The Dynamics of Turbulent Scalar Mixing near the Edge of a Shear Layer

R. M. R. Taveira, C. B. da Silva & J. C. F. Pereira
IDMEC/IST, Technical University of Lisbon, Pav. Mecânica I, 1º Andar, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
E-mail: rodrigo.taveira@ist.utl.pt

Abstract. In free shear flows a sharp and convoluted turbulent/nonturbulent (T/NT) interface separates the outer fluid region, where the flow is essentially irrotational, from the shear layer turbulent region. It was found recently that the entrainment mechanism is mainly caused by small scale ("nibbling") motions (Westerweel et al. (2005)). The dynamics of this interface is crucial to understand important exchanges of enstrophy and scalars that can be conceived as a three-stage process of entrainment, dispersion and diffusion (Dimotakis (2005)). A thorough understanding of scalar mixing and transport is of indisputable relevance to control turbulent combustion, propulsion and contaminant dispersion (Stanley et al. (2002)). The present work uses several DNS of turbulent jets at Reynolds number ranging from $Re_\lambda = 120$ to $Re_\lambda = 160$ (da Silva & Taveira (2010)) and a Schmidt number $Sc = 0.7$ to analyze the "scalar interface" and turbulent mixing of a passive scalar. Specifically, we employ conditional statistics, denoted by $\langle \rangle_I$, in order to eliminate the intermittency that affects statistics close to the jet edge. The physical mechanisms behind scalar mixing near the T/NT interfaces, their scales and topology are investigated detail. Analysis of the instantaneous fields showed intense scalar gradient sheet-like structures along regions of persistent strain, in particular at the T/NT interface. The scalar gradient transport equation, at the jet edge, showed that almost all mixing mechanisms are taking place in a confined region, beyond which they become reduced to an almost in perfect balance between production and dissipation of scalar variance. At the T/NT interface transport mechanisms are the ones responsible for the growth in the scalar fluctuations to the entrained fluid, where convection plays a dominant role, smoothing scalar gradients inside the interface (0.1 $y_\eta$ to 1 $y_\eta$) and boosting them as far as $-2.5 \frac{dy}{\eta}$.

1. Introduction

The interface region between non-vortical flow and fully developed turbulence in free shear flows is a long-standing issue in turbulent research. Coherent structures lying at the turbulent edge between turbulent and non-turbulent regions give birth to a sharp and convoluted interface (Corrsin (1943)), traduced by an alternating behavior between important viscous effects on turbulent regions and the inexistence of enstrophy over non-turbulent flow regions entrained. The study of this "turbulent/non-turbulent (T/NT) interface" is central both form the fundamental and practical points of view (Hunt et al. (2006)) since across the interface important exchanges play a critical role in turbulent mixing, determining the spreading and maintenance of turbulence. Therefore understanding the dynamics of this turbulence region is crucial to understand the exchanges of energy, enstrophy and scalars (turbulent mixing) that can be
conceived as a three-stage process of entrainment, dispersion and diffusion (Dimotakis (2005)). The “turbulent entrainment” process, by which turbulent regions expand through engulfing large packets of irrotational flow and diffusive vorticity communication, is carried out through “nibbling” and “engulfing” mechanisms and governs mass and energy exchanges taking place along the largely distorted surface of the T/NT interface, thus dictating the growth and mixing rates of free shear layers. It was found recently that the entrainment process is mainly accomplished by the small scale (“nibbling”) eddy motions (Westerweel et al. (2005) and Mathew & Basu (2002)), at least for turbulent jets, as early suggested by the pioneering work of Corrsin & Kistler (1955). However, this viscous diffusive mechanism becomes much more efficient at turbulent regimes (compared to the laminar case) because the boundary between turbulent and non-turbulent flow fields becomes highly contorted, and thus with a much larger contact surface, from the motions of large eddies (LVS) close to it, reason why in the past “engulfing” was thought to be the governing entrainment mechanism and nowadays is still believed that total entrainment rate is determined by the largest scales of the flow. These recent results motivated a recent focus in new approaches for studying turbulent entrainment dynamics and the features of the region where turbulent and irrotational fluid interact, giving birth to the T/NT interface. The first and groundbreaking analysis of the interface was done by Corrsin & Kistler (1955). They observed that molecular viscous effects were dominant within such layer and postulated that its properties should be determined by small viscous scales, thus relating the interface thickness and propagation velocity with Kolmogorov length and velocity micro-scales, respectively. Those suggestions were seen to be accurate in the case of an oscillation grid at low Reynolds numbers by Holzner et al. (2007, 2008). However in many of the literature the thickness of the T/NT interface, characterized by the existence of a sharp jump in vorticity and scalar levels, across this thin region, is observer to be of the order of the Taylor micro scale, as previously suggested by Reynolds (1972). Bisset et al. (2002) observed, for a plane wake, a finite jump in the tangential velocity, hence also present in the spanwise vorticity component at the T/NT interface. He noticed this jump to have a width of the order of the Taylor scale. The round jet experiments of Westerweel et al. (2005, 2009) and the planar jet simulations of da Silva & Pereira (2008) and da Silva (2009) also showed the width of the vorticity jump to be of the order of the Taylor micro scale. Westerweel et al. (2009) also performed a control volume analysis to the interface region, showing that the jump in $\Delta U$ at the interface, moving at a given velocity $E_b$, must obey to the condition $E_b \Delta C = F \approx \Delta \tau$, where $F$ is the momentum flux across the control volume, and $\Delta \tau$ is the jump in the Reynolds stresses conditional profile. Expanding this control volume analysis he also related the jump in velocity and scalar conditional profiles, $\frac{\Delta C}{C_b} \approx \frac{\Delta \tau}{\nu}$, with a reasonable agreement. The dynamics of enstrophy and strain near the T/NT interface generated an oscillating grid, was analyzed by Holzner et al. (2007, 2008) noticing the existence of non-negligible strain and kinetic energy dissipation in the non-turbulent regions, near the T/NT interface, and noticing that the net effect of viscosity, at that location, is to promote an increase in the enstrophy levels. Subsequently da Silva & Pereira (2007) and Holzner et al. (2008) observed that this enstrophy increase is caused by viscous diffusion effects, while viscous dissipation remains negative throughout the whole turbulent jet. da Silva & dos Reis (2011) analyzed the role of coherent vortices near the T/NT interface, observing that the presence of IVS, close to the turbulence front, is responsible for the existence of a region of irrotational non-negligible kinetic energy dissipation and a positive enstrophy diffusion along the thin layer bounding turbulent and non-turbulent regions, linking the results of Holzner et al. (2007, 2008) to the IVS in the flow.

