Statistics and scaling of turbulence in a spatially developing mixing layer at Reλ = 250

Antonio Attili and Fabrizio Bisetti

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Statistics and scaling of turbulence in a spatially developing mixing layer at Reₐ = 250

Antonio Attili (a) and Fabrizio Bisetti
Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal 23955, Kingdom of Saudi Arabia
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The turbulent flow originating from the interaction between two parallel streams with different velocities is studied by means of direct numerical simulation. Rather than the more common temporal evolving layer, a spatially evolving configuration, with perturbed laminar inlet conditions is considered. The streamwise evolution and the self-similar state of turbulence statistics are reported and compared to results available in the literature. The characteristics of the transitional region agree with those observed in other simulations and experiments of mixing layers originating from laminar inlets. The present results indicate that the transitional region depends strongly on the inlet flow. Conversely, the self-similar state of turbulent kinetic energy and dissipation agrees quantitatively with those in a temporal mixing layer developing from turbulent initial conditions [M. M. Rogers and R. D. Moser, “Direct simulation of a self-similar turbulent mixing layer,” Phys. Fluids 6, 903 (1994)]. The statistical features of turbulence in the self-similar region have been analysed in terms of longitudinal velocity structure functions, and scaling exponents are estimated by applying the extended self-similarity concept. In the small scale range (60 < r/η < 250), the scaling exponents display the universal anomalous scaling observed in homogeneous isotropic turbulence. The hypothesis of isotropy recovery holds in the turbulent mixing layer despite the presence of strong shear and large-scale structures, independently of the means of turbulence generation. At larger scales (r/η > 400), the mean shear and large coherent structures result in a significant deviation from predictions based on homogeneous isotropic turbulence theory. In this second scaling range, the numerical values of the exponents agree quantitatively with those reported for a variety of other flows characterized by strong shear, such as boundary layers, as well as channel and wake flows. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.3696302]

I. INTRODUCTION

The mixing layer is a canonical flow of great technological relevance to practical devices. In real flows, turbulence is often generated by instabilities and mean flow shear is important. The mixing layer configuration has been studied for over 40 years by theoretical, experimental, and numerical means. For the most part, the existing data on mixing layers documents the dynamics of large organized structures, the process of transition to developed turbulence and the self-similar state for hydrodynamic and passive scalar quantities. Conversely, much less is known about the high order statistical features and scaling of developed turbulence downstream of the instability in free shear configurations.

The seminal work of Brown and Roshko illustrated the existence of two-dimensional, large-scale structures in the mixing layer. Several experimental works provide detailed quantitative knowledge about the mean flow. Bell and Mehta measured turbulent velocity statistics in the self-similar

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(a) Electronic mail: antonio.attili@kaust.edu.sa.
region. Measurements in a number of different configurations have been performed by Dimotakis and coworkers. Both passive and reactive scalar transport in mixing layers have been extensively studied by Konrad, Masutani and Bowman, Clemens and Mungal, and Karasso and Mungal. Substantial effort has been expended in the pursuit of understanding the origin, dynamics, and significance of coherent structures and their role in establishing the mixing layer self-similar state for velocity and scalar fields. Much of the current understanding of the transition from organized structures to developed, three-dimensional, non-organized flow is due to the direct numerical simulations (DNS) of a temporal mixing layer by Rogers and Moser. They showed that the transition to turbulence from laminar initial conditions with simple low wavenumber disturbances displays features that are specific to the type of disturbances introduced in the flow. They identified rollers and rib vortices structures developing during the Kelvin-Helmholtz instability. During the transition, instantaneous features and statistics of the flow field can be well explained by the dynamics of those coherent large structures. The details of the evolution of those structures depend on the initial (or inlet) conditions. Further downstream, the mixing layer achieves a self-similar behavior illustrated by the evolution of the momentum thickness, the total dissipation rate of kinetic energy, and the collapse of mean velocity profiles and Reynolds stresses. However, this self-similar state is often called “apparent,” due to a dependency on the inlet conditions. As highlighted by Rogers and Moser and by Karasso and Mungal, there also exists a link between the hydrodynamic structures, the stage of the transition and the characteristics of scalar mixing. The asymptotic state of the mixing layer is associated with marching probability density function (PDF) for the passive scalar mixing.

Despite the relevance of the mixing layer configuration to the study of turbulence in free-shear flows, the characteristics of developed shear turbulence in a mixing layer are not well documented.

Starting from Kolmogorov’s work, theories describing flow behavior in the turbulent regime have been developed under the hypotheses of homogeneity, isotropy, and high Reynolds number. It is generally accepted that these theories are still applicable if the homogeneity and isotropy hypotheses are verified locally, despite the fact that the large scales of the flow might not be characterized by homogeneous isotropic behavior. The Reynolds number must be high enough for the large, non-isotropic, flow-dependent scales to be separated from the small, isotropic, universal ones. The study of developed turbulence in flow configurations having energetic, coherent, large scale structures such as the mixing layer offers the opportunity to better understand the relation between non-isotropic, flow-dependent fluid motion and isotropic turbulence. Recently, Wang et al. performed a DNS of a spatial mixing layer to investigate the characteristics of fine scale eddies and analyze the dynamics of the tube-like structures typical of homogeneous isotropic turbulence. They described the link between the laminar turbulent transition and coherent fine scales eddies. In the transitional region, large scale rollers and ribs structures interact and fine scale eddies are generated. In the developed region, the rollers and rib structures still exist and the rib structures consist of several eddies.

Statistical analysis of shear flow turbulence has attracted much attention in the last years. Casciola et al. established a new similarity law that extends Kolmogorov’s refined similarity hypothesis to shear flows. Casciola et al. and Gualtieri et al. proposed a double-scaling scenario with exponents depending on the range of scales analyzed. The crossover between the two regimes is assumed to be close to the characteristic shear length scale. Ruiz-Chavarria et al. and Toschi et al. proposed a modified form of structure functions to characterize the effect of shear intensity on the values of the scaling exponents. The scaling properties of mixing layer turbulence have been investigated experimentally by Jiang et al. They describe longitudinal and transverse structure functions and highlight the differences between the scaling exponents for the two. They find that the scaling exponents for the transverse structure functions are smaller than those for the longitudinal ones. In the range of scales analyzed, the scaling exponents reported for the longitudinal structure functions are very similar to those in homogeneous isotropic turbulence.

