EFFECTS OF INITIAL CONDITIONS ON MIXING IN WALL-BOUNDED TURBULENT FLOW

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ABSTRACT
Scalar mixing occurs in a wide variety of environmental and engineering flows. Given that the majority of these flows are turbulent, a more complete understanding of the mechanisms that underlie the scalar mixing process is required to predict and control these flows and the evolution of the concentration(s) of the scalar(s) therein. Direct numerical simulations (DNSs) are particularly useful in the study of turbulence since DNSs resolve the full range of (length and time) scales in turbulent flows. The present work employs a spectral approach for simulating the hydrodynamic field, and a flux integral method for computing the advection and diffusion of the passive scalar. Mixing of the latter is studied in a fully developed turbulent channel flow, and particular attention is paid to the evolution of the scalar dissipation rate and the differences that arise from different scalar-field initial conditions. Observed differences in the evolutions for the three initial conditions investigated are explained by an analysis of the different terms that comprise the scalar dissipation rate budget. To promote mixing in a wall-bounded flow, it is recommended that scalar interfaces be aligned normal to the mean velocity vector, to enhance the stretching of the interface.

INTRODUCTION
Scalar quantities (e.g. temperature, humidity, chemical species concentration) are mixed within a wide range of environmental and engineering flows (e.g. the atmosphere, which transports temperature and humidity; the oceanic mixed layer, in which temperature and salinity are mixed; chemical reactors; heat exchangers, combustion processes, etc.). Given that the vast majority of these flows are turbulent, an understanding of the turbulent scalar mixing process is required to predict (and, ultimately, control) these flows and the evolution of the concentration(s) of the scalar(s) therein. Thus, the present work investigates the turbulent mixing of (passive) scalars, which are governed by the advection-diffusion equation:

$$\frac{\partial \tilde{\theta}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\theta} = \alpha \frac{\partial^2 \tilde{\theta}}{\partial \mathbf{x} \cdot \partial \mathbf{x}_j}$$  \hspace{1cm} (1)

where \( \tilde{\theta} \) represents the instantaneous scalar field, \( \tilde{\mathbf{u}}_j, j = 1, 2, 3 \) are the components of the instantaneous velocity vector field, \( \alpha \) is the scalar’s molecular diffusivity within the fluid, and repeated indices imply Einstein’s summation convention.

The present work focusses on the mixing of scalars within a fully-developed, high-aspect-ratio turbulent channel flow, to model the behavior of real flows and the physical processes therein (as opposed to studying mixing within homogeneous flows). Channel flow is especially appropriate because it is the simplest realization of an inhomogeneous turbulent flow.

Mixing metrics are often used to quantify the efficacy of a scalar mixing process. These include i) the unmixedness parameter \([\text{Danckwerts, 1952}]\ [\text{Dimotakis & Miller, 1990}]: \)  

$$\Xi \equiv \frac{\langle \theta^2 \rangle}{\Theta(1-\Theta)} : 0 \leq \Xi \leq 1$$  \hspace{1cm} (2)

where \( \Theta \) is the average scalar concentration, \( \theta \) is its fluctuation, and angular brackets denote averages, or ii) a multi-scale norm, such as the mix-norm \([\text{Mathew et al., 2005}]: \)  

$$\mu_\theta = \left[ \sum_{|k| \leq Z} \frac{1}{\sqrt{1 + 4 \pi^2 |k|^2}} \left| \hat{\Theta}_k(t) \right|^2 \right]^{1/2}$$  \hspace{1cm} (3)

where \( k \) is the wavevector, and \( \hat{\Theta}_k \) are the Fourier coefficients of a spectral representation of the scalar field. Note that the two metrics are very different: the unmixedness quantifies molecular mixing only, whereas the mix-norm quantifies mixing by accounting for both stirring and molecular mixing. These differences have a notable impact on the results using these metrics. For example, consider the idealized case of mixing in two dimensions of two hypothetical fluids (one white and one black, and both having molecular diffusivities equal to zero). Let one then assume that the fluid could be stirred in such a way that the end result would be a configuration similar to a chessboard, with white and black squares at the smallest scales. In this case, the unmixedness would be maximum (because there is no molecular mixing) whereas the mix-norm will be minimum, because the stirring is complete.

