Transport across stable density interfaces in forced stratified turbulence

Miles M. P. Couchman¹†, Stephen M. de Bruyn Kops² and Colm-cille P. Caulfield¹,³

¹Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, UK
²Department of Mechanical and Industrial Engineering, University of Massachusetts Amherst, Amherst, MA 01003, USA
³Institute for Energy and Environmental Flows, University of Cambridge, Cambridge CB3 0EZ, UK

(Received xx; revised xx; accepted xx)

Understanding how turbulence enhances irreversible scalar mixing in density-stratified fluids is a central problem in geophysical fluid dynamics. Unstable vertical density inversions are often assumed to be an indirect proxy for mixing when direct measurements of scalar diffusion are unavailable. We here investigate this assumption by using a forced direct numerical simulation of stratified turbulence to consider spatial correlations between the vertical density gradient $\partial \rho / \partial z$ and the dissipation rates of kinetic energy $\epsilon$ and scalar variance $\chi$, the latter quantifying scalar mixing. Statistically-steady turbulence is generated by the injection of kinetic energy at large horizontal length scales, leading to a robust vertically-aligned vortex, which in turn induces vertically-layered, opposing horizontal currents in the surrounding flow. Sheared interfaces at the intersection of these currents are correlated with sharp, stable density gradients separating relatively well-mixed layers. While unstable density inversions are most prevalent within the mixed layers, much of the scalar mixing is localized to the intervening interfaces, a phenomenon which would be missed if either local static instability or $\epsilon$ were to be used as a proxy for mixing. We highlight that while the majority of the domain is indeed characterized by the canonical flux coefficient $\Gamma \equiv \chi / \epsilon = 0.2$, often assumed in ocean mixing parameterizations, extreme values of $\chi$ within the statically-stable interfaces, associated with elevated $\Gamma$, strongly skew the bulk statistics. Our findings suggest that current parameterizations of turbulent mixing may be biased by undersampling, such that the most common, but not necessarily the most significant, mixing events are overweighted.

1. Introduction

In a density-stratified fluid, turbulence enhances the rate at which scalars are irreversibly diffused throughout the flow, a process of great interest in a variety of geophysical, environmental and industrial settings (e.g. Fernando (1991)). Of particular importance is characterizing the role of turbulence in the vertical transport of heat within the ocean, a crucial mechanism for driving the required upwelling of cold bottom waters to maintain the ocean’s vertical stratification profile and to complete global circulation currents (Wunsch &
Ferrari (2004). Turbulence in the ocean generates dynamically relevant motions on the order of millimeters, which cannot currently be resolved in numerical circulation models and must therefore be parameterized, with the choice of parameterization found to influence future climate projections strongly (Whalen et al. 2020). Considerable observational, numerical and theoretical work has thus been focused on developing more accurate and universal mixing models which account for the wide range of turbulent processes observed in different flow regimes within the ocean (Caulfield 2020).

The rate at which turbulence mixes a non-uniform density field is often defined in terms of an appropriately-averaged vertical density flux $\overline{B \rho' \omega'}$, where $\rho'$ and $\omega'$ denote fluctuations in density and vertical velocity away from the mean flow, respectively. When considering such a definition, however, it is critical to distinguish between reversible stirring and irreversible diffusive processes (Villermaux 2019). Stirring, occurring on relatively large scales, may be thought of as the adiabatic rearrangement of fluid parcels of different density induced by the underlying turbulence, which in principle is reversible. We here use the term mixing to refer specifically to the diffusive transport of density across gradients that have been enhanced by such macroscopic stirring motions, thus irreversibly leading the system toward a state of greater homogenization. In order to isolate only irreversible contributions to mixing, Lorenz (1955) introduced the concept of an available potential energy (APE). APE quantifies the difference between a system’s current potential energy and its minimum background potential energy (BPE) that could be achieved if fluid parcels were adiabatically sorted into their most stable configuration. For a Boussinesq fluid, Winters et al. (1995) demonstrated that irreversible mixing may be described as the conversion of APE into BPE, with a system’s BPE increasing in time as it homogenizes. Generalizing this mixing framework to compressible flows, Tailleux (2009) argued that mixing of a thermally-stratified fluid should most rigorously be defined as the conversion of APE into internal energy, which in the Boussinesq limit then exactly matches the generation of BPE.