Recently, in order to investigate the role of large and intense vorticity structures (LVS and IVS, respectively) in the context of turbulent entrainment and on the T/NT interface properties, da Silva & Taveira (2010) have shown that the flow coherent vortices near the T/NT interface determine its thickness, $\delta_w$. Indeed, they have shown that $\delta_w$ in a turbulent plane jet the T/NT
Interface thickness is roughly equal to the radius of the LVS lying along the turbulence front, \( \delta_u \sim R_{LVS} \). They showed that radius of the LVS near T/NT interface can be estimated bearing in mind that in long lived vortices the radial viscosity diffusion is roughly balanced by stretching originated by the local strain rate field, \( S' \), as in a Burgers vortex (Jiménez & Wray (1998)). Although LVS are not perfectly described by the Burgers vortex model, these present a rather good approximation and have the same order of magnitude, thus \( R_{LVS} \sim \left( \frac{\nu}{L_{11}} \right)^{\frac{1}{2}} \). In the case of a turbulent jet the magnitude of the strain rate acting on a LVS near the jet edge is \( S \sim \frac{u'}{L_{11}} \), where \( u' \) is the fluctuating velocity field and \( L_{11} \) is the integral scale of turbulence (Hunt et al. (2010)). Hence, \( R_{LVS} \sim \left( \frac{\nu u'}{L_{11}} \right)^{\frac{1}{2}} = L_{11} Re_0^{\frac{1}{2}} \sim \lambda \), where \( Re_0 \) is the Reynolds number associated with the integral scale. Arguably at very high Reynolds and in flows without mean shear the only existing structures are IVS, since LVS are too fragmented. In this case the strain rate field is imposed by the background turbulence \( S \sim \frac{u'}{\lambda} \) and the radius of the vortices, and the thickness of the T/NT interface should reduce to \( R_{LVS} \sim \left( \frac{\nu u'}{L_{11}} \right)^{\frac{1}{2}} = \lambda Re_\lambda^{\frac{1}{2}} \sim \eta \), explaining the differences in the T/NT interface thickness in the experiments by Holzner et al. (2007, 2008).

Turbulent mixing of scalar fields, between gaseous streams, such as temperature, contaminants of chemical species concentration levels, is invariably present in energy generation processes and chemical processes and is undoubtedly one of the largest and primary technological applications of turbulent flows, especially in systems involving combustion of non-premixed or partially premixed reactants streams. The high rates of molecular mixing achievable in turbulent flows allows to attain high and efficient combustion heat release rates, vital in engineering applications ranging from the design of advanced propulsion systems to improvements in traditional combustion processes in industrial facilities (Buch & Dahm (1998)). In many of the cases, environmental regulations impose highly efficient designs that promote the reduction of the emission levels of several potentially harmful trace chemical species resulting from complex mixing and reaction processes in the underlying turbulent flow. Thus a thorough understanding of the mechanisms underlying scalar mixing and transport is of indisputable relevance to control turbulent combustion, propulsion and pollutant/contaminant dispersion in environmental flows (Stanley et al. (2002)). Despite its ubiquitous occurrence and the undisputable value of its understanding very few attempts were performed to model and mimic mixing by means of appealing simplified physical descriptions (Dopazo et al. (2007)). To cope this Dopazo et al. (2007) investigated the mixing characteristics in terms of the principal and Gauss curvatures of isoscalar surfaces of a dynamically passive scalar in an homogeneous field of turbulence, showing that predominant small-scale scalar geometries appear to be flat and tile-like. They also linked the presence of large scalar gradients with these structures characterized by small values in Gauss curvature. Such structures were mostly found along regions dominated by strain, whereas vortical regions are associated with moderate scalar gradients. However their results failed to assess the implications of scalar local structures for mixing models should be scrutinized; neither studied the degree of alignment between maximum dissipation rate sheets and regions of isoscalar surfaces.

Rüetsch & Maxey (1991) analyzed the small scale structures of vorticity and scalar in homogeneous turbulence using a temporal evolution of a passive scalar field in isotropic turbulence. They studied de local topology and the mechanisms responsible for the arise of intense gradient structures, concluding that intense scalar gradient are found to occur in regions of persistent straining flow, such as between neighbor vortex structures of similar circulation or regions of low intensity antiparallel vorticity. They found that it is not the intensity of the strain neither the magnitude of vorticity structures that are responsible for the formation of sheets of strong scalar gradient, but rather regions of persistent strain produced by clusters of vorticity structures with rather equal circulation. Despite the importance of the results the core turbulent zone is less important than the interface region in scalar mixing (Mellado et al. (2009)), and
therefore, the application of results derived from only homogeneous turbulence is limited. Stanley et al. (2002) analyzed the behavior of the pdfs of a passive scalar to study the mixing process in a plane jet over transitional regions and fully developed turbulence and concluded that after the rollup of vortical structures mixing is dominated by large scale engulfing of ambient fluid, whereas in fully developed turbulence small-scale mixing dominates and recently Mellado et al. (2009) proposed to study a passive scalar field in a temporally evolving shear layer using a gradient trajectory analysis. In particular they studied textitpdfs of the scalar field and conditional scalar dissipations rate in the presence of external intermittency, partitioning the turbulence flow into: a turbulent zone and a turbulence interface region. They observed a strong dependence of the conditional dissipation rate on the lateral position and on the conditioning value of the scalar observed, and found that the characteristics of the fields inside the turbulent interfaces determine to a large extent the conventional statistics of the flow. The variation with the scalar level observed for the ratio between the first and second moments of the dissipation rate make invalid certain assumptions commonly employed in turbulence combustion models. An important result for flamelet models in non-premixed turbulent combustion is that there exist large differences in scalar levels, inside turbulent interface regions, along gradient trajectories starting in the outer stream implying that the surface of stoichiometric mixture fraction lies inside turbulence interface for many hydrocarbon-air and hydrogen-air mixtures, and it is the scalar dissipation inside these regions that needs to be accurately modeled, whereas the core turbulent zone is less important, and therefore, the application of results derived from only homogeneous turbulence is limited. Mellado et. al. also showed the mean linear distance between maximum and minimum points, for scalar, to be of the order of the Taylor scale, indicating that there exist anisotropic regions much larger than the Kolmogorov or the Batchelor scales which are diffusely connected.