Motivation for the present study stems from observations by \([\text{Gubanov & Cortelezzi, 2009}]\) and \([\text{Germaine et al., 2018}].\)
who have observed that scalar fields, including the evolution of the scalar dissipation rate, are strongly affected by the initial conditions of the scalar field, even when these initial conditions are mixed by identical hydrodynamic fields. It is therefore of interest to investigate the nature of the physical processes that lead to such different evolutions of the scalar field.

The objective of the present work is therefore to investigate the effect of scalar-field initial conditions on mixing that occurs within fully developed, turbulent channel flow. This will be undertaken by way of an initial comparison between the evolutions of the two aforementioned mixing metrics and the scalar dissipation rate in turbulent flows. However, the primary focus of the present work will be an investigation of the evolution of the scalar fields for the different initial conditions, by way of an analysis of the various terms in the evolution equation (i.e., budget) of the scalar dissipation rate:

\[
\frac{\partial \langle \varepsilon \rangle}{\partial t} + U_j \frac{\partial \langle \varepsilon \rangle}{\partial x_j} = -2\alpha \frac{\partial U_j}{\partial x_i} \left( \frac{\partial \theta}{\partial x_i} \frac{\partial \varepsilon}{\partial x_j} \right) - 2\alpha \frac{\partial \theta}{\partial x_i} \left( \frac{\partial U_j}{\partial x_i} \frac{\partial \theta}{\partial x_j} \right)
\]

\[
-2\alpha \left( \frac{\partial U_j}{\partial x_i} \right) \left( \frac{\partial \varepsilon}{\partial x_i} \right) - 2\alpha \left( \frac{\partial \varepsilon}{\partial x_i} \right) \left( \frac{\partial U_j}{\partial x_i} \right) + \frac{\partial}{\partial x_j} \left( \alpha \frac{\partial \langle \varepsilon \rangle}{\partial x_j} - (\mu_j \varepsilon) \right) - 2\alpha^2 \left( \frac{\partial^2 \langle \varepsilon \rangle}{\partial x_i \partial x_j} \right) \frac{\partial^2 \theta}{\partial x_i \partial x_j}
\]

where \( U_j \) is the mean velocity vector, and \( u_j \) is the velocity fluctuation.

SIMULATIONS

The investigations herein employ numerical simulations of both the turbulent velocity and passive scalar fields, in which the latter is advected by the former. The turbulent velocity field is calculated via direct numerical simulation (DNS), which resolves all scales of the flow by solving the Navier-Stokes equations with constant properties. The DNS of the velocity field is computed using a code entitled CHANNELFLOW (Gibson et al. 2008; Gibson 2010; http://channelflow.org/) which uses spectral discretization in space (Fourier x Chebyshev x Fourier), and a third-order semi-implicit backwards differentiation scheme in time, with no-penetration / no-slip boundary conditions imposed at the walls of the channel \((y = 0 \text{ and } y = 2h)\), where \( h \) is the half-height of the channel, and periodic boundary conditions in the streamwise \((x)\) and spanwise \((z)\) directions. Simulation of the hydrodynamic field is conducted at \( Re_t = 190 \) over a domain of size \( 2\pi h \times 2h \times \pi h \), in the streamwise \((x)\), wall-normal \((y)\) and spanwise \((z)\) directions, respectively, with a resolution of \(256 \times 193 \times 192\). \( Re_t \equiv U_t h / \nu, \ u_t \equiv \sqrt{\nu \times \partial U / \partial y}_{y=0} \), and \( \nu \) is the kinematic viscosity of the fluid.) The resulting turbulent velocity field is statistically steady and statistically one-dimensional, such that \( \langle U \rangle = \langle U \rangle(y) \) only.

