THE INFLUENCE OF ISO-SCALAR SURFACE CURVATURE ON TURBULENT MIXING AND REACTION

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Abstract. The mixing-reaction problem is described in terms of the evolution of iso-scalar surfaces. The scalar diffusive flux is decomposed into a flat-front contribution plus a curvature induced molecular transport. Expressions for the normal propagating velocity of iso-surfaces of a reactive scalar field relative to the fluid are provided making use of the previous decomposition. Transport equations for the scalar-gradient absolute value, as well as for the normal unit vector and for the mean curvature of iso-scalar surfaces are derived.

128³ DNS data for both inert and reactive scalar fields in statistically stationary solenoidal turbulence are used to estimate the flat-front and the curvature induced contributions to the diffusive fluxes. Scalar statistics and, in particular results relevant to molecular mixing models are presented. The influence of the curvature upon scalar dissipation, diffusive fluxes and chemical reaction rate are presented; due to the poor DNS resolution of the iso-scalar surface curvature, these statistical results as well as those for propagation velocity and diffusive length scales should be considered as qualitative.

Key words: Curvature, scalar mixing, reacting flow, combustion, DNS, turbulence.

1. INTRODUCTION

Mixing combined with reaction is ubiquitous in chemical industry, propulsion and power systems, atmospheric and oceanic pollutant dispersion and, even, in some geological and astrophysical flows. Most of the times, the transporting flow is turbulent with strong spatial and temporal inhomogeneities of the thermochemical variables. Scalar fields display complicated patterns, with iso-surfaces being stretched, rotated and
folded by the dynamic structures of the turbulence. The degree of deformation of isoscalar surfaces is apparent from the observation of complicated flow topologies (holes, cusps, saddle points, high curvature regions, ...) [1]-[5].

Flat flame fronts, which form the basis for most laminar flame propagation studies, are uncommon. The influence of the flame curvature upon the burning velocity was considered by Markstein [6], using a linear perturbation technique, and by Pelcé and Clavin [7], via an asymptotic analysis in the limit of large activation energy. Pioneer contributions to the investigation of the relationship between flame curvature and stability are presented in Pelcé [8].

Candel and Poinsot [9] separate curvature and stretch effects on the flame area rate of change and derive an equation for the mean front curvature; through the numerical simulation of a pair of counterrotating vortices interacting with a premixed flame, they estimate that the curvature action may become as important as the straining as time increases. While the tangential stretching may be easily modelled by means of planar stagnation-point laminar flames, the curvature effects are more difficult to treat.

The curvature of isoscalar surfaces has been investigated in connection with flamelets [10] and surface density function models of combustion [11]-[14]. Generally, the assumption is made within the flamelet context, that the Kolmogorov length microscale is much larger than the scalar diffusion thickness in order to justify the neglect of curvature effects. For non-premixed combustion, the validity of the laminar flamelet assumption is limited, among other things, by the curvature effects which modify the one-dimensional flame structure [11]. In fact, the use of some sort of generalised flamelets wherever strong curvatures are present has been proposed.

It is also worth noticing that, in premixed combustion, there is a strong dependence of the curvature effect on the Lewis number [15]; moreover, the correlation between the curvature and the remaining relevant quantities is less important for $Le = 1$.

Kollmann and Chen [3] analytically and numerically (2-D DNS) investigated the production of flame surface density, its dissipation due to diffusion and curvature and its restoration due to normal diffusion and reaction, and scrutinized the effect of saddle points on pocket formation. Vervisch et al.[12] and Vervisch and Veynante [13] clearly established the connections of rigorous PDF methodologies for turbulent combustion with, among others, the flame surface density model; curvature of iso-scalar surfaces explicitly enters theses formulations. Chen and Im [14] correlated burning velocity with tangential strain, curvature and stretch for unsteady premixed hydrogen/air flames using a 2-D DNS study with detailed chemical kinetics.

Zhong, Elghobashi and Boratav [16] studied the influence of the curvature in non-premixed, buoyant and non-buoyant, flames. These authors estimate the mean of the diffusive flux, as well as its normal and curvature contributions, conditional upon the mean curvature of the flame surface.

In the statistical modelling of turbulence, by one-point Probability Density Function (PDF) methods, for example, the relevant quantity is the mean molecular diffusion conditional upon the value of the scalar field. The explicit consideration of the curvature of isoscalar surfaces is absent from the existing formulations of molecular mixing models [17], [18]. Some models mimic the process as one-dimensional diffusion enhanced by an artificial random rearrangement (simulating the action of turbulence) of local and instantaneous scalar values [19]; this redistribution of the scalar field do not require to provide a characteristic mixing time; it only needs length and intensity parameters for the turbulent velocity field.