Buch & Dahm (1998) presented an experimental study of the fine-scale structure of generic passive scalar, for unitary Schmidt number, in an axisymmetric coflowing of a turbulent jet of propane into air, showing that scalar dissipation rate fields consist of entirely strained, laminar, sheet-like diffusion layers, as for high Schmidt cases. However, they observed several differences in the sheet-like structure because the dissipation layers are arranged by the continual stretching and folding of underlying strain rate, and the vortices field bears little resemblance between the two cases. This is mainly visible in lack of similar orientation and in a more contorted sheet structure, due to the comparable sizes between the thickness of the sheets and regions of uniform strain. The thickness of the sheets also presented a bigger span than for high Schmidt, however even the thicker structures still resemble to follow Kolmogorov scaling. Despite these differences the canonical structure does not show dependence on the Reynolds number, however it was shown that the thickness depended on Reynolds or the outer local scale, \( \delta(x) \sim \delta \sim \frac{3}{4} \sim Re^{-3/4} Sc^{-1/2} \). This occurs because these sheets are not remnant of the boundary conditions at nozzle exit, but rather are continually created by the balance and competition between the thinning action of the local strain rate field and the thickening resulting from molecular diffusion. A broad range of flamelet models aim to relate scalar levels and scalar dissipation rates to molecular mass fractions, thus play a key role in turbulent combustion theory and in practical approaches to reducing emissions of regulated trace species from turbulent combustion process. On top of that all major dynamics take place at the intermittent T/NT interface or in its vicinity. Therefore only a thorough analysis and an accurate modeling of the fine-scalar structure involved in the mixing process, close to the T/NT interface, is crucial to establish a rigorous starting point for the development of flamelet models.

The present work employs DNS of turbulent planar jets at Reynolds number ranging from \( Re_{\lambda} = 120 \) to \( Re_{\lambda} = 160 \) (da Silva & Taveira (2010)) with a Schmidt number \( Sc = 0.7 \) to analyze the nature, local topology and properties of the “scalar interface” and to investigate the dynamics of turbulent mixing of a passive scalar near the turbulence front, in a plane jet.
Specifically, we employ conditional statistics in relation to the distance from the T/NT interface, denoted by $\langle I \rangle$, in order to eliminate the intermittency that affects common turbulence statistics close to the jet edge. The physical mechanisms behind scalar mixing near the T/NT interfaces and the associated turbulent scales and topology are investigated in detail.

This work is organized as it follows. In section two the numerical methods are described in detail. Section three presents a description and the analysis of the results. Finally, the paper ends with the summary of the main results and conclusions.

2. Numerical Methods

The present work employs temporal direct numerical simulations (DNS) of turbulent planar jets at Reynolds number ranging from $Re_\lambda = 120$ to $Re_\lambda = 160$ (da Silva & Taveira (2010)) with a Schmidt number $Sc = 0.7$. On table 1, there are listed the physical and computational parameters of the all the simulations used in the present work. All planar jet simulations employ the same numerical algorithm used in the reference simulation $PJET_{120}$ that was previously analyzed and extensively validated in the references (da Silva & Pereira (2009); da Silva (2009)), and therefore only a brief description of the numerics will be made. The numerical code used employs pseudo-spectral methods for spatial discretization while the temporal advancement is done by means of a 3rd order 3 step Runge-Kutta scheme, and the field is fully dialessed using the 3/2 rule (Canuto et al. (1987)). Direct numerical simulations of turbulent flows have been previously to study turbulent entrainment, the mixing process of dynamically passive scalars and the T/NT interface, for instance in wakes by Bisset et al. (2002), in round jets by Mathew & Basu (2002) and plane jets by da Silva & Pereira (2007, 2008) and da Silva & dos Reis (2011).

### Table 1. Simulations analyzed in the present study. $PJET_{120}$ is the simulation used in da Silva & Pereira (2009). $N_x \times N_y \times N_z$ is the number of colocation points along the streamwise ($x$) normal ($y$) and spanwise ($z$) directions, and $L_x \times L_y \times L_z$ is the size of the computational domain.

| Simulation   | $Re_\lambda$ | $L_x \times L_y \times L_z$ | $N_x \times N_y \times N_z$ | Initial Cond.   |
|--------------|--------------|-----------------------------|----------------------------|-----------------|
| $PJET_{120}$ | 120          | $256 \times 384 \times 256$ | $4h \times 6h \times 4h$  | Sint. Noise     |
| $PJET_{120}^{hr}$ | 120          | $648 \times 864 \times 648$ | $4h \times 6h \times 4h$  | Sint. Noise     |
| $PJET_{Chan}$ | 110          | $384 \times 486 \times 384$ | $6.3h \times 6h \times 4.2h$ | DNS Channel    |
| $PJET_{160}$ | 160          | $512 \times 768 \times 512$ | $4h \times 6h \times 4h$  | Sint. Noise     |