In this paper, the results from a DNS of a spatially developing mixing layer with initial vorticity thickness Reynolds number $Re_\theta = 600$ are reported. Data on passive scalar mixing are also available as part of the DNS results. The value of the Reynolds number based on the Taylor microscale
(Re$_t$ $\approx$ 250) allows for a significant separation between large and dissipative scales, and the kinetic energy spectrum displays an inertial range of more than one decade characterized by Kolmogorov scaling. To the authors’ knowledge, the present simulation achieves the highest Reynolds number reported in the literature for the spatially evolving mixing layer.

Turbulence develops from perturbed laminar inlet conditions reaching a self-similar state far downstream of the Kelvin-Helmholtz instability. The very large computational domain used in this study results in a self-similar state being established downstream of the instability. Turbulent statistics are analyzed and compared with data available in the literature for mixing layers in different configurations to assess the existence of a universal self-similar state of the turbulent mixing layer, which is independent of the details of the injection mechanism.

The statistical features of turbulence in the fully developed region are analyzed in terms of structure functions and the scaling exponents are calculated, thus extending recent findings on small scale features in shear dominated turbulence. The degree of homogeneity in the flow is quantified alongside with the details of the isotropy recovery process. The turbulence generated in the mixing layer displays statistical features previously observed in other turbulence flow configurations. The characteristics of small scale turbulence in the mixing layer have been compared to those in homogeneous turbulence and in other shear dominated flows. It is reported that shear can decrease the value of the structure function scaling exponent, which is equivalent to a higher level of intermittency than for homogeneous isotropic turbulence. Furthermore, two ranges for which the scaling is different are reported in this work: one at the large, shear-dominated scales and the other at the small scales, where the mean shear has negligible effects and the homogeneous isotropic turbulence behavior is recovered. In the present work, the effect of shear non-isotropic structures on intermittency and statistics based on Kolmogorov’s theory has been quantified for a wide range of scales.

The paper is organized as follows. In Sec. II, the numerical methods used and initial conditions are discussed. Details on the inlet conditions are provided. Section III presents the large scale statistics of the flow, illustrating the features of coherent structure pairings and transition to self-similarity for both the velocity and scalar fields. High order statistics are shown and discussed in Sec. IV, where the scaling of velocity structure functions is analyzed in detail. Finally, conclusions are presented in Sec. V.

II. PRELIMINARIES

The direct numerical simulation presented in this work is performed by solving the unsteady, incompressible Navier-Stokes equations. An additional transport equation for a passive scalar with Schmidt number equal to 0.7 is also solved. The scalar values are one and zero in the free streams. Constant transport properties are used (kinematic viscosity $\nu = \mu/\rho$ and diffusivity $D$). To facilitate comparison with experiments and allow interaction between the upstream and downstream region, a spatially evolving mixing layer configuration is used in favour of the more common temporally evolving layer.

The parallel flow solver “NGA” developed at Stanford University is used to solve the transport equations. The solver implements a finite difference method on a spatially and temporally staggered grid with the semi-implicit fractional-step method of Kim and Moin. Velocity and scalar spatial derivatives are discretized with a second order finite differences centered scheme. The time step size is calculated in order to have a unity Courant-Friedrichs-Lewy (CFL) number. A pressure-correction step involving the solution of a Poisson equation ensures mass conservation. The code decomposes the computational domain over a number of processors and implements a distributed memory parallelization strategy using the message passing interface. The solution of the Poisson equation on massively parallel machines is performed by the library HYPRE (Ref. 43) using the preconditioned conjugate gradient iterative solver coupled with one iteration of an algebraic multigrid preconditioner.

Along the streamwise direction, the boundary conditions are imposed inflow at $x = 0$ and free convective outflow at $x = L_x$. The boundary conditions are periodic in the spanwise direction $z$ and free-slip in the crosswise direction $y$. The free-slip condition is applied imposing a zero crosswise
velocity component at the boundary. The normal derivatives of the streamwise and spanwise velocity components are set to zero. Consequently, the two velocity components parallel to the wall are free to float. The size of the domain in the crosswise direction is large enough to avoid the turbulent flow field being affected by the free-slip boundary conditions in any significant manner. In the present DNS, the variation of the difference and the average of the free-stream velocities is less than 0.5% between the inlet and outlet planes. Furthermore, the streamwise pressure difference is small according to the mean non-dimensional static pressure gradient \( \langle p(x, y) - p(x = 0, y) \rangle / (1/2 \rho U^2) \), where \( U_c = (u_1 + u_2)/2 \) is the convective velocity and \( u_1 \) and \( u_2 \) are the high- and low-speed stream velocities. At all locations \( (x, y) \), the mean non-dimensional static pressure gradient is less then 0.014, which is comparable to the value 0.012 in the zero-pressure gradient incompressible boundary layer of Wu and Moin.\(^{45} \)

The flow at the inlet \( (x = 0) \) is a hyperbolic tangent profile for the streamwise velocity \( u \) with prescribed vorticity thickness \( \delta_{\omega, 0} \),

\[
u(x = 0, y, z) = U_c + \frac{1}{2} \Delta U \tanh \left( \frac{2y}{\delta_{\omega, 0}} \right),
\]

where \( \Delta U = u_1 - u_2 \) is the velocity difference across the layer. The Reynolds number based on the vorticity (momentum) thickness at the inlet is \( \text{Re}_{\omega} = 600 \) (resp. \( \text{Re}_0 = 150 \)), increasing to \( \text{Re}_{\omega} = 25000 \) (resp. \( \text{Re}_0 = 4250 \)) as the mixing layer develops. The ratio of the two velocities is \( u_1/\delta_{\omega} = 3 \). In a preliminary large-eddy simulation (LES) study, it was observed that more realistic inlet profiles that take into account the presence of a thick splitter plate (i.e., wake/mixing-layer inlet)\(^{45} \) retard the establishment of fully developed turbulence compared to the hyperbolic tangent profile. Low amplitude white noise is superimposed on the hyperbolic tangent profile, resulting in the onset of the Kelvin-Helmholtz instability a short distance downstream of the inlet \( (x \approx 50\delta_{\omega, 0}) \).