Often, it is implicitly considered that a one-dimensional second derivative is a good replacement for the full Laplacian, should the former be calculated in the direction of
the gradient. One-dimensional models, thus, neglect the curvature contribution to micromixing.

In this paper, the different diffusive contributions to the mixing process will be estimated from Direct Numerical Simulation (DNS) data. A pure mixing process and a premixed reactive system undergoing a highly nonlinear reaction, Lewis number unity and constant density isothermal conditions are computed and compared. The details of the governing equations are described in Section 2. Section 3 presents the DNS method and discusses the resolution of the curvature field. Full fields are analysed and statistical results are presented in Section 4. Finally, some conclusions are stated in Section 5.

2. MATHEMATICAL FORMULATION

2.1 Main governing equations.

The transport equations governing the velocity and scalar fields are

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} p_j + \nu \frac{\partial u_i}{\partial x_j} + f_i \tag{2}
\]

\[
\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} = D \nabla^2 C + \omega(C) \tag{3}
\]

where \( u_i \) is the \( i \)th component of the velocity vector, assumed to be a solenoidal, homogeneous and isotropic field undergoing a random forcing, \( f_i \); consequently, the flow is statistically stationary. \( x_i \) is the \( i \)th component of the position vector and \( t \) stands for time. \( p \) is the pressure and \( \nu \) is the kinematic viscosity. Since the density is assumed constant, its value can be taken equal to one. \( C \) represents the fuel mass fraction, bounded between 0 and 1. \( D \) denotes the Fickian diffusivity coefficient.

Two scalar fields, one inert (\( \omega = 0 \)) and another reactive, decaying freely from identical nearly segregated initial conditions with initial mean 0.5 and initial variance 0.1701 have been investigated. The chemical reaction rate, \( \omega(C) \), chosen for the reactive scalar, is highly nonlinear, namely,

\[
\omega(C) = -14C (1 - C)^5 \tag{4}
\]

The chemistry is modelled by a one step reaction which transforms the premixed fuel into products. Arrhenius-like reactions are more realistic than the selected chemical rate. However, this expression was introduced by Picart et al [20] as a highly non-linear term which resembles a realistic one-dimensional Arrhenius-like, and it is much faster to compute.

A molecular mixing model requires representing \( D \left( \nabla^2 C \right) \) in terms of \( C \) and the appropriate characteristics of the velocity field. This diffusive flux can be reexpressed as
where \( \mathbf{n} = \nabla C / |\nabla C| \) is the unit vector normal to the local / instantaneous scalar surface, \( C(x,t) = C_0 \), \( g = |\nabla C| = \partial C / \partial x_n \) is the absolute value of the scalar gradient, \( \nabla C \), with \( x_n \) the coordinate normal to the isoscalar surface, and \( (\nabla \cdot \mathbf{n}) \) is the mean curvature of the isoscalar surface.

The first term on the right side of (5) can be expressed as \( D\left(\partial^2 C / \partial x_n^2\right) \) and represent the molecular diffusion normal to the iso-scalar surface; this is the only contribution for flat iso-surfaces. The effect of the additional diffusive flux caused by the curvature of the iso-scalar surfaces is represented by the last term in (5). As already pointed out in the Introduction, the latter has been systematically neglected in the formulation of molecular mixing models. One of the objectives of this paper is to clarify the relative importance of the flat iso-surface or normal diffusion and the curvature induced one. A turbulent flow is characterized by high velocities of linear dilatation, of angular deformation and of rotation, and strongly stretched and curved isoscalar surfaces are experimentally and numerically visualized. Pope et al [21], via DNS, investigated the curvature of material surfaces in a field of isotropic turbulence; among other things, they found that cylindrical elements are the most probable structures with large curvatures. Brethouwer [1] has used DNS to investigate the dynamics of mixing.

Conservation equation for \( g \), \( \mathbf{n} \) and \( (\nabla \cdot \mathbf{n}) \) are easily obtained

\[
\frac{Dg}{Dt} = -g n_i S_{ij} n_j + \frac{\partial g}{\partial t} \frac{
abla \cdot \mathbf{n}}{\nabla C} \cdot \nabla C + g \frac{\partial}{\partial C} (\mathbf{v} \cdot \mathbf{n}) (6)
\]

\[
\frac{Dn_i}{Dt} = (\delta_{ij} - n_i n_j) S_{jk} n_k + \frac{1}{2} \varepsilon_{ijk} \omega_j n_k + D \left( \nabla^2 n_i \right) + \frac{2D}{g} (\nabla g) \cdot (\nabla n_i) + D (\nabla \cdot \mathbf{n}) \cdot (\nabla \mathbf{n}) (7)
\]

