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A DYNAMICAL SYSTEM FORMALISM FOR THE STUDY OF PASSIVE SCALAR FIELDS

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ABSTRACT

A new dynamical system formalism is proposed for the study of the geometry of passive scalar fields in turbulent flows. This formalism has been employed to investigate the relationship between the topology of diffusing passive scalars and the hydrodynamic topology of homogeneous isotropic turbulence. DNS of forced homogeneous isotropic turbulence at $Re_\lambda \simeq 47$ with $Sc = 1$ in a 128^3 cube was undertaken to generate the data base for this study. This investigation found two principal conclusions: first, the topology of a diffusing scalar (excluding convection) has characteristic length-scales much smaller than hydrodynamic ones, and second, compressible-like topologies are found for the scalar field even for a constant-density fluid flow.

INTRODUCTION

Transport of scalars by turbulent fluid motion is of fundamental importance and is encountered in applications such as pollutant formation, mass and heat transfer and chemical reactions. The physics of many of these applications is extremely complex and not well understood due to the intriguing complex topology of the fluid motions and scalar fields.

In this paper, a new formulation is proposed to study the detailed topology of diffusing scalars and their relationship to the turbulent flow topology. Direct numerical simulations (DNS) of homogeneous isotropic turbulence is used to investigate the relationship between the topology of the diffusing scalar and the hydrodynamic topology.

Yoda *et. al* [2] used a modified concentration gradient field to investigate the topology of the scalar field by calculating the invariants of $\frac{\partial^2 c}{\partial x_i \partial x_j}$, where c is the scalar concentration. However, this formulation has two serious drawbacks: firstly, it cannot be cast in terms of a dynamical system evolution, and secondly no clear physical interpretation emerges from it.

FORMULATION

The guiding idea for the new formulation presented in this paper derives from the observation that a Lagrangian frame is used to obtain the dynamical system associated to the fluid velocity field. With this in mind, the dynamical system associated with the scalar fields develops naturally from a consideration in a Lagrangian frame where the particles are moving "at constant scalar value". The velocity associated with these particles is next shown to be the velocity of the isoscalar surface for a Fick-diffusing, self-reacting scalar.

The evolution of the vector, $\mathbf{y}(t)$, between two neighbouring points, $\mathbf{y}(t)$, located on moving isoscalar surfaces, is given by:

$$\frac{dy_i}{dt} = \frac{\partial V_i}{\partial x_j} y_j, \tag{1}$$

where $\mathbf{V}$ is the isoscalar surface velocity. In the case of a non-diffusing, non-reacting scalar, $\mathbf{V}$ is equal to the local fluid flow velocity $\mathbf{u}$. In this case c is just convected as a constant scalar point, in fact this point is a material point.

In the case of a diffusing/reacting scalar, c is given by

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = D \frac{\partial^2 c}{\partial x_j \partial x_j} + S(c). \tag{2}$$

where $S(c)$ represents a source term of c.
The velocity of an isoscalar surface is implicitly defined by the following relationship

$$\frac{\partial c}{\partial t} + V_j \frac{\partial c}{\partial x_j} = 0. \tag{3}$$

It is apparent that $\mathbf{V} \neq \mathbf{u}$ due to the existence of diffusion and/or chemical reaction. The isoscalar surface velocity, $\mathbf{V}$, can be decomposed into

$$\mathbf{V} = \mathbf{u} + \mathbf{V}_c, \tag{4}$$

where $\mathbf{V}_c$ is the velocity of the isoscalar surface relative to the fluid. This decomposition was introduced by Candel and Poinsot, in the context of flame propagation[3].

There is a degree of freedom, which in principle, does not permit the direct application of this method to the scalar topology. This is due to the fact that the velocity has to be assigned to particles, not just to surfaces. The motions inside the surface are irrelevant regarding the transport of the surface as a whole. In this formulation it is proposed that only the component of the velocity normal to the surface (*i.e.* parallel to the scalar-gradient) is important and needs to be considered, which is also in agreement with the Fickian diffusion hypothesis. Thus, the natural choice for $\mathbf{V}_c$ is the velocity normal to the isosurface; the mass flux due to diffusion is parallel to ∇c and the reaction contribution is due to the existence of ∇c. In this context, $\mathbf{V}$ can then be considered as the velocity of a (non-fluid) particle moving with constant scalar value. As direct consequence, the dynamical system defined by Eq. 1 now has a clear physical interpretation.