2.1. Physical and Computational Parameters

The numerical simulations of plane jets used as initial boundary condition an hyperbolic tangent profile for the mean velocity field, proved to be accurate near the inlet (Stanley et al. (2002) and da Silva & Pereira (2004)),

$$U(x, y, z) = \frac{U_1 + U_2}{2} - \frac{U_1 - U_2}{2} \tanh \left[ \frac{h}{4\delta_\theta} \left( 1 - \frac{2|y|}{h} \right) \right]$$

where the momentum thickness $\delta_\theta/h = 20$, $h$ is the inlet width and $U_1 = 1$ and $U_2 = 0$ are the center line and the far field velocities, respectively. To the mean velocity field was superimposed a 'spectral' synthetic noise, with a relatively high amplitude (8%) in order to speed up the transition process from a laminar regime to turbulence. There was one exception, the simulation
PJET\textsubscript{Chan} that used as initial condition an interpolated turbulent velocity field from a previously run DNS of a turbulent channel flow (Hauet \textit{et al.} (2007)). It is important however to notice the Reynolds number based on the Taylor scale and the initial momentum thickness matched the ones from the reference simulation. The scalar field was initialized in the same manner for all the simulations, including PJET\textsubscript{Chan}, using an hyperbolic tangent profile for the mean field,

\[
\Theta(x,y,z) = \frac{\Theta_1 + \Theta_2}{2} - \frac{\Theta_1 - \Theta_2}{2} \text{tanh} \left[ \frac{h}{4\delta_{\theta}} \left( 1 - \frac{2|y|}{h} \right) \right]
\]

where the scalar deficit thickness $\delta_{\theta} = 20$, and $\Theta_1 = 1$ and $\Theta_2 = 0$ are the center line and the far field scalar levels, respectively.

The Reynolds number based on the inlet width ranged between 3200 and 8000 and the grid sizes varied from 25 million nodes to 360 million nodes. The periodic computational domain of simulation PJET\textsubscript{120} (Fig.1) has a size of $(L_x, L_y, L_z) = (4h, 6h, 4h)$ discretized in a grid of dimensions $(N_x \times N_y \times N_z) = (648 \times 864 \times 648)$ along the streamwise ($x$), normal ($y$) and spanwise ($z$) directions, respectively. The initial Reynolds number is equal to $Re_h = \frac{(U_1-U_2)H}{\nu} = 3200$ and the self-similar regime is obtained at $\frac{T}{T_{ref}} \approx 20$, where $T_{ref} = \frac{h}{2U_1}$, at a moderately high Reynolds number, based on the Taylor scale, of $Re_{\lambda} = \frac{u'\lambda}{\nu} = 120$, where $\lambda$ is the Taylor scale, $u'$ is the \textit{rms} of the streamwise velocity and $\nu$ is the molecular viscosity. The remainder simulations, apart from PJET\textsubscript{Chan}, differ from the reference simulation only on the initial Reynolds number in the case of PJET\textsubscript{160} and on grid resolution for the case of PJET\textsubscript{120}.

2.2. \textit{T/NT Interface Detection and Conditional Statistics} 

One key ingredient of the present study consists in the use of conditional statistics. This are statistics computed in relation to the local distance from the T/NT interface (Bisset \textit{et al.} (2002); Westerweel \textit{et al.} (2005); da Silva & Pereira (2008)). Since the main procedure was already described in detail in reference (da Silva & Pereira (2008)), the current section procedure intends to briefly outline the guiding lines of the procedure employed to obtain these conditional statistics, with special attention to algorithm improvements.

The sketch in Fig.2 shows the T/NT interface separating the turbulent and the irrotational flow regions at the upper shear layer of the plane jet, with the coordinate system ($x, y$) used in the numerical simulation of the turbulent plane jet. The detection of the location of the T/NT interface is done using the vorticity norm threshold $\Omega = (\Omega, \Omega_i)^{1/2}$, where $\Omega_i$ is the vorticity field as in Bisset \textit{et al.} (2002). In the simulations, used in the present study, the detection threshold ranged from $\Omega = [0.7; 1.0] \frac{U_1}{T}$ which are very similar to the ones used by Bisset \textit{et al.} (2002) and Mathew & Basu (2002). The vorticity surface defined by the selected threshold is indicated by a solid line while the T/NT interface envelope is represented by grey dashed lines. As in previous studies (Bisset \textit{et al.} (2002); Westerweel \textit{et al.} (2005); da Silva & Pereira (2008)), due to the extreme complexity of the interface, the statistics are computed in relation to the interface envelope, rather than to the interface itself, without losing important information. Since the plane jet is homogeneous in the streamwise ($x$) and spanwise ($z$) directions, in previous studies, each ($x, y$) plane was treated independently, however in the present work the interface is detected using the entire 3D vorticity field, and the local axis in now normal to the 3D interface envelope, that allows for a better capture of spanwise dynamics close to the interface and therefore an increased accuracy. In the same manner, the computed statistics use data from the 3D data field, instead of using data from 2D \textit{homogeneous planes}.

Summarizing, the entire conditional procedure can be seen as having three independent steps: (i) the procedure starts with the determination of the T/NT interface envelope location $Y_I(x)$, using a cubic interpolation along the $y$ direction, and linear interpolations across the streamwise
and spanwise direction, for each one of the \((N_x, N_y)\) grid points in the original coordinate system; (ii) to which follows the determination of a new local 3D coordinate system \(y_I\), normal to the T/NT interface, defined at the interface location, and finally (iii) the conditional statistics are made in this local coordinate system. The T/NT interface is therefore at \(y_I = 0\), while the irrotational and turbulent regions are defined by \(y_I < 0\) and \(y_I > 0\), respectively. To increase the accuracy of the statistics “holes” of “ambient fluid” that appear inside the jet are removed from the statistical sample. In the first step of the procedure a special care was taken into the definition of a smooth interface, in special dealing with the bursts of turbulent fluid into the non-turbulent side. To perform this operation the algorithm took special care to distinguish these bursts from 3D turbulent structures, by assuring their connection to the turbulent core along at least one of all possible directions. Such procedure allowed the construction of a more accurate and smoother interface, with the additional benefit of reducing the errors in the determination of the local vector normal to the interface.