As it is exceedingly difficult to directly measure the irreversible component of fluxes $B$ within the ocean, a number of indirect methods have been proposed that infer such fluxes from more readily available quantities (Gregg et al. 2018). Two such quantities, associated with what is conventionally referred to as turbulent microstructure, are the dissipation rates of kinetic energy $\epsilon$ and scalar variance $\chi$, 

$$
\epsilon = \frac{\nu}{2} \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right)^2,
\chi = \frac{g \kappa}{\rho_0 N^2} \left( \frac{\partial \rho'}{\partial x_i} \frac{\partial \rho'}{\partial x_i} \right),
$$

representing the rates at which viscosity $\nu$ and molecular diffusivity $\kappa$ smooth gradients in the turbulent velocity $u'$ and density $\rho'$ fields, respectively. In equation (1.1), $g$ denotes the gravitational acceleration, $\rho_0$ a reference background density and $N = \sqrt{-g/\rho_0} \partial \overline{\rho}/\partial z$ the buoyancy frequency, defined by an appropriately averaged ambient density gradient $\partial \overline{\rho}/\partial z$ against which the turbulence acts. The quantities $\epsilon$ and $\chi$ are intimately related to the irreversible processes associated with the conversion of kinetic energy and available potential energy into internal energy, respectively, as is further described by Caulfield (2021). In particular, for the class of direct numerical simulation considered here, characterized by an imposed uniform background stratification $N_0^2$, Howland et al. (2021) demonstrated that $\chi$ computed using $N^2 = N_0^2$ in equation (1.1) provides an excellent approximation to the destruction rate of APE and is therefore a natural measure of local irreversible mixing.

As discussed by Ivey et al. (2018), $\chi$ also arguably provides the most robust method for estimating irreversible mixing from oceanographic measurements, since $B \approx \chi$ in steady-state provided that averaging is performed over sufficiently long times and large volumes so that reversible processes and transport terms are negligible (Osborn & Cox 1972).
Importantly, $\chi$ is both directly proportional to the scalar diffusivity $\kappa$ and sign-definite, effectively filtering out nominally reversible stirring motions to yield a useful estimate of the irreversible fluxes associated with molecular diffusion. Due to a scarcity of $\chi$ measurements, however, $\epsilon$ is more commonly used to infer mixing following the method of Osborn (1980), which requires the introduction of a flux coefficient $\Gamma \equiv \chi/\epsilon$ to prescribe the fraction of turbulent kinetic energy that leads to irreversible mixing, as opposed to being directly dissipated by viscosity. A constant value $\Gamma = 0.2$ is commonly assumed when estimating global patterns of oceanic mixing (MacKinnon et al. 2017), which has been found to be in agreement with tracer release experiments (Gregg et al. 2018). However, there is significant evidence suggesting that $\Gamma$ varies appreciably in different flow regimes (Caulfield 2021) and so a clear physical picture has not yet emerged explaining why $\Gamma = 0.2$ is a reasonable assumption.

In the absence of measurements of $\epsilon$ or $\chi$, mixing locations are primarily inferred from the presence of unstable overturns in vertical density profiles, as proposed by Thorpe (1977). Assuming that the vertical extent of an overturn is correlated with the Ozmidov length $L_O = \sqrt{\epsilon/\mathcal{N}^3}$, $\epsilon$ may be inferred from the measurement of overturns which can then be converted into a flux via $\Gamma$. However, this assumed correlation between the vertical overturning scale and $L_O$ is not always robust, as has recently been discussed, for example, by Ivey et al. (2018), Ijichi et al. (2020) and Mashayek et al. (2021). Using a forced direct numerical simulation (DNS) similar to that considered here, Taylor et al. (2019) quantified the errors associated with the indirect flux estimates of Osborn & Cox (1972), Osborn (1980) and Thorpe (1977) by sparsely sampling vertical profiles of the computational domain in order to mimic oceanographic measurements.

Spatio-temporal intermittency in stratified turbulence greatly reduces the applicability of classical turbulence modeling assumptions, including the common assumption of log-normal distributions for $\epsilon$ and $\chi$ (de Bruyn Kops 2015). Cael & Mashayek (2021) found that global ocean measurements of $\epsilon$ were not well approximated by an assumed log-normal distribution but instead had a skewed right tail, indicating that the most extreme events dominated the bulk statistics. By considering local correlations between direct ocean measurements of $\epsilon$ and $\chi$, Couchman et al. (2021) further emphasized the importance of extreme events, finding that while the majority of the sampled domain was characterized by the canonical flux coefficient $\Gamma = 0.2$, isolated mixing events containing the largest $\chi$ were not reflected by a corresponding local increase in $\epsilon$, yielding a dramatic increase in $\Gamma$.

