Evolution of passive scalar statistics in a spatially developing turbulence

I.Paul,[∗] G. Papadakis, and J.C. Vassilicos

Department of Aeronautics, Imperial College London, London - SW7 2AZ, UK

(Dated: January 9, 2018)

Abstract

We investigate the evolution of passive scalar statistics in a spatially developing turbulence using direct numerical simulation. Turbulence is generated by a square grid-element, which is heated continuously, and the passive scalar is temperature. The square element is the fundamental building block for both regular and fractal grids. We trace the dominant mechanisms responsible for the dynamical evolution of scalar-variance and its dissipation along the bar and grid-element centerlines. The scalar-variance is generated predominantly by the action of mean scalar gradient behind the bar and is transported laterally by turbulent fluctuations to the grid-element centerline. The scalar-variance dissipation (proportional to the scalar gradient variance) is produced primarily by the compression of the fluctuating scalar gradient vector by the turbulent strain-rate, while the contribution of mean velocity and scalar fields is negligible. Close to the grid element the scalar spectrum exhibits a well-defined $-5/3$ power law, even though the basic premises of the Kolmogorov-Obukhov-Corrsin theory are not satisfied (the fluctuating scalar field is highly intermittent, inhomogeneous and anisotropic, and the local Corrsin-microscale-Peclet number is small). At this location, the PDF of scalar gradient production is only slightly skewed towards positive and the fluctuating scalar gradient vector aligns only with the compressive strain-rate eigenvector. The scalar gradient vector is stretched/compressed stronger than the vorticity vector by turbulent strain-rate throughout the grid-element centerline. However, the alignment of the former changes much earlier in space than that of the latter, resulting in scalar-variance dissipation to decay earlier along the grid-element centerline compared to the turbulent kinetic energy dissipation. The universal alignment behavior of the scalar gradient vector is found far-downstream although the local Reynolds and Peclet numbers (based on the Taylor and Corrsin length scales respectively) are low.

[∗] p.immanuvel@imperial.ac.uk

I. INTRODUCTION

A passive scalar is transported by the flow but does not react back, i.e. does not influence the carrier flow. Examples include small variations of temperature, pollutant concentration etc. Understanding the statistical behavior of scalar fluctuations and their gradients is important both from the application as well as the fundamental points of view. Most of the industrial processes (for instance heat exchange, mixing, combustion) involve the transport of scalar by a turbulent flow. Similarly, understanding of micro-mixing, and thus arriving at an effective mixing model, requires knowledge of the fluctuating scalar gradients [1]. The study of passive scalar is also fundamental to the understanding of turbulence itself. Numerous studies on various aspects of scalar turbulence have appeared in the literature and are reviewed in Sreenivasan [2], Sreenivasan and Antonia [3], Majda and Kramer [4], Shraiman and Siggia [5], Warhaft [6], Falkovich et al. [7], Dimotakis [8], Gotoh and Yeung [9].

The dynamics of passive scalar turbulence have been explored theoretically [10, 11], experimentally $[1, 12-15]$, and numerically $[16-21]$ for various flow configurations. Some flows have shear (jets or wakes) and some are shear-free (grid turbulence). In most shear-free flows, a mean scalar gradient is imposed at the inlet [22–26], but there are also studies where the grid is heated [12, 27, 28]. It is important to stress that almost all of the previous studies on shear-free scalar turbulence are either experiments carried out rather far downstream of the grid, or periodic box direct numerical simulations with an imposed mean scalar gradient. Thus, they have analyzed mostly the scalar properties in turbulence which is designed to be close to homogeneous isotropic turbulence (HIT, hereafter).

Last decade has witnessed an interest in turbulent flows generated by fractal grids. Since the work of Seoud and Vassilicos [29], many studies have focused on the turbulent flow generated by multi-scale or fractal grids [30–32]. Recently, Valente and Vassilicos [33], Zhou *et al.* [34, 35, 36] and Paul *et al.* [37] have shown that the turbulence generated by a single square grid-element shares similarities with that generated by a fractal square grid. In both flows, there is an extended turbulent production region followed by a decay region. The production region is characterized by increasing turbulent intensity, which decays further downstream. Previous experimental and numerical studies of Paul et al. [37], Laizet et al. [38], Gomes-Fernandes et al. [39], Laizet et al. [40] have shown that the dynamics of velocity-

gradients in the near-grid region are different from the HIT case. In particular, the velocity spectrum has a $-5/3$ power-law slope even in the near-grid region where the turbulence is highly inhomogeneous and developing. In that region, the $Q - R$ diagrams (where Q and R are the second and third invariants of the velocity gradient tensor) are not developed, and strain dominates enstrophy.

Previous works have demonstrated significantly increased turbulent scalar fluxes in the cross-stream direction in the lee of a fractal grid, and proposed a mechanism to explain this behavior [41–45]. To the best of authors' knowledge, there are no comprehensive studies on the dynamical evolution of scalar-variance and scalar gradients in turbulence generated by fractal or single square grids.

The central aim of this paper is not only to study the statistical behavior of scalar gradients, but also to investigate their relationship with velocity gradients. The turbulence is generated by a single square grid-element which is heated continuously, and the passive scalar is temperature. The present work complements the previous study of the authors on the evolution of velocity gradients in a turbulent flow generated by the same geometry [37]. The scalar gradient analysis aims to answer the following five questions:

- 1. How are the large- and small-scale terms of scalar turbulence generated and transported in this spatially developing turbulence? We identify the dominant mechanisms responsible for the transport of these quantities in §III.
- 2. It is sometimes believed that the evolution of scalar dissipation is similar to that of the mean enstrophy of fluctuations [46]. Do these quantities indeed behave similarly in the examined flow? We report on the similarities and differences along the grid-element and bar centerlines in §III B and §VI. In §V, we explain the observed trends by probing more deeply into the production of these quantities due to turbulent stretching/compressing by strain-rate.
- 3. Does the −5/3 power-law slope of the scalar spectrum appear in the inhomogeneous, near grid-element region? Previous studies have established that for HIT the −5/3 slope appears over a wider range of frequencies than the velocity spectrum (refer to the review of Warhaft [6]). It is not clear if this is also true when the scalar field is highly inhomogeneous and developing. We explore this question in §IV.
- 4. If indeed there is a power-law in the scalar spectrum in the near grid-element region, how do the small-scale scalar dynamics correlate with the scalar cascade? The stretching of vorticity vector is believed to be closely associated with the energy cascade in turbulent flows. The equivalent process in the scalar cascade is the stretching/compressing of the passive scalar gradient vector. In $\S V$, we correlate the behavior of scalar small-scale terms with the −5/3 power-law slope of the scalar spectra.
- 5. How do the scalar spectrum and the scalar gradient dynamics evolve from the near grid-element region to the far-downstream? Since the turbulence is developing, the dynamics of scalar gradients are also expected to vary and we study this evolution throughout this paper.

The rest of the paper is organized as follows. The next section provides the details of the numerical setup. The budgets of large and small scale quantities (scalar variance and dissipation respectively) are discussed in §III. Then we analyze the scalar spectra in §IV and the relation with small scale stretching/compressing $(\S V)$. The evolution of scalar-variance and turbulent kinetic energy dissipation rates are analyzed in §VI. Finally, we summarize the main conclusions in §VII.

II. NUMERICAL METHOD AND COMPUTATIONAL PARAMETERS

Throughout the paper, the instantaneous, mean, and fluctuating velocity fields are denoted as u_i^* , U_i , and u_i respectively (where $i = 1, 2, 3$). The corresponding variables for pressure and temperature are p^* , P, p and T^* , $\langle T^* \rangle$, T. Throughout the paper, the brackets <> are used to represent the time-averaging operation. The continuity, momentum and scalar conservation equations are written as:

$$
\frac{\partial u_i^*}{\partial x_i} = 0 \tag{1}
$$

$$
\frac{\partial u_i^*}{\partial t} + u_j^* \frac{\partial u_i^*}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p^*}{\partial x_i} + \nu \frac{\partial^2 u_i^*}{\partial x_j \partial x_j} \tag{2}
$$

$$
\frac{\partial T^*}{\partial t} + u_j^* \frac{\partial T^*}{\partial x_j} = \alpha \frac{\partial^2 T^*}{\partial x_j \partial x_j} \tag{3}
$$

FIG. 1: Sketch of the computational domain: (a) front view, (b) side view at plane $z/t_0=0$ (the sketches are not to scale).

where ρ, ν, α are the density, kinematic viscosity and thermal diffusivity of the fluid respectively.