The crosswise and spanwise velocity components are perturbed with the same type of disturbance. The low amplitude white noise is added to the laminar profile at the inlet only at crosswise locations \( |y| \leq 4\delta_{\omega, 0} \). The boundary condition and the forcing method used allow a “natural” transition to turbulence without imposing coherent turbulent structures at the inlet. More detailed information about the spectral characteristics of the inlet noise are presented in Fig. 12 (Sec. III), where it is shown that the spectral energy density of the forcing (constant in frequency space) is four orders of magnitude smaller than the energy observed at the most unstable frequency near the onset of the Kelvin-Helmholtz instability around \( x = 50\delta_{\omega, 0} \). Measured in terms of the statistics observed in the self-similar region, the forcing amplitude is 1% of the peak fluctuations. Finally, if measured in terms of mean quantities, the fluctuating kinematic energy injected at the inflow has a maximum value of \( 2 \times 10^{-6} \Delta U^2 = 2 \times 10^{-6} U_c^2 \). The passive scalar at the inlet is unity for \( y \geq 0 \) and zero for \( y < 0 \).

The computational domain extends \( L_x = 473\delta_{\omega, 0}, L_y = 290\delta_{\omega, 0}, L_z = 157.5\delta_{\omega, 0} \) in the streamwise \( (x) \), crosswise \( (y) \), and spanwise \( (z) \) directions, respectively. The domain is discretized with \( 3072 \times 940 \times 1024 \approx 3 \times 10^9 \) grid points \( (N_x \times N_y \times N_z) \). In the region of the domain centered around \( y = 0 \) (\( |y| \leq 45\delta_{\omega, 0} \)), the grid is homogeneous in the three directions: \( \Delta x = \Delta y = \Delta z = 0.15\delta_{\omega, 0} \). Outside the core region for \( |y| > 45\delta_{\omega, 0} \), the grid is stretched linearly until \( \Delta y = 0.6\delta_{\omega, 0} \) at \( |y| = 55\delta_{\omega, 0} \) and then is constant again up to the boundary. In this region, the turbulent kinetic energy is at least three orders of magnitude smaller than its maximum \( (K/\Delta U^2 \approx 0.03 \) in the center of the layer and \( K/\Delta U^2 \approx 10^{-5} \) at \( |y| = 50\delta_{\omega, 0} \)) and fluctuations of the streamwise component of velocity are 3% of their maximum. In this potential flow region, the vorticity and the fluctuating vorticity root-mean-square are, respectively, three and five orders of magnitude smaller than inside the layer. The maximum cell size is kept to a minimum in order to avoid unacceptable loss of performance in the fast parallel iterative solution to the Poisson equation during the pressure correction procedure.

Overall, the spatial resolution is such that \( \Delta x = \Delta y = \Delta z \leq 2.5\eta \) in the whole domain, being \( \eta = v^{3/4} \varepsilon^{-1/4} \) the Kolmogorov scale, and \( \varepsilon \) the turbulent kinetic energy dissipation rate.

A number of highly resolved large-eddy simulations have been performed (results not shown) to select suitable domain sizes in the crosswise and spanwise directions. The large-eddy simulations have a resolution four times coarser in every direction than the DNS. A rather large domain length in the spanwise direction \( L_z (157.5\delta_{\omega, 0} \) was selected to obtain turbulence statistics independent of the domain size.
Preparatory and production simulations were performed on the IBM Blue Gene/P system “Shaheen” available at King Abdullah University of Science and Technology, using up to 65 536 processing cores (16 racks of the Blue Gene/P architecture). The production simulation was advanced in time from the initial conditions until the turbulent flow became statistically stationary. Statistics were accumulated over time for 3500 \( \tau \) (\( \tau = U/\delta \omega \)), 1400 samples of the flow field have been collected to evaluate statistics. A number of time signals have been sampled at several spatial locations in order to calculate spectra and structure functions applying Taylor’s hypothesis. The simulation required around 10 million CPU hours and produced approximately 100 TB of data.

III. STREAMWISE EVOLUTION AND SELF-SIMILAR STATE

It is well known that at a certain distance from the inlet, the mixing layer evolves self-similarly. Appropriate velocity and length scales are the constant velocity difference \( \Delta U \) across the mixing layer and a measure of the local layer thickness. The momentum thickness \( \delta_\theta \) is usually preferred to other quantities (vorticity thickness \( \delta \omega \) or visual thickness) because of its integral nature,

\[
\delta_\theta(x) = \frac{1}{\Delta U^2} \int_{-\infty}^{\infty} (u_1 - \langle u \rangle)(u - u_2)dy.
\]

The local layer momentum thickness is used to define a normalized crosswise coordinate \( y^+ = y/\delta_\theta(x) \). As the profiles of rescaled turbulence statistics collapse on a single curve, the flow is deemed self-similar. Self-similarity implies a linear growth for the total turbulent kinetic energy \( K(x) \) and a constant value for the total dissipation rate \( \varepsilon(x) \), defined as

\[
K(x) = \int_{-\infty}^{\infty} kdy = \frac{1}{2} \int_{-\infty}^{\infty} \langle u'u' \rangle + \langle v'v' \rangle + \langle w'w' \rangle dy,
\]

and

\[
\varepsilon(x) = \int_{-\infty}^{\infty} \epsilon dy = 2\nu \int_{-\infty}^{\infty} \langle S_{ij}S_{ij} \rangle dy,
\]

where \( S_{ij} \) is the rate of strain tensor.

In the remainder of this section, velocity and statistics are reported at selected downstream locations. Table I contains a list of the streamwise coordinates of all stations and corresponding labels.

The streamwise evolution of the normalized momentum thickness \( \delta_\theta(x)/\delta_{\omega,0} \) is shown in Fig. 1. After the initial exponential growth due to the Kelvin-Helmholtz instability, the linear growth set by self-similarity is observed. The thickness compensated with the dimensional scaling \( \chi \) is plotted in the inset. In the self-similar region, the growth rate is \( d\delta_\theta(x)/dx \approx 0.0168 \), obtained with a least-squares fit over the streamwise range \( 300 \times x/\delta_{\omega,0} < 400 \). Rogers and Moser\(^4\) reported a value of 0.014 in a temporal evolving mixing layer simulation. Bell and Mehta\(^6\) and Dimotakis\(^14\) reported experimental values equal to 0.016 and between 0.014 and 0.022, respectively.