The pre-computed velocity field is used as an input to the advection-diffusion solver, and is interpolated from a spectral to a finite-volume representation via spectral (exact) interpolation. A very small correction is applied to the streamwise component of the velocity field to ensure the exact divergence-free condition. The advection-diffusion equation is solved using a fully three-dimensional and cost-effective flux integral method entitled 3DFLUX (Germaine et al. 2013). The fully explicit and multidimensional nature of the approach ensures that it is free of splitting errors, and provides a better convergence rate of the numerical errors when compared to commonly used one-dimensional methods. A semi-Lagrangian approach is implemented in 3DFLUX by discretizing the spatial domain on an Eulerian grid and using a Lagrangian frame of reference for temporal discretization. Solutions for the advection-diffusion equation are obtained using non-overlapping control volumes to discretize the computational domain and estimate the flux exchanged between adjacent cells. DNS of the scalar field is undertaken on the same domain of \( 2\pi h \times 2h \times \pi h \), with a resolution of \( 514 \times 195 \times 194 \) to resolve both the large and small scales of the scalar field. It is assumed that the magnitude of the scalar fluctuations are sufficiently small, such that the dynamics of the velocity field are independent from the scalar field and the scalar is considered as being passive.

As noted above, the evolution of the mixing with time will be studied for three different scalar-field initial conditions, \( IC_x, IC_y, \) and \( IC_z \), as depicted in figure 1. These fields consist of two equal volumes of uniform concentrations, \( \bar{\theta} = +1 \) (black) and \( -1 \) (white), separated by two interfaces (due to the periodic boundary conditions in \( z \)) of total area \( 4\pi h^2 = (2 \times 2h \times \pi h) \) for \( IC_x \) and \( 8\pi h^2 = (2 \times 2h \times 2\pi h) \) for \( IC_y \) and a single interface of area \( 2\pi^2 h^2 = (2\pi \times \pi h) \) for \( IC_z \). All fields have zero mean concentration. Note that all three scalar fields are subjected to identical turbulent velocity fields, and thus any differences in the evolutions of the three scalar fields are the sole result of the orientations of the interfaces defining the initial scalar fields relative to that of the velocity field.

RESULTS

Inspired by the results of Germaine et al. (2018), who investigated the dependence of local anisotropy of passive scalars on their initial conditions, we plot in figure 2 the scalar field distributions that result from the action of the identical turbulent channel flow (velocity field) on scalar fields subjected to the three aforementioned, distinct initial conditions.
scalar-field initial conditions. Imagery generated using VAPOR (Li et al. 2019).

Figure 2: Concentration distributions generated at $\tau = 7$ by the action of the same turbulent channel flow on the three scalar-field initial conditions. Imagery generated using VAPOR (Li et al. 2019).

Figure 3: Time-evolution of the unmixedness parameter (solid line) and the mix-norm (dashed line) for the scalar fields resulting from the three initial conditions.

for a period of $\tau (\equiv tu_i/h) = 7$. From this figure, it is readily observed that the scalar field resulting from the $IC_x$ initial condition is the best mixed, whereas that resulting from the $IC_y$ initial condition is the least well mixed. This is already an intriguing result and indicates that the initial conditions can strongly influence the subsequent mixing. Moreover, it is worth reiterating that all three scalar-field initial conditions were comprised of equal parts “black fluid” (i.e. scalar with an initial concentration $\theta = +1$) and “white fluid” (i.e. scalar with an initial concentration $\theta = -1$). Thus the rate at which mixing will occur in such an inhomogeneous flow (as is the flow in all real devices) is highly dependent on the initial configuration of the two quantities being mixed.

To quantify the mixing, we plot the time-evolutions of the unmixedness parameter ($\Xi$) and the mix-norm ($\mu_b$) for the three scalar-field initial conditions in figure 3. One observes that the unmixedness starts very close to its maximum value of 1, whereas the initial values for the mix-norm fall between 0.3 and 0.4 (because the latter depend on the initial geometry of the scalar field). However, shortly after the velocity field starts mixing the scalar field, the time-evolutions for both mixing metrics follow a similar pattern; i.e. the evolutions of both $\Xi$ and $\mu_b$ decay exponentially with time, with the most efficient stirring and mixing (i.e. fastest rates of decay of $\Xi$ and $\mu_b$) occurring for the $IC_x$ case and the slowest for the $IC_y$ case.