These equations are solved using the in-house parallel solver, *Pantarhei*. The solver is based on unstructured finite volume discretization in a collocated variable arrangement. The convective and diffusive spatial terms are discretized using the second-order centraldifferencing scheme, while the second-order backward scheme is employed for time advancement. The code is parallelized using the PETSc libraries [47]. More details about the solver can be found in Paul *et al.* [37], Paul [48], Paul *et al.* [49, 50].

The front view of the computational domain in the $y - z$ plane is depicted in figure 1a. The origin of the coordinate system is located at the center of the element. The bar has lateral thickness $t_0 = 43mm$, length $L_0 = 229mm$, and streamwise thickness of 6mm. The blockage ratio is 20%. A characteristic wake interaction length scale, defined as $x^* = L_0^2/t_0$ (refer to [30]), is used to normalize the streamwise distance downstream of the grid-element. A side-view of the computational domain at plane $z/t_0 = 0$, with details on the size of the domain and type of boundaries, is shown in figure 1b.

Uniform velocity and temperature profiles are prescribed at the inlet $(U_{\infty} \text{ and } T_{\infty} \text{ respectively})$ tively) and a convective boundary condition is imposed at the outlet. All lateral boundaries are periodic. On the grid-element surface, no-slip condition is applied for velocity and uniform heat flux (\dot{q}_w) for temperature. The *Reynolds* number based on the the free-stream velocity U_{∞} and the bar length L_0 is $Re_{L_0} = 2650$, while based on the lateral thickness t_0 is $Re_{t_0} = 500$. The Prandtl number, $Pr = \nu/\alpha$, is 0.71.

The same mesh employed in our previous study [37] is also used for this paper. It was shown in Paul *et al.* [37] that the ratio of a characteristic mesh size to the Kolmogorov length scale is less than 1 throughout the computational domain. Since $Pr < 1$, the Obukhov-Corrsin scale η_{OC} ($\eta_{OC} = \eta Pr^{-3/4}$ where $\eta = (\nu^3/\epsilon_k)^{1/4}$ is the Kolmogorov length scale and $\epsilon_k = 2\nu \langle s_{ij} s_{ij} \rangle$ where $s_{ij} = \frac{1}{2}$ $rac{1}{2} \left(\frac{\partial u_i}{\partial x_i} \right)$ $\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}$ ∂x_i is the turbulent strain-rate) is larger than the Kolmogorov length scale. Therefore, the mesh resolution is finer for the scalar field compared to the velocity field. At worst, the mesh resolution is $0.63\eta_{OC}$ in the whole domain. More details about the mesh and the numerical setup are presented in Paul et al. [37].

The validation of the solver against experiments for one-point velocity and velocitygradient statistics is presented in Paul *et al.* [37]. We rely upon this validation for the present study since there are no experiments available for the scalar field.

III. BALANCE OF TRANSPORT EQUATIONS

In this section we investigate the dynamics and transport mechanisms of large and small scales of scalar turbulence. The large-scale terms are characterized by fluctuations and the small-scale terms by fluctuation gradients [51]. Scalar-variance is considered a large-scale term while scalar-gradient-variance is a small-scale term. The transport equations of these quantities are studied along the bar and grid-element centerlines because of the different dynamics prevalent at these two locations.

The scalar field under consideration is visualized first. Contours of the instantaneous scalar field are depicted in figure 2a. The scalar is being injected into the wake by heating the grid-element. Vorticity is produced at the walls and shed into the wake. Both scalar and vorticity have therefore initially the same length scale. For the time instant shown in the figure, the scalar wakes behind the bars start meeting at $x/x^* \approx 0.4$. As shown later, the scalar wakes meet at $x/x^* \approx 0.2$ on average, which is similar to the location reported in Paul et al. [37] for the meeting of vortical wakes.

The time-averaged scalar field is shown in figure 2b. The iso-line of normalized mean vorticity vector magnitude is superimposed in order to compare the spreading rate of vor-

FIG. 2: Contours of (a) instantaneous temperature, (b) mean temperature fields. The isocontours range from 1 to 1.5 of T_{∞} . The white colored dotted line in (b) is the isoline of normalized mean vorticity vector magnitude $(\langle |\omega^*| \rangle t_0/U_\infty)$ of 0.18. The black colored dotted-dashed-line is the centerline of the grid-element, while the bar centerline is represented by a pink dotted-dashed-line.

ticity and scalar wakes. The two rates are similar, as expected [52]. A mean recirculation region forms behind the bars and its length is approximately $3.7t_0$ (or $0.13x^*$). The scalar is trapped inside this region, leading to high values in the centerline (depicted as a small circular red area behind the bars in figure 2b).

A. Scalar-variance balance

The transport equation of scalar-variance $\frac{1}{2} \langle T^2 \rangle$ can be written as (refer to [52])

$$
\frac{\partial \left(\langle \frac{1}{2}T^2 \rangle\right)}{\partial t} = -U_j \frac{\partial \left(\langle \frac{1}{2}T^2 \rangle\right)}{\partial x_j} - \langle u_j T \rangle \frac{\partial \langle T^* \rangle}{\partial x_j} - \alpha \langle \frac{\partial T}{\partial x_j} \frac{\partial T}{\partial x_j} \rangle - \frac{\partial}{\partial x_j} \langle \frac{1}{2} u_j T^2 \rangle}{r_v} + \alpha \frac{\partial}{\partial x_j} \left(\frac{\partial \frac{1}{2} \langle T^2 \rangle}{\partial x_j}\right) - \frac{\partial}{\partial x_j} \left(\frac{\partial \frac{1}{2} \langle T^2 \rangle}{\partial x_j}\right)}{r_v}
$$
(4)

where C_v is the mean flow convection, G_v is the production by mean scalar gradient, ϵ_v is the scalar dissipation, T_v is the transport by turbulent fluctuations and D_v is the molecular diffusion. The transient term in the left hand side is 0, as only time-averaged quantities are considered. Note that ϵ_v is proportional to the scalar-gradient variance $\left\langle \frac{\partial T}{\partial x_i} \right\rangle$ ∂x_j ∂T ∂x_j \setminus , the proportionality constant being the thermal diffusivity, α .

Figure 3a presents the evolutions of scalar-variance and turbulent kinetic energy along the

FIG. 3: (a) Evolution of scalar-variance and turbulent kinetic energy along the bar centerline, (b) Evolution of budget terms of scalar-variance along the bar centerline. All terms are normalized by $U_{\infty} T_{\infty}^2 / t_0$.

bar centerline. The scalar-variance increases from $x = 0$ till the end of the mean recirculation region (i.e. $x = 0.13x^*$) and then decays downstream. This trend is very similar to the evolution of the turbulent kinetic energy, but the scalar variance decays slightly faster. The dynamics of scalar-variance is further analyzed through the evolution of the budget terms (figure 3b). Close to the bar, the mean scalar gradients generate scalar-variance, which is transported by the mean flow. The production and transport terms increase until the end of the mean recirculation region, while they are balanced by the turbulent transport and dissipation terms. Downstream of the mean recirculation region, the gradient production and mean transport decrease. After $x/x^* \approx 0.5$, the turbulent transport term becomes negligible and the scalar-variance decays due to dissipation while it is carried by the mean flow.

We now turn our attention to the evolution of scalar-variance and turbulent kinetic energy along the grid-element centerline, figure 4a. Although the variation of these quantities was very similar behind the bars as demonstrated in the previous figure 3a, they exhibit intriguing differences along the grid-element centerline. Firstly, the scalar-variance is negligible for

FIG. 4: (a) Evolution of scalar-variance and turbulent kinetic energy along the grid-element centerline, (b) Evolution of budget terms of scalar-variance along the grid-element centerline. All terms are normalized by $U_{\infty} T_{\infty}^2/t_0$. The transport due to fluctuations of the turbulent kinetic energy is also shown.

 $x/x*$ < 0.2, but the kinetic energy is clearly not. The latter is generated by the work done by pressure [37], a mechanism which is absent for the scalar variance. More specifically, the presence of vortex shedding behind the bars generates a fluctuating pressure field that correlates with the velocity in the grid-element centerline, making the generation term $-\frac{\partial(u_j p)}{\partial x_j}$ ∂x_j for kinetic energy dominant in the lee of the grid. Secondly, the onset of scalar-variance decay occurs upstream compared to that of the turbulent kinetic energy. While the turbulent kinetic energy starts decaying around $x/x^* \approx 0.5$, the decay of scalar-variance starts around 0.4. Comparing figures 3a and 4a, it is interesting that the variation of scalar-variance and turbulent kinetic energy are qualitatively similar, with both quantities reaching a peak value at exactly the same location along the bar centerline, but along the grid-element centerline, their behavior is markedly different. They peak at different locations and the decay rate of scalar variance is significantly faster compared to that of the turbulent kinetic energy.