It then follows that from the scalar gradient direction chosen for $\mathbf{V}_c$, Eq. 3 and Eq. 4, one readily obtains and expression for $\mathbf{V}_c$,

$$V_c = \frac{-D\,\nabla^2 c - S(c)}{|\nabla c|}. \qquad (5)$$

DETAILS OF THE DIRECT NUMERICAL SIMULATION

The DNS of isotropic, homogeneous turbulence were conducted using 128^3 grid points with a fully spectral object-oriented simulation code [1]. The simulation was forced to be statistically stationary with a Reynolds number based on the Taylor microscale of $Re_\lambda \simeq 47$. This value of Re_λ was chosen to minimise numerical and resolution errors, as the V_c calculation involves multiple spatial derivatives. The numerical code to simulate the evolution of a non-reacting scalar has been implemented in the DNS code and tested [1].

The initial scalar field is a "blob" positioned at the centre of the cube with value $c = 1$. The remainder of the computational box has a zero c value. The mean value of c is 0.5. This is a standard set-up for the initial scalar field to study molecular mixing, and the complete procedure may be found in reference [5]. The results presented here relate to Sc number equal to 1.

The results presented in this paper correspond to a non-dimensional time of 2.8, where time has been non-dimensionalised by the "eddy turn-over time". At this stage in the scalar field evolution, the scalar field has reached an approximately uniform distribution.

RESULTS

The invariants P, Q, R for each of the tensors $\frac{\partial V_{ci}}{\partial x_j}$, $\frac{\partial V_i}{\partial x_j}$, $\frac{\partial u_i}{\partial x_j}$ and $\frac{\partial^2 c}{\partial x_i \partial x_j}$, which define the respective topologies of $\mathbf{V}_c$, $\mathbf{V}$, $\mathbf{u}$ and ∇c (this latter was used by Yoda *et al.* [2] to describe the scalar field topology) respectively, have been calculated. The PDF of these quantities conditional on $\mathbf{V}_c$ are shown in Figure 1. An important result observed from this figure is that non-zero values for P are present, which in turn implies that $\nabla \cdot \mathbf{V}_c$ can be different from zero. The physical interpretation of this result is that volume contained among any two iso-surfaces is not preserved, although for the hydrodynamic flow field $\mathbf{u}$ is divergence-free everywhere ($P = 0$ for all space).

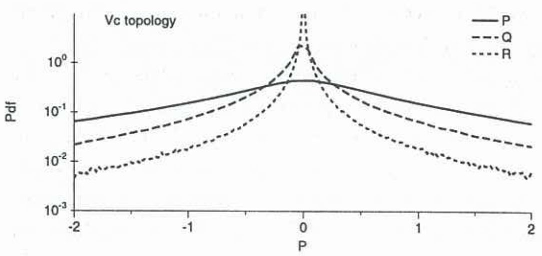

Figure 1: PDF of P, Q and R for the inert scalar field excluding convection ($\mathbf{V}_c$). All quantities shown are normalised by one-fourth of the enstrophy.

According to the topological terminology introduced by Chong *et. al* [4], the following scalar field topologies have been identified as a result of the DNS: 1 stable node - stable node - stable node, 2 unstable node - unstable node - unstable node, 11 stable node - saddle - saddle, 12 unstable node - saddle - saddle, 18 stable focus - stretching, 19 unstable focus - stretching, 20 stable focus - contracting, 21 unstable focus - contracting.