\[
\frac{D(\nabla \cdot \mathbf{n})}{Dt} = -2 S_{ij} n_i n_j + n_i S_{ij} n_j (\nabla \cdot \mathbf{n}) - (\delta_{ij} - n_i n_j) S_{jk} n_k + \frac{1}{2} \varepsilon_{ijk} \omega_j n_k
\]

\[
+ D \nabla^2 (\nabla \cdot \mathbf{n}) - \left( \frac{2D}{g^2} g_{ij} [\nabla g] \cdot (\nabla n_i) \right) + \frac{2D}{g} [\nabla g, i] \cdot (\nabla n_i) + \frac{2D}{g} [\nabla g] \cdot (\nabla \cdot \mathbf{n}) + 2D [(\nabla \mathbf{n}) \cdot (\nabla \mathbf{n})] n_i + D [\nabla \mathbf{n}] (\nabla \cdot \mathbf{n}) (\nabla \cdot \mathbf{n}) (8)
\]

where \( D/Dt = \partial / \partial t + u_i (\partial / \partial x_i) \) is the material derivative operator, \( S_{ij} \) is the rate of strain tensor, \( \varepsilon_{ijk} \) is the Levi-Civita tensor and \( \omega_j \) is the \( j \)-th component of the vorticity vector, \( \mathbf{\omega} \). From (6) a conservation equation for \( \nabla g \) can be readily obtained and, subsequently, transport equations for the two terms on the right side of (5) can be written.

The four terms on the right side of (6) represent the scalar-gradient absolute value, \( g \), enhancement by the straining turbulent field, its molecular transport, the iso-scalar surface square curvature induced dissipation upon \( g \), and its chemical intensification, re-
spectively. While the vorticity does not enter (6), it explicitly appears in (7) for the evolution of $n$, taking into account, for example, the wrapping of iso-scalar sheets around vortex tubes [1]. The rate of strain tensor as well as its gradient contribute to the transport of mean curvature, $(\nabla \cdot n)$, in (8); on the other hand, only the vorticity gradients enter that equation. Both Equs. (7) and (8) for the transport of $n$ and $(\nabla \cdot n)$, respectively, contain diffusion terms expressing pure transport of normal and curvature, cross scalar-gradient/isosurface-curvature diffusive fluxes and square-curvature molecular terms. It is worth pointing out that chemistry do not explicitly contribute to the transport neither of $n$ nor of $(\nabla \cdot n)$, although its implicit contribution to both is obvious through $g$.

A turbulent premixed flame is an example of a propagating surface provided that the flame thickness is much smaller than its radius of curvature [22]. A reaction progress variable can be used to identify the flame location. On the other hand, the stoichiometric mixture fraction could be employed to position a nonpremixed flame; the stoichiometric mixture-fraction iso-surface is a constant property surface [22], [23]. This paper will concentrate on premixed reacting flow. For constant $\rho D$, Eq.(3) for $C(x,t)$, a reaction progress variable, governs the scalar field evolution. Allowing for variable $\rho D$, $C(x,t)$ is governed by

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} = \frac{1}{\rho} \nabla (\rho D \nabla C) + \omega(C)$$

(9)

where the chemical source term, $\omega(C)$, is set equal to zero for inert scalars. Let $C(x,t) = C_0$ be the reaction-progress-variable isosurface defining the premixed flame; the evolution equation for this isosurface is

$$\frac{\partial C}{\partial t} + v^C \frac{\partial C}{\partial x_j} = 0$$

(10)

where $v^C$ is the absolute velocity of the isoscalar surface $C(x,t) = C_0$. Equation (7) can be alternatively written as

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} = -(v^C - u_j) \frac{\partial C}{\partial x_j}$$

(11)

$v^C - \mathbf{u} = -\nabla n$ is the normal propagating velocity relative to the fluid of the premixed flame. With the definitions of the previous section and equating the right sides of (9) and (11) one can easily obtain

$$V = \frac{1}{\rho} \frac{\partial \rho D}{\partial x_n} + \frac{D}{g} \frac{\partial g}{\partial x_n} + D (\nabla \cdot n) + \frac{1}{\rho g} \omega(C)$$

(12)

For constant $\rho D$, the first term on the right side of (12) vanishes. The second term is the normal propagation velocity, $V_{\text{norm}}$, of a flat flame front; the third term is the contribution of the curvature to the propagation speed, $V_{\text{curv}}$, and it is zero for flat flame surfaces; finally, the last term is the chemical addition to the front velocity, $V_{\text{chem}}$. The total
propagation speed, $V_{rot} = V$, is, thus, composed of three additive contributions, two due to diffusive fluxes and one due to reaction.

A natural characteristic diffusion length scale might be $\delta_D = g / (\partial g / \partial x_n) = (\partial C / \partial x_n) / (\partial^2 C / \partial x_n^2)$ or, rather, its absolute value.