The mean streamwise velocity profiles at ten downstream locations (see Table I for the station locations) are plotted in Fig. 2. Starting from \( x/\delta_{\omega,0} \approx 100 \) (station C), the velocity profiles collapse on each other and agree very well with the data of Bell and Mehta.\(^6\) However, self-similarity for

<table>
<thead>
<tr>
<th>Station</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
<th>I</th>
<th>L</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x/\delta_{\omega,0} )</td>
<td>0</td>
<td>50</td>
<td>100</td>
<td>150</td>
<td>200</td>
<td>250</td>
<td>300</td>
<td>350</td>
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turbulent kinetic energy and dissipation rate is achieved further downstream, making the mean velocity profile an unreliable indicator of self-similarity.

Figure 3 shows that the normalized total turbulent kinetic energy grows linearly after a transition region and the self-similar behavior is recovered for \( x > 300 \delta_{\omega,0} \). The streamwise component contribution to the total kinetic energy (\( K_x \)) achieves self-similarity before the two other components (\( K_y \) and \( K_z \)). In the region where strong vortex pairing occurs, the crosswise component (\( K_y \)) of the turbulent kinetic energy undergoes a rapid growth\(^1\) resulting in \( K_y \geq K_x \) for \( 50 \delta_{\omega,0} < x < 100 \delta_{\omega,0} \).

Figure 4 shows that the total dissipation \( \varepsilon \) experiences a rapid growth followed by a slow convergence to self-similarity, which dictates that \( \varepsilon \) is constant. A comparison between Fig. 3 and Fig. 4 reveals that the total dissipation reaches a self-similar state further downstream compared to the turbulent kinetic energy. The asymptotic value of the total dissipation agrees well with the value obtained by Rogers and Moser.\(^1\) The level of agreement is rather remarkable considering the differences between the two studies: spatially versus temporally evolving mixing layer and laminar inlet with noise versus turbulent initial conditions.

**FIG. 1.** Streamwise evolution of the normalized momentum thickness \( \delta_\theta/\delta_{\omega,0} \) defined as in Eq. (2). The solid line is obtained with a least-squares fit in the range \( 300 < x/\delta_{\omega,0} < 400 \); the slope of the line is 0.0168. The inset shows the evolution of the compensated momentum thickness, \( \delta_\theta/(\delta_{\omega,0} \cdot x) \).

**FIG. 2.** Mean streamwise velocity profiles for several downstream locations labeled as in Table I. Measurements from Bell and Mehta\(^6\) (open circles) are shown for comparison.
FIG. 3. Streamwise evolution of normalized total turbulent kinetic energy $K/\Delta U^2$ defined as in Eq. (3) (solid squares). Contributions from the three components of velocity are also shown: $2K_x/\Delta U^2$ (open circles), $2K_y/\Delta U^2$ (open squares), and $2K_z/\Delta U^2$ (open diamonds). Lines indicate least-squares fit over $200 < x/\delta_{w,0} < 400$ ($K_x$) and $300 < x/\delta_{w,0} < 400$ ($K$, $K_y$, and $K_z$).

Figure 4 shows the total production also,

$$P(x) = \int_{-\infty}^{\infty} P dy = \int_{-\infty}^{\infty} - \langle U'_i U'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} dy,$$

where $\{U_i\} = \{u, v, w\}$ is the velocity vector and $\{U'_i\} = \{u', v', w'\}$ its fluctuation. The ratio between production and dissipation becomes constant ($\approx 1.4$) from $x/\delta_{w,0} > 150$ onwards, well before the self-similar state for kinetic energy is established at $x/\delta = 300$. This asymptotic value is in good agreement with the value observed by Rogers and Moser\(^1\) in the self-similar region of a temporal mixing layer. The location $x/\delta_{w,0} = 150$ coincides with the starting point of the linear growth of the mixing layer.

FIG. 4. Streamwise evolution of normalized total dissipation rate $\mathcal{E}/\Delta U^3$ defined as in Eq. (4). Results from Fig. 2(a) in Rogers and Moser\(^1\) are reproduced for comparison (R-M–TBL). The abscissa is a local Reynolds number $Re(x) = \Delta U \delta_{w,0}(x)/\nu$, which allows a direct comparison between the asymptotic behavior of $\mathcal{E}$ in spatially and temporally evolving mixing layers. The total production $P(x)$ defined in Eq. (5) is shown also.
FIG. 5. Evolution of total normalized crosswise component of the turbulent kinetic energy $V$ defined as in Eq. (6). Results from the present simulation shown alongside those in Rogers and Moser. Present simulation (open circles), turbulent boundary layer (TBL) initial conditions (Ref. 1, solid line), laminar initial conditions WHIGH2P (Ref. 9, dashed line), and laminar initial conditions TURB2P (Ref. 9, dotted-dashed line). The quantity $V$ is shown as a function of $x \delta_{a,0}$ for our simulation (bottom axis) and as a function of time $\tau$ for the data of Rogers and Moser (top axis).

streamwise component of kinetic energy. The ratio between production and dissipation is greater than 1.4 for $x \delta_{a,0} < 150$.

Despite the similarity in the asymptotic value of the total dissipation rate $\mathcal{E}$, there exist important differences with respect to the temporally evolving mixing layer (TBL) of Rogers and Moser. Those differences pertain mostly to the transition from the inlet conditions (or initial for the temporal evolving mixing layer) to self-similar, developed turbulence. In our simulation, the turbulent mixing layer develops from a laminar profile and undergoes a natural transition to turbulence. This configuration is similar to the cases described in Moser and Rogers and labeled WHIGH2P and TURB2P in Fig. 5. On the contrary, the same authors described a temporally evolving mixing layer simulation starting from a velocity field constructed by combining two snapshots of a turbulent boundary layer. The integral normalized crosswise component of the turbulent kinetic energy $V$ well characterizes the evolution to self-similarity for a mixing layer, since it can be related to the energy in large coherent structures undergoing pairing events. It is defined as

$$V(x) = \frac{1}{\Delta U^2 \delta_0(x)} \int_{-\infty}^{\infty} v'v' \, dy.$$  

(6)