Vertical layering is also known to be a canonical feature of stratified turbulent flows, with the density field often forming ‘staircases’ of deep, relatively well-mixed layers separated by thin interfaces with strong gradients (Caulfield 2021). For sufficiently stratified environments, vertical shearing induced by the decoupling of horizontal and vertical motions in such a layered structure becomes an important mechanism for triggering instability and the ensuing generation of turbulence (Lilly 1983; Billant & Chomaz 2001). Parameterizations of mixing based on simple domain averages are thus unlikely to be accurate as rare extreme events and spatial heterogeneity within the flow will be missed, a potential cause of the highly-scattered mixing statistics currently reported throughout the literature (Gregg et al. 2018).

In an attempt to classify such intermittency in an automatic, yet robust and interpretable manner, Portwood et al. (2016) devised an algorithm for splitting a snapshot from a forced DNS into three dynamically distinct regions: quiescent regions, intermittent layers and turbulent patches. These regions were distinguished by an increasing degree of local overturning, as determined by computing the fraction of unstable points $\partial \rho / \partial z > 0$ within an extended neighbourhood. Local overturning fractions and dissipation rates $\epsilon$ were found to be strongly correlated, in agreement with the arguments of Thorpe (1977). For the
relatively large filter sizes used to segment the domain, on the order of a buoyancy length $L_B = 2\pi u_h/N$ (where $u_h$ denotes a characteristic horizontal velocity scale), distributions of $\chi$ associated with each region were also found to be correlated with $\epsilon$, although the finer spatial distributions of $\epsilon$ and $\chi$ within each region, and the resulting flux coefficient $\Gamma$, were not considered.

Motivated by the automated flow segmentation of Portwood et al. (2016) in terms of unstable local density gradients $\partial \rho/\partial z > 0$, and the observation of Couchman et al. (2021) that, within the ocean, extreme events in $\chi$ are not necessarily correlated with those in $\epsilon$, we here analyze spatial mixing distributions within a computational domain by considering local correlations between $\epsilon, \chi$ and $\partial \rho/\partial z$. In particular, we wish to probe whether overturning alone provides a robust indicator for local mixing, or if significant mixing as revealed by $\chi$ might occur in other regions that would seem inconspicuous based on consideration of only $\epsilon$ or $\partial \rho/\partial z$.

In line with the previous investigations of Portwood et al. (2016) and Taylor et al. (2019), we consider a forced DNS of stratified turbulence using the methodologies presented in Almalkie & de Bruyn Kops (2012). In §2, we summarize the DNS dataset considered here and highlight the presence of a (previously-unreported) robust vertically-aligned vortex generated by the forcing scheme, that injects energy into the domain at large scales and induces vertical layering in the surrounding flow. In §3, we then consider pointwise correlations between $\partial \rho/\partial z$, $\epsilon$, $\chi$ and the flux coefficient $\Gamma$, which suggests that mixing occurs not only in overturning regions, but also in areas of local static stability. In §4, we move beyond pointwise statistics to consider extended mixing structures within the flow, highlighting two ways in which local static instability in the density gradient fails to be a sufficient indicator of mixing: within the vortex a lateral density gradient is correlated with the majority of $\chi$, and outside the vortex extreme values of $\chi$ are localized to relatively ‘sharp’ stable density interfaces at the bounding edges between overturning layers. Finally, in §5, we summarize our results and discuss implications for parameterizing turbulent mixing within the ocean.

2. Summary of DNS dataset

We consider a statistically-steady, forced DNS of stratified turbulence from the simulation campaign originally reported by Almalkie & de Bruyn Kops (2012), and subsequently analyzed by Portwood et al. (2016) and Taylor et al. (2019). Using a characteristic root-mean-square horizontal velocity scale $u_h$, length scale $L$, and background buoyancy frequency $N_0$, the non-hydrostatic Boussinesq approximation of the Navier-Stokes equations may be written in the following dimensionless form:

$$\nabla \cdot \mathbf{u} = 0, \quad \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\left(\frac{2\pi}{Fr}\right)^2 \rho \mathbf{\hat{z}} \cdot \nabla p + \frac{\nabla^2 \mathbf{u}}{Re} + \mathbf{F}, \quad \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho - w = \frac{\nabla^2 \rho}{Re Pr}. \quad (2.1a, b, c)$$