Given the objective of attempting to tie the evolutions of the mixing metrics to the underlying physics of the turbulence, we first plot the evolutions of the (volume-averaged) scalar dissipation rates ($\langle \epsilon_\theta \rangle$) corresponding to the fields with the three initial conditions as a function of time in figure 4. Although some differences exist at early times ($\tau < 1$), the long term evolution of $\langle \epsilon_\theta \rangle$ is qualitatively similar to the evolutions of both $\Xi$ and $\mu_b$ – the dissipation rates decrease at rates dependent upon the initial conditions of the scalar field, with the fastest decrease in $\langle \epsilon_\theta \rangle$ occurring for $IC_x$, corresponding to the most efficient mixing, and the slowest corresponding to $IC_y$. At shorter times, $\langle \epsilon_\theta \rangle$ increases, presumably due to the stretching and stirring of the interface between the two (i.e. the “black” and “white”) scalar fields, which results in a production of $\langle \epsilon_\theta \rangle$. This is in contrast with the short-time evolutions of both $\Xi$ and $\mu_b$, which are both monotonically decreasing functions of time for all values of $\tau$. Note that the values of $\langle \epsilon_\theta \rangle$ for the $IC_x$ and $IC_y$ cases peak around $\tau \approx 1/3$, whereas the peak in $\langle \epsilon_\theta \rangle$ for the $IC_y$ case occurs later, around $\tau \approx 2/3$.

Before proceeding, we are obliged to discuss the issue of averaging when presenting the results for the individual terms in eq. 4. In particular, the homogeneity (or lack thereof) of both the velocity and scalar fields in this work must be considered in the analysis of the results. Whereas the velocity field is statistically homogeneous in the $x$- and $z$-directions, as well as being statistically stationary, the natures of the scalar fields resulting from the action of the velocity field on the three different initial conditions are all different. The scalar field resulting from the $IC_x$ initial condition is statistically homogeneous in the $x$- and $z$-directions. Lastly, the scalar field resulting from the $IC_z$ ini-
Figure 5: Evolution in time of the space- and time-averages of all 9 terms in the scalar dissipation rate budget in which statistical moments \( \langle \cdot \rangle \) are assessed in planes parallel to the initial location of the interface in the initial condition. (a) \( IC_x \) with \( \frac{1}{L_x^2} \int_{L_x^2} \int_{0}^{L_x} \int_{0}^{L_x} \text{Term} \, d\tau \, dx \), (b) \( IC_y \) with \( \frac{1}{L_y^2} \int_{L_y^2} \int_{0}^{L_y} \int_{0}^{L_y} \text{Term} \, d\tau \, dy \), and (c) \( IC_z \) with \( \frac{1}{L_z^2} \int_{L_z^2} \int_{0}^{L_z} \int_{0}^{L_z} \text{Term} \, d\tau \, dz \).

Table 1: Legend for the various terms in the budget of the scalar dissipation rate.