The large overshoot of $V(x)$ is characteristic of the pairings of large vortices generated via the Kelvin-Helmholtz instability. Such overshoot is present both in our simulation data as well as in the DNS simulations by Moser and Rogers performed starting from a forced laminar profile (the cases labeled WHIGH2P and TURB2P). Conversely, the overshoot is not present for the TBL case. The sudden increase in $V(x)$ followed by the decay towards an asymptotic value delays the establishment of self-similarity. The asymptotic value of $V(x)$ obtained from the present simulation compares extremely favorably with the value from the TBL case of Rogers and Moser showing that despite the different transition dynamics, the same integral value of turbulent kinetic energy in the crosswise velocity component fluctuation is recovered as self-similarity is established. On the contrary, the two cases R-M WHIGH2P and R-M TURB2P do not reach a self-similar final behavior, due to the simulation time being too short. Moreover, the initial conditions for R-M WHIGH2P and R-M TURB2P are obtained by imposed two-dimensional perturbations on a laminar flow field, resulting in persistent “classical” pairing and high levels of $V(x)$. 

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During the initial phase of vortex pairing ($x < 100 \delta_{\omega,0}$), the crosswise velocity fluctuation variance is larger than the streamwise one, as shown in Fig. 6, while further downstream, $\langle v'v' \rangle/\langle u'u' \rangle$ and $\langle w'w' \rangle/\langle u'u' \rangle$ converge to a value less than unity at the crosswise location of peak turbulent kinetic energy. The same evolution of $\langle v'v' \rangle/\langle u'u' \rangle$ has been observed in the experiments by Bell and Mehta and by Browand and Weidman. Very close to the inlet (station B at $x = 50 \delta_{\omega,0}$), crosswise velocity fluctuations are the largest. In the self-similar region, they are everywhere smaller than streamwise velocity fluctuations, with the exception of a small region near the interface between turbulent and non-turbulent flow ($y^+ \approx -5$ and $y^+ \approx 3$).

The transport of a passive scalar ($Z$) with Schmidt number $Sc = 0.7$, is also performed as part of the simulation. Isocontours of the passive scalar concentration are shown in Fig. 7 for two $x$-$y$ planes corresponding to two spanwise positions (the distance between the two $z$ positions is half of the overall domain in the spanwise direction). The streamwise position of the peak of the integral normalized crosswise component of the turbulent kinetic energy $V$ (shown in Fig. 5) is marked with the dashed vertical line labeled A. The two boxes mark the regions shown in Fig. 8, where three-dimensional isocontours of enstrophy are reported. The vortices generated by the Kelvin-Helmholtz instability grow (due to entrainment and pairing) as they evolve in the streamwise direction. In a preliminary study, it was found that the size of the domain has a strong effect on the statistics of turbulence, as discussed by Balaras et al. In particular, we observed that if the domain in the spanwise direction is not large enough, the flow becomes quasi-two-dimensional, with large coherent rollers spanning it in its entirety. Comparing the two passive scalar contour plots in Fig. 7, it is apparent that the flow is three-dimensional throughout the domain. For example, at the location marked with the dashed line labeled with B, a roller is shown in the top panel, while the bottom panel (at a different spanwise position) displays a braid region at the same $x$-$y$ location.

The evolution of three-dimensional structures during the instability, transition, and in the fully developed region is shown in Fig. 8 using isocontours of enstrophy. Only a portion of the domain in the spanwise direction is shown ($0 < z < 59 \delta_{\omega,0}$ out of a total length $L_z = 157.5 \delta_{\omega,0}$). Figure 8(a) shows a top view in the region around the peak of the integral of the normalized crosswise component of the turbulent kinetic energy $\mathcal{V}$ (see Eq. (6)). The transition between qualitatively different behaviors is evident. Upstream of the streamwise location of the $\mathcal{V}$ peak, the mixing layer structure is characterized by coherent rollers and braid regions with large rib vortices. These are the same structures observed by Rogers and Moser in the early stages of the evolution of a temporal mixing layer from laminar initial conditions, forced on its most unstable mode. The axes of the rib vortices do not lie on the $x$-$y$ planes; rather they are inclined. Their inclination correlates with the
FIG. 7. Snapshots of the passive scalar field for two $x$-$y$ planes at two different spanwise positions separated by a distance equal to half of the spanwise domain size. Black (white) regions correspond to a scalar value equal to 0 (1). The whole domain is reported in the streamwise ($x$) direction and only the core region in the crosswise ($y$) direction ($-80\delta_{uv,0} \leq y \leq 60\delta_{uv,0}$).

Sign of the vorticity components $\omega_x$ and $\omega_y$. In the case of rib vortices at a positive angle with respect to the $x$ axis in the $z$-$x$ plane, $\omega_x$ and $\omega_y$ are both positive. Downstream of the location of the peak in $V$, small scale structures dominate the flow field, but rollers and large rib vortices are still present. In the far field, the layer is characterized by the presence of small structures, as shown in Figs. 8(b) and 8(d). Brown-Roshko structures are still apparent (Fig. 8(d) and bottom panel of Fig. 7), but the large rib vortices are absent from the braid regions.

Figures 9–11 show the streamwise evolution of the normalized Reynolds stress tensor components. Convergence to an approximate self-similarity behavior is apparent for all quantities. Also included are the results from the DNS by Rogers and Moser of a temporal evolving mixing layer with turbulent initial conditions and the experiments by Bell and Mehta for a mixing layer originating from turbulent (tripped) splitter plate boundary layers. The results by Rogers and Moser have been shifted to take into account that in the temporal simulation there is no movement of the layer center towards the low-speed stream. In the graphs containing the fluctuations, locations for $x \geq 50\delta_{uv,0}$ are reported. Compared to mean velocity profiles, the Reynolds stress statistics converge to a self-similar state rather slowly.

Figure 12 displays one-dimensional spectra of the streamwise component of velocity obtained using Taylor’s hypothesis starting from time signals of turbulence quantities. Statistics collected at several locations are plotted: the Kelvin-Helmholtz instability develops around $x = 50\delta_{uv,0}$ from the inlet conditions ($x = 0.1\delta_{uv,0}$), which are characterized by low amplitude white noise. The peak position in the spectrum is close to the value predicted by linear stability based on a hyperbolic tangent profile. Downstream of the Kelvin-Helmholtz instability, the flow becomes fully turbulent; the spectra are self-similar with a wide range (more than one decade) of Kolmogorov’s scaling showing a $-5/3$ slope.

