ago [8] and has since been used to simulate homogenous and inhomogeneous, bounded and unbounded flows. The computer program used in this study was written by Bruno Crespo [3], and simulates homogenous, isotropic turbulence and scalar mixing in three dimensions. The program was based on code written by Eswaran and Pope [4, 5] and later modified by Gao [6]. The velocity field is forced such that continuity is satisfied and, on average, energy dissipation and production are equal.

The full Navier-Stokes and scalar equations for incompressible flow are solved, without modeling, on a three-dimensional grid. The scalar transport equation includes a term for the advection of the scalar $\Theta$ by the velocity field $\mathbf{u}$ and another for diffusion of the scalar by molecular effects involving the molecular diffusivity, $\kappa$:

$$\frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta = \kappa \nabla^2 \Theta \tag{1}$$

The scalar is transported by the fluid motion and diffused by molecular effects with no reciprocal action on the flow dynamics (it is passive). In the case where a constant mean gradient, $\beta$, is imposed the scalar is comprised of a component due to the imposed gradient, plus a fluctuating term:

$$\Theta(x) = \theta(x) + \beta \cdot x \tag{2}$$

The transport equation for the scalar fluctuation, $\theta$, then reads:

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \kappa \nabla^2 \theta - \beta \cdot \mathbf{u} \tag{3}$$

The Schmidt number of the scalar ($Sc$) is the ratio $\nu/\kappa$.

Velocity gradient tensor analysis
One of the reasons that the physics of scalar transport is not well understood is due to the complex topology of the fluid motions and scalar fields. In recent years techniques have been developed where the topology of the fluid motions are classified by the invariants of the velocity-gradient tensor, as seen by a non-rotating observer moving at the same velocity as at that point [1]. This has made it possible to classify the topology in many flow-types using consistent criteria.

The velocity gradient tensor (VGT) contains information about the local instantaneous streamline pattern, and is given by the equation:

$$A_{ij} = \frac{\partial u_i}{\partial x_j} \tag{4}$$

where $u_i$ is the velocity vector and $x_j$ is the space vector. The equation $Det(A - \lambda I) = 0$ is used to find the characteristic equation of $A_{ij}$:

$$\lambda^3 + P_A \lambda^2 + Q_A \lambda + R_A = 0 \tag{5}$$

where $\lambda_i$ are the eigenvalues of $A_{ij}$, and $P_A, Q_A, R_A$ are the first, second and third tensor invariants respectively.

$$P_A = -A_{ii} = -tr(A) \tag{6}$$

$$Q_A = -\frac{1}{2} A_{ij}A_{ji} = \frac{1}{2}(P_A - tr(A^2)) \tag{7}$$

$$R_A = -\frac{1}{3} A_{ij}A_{jk}A_{ki} = -det(A) \tag{8}$$

For incompressible flow $P_A = 0$ from continuity and the discriminant of $A_{ij}$ is:

$$D_A = \frac{27}{4} R_A^2 + Q_A^2 \tag{9}$$

The values of $Q_A$ and $R_A$ can be used to detect the topology present at a point in the flow field. Figure 1 shows the two dimensional ($R_A, Q_A$) plane and the four recognised flow topologies defined by the values of $Q_A$ and $R_A$. The tent-like curve is the line $D_A = 0$ and separates the focal topologies at the top of the graph from the strain-dominated topologies at the bottom.

The matrix $A_{ij}$ can be separated into two matrices, one of which is the symmetric rate-of-strain tensor, $S_{ij}$, while the other is the skew-symmetric rate-of-rotation tensor, $W_{ij}$:

$$A_{ij} = S_{ij} + W_{ij} \tag{10}$$

As with $A_{ij}$, $S_{ij}$ has three corresponding invariants ($P_S, Q_S$ and $R_S$), as does $W_{ij}$ ($P_W, Q_W$ and $R_W$). For incompressible flow...
relations were run with different space- and time-averaged quantities. The averaging was under-
is given in Table 1. The run data are ensemble averages, i.e. of the input parameters and run data for these two simulations

dissipation.

cally achieved after 5-10 integral times as ascertained by mon-
state. Statistical stationarity of the scalar distribution was typi-

In summary, the velocity gradient tensor contains all the infor-
mation on the rotation, stretching and angular deformation of the infinitesimal fluid elements.

Details of DNS

This work was carried out on a 128³ mesh grid with periodicity length of 2π, so the wavenumbers are integers. Several simulations were run with different Reₜ and Sc values, but in this paper we will concentrate on the results for a constant Sc of 0.25 and for two average Reₜ values of 66 and 79. A summary of the input parameters and run data for these two simulations is given in Table 1. The run data are ensemble averages, i.e. space- and time-averaged quantities. The averaging was under-

Both the Corrsin-Oboukhov length scale and the Kolmogorov microscale exceed the smallest resolved length of 0.0165 for both simulations. Therefore, both the velocity and scalar fields are resolved.