The ratio of $V_{norm}$ due to the diffusion normal to the front, the second term in (12), and of $V_{curv}$ due to that induced by the curvature, the third term in (12), is

$$R_{nic} = \frac{D(\partial g / \partial x_n)}{g} \sim \frac{R}{\delta_D}$$

where $R = (\nabla \cdot n)^{-1}$ is the mean radius of curvature of the isosurface. The ratio $\delta_D / R$ could be similar to a Markstein number [7], [8] and [24].

For turbulent flows all the variables in (12) are random. $V$ must be properly averaged to obtain mean values. Zhong et al [16] obtain the averaged values of $D(\partial g / \partial x_n)/g$ and of $D(\nabla \cdot n)$ conditioned upon the curvature, $\nabla \cdot n$, for the mixture fraction of a nonpremixed flame; for a nonbuoyant flame, they estimate that the diffusion due to curvature is approximately one order of magnitude larger than that for a flat-front, when both diffusive fluxes are conditioned on the value of the curvature.

2.2 A simple analytical study.

In order to illustrate a case in which the curvature induced diffusion can dominate over the normal diffusive flux, the evolution of a scalar field, $C(x, y, t)$, in a two-dimensional (2-D) stagnation point is considered. Apart from being the flow investigated by Liñán [25] in order to unveil the extinction of premixed flames, this also corresponds to one of the small scale topologies in turbulent flows and, therefore, one to be investigated as far as mixing characteristics is concerned [34]. Starting from the initial condition $C(x, y, 0) = 1 / g (x) g (y)$ and undergoing the velocity field $u = (y, x, -y, y, 0)$, $C(x, y, t)$ evolves according to

$$C(x, y, t) = C_{max}(t) \exp \left[ -\frac{x^2}{2 D(D^2 e^{2x t} - 1)} - \frac{y^2}{2 D(D^2 e^{2x t} - 1)} \right]$$

where

$$C_{max}(t) = 1 / \sqrt{2 \pi (D / \gamma) \sqrt{2 \gamma^2 + 2 [c^2 (2 \gamma^2 t) - 1]}}$$

The iso-scalar surface $C(x, y, t) = C_0$, with a unit normal vector $n = (n_x, n_y)$ has a mean curvature
\[ \nabla \cdot \mathbf{n} = \frac{n_x}{x} \left(1 - n_x^2 \right) + \frac{n_y}{y} \left(1 - n_y^2 \right) \] (16)

The ratio of flat-front to curvature-induced diffusion contributions can be also analytically evaluated. For \( I = 10^{-4} \left( C_0^2 \cdot m^1 \right) \), \( D = 10^{-5} \left( m^2 / s \right) \) and \( \gamma = 0.1 \left( s^{-1} \right) \), the isoscalar surface \( C_0 = 0.005 \) exists for \( 0 < t < 12.3 \) s [23]. The initial circular blob becomes an ellipse as time evolves, with major and minor axis, \( a(t) \) and \( b(t) \), respectively. The mean curvatures at point \( x = a(t) \) continuously increase, while at \( y = b(t) \) continuously decrease. The ratio, \( R_{\text{sc}} \), of the flat-front to the curvature-induced diffusive contributions, before the isoscalar surface \( C(x, y, t) = 0.005 \) disappears, takes asymptotically very small values at \( x = a(t) \), while the flat-front contribution dominates at \( y = b(t) \).

3. NUMERICAL SIMULATION

3.1 Methodology description

A Direct Numerical Simulation (DNS) of Equs.(1)-(4) is performed in a cubic box with 128³ grid points and periodic boundary conditions. The length of each edge of this cube is \( 2\pi r \). A second-order Runge-Kutta numerical scheme advances the transport equations in time, whereas a pseudo-spectral code [26], [27] and [28] is used in the spatial domain.

The forcing scheme is that of [29] with a zero correlation time. To be more specific, all the nodes with a modulus less than \( 2\sqrt{2} \), except the zero node which has no contribution, receive at each time step a random Gaussian forcing contribution with an intensity such that the Reynolds number (based on the Taylor microscale) is close to 70; the phase is adjusted so that the forcing is incompressible.

The Damköhler number is approximately one, so that the characteristic time and spatial scales due to chemistry are of the same order of those due to turbulent mixing; the numerical complexity of solving a stiff problem with widely different characteristic scales is, thus, avoided. The Schmidt number was set equal to 0.7.

In order to reduce aliasing, a spherical filter is applied to the data in Fourier space; all nodes corresponding to a wave number larger than \( 64 \times 0.942 = 60.288 \) are set equal to zero. This filter was chosen [26] in order to get rid of the double and triple aliasing contribution [30] caused by the convective terms. Some amount of aliasing due to the single contribution of the convective terms and the chemical term still remains; however, it may be neglected according to the criterion of Kida and Murakami [31], since the spatial resolution is such that the value of the largest wave number times the Kolmogorov length microscale is of order two (around 1.95); a value greater than one is considered sufficient to resolve the field [32].