The Pdf of the passive scalar concentration has been evaluated at several cross stream positions, corresponding to different values of the mean concentration $\langle Z \rangle$. The position of the peaks of the Pdf in sample space with respect to its mean is of great interest, since two behaviors are typically observed. If the peak location is independent of the mean, the Pdf is called non-marching, while if the peak position changes with the mean and coincides with the value of $\langle Z \rangle$, the Pdf is called...
FIG. 8. Local enstrophy $\omega^2$ isocontour ($0 < z < 59\delta_{u,0}$). The value of the isocontour is the same for all the figures and equal to $0.1\omega_{\text{max}}^2$.

FIG. 9. Normalized streamwise velocity fluctuation variance $\langle u'u' \rangle/\Delta U^2$ for several downstream locations (solid lines) labeled as in Table I. The DNS results from Rogers and Moser (dashed line) and measurements from Bell and Mehta (open circles) are shown for comparison.
FIG. 10. Normalized crosswise velocity fluctuation variance $\langle v'v' \rangle / \Delta U^2$ for several downstream locations (solid lines) labeled as in Fig. 9. The DNS results from Rogers and Moser (dashed line) and measurements from Bell and Mehta (open circles) are shown for comparison.

Marching. Figures 13 and 14 show the Pdf of the passive scalar at two streamwise positions, i.e., $x = 100\delta_{w,0}$ and $x = 400\delta_{w,0}$, respectively. Both graphs display the results for three different cross stream positions, where $\langle Z \rangle = 0.3$, $\langle Z \rangle = 0.5$, and $\langle Z \rangle = 0.7$. In the transitional region of the mixing layer the Pdf is non-marching, while the Pdf becomes marching in the far field. The marching behavior is associated with developed turbulence after the mixing transition, confirming that the far field turbulence is well developed.

IV. SMALL SCALES STATISTICS

The statistical properties of turbulence in the inertial range can be characterized in terms of longitudinal velocity structure functions. The $n$th-order longitudinal structure function for the
streamwise component of velocity is defined at position \( x \) as

\[
S_n(x, r) = \langle |u(x + r) - u(x)|^n \rangle,
\]

where the separation \( r \) is a distance in the streamwise direction. Theoretical, experimental, and numerical studies support the hypothesis that \( S_n \) has a universal, power-law dependence on \( r \) in the inertial range, i.e., \( S_n(r) \sim r^{\zeta(n)} \). Universality refers to the scaling exponent being independent of the details of turbulence generation. A number of studies (see Frisch\textsuperscript{23} for a detailed review) established that the functional form of the exponent \( \zeta(n) \) differs from the one implied by Kolmogorov’s 1941 theory\textsuperscript{21, 22, 51} (henceforth referred to as K41), i.e., \( \zeta(n) = \zeta_{K41}(n) = n/3 \).

The longitudinal velocity structure functions up to 6th order are evaluated in the mixing layer using velocity signals sampled in time and applying Taylor’s hypothesis. The velocity probes are

![FIG. 12. Longitudinal one-dimensional energy spectra \( E_{11} \) at selected streamwise locations. Inlet condition with low amplitude white noise \( (x = 0.1\delta_{\omega,0}) \), Kelvin-Helmholtz instability \( (x = 50\delta_{\omega,0}) \) where the vertical line indicates the value of the wavenumber of the most unstable mode from linear stability analysis of the hyperbolic tangent profile.\textsuperscript{2, 3} The dashed line indicates a \(-5/3\) slope showing a wide inertial range in the self-similar region.](image)

![FIG. 13. Probability density function of the passive scalar at \( x = 100\delta_{\omega,0} \) for several cross stream positions, corresponding to different values of mean scalar value. Squares: \( \langle Z \rangle = 0.3 \). Circles: \( \langle Z \rangle = 0.5 \). Triangles: \( \langle Z \rangle = 0.7 \).](image)
FIG. 14. Probability density function of the passive scalar at $x = 400\delta_{x=0}$ for several cross stream positions, corresponding to different values of mean scalar value. Squares: $\langle Z \rangle = 0.3$. Circles: $\langle Z \rangle = 0.5$. Triangles: $\langle Z \rangle = 0.7$.

located in a region of fully developed turbulence at $x = 400\delta_{x=0}$ and $y = -4\delta_{x=0}$. The crosswise coordinate was selected to coincide with the location of maximum turbulent kinetic energy at the given streamwise location. Time signals have been used in a number of experimental studies\textsuperscript{31, 52–54} to evaluate structure functions and characterize their scaling behavior. The results agree with those obtained analyzing spatial flow field\textsuperscript{55} directly. A detailed analysis of the applicability of Taylor’s hypothesis in the context of structure functions can be found in Lávov et al.\textsuperscript{56} Within the range of parameters in our configuration, the systematic error due to the use of temporal surrogates instead of spatial statistics is of the order of 0.01 for the 2nd-order structure function exponent. Thus, the approximation errors related to the use of Taylor’s hypothesis do not affect the overall conclusions of our analysis.

The analysis of structure functions based on numerical DNS databases is complicated by Reynolds number effects, since the Reynolds number of flow regimes accessible via computations is typically rather low. Recently, Antonia and Burattini\textsuperscript{57} analyzed Reynolds number ($Re_\lambda$) effects on the 2nd- and 3rd-order structure functions for grid turbulence (with energy decay in the streamwise direction) and a DNS of a forced periodic box. They used the following description for the 2nd-order structure function as a function of $Re_\lambda$ (see also Antonia et al.\textsuperscript{58} and Kurien and Sreenivasan\textsuperscript{59}):

$$ S_2(r^*) = \frac{r^{2\gamma}}{15} \frac{(1 + \beta r^*)^{2\gamma - 2}}{(1 + (r^*/r_{cu}^*)^2)^{\gamma}}. \quad (8) $$