<table>
<thead>
<tr>
<th>Color</th>
<th>Term #</th>
<th>Term</th>
<th>Physical interpretation</th>
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<tbody>
<tr>
<td></td>
<td>(i)</td>
<td>( \frac{\partial}{\partial \tau} \langle \epsilon \theta \rangle )</td>
<td>time rate of change of ( \langle \epsilon \theta \rangle )</td>
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<td></td>
<td>(ii)</td>
<td>( \langle U_i \rangle \frac{\partial}{\partial x_j} \langle \epsilon \theta \rangle )</td>
<td>mean flow advection of ( \langle \epsilon \theta \rangle )</td>
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<td></td>
<td>(iii)</td>
<td>( 2\alpha \frac{\partial \langle \theta \rangle}{\partial x_i} \frac{\partial \langle \epsilon \theta \rangle}{\partial x_j} )</td>
<td>production of ( \langle \epsilon \theta \rangle ) by mean velocity gradients</td>
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<td></td>
<td>(iv)</td>
<td>( 2\alpha \frac{\partial \langle \theta \rangle}{\partial x_i} \frac{\partial \langle \epsilon \theta \rangle}{\partial x_j} )</td>
<td>production of ( \langle \epsilon \theta \rangle ) by mean scalar gradients</td>
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<td></td>
<td>(v)</td>
<td>( \alpha \frac{\partial^2 \langle \theta \rangle}{\partial x_i \partial x_j} \langle u_i \rangle \langle u_j \rangle )</td>
<td>mixed production of ( \langle \epsilon \theta \rangle )</td>
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<td></td>
<td>(vi)</td>
<td>( 2\alpha \langle \frac{\partial \epsilon}{\partial x_i} \frac{\partial \theta}{\partial x_j} \rangle )</td>
<td>production of ( \langle \epsilon \theta \rangle ) by turbulent vortex stretching</td>
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<td></td>
<td>(vii)</td>
<td>( -\alpha \frac{\partial^2}{\partial x_i \partial x_j} \langle \theta \rangle )</td>
<td>molecular transport of ( \langle \theta \rangle )</td>
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<td></td>
<td>(viii)</td>
<td>( \frac{\partial}{\partial x_i} \langle u_i \rangle \langle \epsilon \theta \rangle )</td>
<td>turbulent advection of ( \langle \epsilon \theta \rangle )</td>
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<td></td>
<td>(ix)</td>
<td>( 2\alpha^2 \frac{\partial^2 \theta}{\partial x_i \partial x_j} \frac{\partial^2 \epsilon}{\partial x_i \partial x_j} )</td>
<td>molecular dissipation of ( \langle \epsilon \theta \rangle )</td>
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ulnar dissipation of \( \langle \epsilon \rangle \) peak at later times for \( IC_x \) (at \( \tau > 1 \)) than they do for the \( IC_z \) and \( IC_y \) cases (which peak at \( \tau < 1 \)). This behaviour is also consistent with the evolutions of \( \langle \epsilon \rangle \) in figure 6 noted above.

We further investigate the budget of the scalar dissipation rate for the three initial conditions by plotting the time evolution of terms when spatially averaged over a single y-z plane in figure 7. Note that the plane over which the spatial averaging is performed in figure 7 is parallel to the interface between the “black” and “white” fluids in the \( IC_z \) initial condition, and located at the mid-plane of the channel in the z-direction (i.e. \( h/L_y = 0.5 \)), i.e. the location of one of the two interfaces between the “black” and “white” fluids at \( \tau = 0 \) for \( IC_z \). In figure 6 it is first worth noting the qualitative similarities of the evolutions of the terms in \( \langle \epsilon \rangle \) budget for the \( IC_y \) and \( IC_z \) initial conditions. These two subfigures exhibit similar behaviours due to the absence of terms associated with spatial gradients of statistical moments in the directions of the averaging in the respective figures. We also note that analogous similarities are observed when reproducing the equivalent of figure 6 but spatial averaging in the other two (x-z and x-y) mid-planes (not shown). However, in contrast to figures 6(b) and 6(c), figure 7(a) is dominated at early times by mean-flow advection of \( \langle \epsilon \rangle \) and turbulent advection of \( \langle \epsilon \rangle \). This will be further discussed with respect to figure 7, which follows.