The time step is chosen as the smallest value between that which guarantees a Courant number equal to 0.8 (it must be less than 1) and 0.001; the last value is selected in order to yield a well resolved chemical term. The Courant number, \( C_o \), is defined as

\[ C_o = \frac{dt}{dx \max \{|u_1|, |u_2|, |u_3|\}} \] (17)

The parameters are adjusted so that the integral length scale of the velocity field is less than one sixth of the length of each edge of the computational box. A value less than one third is sufficient to guarantee that the resulting flow is homogeneous.
The initial velocity field evolves for ten eddy turn-over times, reaching a stationary state where the spectrum presents small fluctuations. Then, an initial scalar field as close as possible to a homogeneously random bimodal distribution of 0 and 1 values is taken. The mean of this initial field is approximately 0.5 and its values are not exactly 0 and 1; they are smoothed, to avoid strong aliasing effects during the initial time steps. The inert and the reactive scalar fields are identical at the initial stage.

To avoid a rapid mixing of the initial scalar field, it is necessary that its integral scale is not too small. This is guaranteed by choosing, first, a random spectrum where the only non-zero contributions are those of wave numbers with a modulus less than 4. In the subsequent step of the scalar field initialisation, a cut-off is chosen and the values of the previous pseudo-field for wave-numbers smaller than the cut-off are set equal to zero, whereas those scalar values for wave-numbers greater than or equal to the cut-off are set to one. To end the initialization, the resulting scalar field is smoothed.

The full characterization of the initial velocity field at time $t=0$ is given by the Reynolds number based on the Taylor microscale ($Re_t = 66.66$), the integral length scale ($L = 2\pi$), the kinematic viscosity ($v = 0.012$), the Taylor microscale ($\lambda = 0.5139$), the Kolmogorov microscale $\eta = 0.03198$, the total kinetic energy ($k = 3.635$) and the energy dissipation rate ($\epsilon = 1.652$).

The initial scalars, identical for both the inert and the reactive fields, are characterised by a diffusivity coefficient ($D = 0.017143$), a Schmidt number ($Sc = 0.7$), scalar mean ($\langle C \rangle = 0.4971$), scalar variance ($\langle C^2 \rangle = 0.1395$), $C_{\min} = 0.000861$ and $C_{\max} = 0.9996$.

3.2 Resolved and unresolved fields

As it has already been said in Subsection 3.1, the maximum wave number times the Kolmogorov length microscale is assigned a value such that a good resolution of the gradient fields can be guaranteed. However, in order to investigate the topological properties of iso-scalar surfaces, that resolution may be too coarse. In effect, the iso-scalar surface curvature is related to second order derivatives instead of first order ones. Moreover, to obtain the mean curvature from Eq. (5), one has to divide second order derivatives by $g = |\nabla C|$; that makes things even worse since, wherever the gradient of the scalar field is close to zero, this division will, in general, yield a large number; as a result the curvature will be a highly intermittent variable, with a significant amount of energy in the high wave numbers. In other words, computing the curvature near to zero-gradient points may be subject to large errors.

A possible way of knowing whether a periodic field is well resolved is by looking at its spectrum [33]. The smaller the spectral content at high wave numbers, the better the field is resolved. The amount of "energy" in the resolved high wave numbers serves as a qualitative estimator of the spectral content in the unresolved scales. Hierro et al [33] provide examples of spectra for well resolved fields, such as turbulent kinetic energy and the scalar fluctuations; they also present the spectrum of the curvature field, as an example of a poorly resolved variable. The Laplacian of the scalar field, for instance, is clearly inside a sharp decay zone at the cutoff wave-number; thus, it is likely that Laplacian-like variables may be reasonably well resolved [33].

An alternative way of finding whether a field is well resolved consists of separately computing the two sides of a balance equation. An example is Eq.(5), where the left-hand term is the total diffusive flux, while its right-hand term is the addition of the normal and the curvature diffusions, respectively. The three terms may be computed separately, and Eq.(5) should be satisfied, provided that all the terms are well resolved.
Hierro et al. [33] clearly show how conditioning the two sides of (5) upon the scalar value leads to small deviations between the independently estimated left and right sides. On the other hand, conditioning on the curvature values yields non-negligible differences between the two sides of (5).

When computing a mean conditional upon the scalar, close points in the physical space have associated close values in the composition space and contribute to the same bin in the histogram which approximates the conditional mean. On the other hand, the larger the intermittency, implies that close points in the physical space may have widely different values in the curvature space and contribute to different bins in the histogramic reconstruction of the conditional mean. Balance behavior is more sensitive to the conditioning variable than to the added quantities: when one considers close points in the physical space, errors are alike in all the terms of Eq. (5), so that the balance is preserved.