In step (ii) previous works followed different paths in the determination of the local frame. Apart from being 2D procedures, works as the one of Bisset et al. (2002) followed a similar procedure to ours, using a frame normal to the turbulence front surface, whereas in works by Westerweel et al. (2005, 2009) the conditional statistics are computed in a frame aligned with the reference frame, although centered at the interface location. Finally, to improve the degree of convergence several instantaneous fields taken from the fully developed turbulent regime were also used to improve the statistics.

With this procedure conditional statistics of any flow quantity can be made in relation to the distance from the T/NT interface. We denote these conditional statistics by \(\langle \rangle_I\) whereas \(\langle \rangle\) denotes the classical statistics computed using spatial averaging over the \((x, z)\) planes.

2.3. Conditional Statistics of the Vorticity Components near the T/NT Interface

Figure 3 shows conditional mean profiles of \(\langle |\Omega_x| \rangle_I\), \(\langle |\Omega_y| \rangle_I\), \(\langle |\Omega_z| \rangle_I\), and \(\langle \Omega_z \rangle_I\) in relation to the distance from the T/NT interface non dimensionalized by \(u_\lambda/\lambda\) where \(\lambda\) and \(u_\lambda\) are the Taylor micro-scale and velocity-scale associated with the taylor scale respectively, inside the turbulent region i.e. \(u_\lambda = (\varepsilon \lambda)^{1/3}\) where \(\varepsilon = 2\nu S_{ij}S_{ij}\) is the viscous dissipation rate. In agreement with other numerical and experimental works (Westerweel et al. (2005); Mellado et al. (2009)) all the
vorticity components display a sharp jump at the T/NT interface and the thickness of this jump is roughly equal to the Taylor micro-scale.

3. Results

3.1. Turbulence and Vorticity Structure near the T/NT Interface

The conditional mean streamwise $\langle u \rangle_I$ and normal $\langle v \rangle_I$ velocity profiles are displayed in Fig. 4. The conditional streamwise velocity is quite different from the classical streamwise velocity in a jet $\langle u \rangle$ which grows continually from the outer to the inner jet region. In contrast $\langle u \rangle_I$ is roughly constant in the irrotational region $y_I/\lambda < 0$ and increases sharply near the T/NT interface $y_I/\lambda = 0$. Moreover, the normal velocity gradient $\partial \langle u \rangle_I / \partial y_I$ has two distinct values inside the turbulent region: a stronger velocity gradient $\partial \langle u \rangle_I / \partial y_I$ in the region $0 < y_I/\lambda < 1.5$ is followed by a weaker gradient for $y_I/\lambda > 1.5$, as found in the conditional mean streamwise velocity from the experimental round jet from Westerweel et al. (2005, 2009). The conditional normal jet velocity $\langle v \rangle_I$ is negative in the irrotational flow and is positive in the turbulent region. In the present case $\langle v \rangle_I < 0$ for $y_I/\lambda < 0$ implies a transport of irrotational fluid into the turbulent region and $\langle v \rangle_I > 0$ for $y_I/\lambda > 0$ underlines the shear layer expansion due to momentum diffusion inside the turbulent region. Right at the T/NT interface $y_I/\lambda = 0$ we have $\langle v \rangle_I < 0$ which means that the velocity of the entrainment wind is bigger than the velocity of expansion of the turbulent front in agreement with Corrsin & Kistler (1955). The shape and magnitude of this profile is in excellent agreement with Westerweel et al. (2005, 2009).

The conditional mean profiles of mean pressure $\langle p \rangle_I$ and pressure variance $\langle p'p' \rangle_I$ for the present simulation are shown in figure 5. The mean pressure over the irrotational region, as inside the turbulent region is roughly constant. These two regions are connected by a sharp gradient with a thickness close to one Taylor scale, where the mean pressure inside the turbulent plane jet is considerably smaller than the surrounding pressure. This is explained by the presence of large...
vorticity structures with a radius of the order of one Taylor scale (da Silva & Taveira (2010)), along the jet shear layer, which are well known for being characterized by a local minima of the pressure field. In isotropic turbulence it is the presence of intense vorticity structures that is responsible for the negatively skewed shape of the pressure probability density function (Lesieur (1997)). The evolution captured for pressure variance over the conditional profiles \( \langle p'^2 \rangle_I \) shows a more surprising result, displaying a maximum inside the turbulent region at between one and two Taylor scales from the T/NT Interface. Pressure variance appears to be higher at the region where the large vorticity structures, in the jet shear layer, have their cores located. This can be explained both by the maximum in the induced velocity at the LVS perimeter and by the fact that near the T/NT interface pressure as local minimums streamwisely separated by at least a minimum distance of two core radius. The pressure variance grows quite rapidly inside the irrotational regions as one approaches the T/NT interface, however it decreases more slowly as the jet centre is approached. These two facts can be explained by the fact that close to the interface significant velocity and thereby pressure fluctuations are induced by the LVS lying around the T/NT interface, whereas pressure fluctuations decrease as the degree of isotropy increases towards the center of the jet.