To investigate the evolution of the terms in the \( \langle \epsilon \rangle \) budget that are not subjected to such an artefact, we plot in figure 7 their evolution in time at mid-plane corresponding to the initial location of the interface for the three initial conditions. It reveals that figure 7(a), which corresponds to the \( IC_z \) initial condition, is significantly different from those corresponding to \( IC_y \) (7(b)) and \( IC_x \) (7(c)), which are quite similar. The dominant terms in figures 7(b) and 7(c) are the molecular dissipation of \( \langle \epsilon \rangle \), the production of \( \langle \epsilon \rangle \) by turbulent vortex stretching, production of \( \langle \epsilon \rangle \) by mean scalar gradients, the rate of change of \( \langle \epsilon \rangle \) with time, and turbulent advection of \( \langle \epsilon \rangle \); figure 7(a) is distinctly different. Of particular note is the importance played by mean-flow advection of \( \langle \epsilon \rangle \) at early times, which is dominant for \( \tau < 0.2 \), and balanced by turbulent advection of \( \langle \epsilon \rangle \). Given that fully developed turbulent channel flow must be unidirectional, the absence of the mean-flow advection term in the other directions is to be expected. However, the early dominance of this term is noteworthy. In this respect, consideration of the evolution time of the interface(s) between the “black” and “white” fluids is beneficial. For the \( IC_y \) case, the \( \Theta = 0 \) plane will not change in time and will be advected along the \( y/h = 1 \) plane as the flow evolves, but remaining at the same location as the initial interface. However, the evolution of the scalar field in time is quite different for \( IC_x \). The interface remains “anchored” to the walls due to the no-slip condition, and is strongly stretched in the x-direction by the mean flow, while being stirred by the turbulence. Thus as the interface is advected downstream, it can “blow by” a given downstream location multiple times. This effect can be observed by the oscillations in the unsteady term (dark blue line), and to a lesser degree the mean flow advection terms (red line) in figure 7(a).

It is worth noting that the period of the observed oscillation is indeed equal to half of the channel’s “flow-through” time (i.e. \( \frac{1}{2} \frac{x}{L_y} \approx \frac{1}{2} \frac{L_y}{(U_{\text{avg}})} \), \( \mu_x/h = 0.17 \)). With respect to \( IC_z \), the \( (\Theta = 0) \) plane will be advected downstream the mid-plane of the channel (\( z = 0.5L_z \)), although its top and bottom edges will remain anchored to the walls of the channel, thus emulating aspects of both \( IC_y \) and \( IC_x \).

Given that the results in figure 7 are all averages taken at the three midplanes of the channel, they are somewhat anomalous. For example, when averaging in the x- and z-directions at \( y/h = 1 \) (as is the case in figure 7(b)), there can be no contribution to \( \langle \epsilon \rangle \) arising from production by the mean velocity gradient because \( \partial U/\partial y = 0 \) at that one location (and no other). Thus it bears investigating the budget of the scalar dissipation rate for the three initial conditions at non-mid-plane locations. To this end, the evolutions of the terms in the budget of the scalar dissipation rate are plotted for \( IC_z \) spatially averaged over a y-z plane located at \( x/L_x = 0.25 \) in figure 8(a), for \( IC_y \) spatially averaged over an x-z plane located at \( y/h = 0.5 \) in figure 8(b), and for \( IC_x \) spatially averaged over an x-y plane located at \( z/L_z = 0.25 \) in figure 8(c). The aforementioned periodic passing of the interface over the measurement plane for the \( IC_x \) case is even more prominent in figure 8(a). However, figures 8(b) and 8(c) also reveal another phenomenon that explains the slower evolutions of \( \langle \epsilon \rangle \) for the \( IC_y \) and \( IC_z \) cases. In these two non-mid-plane cases, one observes an initial period of “inactivity.” The initial period in which the terms in the budget of \( \langle \epsilon \rangle \) are effectively zero results from the interface having not yet “reached” the measurement location. In these two cases, the interface can only travel laterally by the action of the turbulence, given that there is no mean velocity in the y- and z-directions. This phenomenon i) is not observed for the \( IC_x \) case, because the interface can be advected by the non-zero mean flow, and ii) further explains the slower evolutions of \( \langle \epsilon \rangle \) for the \( IC_y \) and \( IC_z \) cases, given that regions located increasingly far away from the interface experience a delay before they begin to mix. This latter effect therefore serves to retard the total mixing, because the interface surface is not normal to the mean velocity vector.
REFERENCES