4. RESULTS

DNS results at time, $t=1.135$ will be presented and discussed in this Section. The variables characterising the velocity field are, $\langle k \rangle = 5.336$, $\langle \varepsilon \rangle = 3.257$, $Re_x = 69.68$, $l_{im}=0.4433$, $\eta = 0.02699$. Similarly, for the inert scalar field $\langle C \rangle = 0.497061$, $\langle C^2 \rangle = 0.008833$, $C_{min}=0.09804$ and $C_{max}=0.89779$. For the reactive scalar field, $\langle C \rangle = 0.063858$, $\langle C^2 \rangle = 0.012655$, $C_{min}=0.0$ and $C_{max}=0.864635$.

4.1 Results and discussions of Scalar Field

Fig. 1 depicts a 2-D cross section of the DNS cube with iso-scalar zones; it is evident that the reactive scalar is significantly depleted. Figs. 2 and 3 portray 2-D cross sections with iso-dissipation and iso-reaction zones, respectively, corresponding to the previous scalar field. The scalar dissipation rate is only important around the pockets of remaining fuel. Chemical activity is important even for low scalar values, as the maximum reaction rate occurs at $C = 1/6$. Fig. 4 is a 3-D snapshot of the iso-scalar surface $C=0.1$; complicated surface geometry is apparent, with large curvature regions, saddle points, etc.

The scalar probability density function (PDF) is plotted in Fig. 5 for both the inert and the reactive fields. Chemistry drives the reactant towards zero, with large values of the PDF near that value. Pure mixing, on the other hand, leaves the mean unaltered, clustering the probability about it.

In order to test the hypothesis of replacing the scalar dissipation rate, $\varepsilon_c$, by the turbulent kinetic energy dissipation rate, $\varepsilon$, commonplace in many mixing models, the joint PDF of the second invariant of the strain rate tensor, $-Q_3 = 4\nu \varepsilon$, and $\varepsilon_c$ is plotted in Figs. 6 and 7 for the inert and the reactive cases, respectively. The arrows indicate the dynamics in the phase-plane of that pair of variables, obtained from the corresponding transport equations [34]. It is apparent from the results shown that, in general, the decreasing of the scalar dissipation is strongly related to low values of the strain; however, for the reactive case, the chemistry coupled to the turbulence causes that reduction to occur even for moderate strain values. Figure 8 depicts the result for the scalar dissipation rate conditional on $-Q_3$, for both the inert and the reactive cases; although the statistical proportionality of scalar and energy dissipation rates is far from satisfactory,
even for the pure mixing problem, it is observed the well known correlation between large values of the strain and of the scalar dissipation.

4.2 Results and discussions relevant to Molecular Mixing Models

The critical issue in the development of molecular mixing models is to express the diffusive term, \( D \nabla^2 C \), conditioned upon the scalar value, \( C \), in terms of known statistical variables. Figs 9, Fig 10 and Fig 11 are 2-D cross sections of the DNS cube with iso-value zones for the total diffusive flux, and for the normal and the curvature diffusions, respectively. Comparison of the three Figures with the iso-scalar zones in Fig. 1 confirm that normal diffusion dominates about low curvature lines, while the curvature induced diffusion has a leading role near bent scalar iso-lines. Notice, however, that 3-D topologies will be surely masked by these 2-D pictures.

Figs 12 and 13 are plots of the total diffusive flux, and the normal and curvature diffusions conditional upon \( C \) for the inert and for the reactive scalars, respectively. The conventional shapes for the inert case are reproduced, with the curvature diffusion accounting for about one third of the contribution to the total diffusive flux, displaying the same sign as the normal diffusion over the whole range of scalar values. On the other hand, the reaction induces negative conditional diffusive fluxes over most scalar values; only for \( C < 0.2 \) the total and the normal diffusions display positive values. In any event, the effect of the curvature upon the conditional diffusive fluxes is seldom negligible.

4.3 Curvature Influence

The poor resolution for the curvature of iso-surfaces has been pointed out in sub-Section 3.2. The following results must be taken with some caution and should be considered of a qualitative nature. Numerical simulations with mesh 256\(^3\) are in progress in order to achieve better resolved fields.

Fig. 14 is a plot of the PDF of the curvature, \( V \cdot n \), of iso-scalar surfaces for inert and for reactive fields. As anticipated, the curvature displays a high degree of intermittency. Chemical reaction apparently creates surfaces with larger curvatures, as shown by the slowly decaying tails of the PDF. The scalar mean conditioned upon the curvature values is presented in Fig. 15 for both the inert and the reactive cases; for the inert scalar, concave surface topologies \((V \cdot n < 0)\) yield a conditional average around 0.56, while that value for convex fronts \((V \cdot n > 0)\) is about 0.44, with an unconditional average close to 0.50.