The budget terms, shown in figure 4b, provide insight into the evolution of scalar-variance along the grid-element centerline. The first term that becomes active is the turbulent trans-

port term, $T_v = -\frac{\partial}{\partial x}$ $\frac{\partial}{\partial x_j}\Big\langle \frac{1}{2}$ $\frac{1}{2}u_jT^2$. The two lateral directions $(j = 2, 3)$ make the largest contribution to this term, indicating that the scalar-variance, which was produced by the mean scalar gradients near the bar, is brought to the grid-element centerline through the lateral motion of the bar wakes. The average meeting point of the thermal wakes is $x/x^* \approx 0.2$, and this marks the location of rapid growth of turbulent transport (and consequently scalar variance). The turbulent transport term is balanced by the mean convection and dissipation. Turbulent transport becomes negligible around $x/x^* \approx 0.5$. Further downstream, the scalar-variance is carried by the mean flow while it is dissipated.

The differences in the decay rate of turbulence kinetic energy and dissipation have been studied before, but mainly for homogeneous isotropic turbulence [12, 53, 54]. Theoretical analysis shows that, if the spectra of kinetic energy and scalar peak at wavenumbers that are of the same order, the exponents of the decay equation are similar (values 1.38 and 1.48 are reported in Lesieur *et al.* [54]). If however, the scalar is injected at a much larger wavenumber, then the instantaneous decay rate of scalar variance is much larger compared to the aforementioned values. Such a behavior was observed by [12] on heated grid experiments and a theoretical explanation was proposed by Lesieur *et al.* [54]. The (initially small) temperature integral scale grows to approach the velocity integral scale, and during this time larger decay rates are predicted. It is unlikely that this explanation is valid also for our case. First, the anomalous behavior was measured when the scalar was introduced by placing a heated parallel array of fine wires (a mandolin) downstream of the unheated grid. This results in the scalar and velocity spectra to have different spectral peaks, but in our case vorticity and scalar are both injected at the grid location. Secondly, the measurements of [12] were carried out far from the grid (at location 80 times the grid size, as mentioned in their figure 15), while our analysis focuses very close to the grid.

In the present case, the budget analysis reveals that the evolution of scalar-variance along the grid-element centerline is controlled by two terms, turbulent transport and dissipation. Although the turbulent transport of turbulent kinetic energy (also shown in figure 4b) and that of scalar-variance reach a peak value around $x/x^* \approx 0.3$, their evolution downstream of $x/x^* \approx 0.3$ differs. In particular, the turbulent transport of of scalar variance is negligible after $x/x^* \approx 0.45$, while that of kinetic energy persists further downstream. It is interesting to notice that the spatial shape of the two turbulent transport terms shares many similarities with the shape of scalar variance and kinetic energy. To get a more detailed picture of scalar

FIG. 5: (a) Evolution of scalar-gradient-variance and enstrophy along the bar centerline, (b) Evolution of budget terms of scalar-gradient-variance along the bar centerline. All the terms are normalized by $U_{\infty} T_{\infty}^2 / t_0^3$.

dynamics for our configuration, in the next section we examine the evolution of scalargradient variance.

B. Scalar-gradient-variance balance

This subsection focuses on the evolution of the small-scale term, the scalar-gradient variance $\langle G_i G_i \rangle$, where $G_i = \frac{\partial T}{\partial x_i}$ $\frac{\partial T}{\partial x_i}$. As mentioned earlier, the scalar dissipation ϵ_v is proportional to this term.

Denoting the gradient of instantaneous scalar (i.e. mean plus fluctuation) as $G_i^* = \frac{\partial T^*}{\partial x_i}$ $\frac{\partial T^*}{\partial x_i},$ the transport equation can be written as (see [55]):

$$
\frac{\partial \left(\langle \frac{1}{2}G_i G_i \rangle\right)}{\partial t} = -U_j \frac{\partial \left(\langle G_i G_i \rangle\right)}{\partial x_j} - \langle G_i u_j \rangle \left\langle \frac{\partial G_i^*}{\partial x_j} \right\rangle - \left\langle G_i \frac{\partial u_j}{\partial x_i} \right\rangle \left\langle \frac{\partial G_i^*}{\partial x_j} \right\rangle
$$
\n
$$
- \langle G_i G_j \rangle \frac{\partial U_j}{\partial x_i} - \left\langle G_i s_{ij} G_j \right\rangle - \frac{1}{2} \frac{\partial}{\partial x_j} \langle G_i G_j u_j \rangle
$$
\n
$$
+ \frac{\alpha}{2} \frac{\partial^2}{\partial x_j \partial x_j} (\langle G_i G_i \rangle) - \alpha \left\langle \frac{\partial G_i}{\partial x_j} \frac{\partial G_i}{\partial x_j} \right\rangle
$$
\n(5)

where C_G is the convection by mean flow, G_G and β_G are the production terms by mean scalar and velocity gradient respectively, α_G is the mixed production, P_G is the production by turbulent stretching/compression, T_G is transport by turbulent fluctuations, D_G is the diffusion, and finally ϵ_G is the dissipation.

The evolution of scalar-gradient-variance along the bar centerline is presented in figure 5a. It is very similar to that of the mean enstrophy, also shown in the same figure, with values reaching a peak at the end of the mean recirculation region and then monotonically decaying further downstream. The corresponding budget terms, shown in figure 5b, reveal that the growth of $\langle G_i, G_i \rangle$ is due to the stretching/compression of the gradient vector G_i by the fluctuating strain field (term P_G). This is balanced by the dissipation throughout the bar centerline, while the contribution of all the other terms is negligible. In the field experiments of Gulitski *et al.* [1], the contribution of mean fields (both velocity and scalar) to the generation of small scales was also found to be negligible.

The spatial evolution of scalar-gradient-variance and mean enstrophy however differ along the grid-element centerline. As expected, the scalar-gradient-variance is negligible in the region upstream the meeting of the wakes. It starts increasing at $x/x^* \approx 0.2$ until $x/x^* \approx 0.4$, and the growth is faster than that of enstrophy (figure 6a). Also decay starts earlier compared to enstrophy; this difference is further discussed in §VI.

The budgets along the grid-element centerline are plotted in figure 6b. The first term to initiate the growth of $\langle G_i, G_i \rangle$ is the turbulent transport term; this is similar to scalarvariance. Once scalar gradients appear in the centerline, the background strain, which is mainly due to pressure Hessian and turbulent transport [37], activates the production stretching/compression term P_G , which takes over and becomes the main growth mechanism. The two production terms are balanced by mean convection and dissipation. After

FIG. 6: (a) Evolution of scalar-gradient-variance and enstrophy along the grid-element centerline, (b) Evolution of budget terms of scalar-gradient-variance along the grid-element centerline. All the terms are normalized by $U_{\infty} T_{\infty}^2 / t_0^3$.

 $x/x^* \approx 0.4$, the mean convection and production are balanced by turbulent transport and dissipation. Far downstream, the transport terms (both mean and turbulent) become negligible, and only the production and dissipation terms remain that balance each other. A more detailed analysis of the production due to stretching/compression is presented in section V.

IV. SPECTRUM OF THE FLUCTUATING SCALAR

Results are presented only along the grid-element centerline. As demonstrated in §III B, the scalar and turbulent kinetic energy dissipation evolve differently along the grid-element centerline, and secondly both intermittent as well as fully-turbulent regions exist (see figure 2a). As will be shown in the rest of this study, scalar gradient dynamics also exhibit intriguing behavior along the grid-element centerline.

The values of the Taylor-scale Reynolds number (Re_{λ}) and the Corrsin-scale Peclet number (Pe_{λ_T}) at different stations are provided in table I. Note the low values of Re_λ and Pe_{λ_T} . Such values allow for very well resolved numerical simulation and long time integration, both

x/x^* 0.1 0.25 0.35 0.5 0.75 0.95				
$Pe_{\lambda T}$ 5.21 12.31 19.45 25.6 24.71 23.89				
		Re_λ 10.21 22.01 34.49 37.58 39.12 33.12		

TABLE I: Values of Pe_{λ_T} and Re_{λ} at different locations along the grid-element centerline. Here, $Re_{\lambda} = \frac{\lambda}{\nu}$ ν $\sqrt{\frac{\langle u_i u_i \rangle}{3}}$ where λ is the Taylor microscale defined as $\lambda = \sqrt{\frac{5\nu \langle u_i u_i \rangle}{\epsilon_k}}$ $\frac{u_i u_i}{\epsilon_k}$ and $Pe_{\lambda_T} = \frac{\lambda_T}{\alpha}$ α $\sqrt{\frac{\langle u_i u_i \rangle}{3}}$ where λ_T is the Corrsin microscale, defined as $\lambda_T = \sqrt{\frac{6\alpha \langle T^2 \rangle}{\epsilon_v}}$ ϵ_v

of which are conducive to the statistical convergence of second and third order correlations as well as good balance of transport equations. In the following we assess whether turbulence properties that are found for high Reynolds and Peclet number flows can be also detected in flows with low values of these parameters. To this end, we analyze the scalar spectra along the grid-element centerline.