The star superscript (*) indicates non-dimensionalization with Kolmogorov scales, $r_{cu}^*$ is the crossover size between the dissipative and inertial ranges, $c = 1 - \xi(2)/2$ and $\beta = 1/L^*$, with $L$ indicating the integral length scale. Equation (8) modifies the model proposed by Batchelor\textsuperscript{60} to account for finite Reynolds number effects.\textsuperscript{57, 59} For isotropic turbulence, the non-dimensional Taylor microscale is $\lambda^* = 15^{1/4}Re_\lambda^{1/2}$, $\langle u'^*u'^* \rangle = Re_\lambda/15^{1/2}$, and $L^* = 15^{-3/4}C\epsilon Re_\lambda^{3/2}$ with $L = C\epsilon\langle u'u' \rangle^{3/2}/\langle \epsilon \rangle$. The crossover size is $r_{cu}^* = (15C\epsilon)^{1/4}$. The dimensionless energy dissipation $C\epsilon$ is assumed to be unity and the Kolmogorov constant $C_{\epsilon 2} = 2$. Figure 15 shows a comparison of the model in Eq. (8) with the compensated second order structure function obtained from the DNS data. In the limit of $Re_\lambda \to \infty$, Kolmogorov’s theory indicates that the compensated 2nd-order structure function tends to the asymptotic value 2. Our DNS data are characterized by $Re_\lambda = 250$, which is not high enough to fully recover inertial range behavior, i.e., a region of constant compensated structure function. The agreement between the DNS data and the model is rather satisfactory, especially for $r/\eta < 100$. We conclude that the turbulence generated by the mixing layer is remarkably similar to homogeneous isotropic turbulence as long as the separation distance is small enough,
FIG. 15. Comparison of the second order structure function (circles) with the model in Eq. (8) for isotropic turbulence (solid lines); the model equation is plotted for several values of $R_e \lambda$.

$e.g. \ r/\eta < 100$. At larger scales, the apparent discrepancy can be attributed to mean shear, to the evolution of the Kelvin-Helmholtz instability, to the dynamics of large coherent structures, and vortex pairing.

Figure 16 shows the normalized, longitudinal, one-dimensional energy spectrum of the streamwise velocity component. The Taylor microscale and the mixing layer vorticity thickness are also indicated for reference. As it is apparent in the compensated spectrum reported in the inset of Fig. 16, the whole inertial range is affected by the “bump” related to predissipative bottleneck effects. This characteristic further indicates lack of full convergence to high Reynolds number asymptotic behavior.

Structure functions have been analyzed in a range of scales extending from a few Kolmogorov scales up to scales as large as the mixing layer vorticity thickness. In moderate Reynolds number flow, the extended self-similarity (ESS) concept introduced by Benzi et al. has been widely applied to analyze scaling properties of turbulence. The ESS concept relies on analyzing $S_n(r)$.
as functions of $S_2(r)$ or $S_3(r)$, rather than $S_n(r)$ as functions of $r$. The data in ESS form display wider scaling ranges that can be used to fit exponents accurately. The relative exponents $\gamma_{n,2} = \frac{\zeta(n)}{\zeta(2)}$ and $\gamma_{n,3} = \frac{\zeta(n)}{\zeta(3)}$ are computed instead of direct ones $\zeta(n)$.

Figure 17 shows the value of the relative logarithmic derivative of three structure functions ($n = 4, 5, 6$) plotted versus the normalized separation distance $r/\eta$. The value of the relative exponents $\gamma_{n,3}$ fluctuates over the whole range of separation distances considered. As expected, the fluctuations are more pronounced for high-order structure functions (e.g., compare structure functions $n = 4$ and $n = 6$). Despite the fluctuations, it is possible to identify a wide range of scales ($60 < r/\eta < 250$) with approximately constant exponents. The values of the exponents averaged over this range are in very good agreement with those in homogeneous isotropic turbulence (see Table II). In this range of "small" scales ($60 < r/\eta < 250$), it appears that the set of exponents is independent of the flow configuration, large scale features, and the means of turbulence generation. These conclusions are in agreement with the results by Jiang et al.\textsuperscript{31} They reported an experimental study of several turbulent mixing layers up to $Re_\lambda = 237$, close to this in our simulation ($Re_\lambda = 250$). The authors considered

\begin{equation}
\gamma_{n,\alpha} = \frac{\zeta(n)}{\zeta(\alpha)} = \frac{d \log S_n(r)}{d \log S_\alpha(r)} \quad \text{with} \quad \alpha = 2, 3,
\end{equation}

where $d \log S_n(r)/d \log S_2(r)$ and $d \log S_n(r)/d \log S_3(r)$ are the relative logarithmic derivatives.

### Table II. Relative scaling exponents of velocity structure functions $\gamma_{n,3} = \frac{\zeta(n)}{\zeta(3)}$ for the turbulent mixing layer.

Comparison with homogeneous isotropic turbulence\textsuperscript{23,54,55} and shear dominated turbulence\textsuperscript{32–34,37,39,40} The strong shear turbulence exponents are summarized in one column, since they are not available for every order $n$ in all of the configurations reported. The range of variation reflects the differences among the various flow configurations.

<table>
<thead>
<tr>
<th>$\gamma_{n,3}$</th>
<th>DNS data ($60 &lt; r\eta &lt; 250$) (using ESS)</th>
<th>Homogeneous isotropic turbulence</th>
<th>DNS data ($400 &lt; r\eta &lt; 460$) (using ESS)</th>
<th>Shear turbulence</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.695</td>
<td>0.69</td>
<td>0.74</td>
<td>0.74–0.77</td>
</tr>
<tr>
<td>4</td>
<td>1.28</td>
<td>1.28</td>
<td>1.19</td>
<td>1.17–1.22</td>
</tr>
<tr>
<td>5</td>
<td>1.55</td>
<td>1.54</td>
<td>1.32</td>
<td>1.31–1.35</td>
</tr>
<tr>
<td>6</td>
<td>1.79</td>
<td>1.78</td>
<td>1.44</td>
<td>1.43–1.48</td>
</tr>
<tr>
<td>7</td>
<td>1.99</td>
<td>2</td>
<td>1.57</td>
<td>1.55</td>
</tr>
</tbody>
</table>
scales in the range $50 < r/\eta < 250$ and recovered the homogeneous isotropic turbulence scaling of longitudinal structure functions.