Fig. 16 represents the scalar dissipation, \( E_C \), conditioned on the curvature values, \( V \cdot n \), for both the inert and the reactive concentrations; the symmetry of the curve for the inert case indicates that convex and concave topologies are equally dissipative, whereas the concave structures seems to increase the scalar dissipation when chemical reaction is present.

The scalar diffusive flux, as well as its two components, the normal and the curvature diffusions, conditional upon the curvature \( V \cdot n \), are displayed in Figs. 17 and 18 for both the inert and the reactive fields. Concave topologies contribute negatively to the three diffusive fluxes, while convex structures show positive values. This implies scalar profiles in the direction normal to the iso-surfaces, displaying convex and concave curves for negative and positive iso-scalar surface curvatures, respectively. This trend is common for both the inert and the reactive cases. However, while the curves have the same absolute values for the same positive and negative curvature values for the inert
The chemical reaction apparently favors larger negative diffusive fluxes associated to concave fronts than those related to the positive curvature.

Fig. 19 is a plot of the joint PDF of the curvature, $\nabla \cdot n$, and the chemical reaction rate, $\omega(C)$. A slightly preferential chemical activity is associated with negative curvatures, namely, concave fronts. This fact is more clearly shown in Fig. 20, where the average reaction rate conditioned upon the curvature values is plotted; concave fronts seem to be chemically more active than convex ones, with a maximum value for slightly negative curvatures.

### 4.4 Relative importance of diffusive fluxes

In order to evaluate the relative importance of the normal and curvature diffusive fluxes, the ratio, $R_{nic}$, defined by Eq. (13), of these two diffusion terms is used. Fig. 21 presents the PDF of $R_{nic}$ for both the inert and the reactive cases. The tails display some degree of intermittency. The probability of encountering values of $R_{nic} < -10$ and $R_{nic} > 10$, namely, points for which the normal diffusion dominates over the curvature flux is about 14% for both the inert and the reactive scalar fields. Probability of finding values of $R_{nic} < -10$ is 6.5%, while probability of values $R_{nic} > 10$ is about 7.5%. This is an indication that for a significant percentage of the points, the curvature diffusion should be retained compared to the normal diffusive flux.

### 4.5 Propagation Velocity

Although the calculation of the propagation velocity of iso-scalar surfaces is affected by the intermittency and the poor resolution of $\nabla \cdot n$, discussed in Section 3.2, some qualitative results are presented. Fig. 22 is a plot of the PDF of $V_{tot}$, $V_{norm}$, $V_{curv}$ for an inert scalar. Identical curves are presented in Fig. 23 for a reactive field, adding the PDF of $V_{chem}$. The inert scalar displays nearly symmetric curves, with equally probable positive and negative values of the various velocities. On the other hand, the reaction seems to produce slowly decaying tails and clearly favors negative velocity propagation values of $V_{chem}$.

The expected values of the different velocities conditional on the scalar value are plotted in Figs. 24 and 25. The curve of $V = V_{tot}$ is a qualitative indication that iso-scalar surfaces, about the maximum reactivity surface, $C = 1/6$, can significantly vary its propagation velocity, making the choice of a single characteristic speed a difficult task.

### 4.6 Length Scales

The evaluation of the diffusive length, $\delta_D$, and of the radius of curvature, $R$, are subject, once more, to the poor curvature resolution already mentioned. In any case, a qualitative discussion of some preliminary results is presented. The PDF of $|\delta_D|$ is given in Fig 26 for both the inert and the reactive cases. The presence of chemistry reduces the PDF tails, structuring the reactive fronts with smaller diffusive zones. The average value of the absolute value of $\delta_D$ is $\langle |\delta_D| \rangle = 0.255$, as compared to a value of 0.027 for the Kolmogorov length micro-scale. Fig. 27 presents the average value of $|\delta_D|$ conditioned on the scalar content.

Fig. 28 plots the PDF of $R$ for both inert and reactive fields. Reaction acts on $R$ similarly to its effect on $\delta_D$. 

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C. Dopazo et al. / Iso-scalar surface curvature in turbulent mixing and reaction
5. CONCLUSIONS

DNS results have been used to characterise the scalar field statistics, as well as some topological features related to iso-scalar surface curvature. The statistical variables involving that curvature are mainly qualitatively estimates, due to the poor resolution of the curvature computation. $256^3$ DNS are in progress in order to improve the resolution problem.