Oboukhov [10] and Corrsin [11] extended the phenomenology of Kolmogorov [56] to the scalar field, and developed what is known as $Kolmogorov - Obukhov - Corrsin$ (or KOC) theory. It is concerned with locally HIT at very high Reynolds and Peclet numbers. One of its main predictions when $Pr < 1$ is that a range of wavenumbers exists where the scalar spectrum (E_{TT}) takes the form

$$
E_{TT}(\kappa) = C_{\epsilon T} \epsilon_k^{-1/3} \epsilon_v \kappa^{-5/3}
$$
\n(6)

where $C_{\epsilon T}$ is the Obukhov-Corrsin constant and κ is the wavenumber. It is important to stress that the claim of KOC theory is that $E_{TT}(\kappa) \sim \kappa^{-5/3}$ is only applicable to fullydeveloped homogeneous, isotropic turbulence (HIT) at high Re_λ and Pe_{λ_T} .

The computed and compensated spectra at different locations along the grid-element centerline are illustrated in figure 7. At $x/x^* = 0.25$, where the velocity spectrum was reported to exhibit a $-5/3$ slope for the first time along the grid-element centerline (refer to Paul *et al.* [37]), the scalar spectrum has a well-defined $-5/3$ slope for about a decade of frequencies (see the compensated spectra for $x/x^* = 0.25$ in figure 7b). It is indeed surprising that such a well-defined power-law appears at a location where the local Re_λ and Pe_{λ_T} numbers are too low for an inertial subrange to exist. In fact, Re_λ is only 22.01 and $Pe_{\lambda T}$ is a mere 12.31 (see table I). Due to these very small values and the developing nature of the turbulence, the scalar spectrum is not at all expected to have any power-law

FIG. 7: (a) Spectra of the fluctuating scalar at different locations along the grid-element centerline, (b) Compensated spectra plotted in linear-logarithmic axes at the same locations. The dotted lines in (a) indicate the $-5/3$ slope, while in (b) they represent a constant value of $E_{TT}(ft_0/U_\infty)^{5/3}$.

scaling at this location. Yet, the spectrum does exhibit a definite -5/3 power-law slope for just under a decade of frequencies. Note also that, $x/x^* = 0.25$ is the location where the fluctuating scalar and its gradients have just been brought to the grid-element centerline by the turbulent transport from the bar wakes (see §III).

The power-law behavior observed in the near-grid-element region is not related to the KOC theory. The relationship between the small scales of scalar and the well-defined $-5/3$ power-law slope is further analyzed in §V. Note that this is the first study that reports a well-defined $-5/3$ power-law in the scalar spectrum for a flow characterized by intermittent switching between turbulent and potential flow region at such low overall Re_λ and Pe_{λ_T} numbers.

The scalar spectra in the more homogeneous decay region are also plotted in figures 7a and 7b. The frequency range of $-5/3$ slope appears to be decreasing in these locations compared to that of the near-grid-element region. This is consistent with the observations made for the velocity spectra in Paul et al. [37]. At these fully-turbulent locations, Paul

FIG. 8: PDF of scalar gradient production at different locations along the grid-element centerline: (a) x/x^* =0.25, (b) x/x^* =0.5, (c) x/x^* =0.95.

et al. [37] reported that the velocity spectra have power-law slope defined only for a limited range of frequencies. The scalar spectra however have a more clearly defined power-law for a wider range of frequencies. This observation has also been reported in the literature on heated-grid fully developed homogeneous turbulence, but for high Re_λ and $Pe_{\lambda T}$ values [12, 27]. The −5/3 range of scalar spectra with respect to velocity spectra is also reported in Lee et al. [57].

V. EIGEN-CONTRIBUTIONS OF STRAIN-RATE TO THE SCALAR GRADI-ENT PRODUCTION

In this section, we explore further the relation of small scales with the spectra. To this end, the stretching/compressing of scalar-gradient vector, $-G_i s_{ij} G_j$, which is the main production term of scalar dissipation is analyzed. This term can be written as,

$$
-G_i s_{ij} G_j = -|\mathbf{G}|^2 \lambda_1 \cos^2(\mathbf{G}, \mathbf{e}_1) - |\mathbf{G}|^2 \lambda_2 \cos^2(\mathbf{G}, \mathbf{e}_2) - |\mathbf{G}|^2 \lambda_3 \cos^2(\mathbf{G}, \mathbf{e}_3)
$$
(7)

where G is the scalar gradient vector, while λ_i and \mathbf{e}_i (where i=1,2,3) are the strain-rate eigenvalues and eigenvectors respectively. Equation (7) shows that the production of scalar dissipation depends on the strain-rate eigenvalues and the alignment between the scalar gradient vector and the strain-rate eigenvectors. The statistical behavior of the production term is discussed first, followed by an analysis of the contribution of the individual eigenvalues and eigenvectors.

x/x^*		$\begin{array}{ccc} \begin{bmatrix} 0.1 & 0.25 & 0.35 & 0.5 & 0.75 & 0.95 \end{bmatrix} \end{array}$		
$-\langle G_i s_{ij} G_j \rangle / \langle G^2 \rangle \langle s^2 \rangle^{1/2}$ - 0.11 0.195 0.19 0.18 0.17				

TABLE II: Values of normalized stretching/compressing at different locations along the grid-element centerline.

The PDFs of scalar gradient production are plotted at different locations in figure 8. The PDFs are skewed towards positive at all stations. The positive value of $-\langle G_i s_{ij} G_j \rangle > 0$ is considered a universal behavior of small-scale scalar turbulence [1, 21, 51, 58–60]. The same behavior is observed also here, at locations where the local Re_λ is very small and the flow is intermittent.

Table II records the values of production term normalized by the product $\langle s^2 \rangle^{1/2} =$ $\langle s_{ij} s_{ij} \rangle^{1/2}$ and $\langle G^2 \rangle = \langle G_i G_i \rangle$. This ratio initially increases rapidly from $x/x^* \approx 0.2$ to 0.35. This increase shows that $-\langle G_i s_{ij} G_j \rangle$ increases faster than the product $\langle G^2 \rangle \langle s^2 \rangle^{1/2}$. Further downstream, the ratio decreases gradually. This is because $\langle s^2 \rangle$ increases slightly in this region (i.e. from $x = 0.35x^*$ to $0.5x^*$, see figure 10 of Paul *et al.* [37]). Far downstream the ratio again decreases slowly, ascertaining that the decay of $-\langle G_i s_{ij} G_j \rangle$ is similar to that of $\langle G^2 \rangle$ and $\langle s^2 \rangle^{1/2}$. Therefore, the growth of $-\langle G_i s_{ij} G_j \rangle$ is faster than $\langle s^2 \rangle^{1/2} \langle G^2 \rangle$, while its decay is similar to that of $\langle s^2 \rangle^{1/2} \langle G^2 \rangle$. The reason for this behavior will become clearer later in this section.

A. The role of strain-rate eigenvalues in scalar gradient production

The strain-rate eigenvalues are ordered as $\lambda_1 > \lambda_2 > \lambda_3$. The incompressibility constraint implies that $\lambda_1 + \lambda_2 + \lambda_3 = 0$. The largest strain-rate eigenvalue is always positive (i.e. $\lambda_1 > 0$), and the third eigenvalue is always negative (i.e. $\lambda_3 < 0$). The intermediate eigenvalue can be either positive or negative. For many turbulent flows, the intermediate eigenvalue is positive on average, and this is one of the universal properties of small-scale turbulence [16, 39, 61, 62]. These strain-rate eigenvalues influence the scalar gradient production as indicated in (7) (refer also to Gulitski *et al.* [1]). It is known from Paul *et al.* [37] that in the grid-element centerline region $0.25 < x/x^* < 1$, the PDF of the intermediate strain-rate eigenvalue is skewed positive resulting in two stretching directions and one compressive direction. More