As shown in Fig. 17, there exists an additional scaling range at larger scales ($400 < r/\eta < 460$). This second scaling is characterized by a more pronounced deviation from the linear predictions due to K41. Two observables used\textsuperscript{29, 32} in the context of ESS aid the understanding of this second scaling at larger scales: $\sigma_n = S_n/S_2^{\alpha_2}$ and $\rho_n = S_n/S_3^{\alpha_3/3}$. The observable $\sigma_n$ (resp. $\rho_n$) is plotted in logarithmic scale versus the structure functions $S_2(r)$ (resp. $S_3(r)$); its logarithmic derivative is related to relative exponents and their deviation from K41,

$$
\frac{\text{d} \log \sigma_n}{\text{d} \log S_2} = \gamma_{n,2} - \frac{n}{2} = \gamma_{n,2} - \frac{\zeta_{K41}(n)}{\zeta_{K41}(2)}
$$

and

FIG. 18. The observable $\sigma_n = S_n/S_2^{\alpha_2}$ is plotted as a function of $S_2$ in logarithmic scale. For $60 < r/\eta < 250$, the data are fitted by a power law with slope equal to $-0.43$ ($\gamma_{n,2} = 2.57$). For larger scales ($400 < r/\eta < 460$), the slope is $-1.06$ ($\gamma_{n,2} = 1.94$). Inset: slope versus separation.

FIG. 19. The observable $\rho_n = S_n/S_3^{\alpha_3/3}$ is plotted as a function of $S_3$ in logarithmic scale. For $60 < r/\eta < 250$, the data are fitted by a power law with slope equal to $-0.22$ ($\gamma_{n,3} = 1.78$). For larger scales ($400 < r/\eta < 460$), the slope is $-0.56$ ($\gamma_{n,3} = 1.44$). Inset: slope versus separation.
Figures 18 and 19 illustrate the behavior of $\sigma_6$ and $\rho_6$ as a function of $S_2$ and $S_3$ recovered from the DNS data. The logarithmic derivative is shown in the insets. The homogeneous isotropic turbulence scaling is observed in the range $60 < r/\eta < 250$. At larger scales, a different exponent is obtained with a least-squares fitting over the range of $S_2$ and $S_3$ corresponding to $400 < r/\eta < 460$. The scale $r/\eta = 400$ corresponds to approximately 10 shear length scales $L_S = \sqrt{\varepsilon/S^3}$, $S$ being the local mean shear. This estimate for the shear length scale is derived from dimensional analysis, so that there may be a multiplicative prefactor of order unity in its expression. Furthermore, it is assumed that production and dissipation are in equilibrium. Thus, it is only an approximation in the mixing layer configuration. Ruiz-Chavarria et al.\textsuperscript{32} reported very similar values of relative exponents for large scales ($r > 10L_S$) in a boundary layer experiment. The values of the large-scale exponents recovered from the mixing layer data in our study compare very favorably with those from a number of other studies on strong shear flows. Table II summarizes the values of the relative exponents in the two ranges from our data and several experimental and numerical studies published in the literature. Available data include scaling exponents in homogeneous isotropic turbulence\textsuperscript{23,54,55} and in strong shear flows: the near-wall region in a channel DNS,\textsuperscript{33,38} a channel flow experiment,\textsuperscript{34} the logarithmic sublayer of a boundary layer flow,\textsuperscript{32} a wake flow experiment,\textsuperscript{39} and a Kolmogorov flow with anisotropic forcing.\textsuperscript{40} Figure 20 shows the difference of the relative exponent $\gamma_n$ and the linear scaling implied by K41. The agreement among our data in a turbulent mixing layer at $Re_\lambda = 250$ and a number of other studies is apparent for structure functions up to order 7.

V. CONCLUSIONS

A direct numerical simulation of a turbulent, spatially developing mixing layer has been performed. The DNS dataset describes the momentum and passive scalar mixing in a turbulent free-shear flow at $Re_\lambda = 250$ and constitutes the highest Reynolds number dataset for a spatially developing mixing layer available in the literature.
Turbulence develops downstream of the Kelvin-Helmholtz instability and a self-similar state is achieved from laminar boundary conditions forced with random noise. In this respect, turbulence develops "naturally" from a laminar flow configuration. The coherent structures characteristic of the transitional region have been found to be very similar to those in mixing layers initiated with laminar conditions. These structures are not usually observed in numerical simulations of mixing layers with turbulent initial or inlet conditions. The self-similar state is recognized by observing the streamwise evolution of Reynolds stresses, mixing layer thickness, turbulent kinetic energy, dissipation, and mixing characteristics (i.e., the passive scalar $\text{Pdf}$). Once the self-similar state is achieved, the turbulence statistics profiles, rescaled with the appropriate velocity and length scales, are in good agreement with well-established experimental and numerical results available in the literature for mixing layers. In particular, the self-similar behavior achieved in our simulation agrees well with the behavior of spatial and temporal mixing layers evolving from turbulent flow inlet conditions (turbulent initial conditions for the temporal mixing layer). This agreement is particularly apparent for the integral of the crosswise component of the turbulent kinetic energy, which is a good indicator of the evolution of the large coherent structures undergoing pairing events. We also observed that the streamwise evolution of the integral of the crosswise component of the turbulent kinetic energy is similar to that in flows with laminar initial or inlet conditions. This finding is coherent with the dynamics of three-dimensional structures observed during the transition, prior to the integral of the crosswise component of the turbulent kinetic energy converging to an asymptotic value characteristic of turbulent initial conditions.

The statistical features of turbulence in the self-similar region have been studied in terms of longitudinal velocity structure functions. In order to overcome finite Reynolds number effects, the extended self-similarity approach has been used to evaluate scaling exponents. The exponent behavior is found to depend on the range of scales considered. A wide scaling range with exponents that compare well with those typical of homogeneous isotropic turbulence is recovered for scales $60 < r/\eta < 250$. At larger scales, the exponents take values similar to those reported for strong-shear flow configurations. A detailed comparison with literature data reveals a remarkable level of agreement across rather different flow configurations, such as other free-shear configurations and wall flows.

Highly anisotropic Brown-Roshko structures persist in the region characterized by fully developed turbulence, where homogeneous isotropic turbulence scaling is observed at scales $r/\eta < 250$.

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