Complicated flow topologies are apparent from the 2-D and 3-D plots of iso-scalar surfaces. Flat surface portions are relatively infrequent, predominating holes, pockets, saddle points and, in general, highly curved surfaces. Apart from the effect of saddle points on pocket formation analysed by Kollmann and Chen [3], these configurations may have a role in scalar mixing; some preliminary indications have been obtained by Hierro [35] through the use of simple analytical purely molecular diffusion models with stochastic initial conditions; while the PDF evolution is anomalous for 1-D cases, the mixing in probability space is closer to reality for 2-D and 3-D cases where saddle points appear. Neither flamelet models nor molecular mixing models in the PDF methodology include the curvature of iso-scalar surfaces. The results presented show that the curvature induced diffusion is not, generally, negligible. The Physics of surface deformation and curving due, for example, to wrapping and folding in intense vorticity regions seems to be an important ingredient to parametrise the curvature effects upon diffusion fluxes in turbulent flows.

DNS accounting for variable density and thermal effects would be a better approximation for more realistic turbulent combusting scalars. For initially segregated scalars the influence of curvature may be small. However, for moderately mixed inert scalars, the effect of curvature could contribute about one third of the total diffusive flux. Under reactive conditions, the curvature has almost everywhere a negative contribution, acting as a soft chemical reaction which consumes premixed fuel, and can be the dominant contribution to micromixing for some values of the scalar field.

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Figure 1. Iso-concentration zones of the reactive scalar, C, in a plane of the simulation cube.

Figure 2. Iso-zones of the reactive scalar dissipation rate in a plane of the simulation cube.
Figure 3. Iso-zones of the chemical reaction rate in a plane of the simulation cube.

Figure 4. Reactive scalar. Iso-scalar surface C=0.1 in the 3-D simulation domain.
Figure 5. Probability density function (PDF) of the concentration C for both the inert and the reactive scalars.

Figure 6. Joint PDF of minus the strain rate tensor second invariant, $-Q_s = 4\nu \varepsilon$, and the scalar dissipation rate, $\varepsilon_C$, for the inert scalar. Arrows indicate the averaged motions of the variables in the phase-plane.
Figure 7. Joint PDF of $-Q_s$ and $\varepsilon_c$ for the reactive scalar. Arrows indicate the averaged dynamics, as in Fig. 6.

Figure 8. The scalar dissipation rate, $\varepsilon_c$, conditional on $-Q_s$ for both the inert and the reactive scalars.
Figure 9. Reactive scalar. Iso-zones of the scalar diffusion in a plane of the simulation cube.

Figure 10. Reactive scalar. Iso-zones of the normal diffusion in a plane of the simulation cube.
Figure 11. Reactive scalar. Iso-zones of the curvature diffusion in a plane of the simulation cube.

Figure 12. Inert scalar. The total scalar diffusion, and its normal and curvature contributions, conditional upon the scalar concentration value, C.
Figure 13. Reactive scalar. The total scalar diffusion, and its normal and curvature contributions, conditional upon the scalar concentration value, C.

Figure 14. PDFs of the isoscalar surface curvatures, $\nabla \cdot \mathbf{n}$, for the inert and the reactive scalar fields.
Figure 15. The average scalar concentration conditional upon the curvature, $\nabla \cdot n$, for both the inert and the reactive scalars.

Figure 16. The average scalar dissipation rate, $\varepsilon_c$, conditional upon the curvature, $\nabla \cdot n$, for both the inert and the reactive scalars.
Figure 17. Inert scalar. The average scalar diffusion, and its normal and curvature contributions, conditional on the curvature values.

Figure 18. Reactive scalar. The average scalar diffusion, and its normal and curvature contributions, conditional on the curvature values.
Figure 19. Joint PDF of the curvature and the chemical reaction rate.

Figure 20. The average chemical reaction rate conditioned on the curvature values.
Figure 21. PDFs of the ratio $R_{nc}$ for both the inert and the reactive cases.

Figure 22. Inert scalar. PDFs of the local iso-scalar surface velocities due to the normal and the curvature diffusions. The PDF of the total velocity is also shown.
Figure 23. Reactive scalar. PDFs of the local iso-scalar surface velocities due to the normal and the curvature diffusions, as well as to the chemical reaction. The PDF of the total velocity is also depicted.

Figure 24. Inert scalar. The different local iso-scalar surface average velocities conditional upon the scalar concentration.
Figure 25. Reactive scalar. The different local iso-scalar surface average velocities conditional upon the scalar concentration.

Figure 26. PDFs of the absolute value of the characteristic diffusion length-scale, $|\delta_D|$, for both the inert and the reactive scalars.
Figure 27. The absolute value of the average diffusion length scale, $|\delta_s|$, conditional upon the concentration, $C$, for both the inert and the reactive scalars.

Figure 28. PDFs of the radius of curvature, $R$, for both the inert and the reactive scalars.