Figures ?? show the conditional mean profiles of the Taylor and Kolmogorov micro-scales in the jet. In inhomogeneous turbulence it is interesting to define a longitudinal \( \lambda_x^2 = \langle u'^2 \rangle / \langle (\partial u' / \partial x)^2 \rangle \), a normal \( \lambda_y^2 = \langle v'^2 \rangle / \langle (\partial v' / \partial y)^2 \rangle \), and a transverse \( \lambda_z^2 = \langle w'^2 \rangle / \langle (\partial w' / \partial z)^2 \rangle \) Taylor micro-scale. \( \lambda_x \), \( \lambda_y \) and \( \lambda_z \) are similar \( \approx 0.15H \), but not exactly equal inside the turbulent region of the jet, which indicates some level of anisotropy of the jet inside the shear layer. This anisotropy is clearly important in the irrotational region where \( \lambda_x \) and \( \lambda_y \) are much bigger than \( \lambda_z \). The most interesting fact is that the Taylor scales are roughly constant inside the turbulent region and therefore can be used to characterize this region. In this work, the distance from the T/NT interface is non-dimensionalized by the ‘mean’ Taylor micro scale \( \lambda = (\lambda_x + \lambda_y + \lambda_z) / 3 \) inside the turbulent region. The conditional Kolmogorov micro-scale shown in Fig.?? is computed using the conditional viscous dissipation rate \( \eta = (\nu^3 \varepsilon)^{1/4} \) and is constant \( \eta = 0.008H \) inside the turbulent region, and for this fact can be used also as a characteristic turbulent length in the conditional statistics. These results are in agreement with da Silva & Taveira (2010), where it was seen the size of the LVS and thereby the interface thickness to be of the order of the Taylor scale. \( R \sim (\frac{S' u'}{L_{11}})^{1/2} \) and the strain rate acting on a LVS near the jet edge is given by \( S' \sim u' / L_{11} \), where \( u' \) is the \( rms \) of the streamwise velocity and \( L_{11} \) is the integral scale of turbulence, from which results \( R \sim (\frac{\nu}{u' / L_{11}})^{1/2} = L_{11} Re_0^{-1/2} \sim \lambda \).
3.2. Passive Scalar Structure near the T/NT Interface

As important as studying the fine scale structures of vorticity in turbulent flows, is to unveil the local structure of scalar involved in scalar mixing. This mixing process occurs at the intermittency region of shear layers and therein is crucial to understand the implications of local dynamics and turbulence structures in the topology of scalar coherent structures and the dynamics of scalar mixing.

A local conditional approach must be followed in order to shade light over a definite answer to these questions. This matter becomes even more important when one realises that scalar dynamics are even sharper than the ones of vorticity field when we cross the interface between the non-turbulent fluid and the turbulent region. Figures ?? show some conditional statistics from a-priori tests at the edge of a turbulent plane jet. From the rms of velocity and scalar fluctuations, it becomes obvious that the presence of the interface has a much larger local impact over the scalar field when compared to the velocity. This is essentially true because important velocity fluctuations arise at the T/NT interface and over non-turbulent region by means of inviscid kinetic energy transport, namely by pressure diffusion Taveira et al. (2009). Figures ?? present a comparison between sub-grid production and dissipation for the cases of the velocity and scalar fields. Once again it becomes obvious that close to the T/NT interface the particular dynamics of the scalar field become much more intense at small scales than the velocity and vorticity field. Both subgrid scales production and dissipation are almost ten times larger than the ones observed for the core more homogeneous turbulence. Modeling the mixing mechanisms for scalar become thereby much more demanding over refinement requirements or have to account for a much larger share of the mixing dynamics. Since the first alternative is unpractical on the engineering point of view, a deep and accurate understanding of local interface topology and transport mechanisms are vital to establish a starting point to LES models.

![Image](image1.png)

**Figure 8.** Scalar gradient sheets (red) involving the IVS and LVS close to the jet edge.

![Image](image2.png)

**Figure 9.** Scalar gradient field at the jet center.

From an instantaneous visualization of the flow field (Fig.8) one can see sheets of scalar gradient involving the IVS and LVS close to the jet edge, showing clearly that the fine scale structures of scalar is organized under a sheet-like topology, rather than in tubes. In figure 9, as seen by Buch & Dahm (1998) at unitary Schmidt, the sheets are not flat as expected for high Schmidt numbers, but somewhat contorted. In particular the sheets follow perfectly the highly contorted shape of the interface, presenting preferential directions of alignment that may influence scalar dynamics when compared to homogeneous turbulence. As in Buch & Dahm (1998) these sheets present different thickness at a local level but remain of the same order of magnitude. The thickness of such structures varies along the jet due to their particular sensitivity to the local characteristics of persistent strain and scalar gradients at the interface. Figure 10 shows a local profile of scalar gradient over one of these structures, where one can see an extremely steep and intense jump right at the T/NT interface. This jump appears to have a thickness of the order of the Kolmogorov length scale and close to $\delta_\theta \sim 0.2\lambda \approx 3\eta$, clearly much thinner than the LVS defining the bounds of the T/NT interface. This raises the question about the existence of a scalar interface layer, rather than a common interfacial structure for both the velocity and scalar fields, as commonly suggested Westerweel et al. (2009). To analyze this question one may...
look at the classical and conditional profiles of mean scalar level, scalar fluctuations and scalar gradient.

Figure 10. Local evolution of the scalar field, $\theta$.

Figure 11. Classical mean scalar $\langle \theta_I \rangle$ and scalar variance $\langle \theta_I'^2 \rangle$.

Figure 12. Conditional mean scalar $\langle \theta_I \rangle$ and scalar variance $\langle \theta_I'^2 \rangle$.