Quantity / x/x^*			0.1 0.25 0.35 0.5 0.75 0.95		Field experiment
$\langle \lambda_1 \rangle / \langle s^2 \rangle^{\frac{1}{2}}$			$-$ 0.40 0.48 0.54 0.55 0.56		0.53
$\langle \lambda_2 \rangle / \langle s^2 \rangle^{\frac{1}{2}}$				$-$ 0.09 0.09 0.12 0.13 0.13	0.09
$\langle \lambda_3 \rangle / \langle s^2 \rangle^{\frac{1}{2}}$				$-$ -0.49 -0.57 -0.66 -0.68 -0.69	-0.62
$\langle \lambda_1^2 \rangle / \langle s^2 \rangle$			$-$ 0.36 0.38 0.37 0.36 0.36		0.4
$\langle \lambda_2^2 \rangle / \langle s^2 \rangle$				$-$ 0.05 0.05 0.05 0.05 0.05	0.04
$\langle \lambda_3^2 \rangle / \langle s^2 \rangle$		$- \ \ \, 0.59 \ \ \, 0.57 \ \ \, 0.58 \ \ \, 0.59$		0.59	0.56
$\langle \lambda_1^3 \rangle / \langle s^2 \rangle^{\frac{3}{2}}$			$-$ 0.74 0.43 0.32 0.28 0.28		0.48
$\langle \lambda_2^3\rangle/\langle s^2\rangle^{\frac{3}{2}}$				$-$ 0.05 0.02 0.02 0.05 0.05	0.01
$\langle \lambda_3^3 \rangle / \langle s^2 \rangle^{\frac{3}{2}}$				$-$ -1.57 -0.86 -0.66 -0.60 -0.60	-0.73

TABLE III: Values of normalized eigenvalues of strain-rate tensor at different locations along the grid-element centerline. The values are compared against the field experiments of Gulitski et al. [1].

statistics of the normalized strain-rate eigenvalues are provided in table III. The normalized values of $\langle \lambda_i^2 \rangle$ (where i=1,2,3) remain remarkably constant, while the normalized values of $\langle \lambda_1 \rangle$ and $\langle \lambda_3^3 \rangle$ increase and $\langle \lambda_3^3 \rangle$ and $\langle \lambda_3 \rangle$ values decrease. The downstream evolution of $\langle \lambda_2 \rangle$, $\langle \lambda_2^2 \rangle$ and $\langle \lambda_2^3 \rangle$ remains insensitive to any kind of normalization, although the PDF of λ_2 showed remarkable difference from the near-grid-element to the decay regions as reported in Paul *et al.* [37]. In the same table III, the values from an atmospheric boundary layer field experiment [63] are also provided. Although the Reynolds number of the field experiment is too large ($Re_\lambda \approx 10^4$), the computed values of normalized mean strain-rate eigenvalues are surprisingly close, in particular for $\langle \lambda_i \rangle$ and $\langle \lambda_i^2 \rangle$.

We turn now our attention to the contribution of the strain-rate eigenvalues on the scalar gradient production. Figure 9 shows the joint probability distribution (JPDF) between the strain-rate eigenvalues and the scalar gradient production. The analysis is carried out at two stations along the grid-element centerline: (i) at $x/x^* = 0.25$ located in the near-gridelement region (figures 9a-9c) and (ii) at $x/x^* = 0.95$ located in the far-downstream decay

FIG. 9: JPDF of eigenvalues of strain-rate tensor against the scalar gradient production: (a-c) at x/x^* =0.25 (near-grid-element inhomogeneous region), (d-f) at x/x^* =0.95 (decay region). The isocontours range from 10^1 to 10^{-1} .

region (figures 9d-9f). Figures 9d-9f also look similar to those reported in Gulitski et al. [63] (see figure 16 of their paper) for the atmospheric boundary layer. It is evident from figure 9 that the extensive λ_1 and compressive λ_3 strain-rate eigenvalues are positive and negative respectively, while the tendency for the intermediate strain-rate eigenvalue λ_2 to skew towards positive is apparent in both the near-grid-element and far-downstream regions.

The preference for the positive scalar gradient production is only marginal at a location where the scalar spectrum exhibits the best −5/3 power-law slope. Since stretching/compression is believed to have a close relationship with the scalar cascade, it might be intuitive to expect a stronger preference for the production term of scalar gradients, but in reality that does not occur. This indicates that the stretching/compression process of scalar gradients may not be the most fundamental process behind the -5/3 power-law slope. This is further ascertained in figures 9d-9f where the production of scalar gradient is strongly preferred (as evident from the asymmetry in the JPDF with respect to

FIG. 10: PDF of cosine of the angle between scalar gradient vector and strain-rate eigenvectors at different locations along the grid-element centerline: (a) x/x^* =0.25, (b) x/x^* =0.35, (c) x/x^* =0.5. The dotted lines in (c) are the results from Vedula *et al.* [21].

 $-G_i s_{ij} G_j/\langle G_i s_{ij} G_j \rangle = 0$, yet the spectrum at this location has a power-law defined for a more narrow range of frequencies than that of the near-grid-element region. Figures 9d-9f also reveal that there is a correlation between the strain-rate eigenvalues and the positive skewness of scalar gradient production in the homogeneous decay region.

B. The role of geometrical alignments in scalar gradient production

The other factor that affects the production of scalar gradient, the geometrical alignments (refer to equation 7), is analyzed in this subsection. These alignments were first reported by Ashurst et al. [16] for a periodic homogeneous isotropic turbulence. It was observed that the fluctuating scalar gradient vector aligns with the compressive strain-rate eigenvector, and it is perpendicular to the intermediate strain-rate eigenvector. The extensive strain-rate eigenvector aligns 45° with the fluctuating scalar gradient vector. These observations were also verified in subsequent studies of Gulitski et al. [1], Abe et al. [17], Vedula et al. [21]. These alignment properties are also considered universal characteristics of small-scale scalar turbulence.

The PDFs of the absolute value of the cosine of the angle between the fluctuating scalar gradient vector and the strain-rate eigenvectors are plotted for different grid-element cen-

FIG. 11: (a) PDF of cosine of the angle between fluctuating scalar gradient and vorticity vectors at different locations along the grid-element centerline, (b-c) Comparison between alignments of instantaneous versus fluctuating scalar-gradient and vorticity vectors at: (b)

 x/x^* =0.25, (c) x/x^* =0.5.

terline locations in figure 10. The alignment behavior at $x/x^* = 0.25$ and 0.35 is shown in figures 10a and 10b respectively. The scalar gradient vector aligns with the compressive strain-rate eigenvector but is normal to the other two eigenvectors. This is not the universal alignment behavior reported in the previous studies [1, 17, 21]. Note that at the same locations the alignment behavior of vorticity was also found by Paul *et al.* [37] to be anomalous; the vorticity vector aligned with both the extensive and intermediate strain-rate eigenvectors. Note also that the alignment of the compressive strain-rate eigenvector with the scalar gradient vector becomes stronger from $x/x^* = 0.25$ to 0.35 giving a possible answer as to why the scalar-gradient-variance increase in the region $0.2 < x/x^* < 0.35$ (refer to figure 6a). The alignment behavior for the region $0.2 < x/x^* < 0.35$ agrees with the results of Brethouwer *et al.* [60] who reported that strain-dominated regions strengthen the alignment of the scalar gradient vector with the compressive strain-rate eigenvector. The alignment behavior after $x/x^* \approx 0.4$ starts to exhibit the universal trend reported in the literature as the PDFs in figures 10c, plotted for $x/x^* = 0.5$, are very similar to the results of Vedula et al. [21]. This universal alignment behavior prevails throughout the decay region although the values of Pe_{λ_T} and Re_{λ} are significantly low.

Unlike the alignment behavior of the fluctuating scalar-gradient vector with the strain-

FIG. 12: PDF of eigen-contribution to scalar gradient production at different locations along the grid-element centerline: (a) x/x^* =0.25, (b) x/x^* =0.5, (c) x/x^* =0.95.

rate eigenvectors that changes along the grid-element centerline, the alignment with the fluctuating vorticity vector remains the same as noted in figure 11a. The figure also shows that homogeneity in fluctuating vorticity statistics is attained only in the downstream of $x/x^* \approx 0.35$. The fluctuating scalar-gradient vector aligns perpendicular to the vorticity vector throughout the grid-element centerline. This result closely follows the mathematical fact that the instantaneous scalar product between vorticity and scalar-gradient vectors is a Lagrangian inviscid invariant. We also noted some difference between instantaneous and fluctuating alignment characteristics of scalar-gradient and vorticity vectors only in the inhomogeneous region where the mean gradients are strong (see figure 11b). On the other hand, the alignments results of instantaneous and fluctuating scalar-gradient and vorticity vectors are nearly similar in the homogeneous region starting from $x/x^* \approx 0.5$ as shown in figure 11c.