Figure 2 shows that due to the "compressible"-like behaviour of the scalar field, additional topologies which are not present in the hydrodynamic field are found in the scalar field (*i.e.* topologies 1, 2, 19 and 20). As $\mathbf{V}_c$ includes scalar-gradients in its definition, its topological regions should have a smaller characteristic length than the topology associated with $\mathbf{u}$. A more dominant effect of $\mathbf{V}_c$ on the contribution of $\mathbf{V}$ is thus expected, which is in agreement with results shown in Figure 2. A consequence of this re-

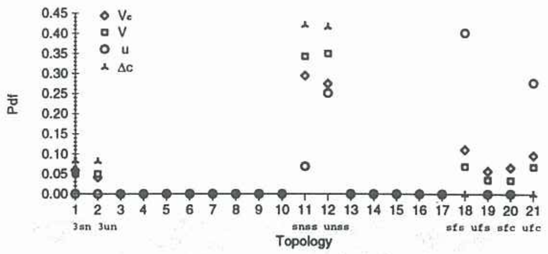

Figure 2: Normalized histogram of the appearance of each topological region associated with the velocity field $\mathbf{u}$, inert scalar field excluding convection $\mathbf{V}_c$, inert scalar field including convection $\mathbf{V}$, and ∇c

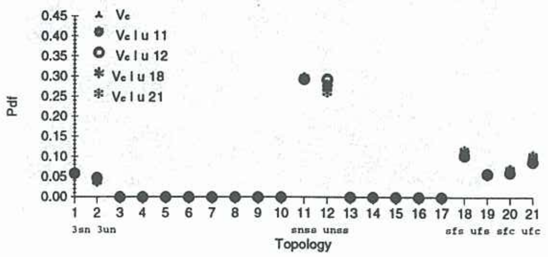

Figure 3: Normalized histogram of the appearance of each topological region associated with the inert scalar field excluding convection $\mathbf{V}_c$, conditioned on the local topology associated with the velocity field $\mathbf{u}$.

sults is that statistical independence between the hydrodynamic and scalar field topologies is suggested. A result which is supported by the data presented in Figure 3.

Figure 4 and 5 shows isocontours of the joint PDF (JPDF) of R and Q conditional on different values of P derived from $\mathbf{V}_c$ and $\mathbf{u}$. In Figure 4, the case $P = 0$ is shown for $\mathbf{V}_c$ and compared to JPDF for $\mathbf{u}$. The line $D = 0$ at constant P, where D is the discriminant of the characteristic equation, given by

$$D = \frac{R^2}{4} + (\frac{P^3}{27} - \frac{PQ}{6})R + (\frac{Q^3}{27} - \frac{P^2Q^2}{108}) \quad (6)$$

is also shown. No asymmetries arise in the scalar topology, which is in accordance with the geometrical nature of $\mathbf{V}_c$ and the statistical homogeneity of the turbulent field. However, for $P \neq 0$, this symmetry is broken. Figure 5 shows that for $P \neq 0$, stable scalar topologies are more probable when $P > 0$ ("compression"), while for $P < 0$, ("expansion") unstable scalar topologies are more probable.

CONCLUSION

- A new physical description of the topology of the scalar field undergoing turbulent convection has been introduced via the velocity associated with isoscalar surfaces.
- This scalar topology description includes the effect of diffusion and reaction through scalar derivatives, which implies topological regions of smaller characteristic lengths.
- A consequence of this formulation is thus statistical independence between scalar (excluding convection) and hydrodynamic topologies.
- Therefore, the scalar topology is mostly governed by the geometrical isosurface configuration at a given time.