Figure 11 shows the classical well known near Gaussian profile of mean scalar and the double hump distribution in the scalar fluctuation. However as expected, from the previously shown results, these are much different than the local real dynamics displayed in the conditional profiles (Fig.12). Here one can observe the existence a very sharp jump, right at the T/NT interface, both for scalar mean and fluctuations levels. It is important to notice that this jump is much sharper than the one observed in the conditional profiles of streamwise velocity. Unlike the classical mean, $\langle \theta_I \rangle$, scalar profile displayed in figure 11 which grows continually from the outer to the inner jet region, $\langle \theta_I \rangle$ is roughly constant at the irrotational region $y_I/\lambda < 0$ and increases sharply near the T/NT interface $y_I/\lambda = 0$. Moreover, the normal velocity gradient $\partial \langle \theta_I \rangle/\partial y_I$ has two distinct values inside the turbulent region: a stronger velocity gradient $\partial \langle \theta_I \rangle/\partial y_I$ in the region $0 < y_I/\lambda < 1$ is followed by a weaker gradient for $y_I/\lambda > 1$, as found in the conditional profiles from the experimental round jet of Westerweel et al. (2009). This first region roughly corresponds to the T/NT interface region, and is a reason supporting a common interface structure. In the case of the $P_{JET_{Chan}}$, displayed in figure 12 one can even see the jump in the scalar level to end at approximately $[0.55; 0.6]\lambda$, right at the end of the jump in the vorticity norm, and of course in agreement with the radius of the LVS lying at the interface. As for the scalar variance, one can see that scalar fluctuations also display two distinct, roughly constant, gradient regions. The first one located at the interface, whereas and the second one ends at the maximum fluctuations level at $y_I/\lambda \sim 4$. This region appears to be the length required by the turbulence to reach a more homogeneous state, also verified in the balances of
vorticity and kinetic energy, close to the T/NT interface, by Taveira et al. (2009). However, perhaps a more important quantity to study in order to analyze the topology of scalar is the scalar gradient, as this quantity stands for the scalar as vorticity, or enstrophy, for the velocity field. As seen in the flow visualizations, unlike vorticity sheets that roll up due to the strain field and collapse into tube-like structures, intense gradient sheets, arising from persistent strain, maintain their sheet-like structure. Despite so, locally, at the T/NT interface this structures display rather complex geometries due to the similar length scale between their dimensions, namely their thickness, and the length of coherent strain regions. Scalar gradient statistics may therefore help to shade some light over the global topology of the scalar interface. Figures 13 and 14 establish a comparison of classical and conditional profiles, where clearly one can see that only conditional statistics are able to capture the local topology seen in figures ??.

In the conditional profile one can see an extremely sharp jump, right at the T/NT interface, with a thickness close to the Kolmogorov scale, \( \delta \theta \sim 0.2 \lambda \approx 3 \eta \), as seen in the instantaneous profile. This evidence contrarily to the jump in the scalar level may indicate the existence of a thinner region, when comparing to the T/NT interface, central to the process of scalar mixing.

![Figure 13. Classical profile of the scalar gradient \( \langle G_i G_i \rangle \).](image)

![Figure 14. Conditional profile of the scalar gradient \( \langle G_i G_i \rangle \).](image)

![Figure 15. Conditional profile of \( \langle G_y \rangle \).](image)

All three components of the gradient (not shown) display the same behavior, despite one notices \( |G_y| \) to be more intense at the turbulence front. This is expected because in a jet plane, close to the T/NT interface, the normal direction \( (y) \) presents the higher degree of anisotropy. However, the important fact is that all components display a peak at a distance close to \( 3 \eta \), considerably smaller than the LVS dimensions, but typical from the sheets observed at the interface Buch & Dahm (1998). From one Taylor scale onwards, \( y_I / \lambda \gtrsim 1 \), all components fall to approximate mean values that remain rather constant along the entire turbulence core, showing that turbulence and scalar dynamics undergo a fast transition across the interface defined by the LVS. Fig.15 represents \( G_y \) and shows that the local dynamics takes place at even finer scales as one sees to take the most intense value a distance smaller than two Kolmogorov scales, \( y_I / \eta \lesssim 2 \).

To finalize this section it is interesting to depict how the dimensions of the fine scale scalar structures relate with the characteristic scales for a scalar field, rather the ones deeply related with the velocity and vorticity fields. For this purpose one calculated the following scalar micro scales, displayed in Figs.16, 17 and 18: the Batchelor scale, \( \eta_B^\theta = \left( \nu \lambda^2 \frac{2}{\epsilon} \right)^{1/4} \), the Corrsin scale, \( \eta_C^\theta = \left( \frac{2}{N} \right)^{1/4} \), and generalized Taylor scale for a scalar field, \( \lambda_y^2 = \frac{2 \langle \theta \theta' \rangle}{\langle \partial \theta / \partial y \rangle} \). One can see that Batchelor and Corrsin scales fall to very similar values due to the unitary Schmidt number. These are also from the same order of the Kolmogorov scale, therefore at this low Schmidt
number one is unable to point out a scale over another to consider the most characteristic of the scalar interface. On the other hand from the Taylor scale one can see that this one is about ten times smaller than one for the velocity field, \( \lambda_\theta \approx 0.1 \lambda \), which is very close to the thickness of the jumps in the scalar gradient conditional profiles and also related with the range of action of local transport mechanism as one will see ahead. This fact unveils a reality that is much more convenient for the explanation and reasoning of the gradient sheets thickness and the confinement local transport mechanisms, however results at higher Schmidt numbers are needed in order to confirm these results.

3.3. Scalar Gradient Transport Equation at the T/NT Interface Vicinity

Understanding the dynamics of scalar transport and mixing at the T/NT interface is of extreme importance to combustion modeling. The local mechanisms responsible for scalar mixing, at fine scales, are depicted by the analysis of all terms involved in the scalar gradient balance in the vicinity of the turbulence front. This is done by means of visualizations of the instantaneous flow field and conditional profiles of the scalar gradient budget.

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} G_i G_i \right) + u_j \frac{\partial}{\partial x_j} \left( \frac{1}{2} G_i G_i \right) = -G_i G_j S_{ij} - \gamma \left( \frac{\partial G_i}{\partial x_j} \right)^2 + \gamma \frac{\partial^2}{\partial x_j^2} \left( \frac{1}{2} G_i G_i \right)
\]

Figure 19 shows the mean evolution of the transport equation for unconditioned ensemble averages. It shows the well-known classical picture of almost perfect balance between production and dissipation mechanisms, whereas transport mechanisms are almost negligible. Such dynamics are also similar to the classical ones observed previously for enstrophy transport. Also, as observed for enstrophy in previous works (Taveira et al. (2009)), local instantaneous profiles presented in figure 21 do not agree with this classical view, evidencing important events located at the edge of the jet. Indeed, these highlight the role of transport mechanisms over the production and dissipation ones.