C. The combined effects of strain-rate eigenvalues and eigenvectors to scalar gradient production

The combined effect of strain-rate eigenvalues and eigenvectors on the scalar gradient production is plotted in figure 12. At $x/x^* = 0.25$, where the scalar-gradient-variance has just started to develop and the scalar spectrum has the best-defined −5/3 power-law slope, the production of scalar gradient is predominantly due to the compressive strainrate eigenvalue and eigenvector as only the PDF of $-|G|^2\lambda_3\cos^2(G, e_3)$ is skewed to the

Quantity/ x/x^*				
$\langle \mathbf{G} ^2 \lambda_1 \cos^2(\mathbf{G}, \mathbf{e}_1) \rangle / \langle G_i s_{ij} G_j \rangle$ - -0.18 -0.31 -0.27 -0.25 -0.22 -0.64				
$\langle G ^2 \lambda_2 \cos^2(G, e_2) \rangle / \langle G_i s_{ij} G_j \rangle$ - -0.03 -0.04 -0.04 -0.04 -0.04 -0.04				-0.05
$\langle G ^2 \lambda_3 \cos^2(G, \mathbf{e}_3) \rangle / \langle G_i s_{ij} G_j \rangle$ - 1.21 1.35 1.31 1.29 1.26				1.69

TABLE IV: Contribution of strain-rate eigenvalues to scalar gradient production. The values are compared with the field-experiments of Gulitski et al. [1].

positive. A similar finding was reported in Gulitski *et al.* [1] but for a homogeneous isotropic turbulence. Therefore, the small scales of scalar are due to compressing of fluid elements, although the small scales of velocity fluctuation are due to vortex stretching. As a novelty, this study takes this result one step further and shows that this compressing of fluid elements is mostly associated with the strain-rate eigenvectors for the developing inhomogeneous turbulence. In the decay region, some portion of the PDF of $-|\mathbf{G}|^2 \lambda_2 \cos^2(\mathbf{G}, \mathbf{e_2})$ is in the positive x-axis, but the overall contribution is negative.

The observations noted in figure 12 are further analyzed through the mean values of individual components of the eigen-contribution to the scalar gradient production (see table IV). The values of $\langle |G|^2 \lambda_1 \cos^2(G, e_1) \rangle$ and $\langle |G|^2 \lambda_2 \cos^2(G, e_2) \rangle$ are negative and the only positive component is $\langle |G|^2 \lambda_3 \cos^2(G, e_3) \rangle$. This observation ascertains that the production of scalar gradient is due to the compressive action of strain-rate eigenvalues and eigenvectors [1]. The mean eigen-contribution values are compared against the very high Reynolds number field experiments of Gulitski *et al.* [1]. Although the values of $\langle |G|^2 \lambda_2 \cos^2(G, e_2) \rangle$ and $\langle |G|^2 \lambda_3 \cos^2(G, \mathbf{e_3})\rangle$ are closer to the literature values, the values of $\langle |G|^2 \lambda_1 \cos^2(G, \mathbf{e_1})\rangle$ show some significant discrepancy. Recall that the present simulation is carried out for a low Reynolds number, and the observed discrepancy could well be a Reynolds number effect.

Concerning the evolution of $\langle |G|^2 \lambda_3 \cos^2(G, e_3) \rangle$ with respect to $-\langle G_i s_{ij} G_j \rangle$, it can be noted that the behavior of these two terms are similar; both terms increase from x/x^* =0.2 to 0.4, and then they decay gradually. Noting from table III that the values of $\langle \lambda_3 \rangle$ decrease from $x=0.25x^*$ to $0.4x^*$, the rapid increase of $-\langle G_i s_{ij} G_j \rangle$ compared to $\langle G_i G_i \rangle$ and $\langle s_{ij} s_{ij} \rangle$ is the result of rapid increase in the strong alignment between the compressive strain-rate eigenvector and the scalar gradient vector. In simple terms, the asymmetric evolution of $-\langle G_i s_{ij} G_j \rangle$ compared to $\langle G_i G_i \rangle$ and $\langle s_{ij} s_{ij} \rangle$ is the result of asymmetric evolution of the

FIG. 13: Evolution of turbulent kinetic energy and scalar-variance dissipations along: (a) the bar centerline, (b) the grid-element centerline. (c) Evolution of the time-averaged quantities χ and Υ (defined in the text) along the grid-element centerline.

alignment behavior between the strain-rate eigenvector and the scalar gradient vector.

VI. STRETCHING OF VORTICITY VECTOR VERSUS STRETCHING OF A PASSIVE VECTOR

The aim of this final section is to provide an explanation as to why the scalar dissipation $(\epsilon_v = \alpha \langle G_i G_i \rangle)$ starts decaying earlier along the grid-element centerline compared to kinetic energy dissipation $(\nu \langle \omega_i \omega_i \rangle)$, as demonstrated in figure 6a. The dissipation quantities are sometimes believed to have similar behavior [46] and the relationship is given as $\langle G_i G_i \rangle^{1/2} =$ $C \langle \omega_i \omega_i \rangle^{1/2} Pr^{1/2}$, where C is a constant that depends on the flow conditions. In periodic box simulation, Pumir [19] found that this relation is very well satisfied, with a value of constant C close to 2.

The spatial evolution of these two dissipation rates along the bar and the grid-element centerlines is plotted in figures 13a and 13b respectively. The relationship $\langle G_i G_i \rangle^{1/2} \sim$ $\langle \omega_i \omega_i \rangle^{1/2} Pr^{1/2}$ is valid only along the bar centerline and for $x/x^* > 0.6$ on the grid-element centerline. Indeed, figure 13a demonstrates that the qualitative behavior of the two dissipation profiles is similar along the bar centerline, with values peaking at the same position. The value of the constant C in the current simulation is approximately 0.2. At the grid-

FIG. 14: PDF of scalar gradient production rate and enstrophy production rate at different locations along the grid-element centerline: (a) x/x^* =0.25, (b) x/x^* =0.5, (c) x/x^* =0.95.

element centerline however, the onset of scalar dissipation decay occurs earlier than the decay of kinetic energy dissipation (see figures 13b and 6a). A similar behavior between the dissipation rates of kinetic energy and scalar-variance is also reported in Lesieur [53], Lesieur et al. [54].

In order to provide an explanation for the aforementioned behavior, we explore below in more detail the turbulent stretching/compression of the vorticity and the scalar gradient vectors. This is motivated by the fact that the dominant production terms are $-G_i s_{ij} G_j$ and $\omega_i s_{ij} \omega_j$ respectively. As noted in Tsinober [51], the vorticity vector and turbulent strainrate are coupled. It can be seen from the governing equations of enstrophy $(\omega_i \omega_i)$ and strain-product $(s_{ij}s_{ij})$ (refer to equations (5.4) and (5.7) of Paul *et al.* [37]) that the vortex stretching/compression term appears in both equations: as a source term for enstrophy and a sink for strain-product. This means that the growth of enstrophy reduces the strain-rate and thus weakening the stretching/compression which eventually leads to the enstrophy damping. On the other hand the stretching of the scalar gradient vector is determined by strain only (i.e. does nor react back). It is thus expected that the statistics of the stretching/compression of the two vectors will be different.

In Ohkitani [64], the normalized stretching/compression rates of vorticity and scalar gradient were defined as $\chi = \frac{\omega_i s_{ij} \omega_j / \omega_i \omega_i}{\sqrt{N}}$ $\frac{\omega_j/\omega_i\omega_i}{\langle\omega_i\omega_i\rangle}$, and $\Upsilon = \frac{-G_is_{ij}G_j/G_iG_i}{\sqrt{\langle\omega_i\omega_i\rangle}}$. The variation of χ and Υ along the different grid-element centerline is shown in figure 13c. Clearly, the stretching/compression rate of the passive vector is stronger than that of the vorticity vector throughout the grid-element centerline. The dominance of passive vector stretching/compression over vorticity vector was first reported in Ohkitani [64]. The current results, however, cannot be directly compared with the study of Ohkitani [64], as the latter considers 'frozen' passive vectors that satisfy the continuity equation. For the distinction between the two types of passive vectors refer to the book of Tsinober [51].

The reason for the observed difference lies in the two-way coupling between strain and vorticity. When the mean enstrophy increases in the region of $0.2 < x/x^* < 0.5$ (see figure $8(a)$ of Paul *et al.* [37]), the stretching of vorticity also increases in this region, but this increase weakens the strain-rate magnitude (because the stretching/compression term acts as a sink for the strain) which in turn reduces the strength of vortex stretching/compression (that depends on the strain magnitude). This can explain why the stretching/compression rate of vorticity vector is smaller than that of a passive vector. Although the comparison of stretching/compression rates between the vorticity vector and the scalar gradient vector confirms the validity of Ohkitani's observation for the current case, it cannot explain why the onset of scalar-variance dissipation decay occurs much earlier along the grid-element centerline.