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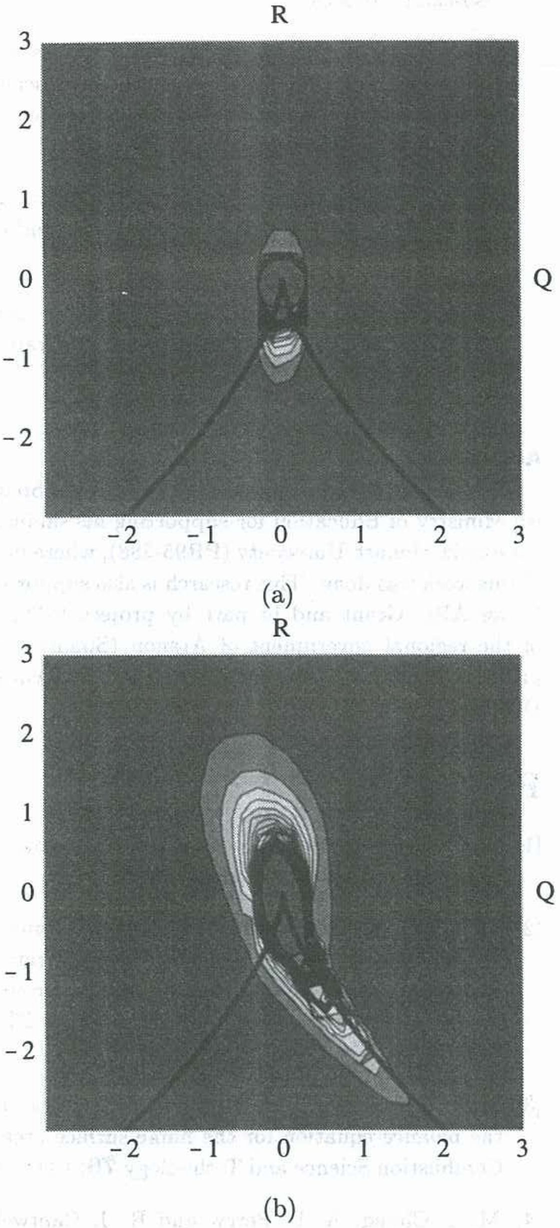

Figure 4: Isocontours of the joint PDF of R and Q conditional on $P = 0$ for the topology associated with the inert scalar field excluding convection $(\mathbf{V}_c)$(a) and for the topology associated with the fluid velocity field $(\mathbf{u})$(b). The line $D = 0$ is indicated by the solid black curve.

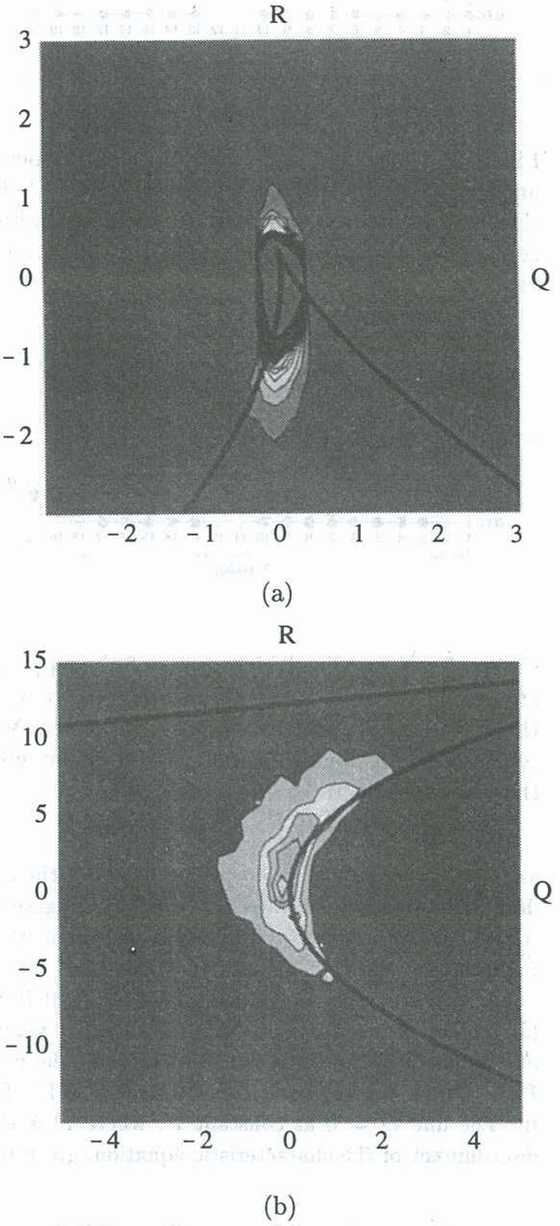

Figure 5: Isocontours of the joint PDF of R and Q conditional on $P = -1$("small expansion") (a) and $P = 7$ ("compression") (b) for the topology associated with the inert scalar field excluding convection. The velocity field is incompressible($P = 0$). The line $D = 0$ is indicated by the solid black curve.