Results

Statistical stationarity of the velocity and scalar fields

Figure 2 shows the values for Reₜ and the variance of the fluctuating part of the scalar (s²) over the last five eddy turnover times for each of the simulations. The higher Reynolds number simulation has a higher variance of the fluctuating part of the scalar compared to the lower Reynolds number simulation.

Joint probability distribution functions

Numerical results from the simulations are presented as joint probability distribution functions (joint-PDFs). This way of presenting the results has previously been used to investigate the structure of the invariants and the geometry of turbulent motions in isotropic homogeneous turbulence (e.g. [10]) as well as in investigations of the distribution of a passive scalar with imposed mean gradient in isotropic homogeneous turbulence (e.g. [10]).

The joint-PDFs shown in Figure 3 are of the scalar fluctuation and discriminant for the two Reynolds numbers. Note that the contours of the joint-PDFs have been chosen as exponential values because of the large range of probabilities that occur. The data for the joint-PDFs was obtained by combining the results at random intervals in the simulation. To allow direct comparison with simulations of different Reₜ, the ensemble averaged value of QW cubed ((QW)³) is used to normalise the discriminant, as was done in [7].

The reason for plotting the joint-PDF of the scalar fluctuation and the discriminant is to observe if any scalar fluctuation values are particularly associated with discriminant values that are greater than or less than zero, i.e. the division between focal and strain dominated structures as shown in Figure 1. From the two joint-PDFs in Figure 3 it does not appear that there is any particular association between scalar fluctuation values and local topology. The only difference appears to be the slightly wider range of scalar fluctuation values that occur at the specified probabilities for the higher Reynolds number simulation.
<table>
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Table 1: Input parameters and run data for the two simulations

The joint-PDFs in Figure 4 are of the gradient of the scalar fluctuation in the direction of the applied mean gradient and the discriminant for the two ReL values. A similar graph was presented by Pumir [10], except that the results were for the absolute value of the scalar gradient fluctuation. In that paper, Pumir noted that there appeared to be a correspondence between the highest scalar gradients and regions of weakly strain-dominated topologies. From our joint-PDFs we can see that for high positive scalar gradients the results are fairly evenly distributed between the focal and strain-dominated topologies, however for the high negative scalar gradients there is a bias towards strain-dominated topologies, although this bias tends to decrease with increasing ReL.

Not included here are the joint-PDFs for the gradient of the scalar fluctuation in the direction normal to the applied mean gradient and the discriminant. These show a similar relationship between high negative scalar gradients and strain-dominated...
From Figure 4 for correspond to regions where zero. This also corresponds to regions where structure depending on the local values of Chong to produce Figure 5 which shows the variation in flow stretching. These relationships have been applied by Perry and respectively to the local enstrophy density and local irrotational topologies, although the effect is less pronounced compared to those in Figure 4.

Individual results
As described previously, the invariants $Q_W$ and $Q_S$ are related respectively to the local enstrophy density and local irrotational stretching. These relationships have been applied by Perry and Chong to produce Figure 5 which shows the variation in flow structure depending on the local values of $Q_W$ and $Q_S$ [9].

From Figure 4 for $Re_\lambda = 79$, the large negative scalar gradients correspond to regions where $D_3$ is equal to or slightly less than zero. This also corresponds to regions where $Q_A$ is less than zero and, since $Q_A = Q_W + Q_S$, where $Q_W \leq -Q_S$. According to Figure 5 these would be regions dominated by irrotational stretching and possibly the formation of vortex sheets. To test this analysis Figure 6 was constructed. This shows where in the $(Q_W, -Q_S)$ plot those data points fall that have scalar gradient $(\partial \theta / \partial x)$ less than -20, compared to those that have scalar gradient greater than 10. In both cases the number of points plotted represent approximately 0.5% of the total data points in the simulation. It can be seen that the data points for the large negative scalar gradient are concentrated in the regions dominated by irrotational stretching, while for the large positive scalar gradients the data is distributed across the $(Q_W, -Q_S)$ plane, and into regions of high vorticity.

Conclusion
In this paper we have analysed data from a DNS simulation of turbulence incorporating a passive scalar with imposed mean gradient using the topological technique of Chong, Perry and Cantwell [1]. This approach provides quantitative results that can be used to infer the relationship between the distribution of the scalar and the local flow topology. We have concentrated primarily on the relationship between the scalar gradient and the location of vortical or strain dominated structures and found that large negative scalar gradients correspond to regions dominated by irrotational stretching. Many other paths for investigating the relationships between the scalar and velocity fields are available using the topological approach, and these will be developed in the future.

Acknowledgements
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References