Figure 13c demonstrates that the growth of both χ and Υ is suddenly hampered. This occurs earlier for the passive scalar field compared to the vorticity field. What is the process that suddenly impedes the growth of stretching/compression rates? It is intuitive that this process should be related to the stretching/compression term. Indeed, as shown in the next paragraph, the decay of scalar dissipation starts earlier than that of the kinetic energy dissipation due to the difference in alignments between the scalar gradient vector and the strain-rate eigenvector. The production of the two dissipation quantities depends on the strain-rate eigenvalues and the alignment of the eigenvectors with the vorticity and scalar gradient vector (equation (7)). Since the strain-rate eigenvalues appear in the same way in both production terms, the difference in evolution should originate from the geometrical alignments.

For the kinetic energy dissipation, the extensive and intermediate eigenvectors aid the growth of $\langle \omega_i \omega_i \rangle$ (see figure 20 of Paul *et al.* [37]). On the other hand, as reported in many studies (and confirmed in figure 12), the growth of $\langle G_i, G_i \rangle$ occurs predominantly due to the compressive eigenvector. This is because, as was noticed earlier, the extensive eigenvector has a negative effect on the growth of scalar-gradient-variance, and the intermediate eigenvector aligns perpendicular to the scalar gradient vector. The vorticity vector aligns with both the extensive and intermediate eigenvectors in the region $0.2 < x/x^* \leq 0.5$, and thus acting as a main agent to increase $\langle \omega_i \omega_i \rangle$ in that region (see figure 22 of Paul *et al.* [37]). If $\langle G_i G_i \rangle$ has to increase in $0.2 < x/x^* \leq 0.5$, then the scalar gradient vector is expected to align only with the compressive eigenvector. Yet, such an alignment behavior is noticed only in the region $0.2 < x/x^* < 0.4$ where the extensive and intermediate eigenvectors align perpendicular to the scalar gradient vector and thus they do not hamper the growth of scalar-gradientvariance due to the compressive eigenvector. When the extensive strain-rate eigenvector aligns 45^o to the scalar gradient vector (i.e after $x/x^* > 0.4$), the negative effect due to this alignment on the scalar-gradient-variance is felt in the form of decreasing the scalar-gradientvariance. Comparing the alignment behavior of the scalar gradient vector with that of the vorticity vector, it is observed that the vorticity vector changes its alignment behavior later along the grid-element centerline (it occurs only after $x/x^* = 0.5$) than that of the scalar gradient vector. Thus, the delayed change in alignment behavior of vorticity vector causes the scalar-variance dissipation to decay earlier along the grid-element centerline than the turbulent kinetic energy dissipation.

VII. CONCLUSIONS

This paper presents a statistical analysis of a passive scalar (in the form of temperature) injected into a spatially developing turbulence. The turbulence is generated by a single square grid-element which is heated continuously. The main objective of this study was to seek answers to the five questions raised in §I. The answers for those questions are given below:

1. The large-scale quantity (scalar-variance) is generated mainly behind the bars due to the action of mean scalar gradients. It is then laterally transported to the grid-element centerline through turbulent transport due to the intermittent meeting of the bar wakes (external intermittency). The mean velocity and scalar fields have minimal effect on the production of the small-scale quantity (scalar-gradient-variance, proportional to scalar dissipation), even behind the grid-element bars. Instead, this is produced by the turbulent strain rate via the stretching/compressing process. This study has shown that the production of scalar dissipation is due to compressive action of strain-rate, while it is the stretching action that produces the kinetic energy dissipation.

- 2. Although the evolution of scalar dissipation is similar to the turbulent kinetic energy dissipation along the bar-centerline, they behave differently along the grid-element centerline. The different alignment behavior of the scalar gradient vector and the vorticity vector with the strain-rate eigenvectors explains why the scalar dissipation decays much earlier along the grid-element centerline than that of the turbulent kinetic energy dissipation.
- 3. The scalar spectrum is observed to exhibit the best −5/3 power-law slope in the neargrid-element region. This slope occurs even in the highly-intermittent, non-Gaussian and inhomogeneous region where the local Re_{λ} and Pe are significantly low.
- 4. The −5/3 slope in the scalar spectrum is most clearly observed in the regions where the small-scale terms of scalar have just started developing. The scalar spectrum has a well-defined $-5/3$ power-law slope for at least a decade of frequencies in the locations where the strength of stretching/compressing of scalar gradient by strain-rate is weak. On the other hand, in the locations where the stretching/compressing strength is high, the frequency range becomes narrower. Hence, the stretching/compressing process of scalar gradients by strain-rate (equivalent to the vortex stretching process in velocity field) is not necessarily the cause of the -5/3 power-law behavior.
- 5. Moving from the near-grid-element centerline region to the far-downstream, it is noted that the -5/3 slope in the scalar spectrum slowly erodes, and the alignment between the scalar gradient vector and the strain-rate eigenvector morphs to the universal alignment behavior reported in the literature.

ACKNOWLEDGMENTS

This research project was funded by the European Commission under the Innovative Doctoral Program (IDP) in Marie Curie framework through MULTISOLVE (Grant Agreement Number 317269). The simulations were carried out on the facilities of Archer, the UK national high-performance computing service under the grant EP/L000261/1 of the UK Turbulence Consortium (UKTC), and on the High Performance Computing Service of Imperial College London. JCV acknowledges support from ERC Advanced Grant 320560.