Fig. 20, illustrates the mean conditional profiles of all mechanisms in the scalar gradient balance, where is possible to observe radical differences in local dynamics when comparing to the classical view, clearly unsuited to study such fine scale dynamics. The conditional statistics are able to overtake the obstacles posed by local intermittency in the region bounding turbulence unveiling the true about the T/NT interface scalar mixing. These results are in remarkable agreement with the instantaneous profiles, at least in a qualitative point of view. The quantitative differences
can be easily explain by the fact that the profiles displayed in figure 21 are computed over an extremely intense structure with the purpose of reinforcing the local importance of both small and large scale transport mechanisms. Although extremely important close to this intense structure, it is easily observable that in average the influence of these transport mechanisms fades rapidly. This can also be observed in the conditional profiles from figure 20. One can even notice that these mechanisms almost appear to cease their action from one Taylor scale inwards, \( \frac{y}{\lambda} > 1 \), giving place to the well-known balance between production and dissipation. A closer look into each mechanism shows that both transport mechanisms action becomes almost negligible, in average, after one Taylor scale \( \frac{y}{\lambda} \gtrsim 1 \), whereas production and dissipation only reach their turbulent values at \( \frac{y}{\lambda} \gtrsim 4 \) suggesting turbulent processes need some time to become fully effective, in agreement with the fact that along this first two Taylor scales lye the anisotropic structures defining the T/NT interface layer. Perhaps a more important observations is that the characteristic scale of all mechanisms seems to be of the order of the Kolmogorov scale, in agreement with the small scale mixing structure studied by Buch & Dahm (1998). Right at the T/NT interface one can see that convection is the dominant term, accounting for the biggest part in scalar mixing and communication to the external non-turbulent regions. Diffusive transport is also clearly responsible for scalar mixing, making its action felt even at further outer regions when compared to the advection mechanism promoted by the LVS that define the T/NT Interface. Both transport mechanisms can be seen to communicate scalar by mixing it from regions of high scalar gradient production, arising from the interaction of persistent strain fields produced by the long lived counter-rotating LSV with similar circulation, lying at the vicinity of the T/NT interface and responsible for its highly contorted shape, and the obvious presence of scalar gradient at the T/NT interface, as observed by Ruetsch & Maxey (1991) in homogeneous turbulence. Finally, it is also important to bear in mind that this characteristic length scale is also of the order of magnitude obtained for the scalar Taylor scale and the classical Corrsin and Batchelor scales. More data, from simulations at different Schmidt numbers is needed before a definitive answer can be proposed. Also important is to notice the existence of production and dissipation outside the turbulent region, close to the T/NT interface. This is easily explainable
by the presence of non-negligible persistent strain and scalar fluctuation (due to high diffusive
effects and small Schmidt numbers) at these regions.

4. Conclusions

In this work several direct numerical simulations (DNS) of turbulent plane jets were used to
study in depth the properties of the T/NT interface and the topology of the vorticity and scalar
fields. To accomplish these objectives it were studied, by mean of classical and conditional
statistics, important turbulent quantities, as for instance pressure, velocity, and kinetic energy,
along with the analysis of the transport equation of scalar gradient across the T/NT interface.
From the analysis of turbulence features it was confirmed the existence of sharp jumps at velocity,
scalar and vorticity norm at the T/NT interface region. These jumps have a thickness of the
order of the Taylor scale in the case of a turbulent plane jet, also seen to be the one that allows
for the best fitting and scaling of the vorticity norm, at the T/NT interface vicinity, for velocity
fields at different Reynolds numbers. This leads to the verification that the thickness of the
interface was dependent on the local topology of the coherent vorticity structures, suggesting
the interface to be, in fact, made of the boundaries of the large vorticity structures (LVS), and
therefore its thickness is equal to the radius of the biggest long lived coherent structures at the
interface outer boundary, namely $\delta_\omega \sim R_{LV S}$, which is found to be of the order of the Taylor
scale. As for the pressure field, it was seen to have a minimum close to one Taylor scale from the
interface in agreement with the presence of the cores of the LVS defining the T/NT interface. It
was also found that this location coincided with the presence of maximum pressure fluctuations
responsible for the spread of velocity fluctuations and Reynolds stresses to the entrained and
irrotational fluid.

From the analysis of a dynamically passive scalar, close to the jet edge, it was verified that
the exchanges in the turbulent mixing occur due to the presence of high scalar gradient regions,
spatially arranged in coherent sheet-like structures, whose thickness was found to be of the order
of the Kolmogorov scale, rather than the Taylor scale. Therefore one may suggest the existence
of a "scalar interface" with a thickness of the order of the Kolmogorov scale. It is also very
important to notice that from the analysis of the characteristic scales for a scalar fields one saw
that the generalized scalar Taylor scale, $\lambda_\theta$ to be of the order of the Kolmogorov scale, and
therefore more data from simulations at different Reynolds and Schmidt numbers are needed
in order to reach a definite conclusion. However the conditional profiles for the mean scalar
field and scalar fluctuations showed these quantities to have a jump across a region of the same
thickness of the T/NT interface evidencing that despite gradient sheets are much thinner the
scalar fields undergoes a steep transition across the entire T/NT interface. From the analysis
of the mixing and transport of scalar it was find that the all mechanisms of the scalar gradient
balance are found at a very confined region, close to the T/NT interface, with a thickness of the
order of the generalized scalar Taylor scale, $\lambda_\theta$. The most important realization is that unlike
suggested by classical statistics, close to the T/NT interface, the transport mechanisms are not
only non-negligible but the dominant ones. From the analysis of each mechanism involved in
the balance it was observed that small scale processes such as molecular diffusion present an
importance similar to the ones connected to larger scales of the flow, but nevertheless advection
is seen to play the dominant in mixing of a passive scalar near the T/NT interface, smoothing
scalar gradients inside the interface ($0.1 \lambda$ to $1 \lambda$) and boosting them as far as $-2.5 \gamma_{\eta}$. However,
the results suggest scalar mixing to result from a complex interaction between large and small
scale mechanisms. It was also verified that production and dissipation mechanisms take one
Taylor scale to become dominant and all mechanism need about four Taylor scales, $y_1/\lambda \gtrsim 4$,
before reaching their turbulent regimes, where a near perfect balance between production and
dissipations becomes established.
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