- [1] G Gulitski, M Kholmyansky, W Kinzelbach, B Lüthi, A Tsinober, and S Yorish, "Velocity and temperature derivatives in high-reynolds-number turbulent flows in the atmospheric surface layer. part 3. temperature and joint statistics of temperature and velocity derivatives," J. Fluid Mech. 589, 103–123 (2007).
- [2] KR Sreenivasan, "On local isotropy of passive scalars in turbulent shear flows," in Proc. R. Soc. Lond. A, Vol. 434 (The Royal Society, 1991) pp. 165–182.
- [3] KR Sreenivasan and RA Antonia, "The phenomenology of small-scale turbulence," Annu. Rev. Fluid Mech. 29, 435–472 (1997).
- [4] AJ Majda and PR Kramer, "Simplified models for turbulent diffusion: theory, numerical modelling, and physical phenomena," Phys. Rep. 314, 237–574 (1999).
- [5] BI Shraiman and ED Siggia, "Scalar turbulence," Nature 405, 639–646 (2000).
- [6] Z Warhaft, "Passive scalars in turbulent flows," Annu. Rev. Fluid Mech. 32, 203–240 (2000).
- [7] G Falkovich, K Gawdzki, and M Vergassola, "Particles and fields in fluid turbulence," Rev. Mod. Phys. 73, 913 (2001).
- [8] PE Dimotakis, "Turbulent mixing," Annu. Rev. Fluid Mech. 37, 329–356 (2005).
- [9] T Gotoh and PK Yeung, "Passive scalar transport in turbulence," Ten Chapters in Turbulence (ed. Y. Kaneda, P.A Davidson & K. R. Sreenivasan) (2013).
- [10] AM Oboukhov, "Structure of the temperature field in turbulent flows," Izv. Akad. Nauk SSSR Geogr. Geophys 13, 58–69 (1949).
- [11] S Corrsin, "On the spectrum of isotropic temperature fluctuations in an isotropic turbulence," J. App. Phys. 22, 469–473 (1951).
- [12] Z Warhaft and JL Lumley, "An experimental study of the decay of temperature fluctuations in grid-generated turbulence," J. Fluid Mech. 88, 659–684 (1978).
- [13] KR Sreenivasan and RA Antonia, "Skewness of temperature derivatives in turbulent shear flows," Phys. Fluids 20, 1986–1988 (1977).
- [14] KR Sreenivasan, RA Antonia, and D Britz, "Local isotropy and large structures in a heated turbulent jet," J. Fluid Mech. 94, 745–775 (1979).
- [15] RA Antonia and CW Van Atta, "On the correlation between temperature and velocity dissipation fields in a heated turbulent jet," J. Fluid Mech. 67, 273–288 (1975).
- [16] WMT Ashurst, AR Kerstein, RM Kerr, and CH Gibson, "Alignment of vorticity and scalar gradient with strain rate in simulated navier–stokes turbulence," Phys. Fluids 30, 2343–2353 (1987).
- [17] H Abe, RA Antonia, and H Kawamura, "Correlation between small-scale velocity and scalar fluctuations in a turbulent channel flow," J. Fluid Mech 627, 1-32 (2009).
- [18] H Abe and RA Antonia, "Scaling of normalized mean energy and scalar dissipation rates in a turbulent channel flow," Phys. Fluids 23, 055104 (2011).
- [19] A Pumir, "A numerical study of the mixing of a passive scalar in three dimensions in the presence of a mean gradient," Phys. Fluids 6, 2118–2132 (1994).
- [20] M Holzer and ED Siggia, "Turbulent mixing of a passive scalar," Phys. Fluids 6, 1820–1837 (1994).
- [21] P Vedula, PK Yeung, and Rodney O Fox, "Dynamics of scalar dissipation in isotropic turbulence: a numerical and modelling study," J. Fluid Mech. 433, 29–60 (2001).
- [22] KR Sreenivasan, S Tavoularis, R Henry, and S Corrsin, "Temperature fluctuations and scales in grid-generated turbulence," J. Fluid Mech. 100, 597–621 (1980).
- [23] C Tong and Z Warhaft, "On passive scalar derivative statistics in grid turbulence," Phys. Fluids 6, 2165–2176 (1994).
- [24] R Budwig, S Tavoularis, and S Corrsin, "Temperature fluctuations and heat flux in gridgenerated isotropic turbulence with streamwise and transverse mean-temperature gradients," J. Fluid Mech. 153, 441–460 (1985).
- [25] L Mydlarski and Z Warhaft, "Passive scalar statistics in high-Péclet-number grid turbulence," J. Fluid Mech. 358, 135–175 (1998).
- [26] C Jayesh, Tong and Z Warhaft, "On temperature spectra in grid turbulence," Phys. Fluids 6, 306–312 (1994).
- [27] TT Yeh and CW Atta, "Spectral transfer of scalar and velocity fields in heated-grid turbulence," J. Fluid Mech. 58, 233–261 (1973).
- [28] RA Antonia, SK Lee, L Djenidi, P Lavoie, and L Danaila, "Invariants for slightly heated decaying grid turbulence," J. Fluid Mech 727, 379–406 (2013).
- [29] RE Seoud and JC Vassilicos, "Dissipation and decay of fractal-generated turbulence," Phys. Fluids 19, 105108 (2007).
- [30] N Mazellier and JC Vassilicos, "Turbulence without richardson–kolmogorov cascade," Phys. Fluids 22, 075101 (2010).
- [31] PC Valente and JC Vassilicos, "The decay of turbulence generated by a class of multiscale grids," J. Fluid Mech. 687, 300–340 (2011).
- [32] R Gomes-Fernandes, B Ganapathisubramani, and JC Vassilicos, "Particle image velocimetry study of fractal-generated turbulence," J. Fluid Mech. 711, 306–336 (2012).
- [33] PC Valente and JC Vassilicos, "Universal dissipation scaling for nonequilibrium turbulence," Phys. Rev. Lett. 108, 214503 (2012).
- [34] Y Zhou, K Nagata, Y Sakai, H Suzuki, Y Ito, O Terashima, and T Hayase, "Development of turbulence behind the single square grid," Phys. Fluids 26, 045102 (2014).
- [35] Y Zhou, K Nagata, Y Sakai, Y Ito, and T Hayase, "Enstrophy production and dissipation in developing grid-generated turbulence," Phys. Fluids 28, 025113 (2016).
- [36] Y Zhou, K Nagata, Y Sakai, Y Ito, and T Hayase, "Spatial evolution of the helical behavior and the 2/3 power-law in single-square-grid-generated turbulence," Fluid Dyn. Res. 48, 021404 (2016).
- [37] I Paul, G Papadakis, and JC Vassilicos, "Genesis and evolution of velocity gradients in near-field spatially developing turbulence," J. Fluid Mech. 815, 295–332 (2017).
- [38] S Laizet, JC Vassilicos, and C Cambon, "Interscale energy transfer in decaying turbulence and vorticity–strain-rate dynamics in grid-generated turbulence," Fluid Dyn. Res. 45, 061408 (2013).
- [39] R Gomes-Fernandes, B Ganapathisubramani, and JC Vassilicos, "Evolution of the velocitygradient tensor in a spatially developing turbulent flow," J. Fluid Mech. 756, 252–292 (2014).
- [40] S Laizet, J Nedić, and JC Vassilicos, "The spatial origin of- 5/3 spectra in grid-generated turbulence," Phys. Fluids 27, 065115 (2015).
- [41] H Suzuki, K Nagata, Y Sakai, and T Hayase, "Direct numerical simulation of turbulent mixing in regular and fractal grid turbulence," Phys. Scripta 2010, 014065 (2010).
- [42] H Suzuki, K Nagata, Y Sakai, and R Ukai, "High-schmidt-number scalar transfer in regular and fractal grid turbulence," Phys. Scripta 2010, 014069 (2010).
- [43] S Laizet and JC Vassilicos, "Stirring and scalar transfer by grid-generated turbulence in the presence of a mean scalar gradient," J. Fluid Mech. 764, 52–75 (2015).
- [44] Y Ito, T Watanabe, K Nagata, and Y Sakai, "Turbulent mixing of a passive scalar in grid turbulence," Phys. Scripta 91, 074002 (2016).
- [45] T Watanabe, Y Sakai, K Nagata, Y Ito, and T Hayase, "Implicit large eddy simulation of a scalar mixing layer in fractal grid turbulence," Phys. Scripta 91, 074007 (2016).
- [46] S Corrsin, "Remarks on turbulent heat transfer: an account of some features of the phenomenon in fully turbulent regions," in *Proc 1st Iowa Symp on Thermodynamics* (1953) pp. 5–30.
- [47] S Balay, S Abhyankar, M Adams, J Brown, P Brune, K Buschelman, V Eijkhout, W Gropp, D Kaushik, and M Knepley, *Petsc users manual revision 3.5*, Tech. Rep. (Technical report, Argonne National Laboratory (ANL), 2014).
- [48] I Paul, Evolution of velocity and scalar gradients in a spatially developing turbulence, Ph.D. thesis, Imperial College London UK (2017).
- [49] I Paul, G Papadakis, and JC Vassilicos, "DNS of heat transfer from a cylinder immeresed in the production and decay regions of grid-element," J. Fluid Mech. Under review (2018).
- [50] I Paul, G Papadakis, and JC Vassilicos, "On the skewness of passive scalar gradients in heated grid-element turbulence," J. Fluid Mech. Under review (2018).
- [51] A Tsinober, An informal conceptual introduction to turbulence, Vol. 483 (Springer, 2009).
- [52] H Tennekes and JL Lumley, A first course in turbulence (MIT press, 1972).
- [53] M Lesieur, Turbulence in fluids, Vol. 40 (Springer Science & Business Media, 2012).
- [54] M Lesieur, C Montmory, and JP Chollet, "The decay of kinetic energy and temperature variance in three-dimensional isotropic turbulence," Phys. Fluids 30, 1278–1286 (1987).
- [55] BE Launder, "On the computation of convective heat transfer in complex turbulent flows," J. Heat Transfer 110, 1112–1128 (1988).
- [56] AN Kolmogorov, "The local structure of turbulence in incompressible viscous fluid for very large reynolds numbers," in Dokl. Akad. Nauk SSSR, Vol. 30 (1941) pp. 299–303.
- [57] SK Lee, A Benaissa, L Djenidi, P Lavoie, and RA Antonia, "Scaling range of velocity and passive scalar spectra in grid turbulence," Phys. Fluids 24, 075101 (2012).
- [58] GR Ruetsch and MR Maxey, "Small-scale features of vorticity and passive scalar fields in homogeneous isotropic turbulence," Phys. Fluids 3, 1587–1597 (1991).
- [59] GR Ruetsch and MR Maxey, "The evolution of small-scale structures in homogeneous isotropic turbulence," Phys. Fluids 4, 2747–2760 (1992).
- [60] G Brethouwer, JCR Hunt, and FTM Nieuwstadt, "Micro-structure and lagrangian statistics of the scalar field with a mean gradient in isotropic turbulence," J. Fluid Mech. 474, 193–225 (2003).
- [61] R Betchov, "Numerical simulation of isotropic turbulence," Phys. Fluids 18, 1230–1236 (1975).
- [62] B Ganapathisubramani, K Lakshminarasimhan, and NT Clemens, "Investigation of threedimensional structure of fine scales in a turbulent jet by using cinematographic stereoscopic particle image velocimetry," J. Fluid Mech. 598, 141–175 (2008).
- [63] G Gulitski, M Kholmyansky, W Kinzelbach, B Lüthi, A Tsinober, and S Yorish, "Velocity and temperature derivatives in high-reynolds-number turbulent flows in the atmospheric surface layer. part 1. facilities, methods and some general results," J. Fluid Mech. 589, 57–81 (2007).
- [64] K Ohkitani, "Numerical study of comparison of vorticity and passive vectors in turbulence and inviscid flows," Phys. Rev. E 65, 046304 (2002).