The governing equations (2.1) are numerically integrated using a pseudospectral technique in a triply-periodic domain, as detailed by Almalkie & de Bruyn Kops (2012). The dimensionless parameters governing the flow are the Prandtl number $Pr = \nu/\kappa$, Froude number $Fr_h = 2\pi u_h/(N_0 L)$ and Reynolds number $Re_h = u_h L/\nu$. The density field satisfies $\rho(x,t) = \rho_0(1 - N_0^2 z/g) + \rho'(x,t)$, as is defined by a reference density $\rho_0$, an imposed constant background buoyancy frequency $N_0$, and density perturbation $\rho'$ satisfying the periodic boundary conditions. The imposed background buoyancy frequency $N_0$ is used as the characteristic ‘appropriately-averaged’ buoyancy frequency $\bar{N}$ required to compute $\chi$ in equation (1.1), as is widely considered the natural choice when quantifying irreversible mixing in numerical simulations with an imposed background stratification (see e.g. Shih
Transport across stable density interfaces

et al. (2005); Maffioli et al. (2016); Garanaik & Venayagamoorthy (2019); Portwood et al. (2019)). By explicitly computing the available potential energy (APE) of a triply-periodic domain with an imposed uniform background stratification $N_0$, Howland et al. (2021) confirmed that normalizing $\chi$ by $N_0$ indeed provides an excellent approximation to the true irreversible mixing rate as computed through changes in the system’s APE. The forcing term $F$ is governed by the deterministic scheme denoted ‘Rf’ in Rao & de Bruyn Kops (2011), which adds energy to horizontal motions larger than 1/8th of the horizontal box size so as to match a target kinetic energy spectrum at small wavenumbers. We consider a simulation characterized by $Pr = 1$, $Fr_h = 2.23$ and $Re_h = 1271$, in a domain of size $2\pi \times 2\pi \times \pi$ with $4096 \times 4096 \times 2048$ grid points, resulting in a grid spacing of $\Delta \approx L_K/2$, with $L_K$ denoting the Kolmogorov length scale. We consider a single snapshot of the flow in time and all figures are displayed on grids that have been sparsed by a factor of eight in each dimension.

The main characteristics of the dataset are summarized in Figure 1. The vertically-averaged dissipation rate $\varepsilon$ (Figure 1a) reveals a dominant patch of elevated turbulence that is generated by a large-scale vertically-aligned vortex in the velocity field, rotating counter-clockwise (Figure 1b). Radial averages, centered on the vortex, of the angular velocity $u_\theta$ and vertical component of vorticity $\omega_z = \partial v/\partial x - \partial u/\partial y$ are plotted in Figure 1c, indicating a Rankine-type vortex that is approximately characterized by rigid body rotation at small radii $r$ from the vortex core, followed by a transition to roughly irrotational flow at larger $r$. It is important to note that such a description characterizes the radially-averaged flow, and that smaller-scale vortical motions will still certainly be present in the turbulent patch surrounding the vortex. A series of horizontal currents traveling in alternating directions are found to emanate from the vortex, characterized by a vertical scale on the order of a buoyancy length $L_B$. In Figure 1d, we plot the vertical slice of the density field that corresponds to the velocity field shown in Figure 1b, highlighting an analogous vertically-layered structure outside of the vortex, with relatively well-mixed density layers separated by sharp, stable interfaces. The approximate locations of these density interfaces (delineated by green contours) correspond to minima in the histogram of $\rho$ (Figure 1e), which highlights a strong perturbation of the density field away from its uniform background gradient. Superimposing these density contours on the velocity field in Figure 1b highlights that the sheared interfaces in the velocity field are strongly correlated with the stable interfaces in the density field. This correlation is further demonstrated in Supplementary Video 1, where rotations of the slices in Figures 1b,d around the center of the vortex are shown. In §4, we demonstrate that these interfaces, characterized by both high shear and a strong statically-stable density gradient, are critically important for the mixing generated outside of the vortex.

The spontaneous formation of a persistent vortex is a key, yet previously unreported feature of the forcing scheme of Rao & de Bruyn Kops (2011) used to generate statistically-steady turbulence. In particular, the identification of the vortex in Figure 1 provides insight into how the segmentation results of Portwood et al. (2016) (see their Figure 2c), who used an identical forcing scheme, are related to the background flow field. Specifically, the roughly cylindrical patch of most vigorous turbulence detected by Portwood et al. (2016), using a filter of size $L_B$, extends across the entire vertical domain and almost certainly corresponds to an analogous vortical structure in their DNS. Similarly, their ‘intermittent layers’ are primarily composed of horizontal offshoots from the central vertically-aligned turbulent patch, and are shaped by a similar pattern to the sheared velocity interfaces observed in Figure 1b. As it is now evident that Portwood et al. (2016) have broadly identified such a vortex to be a turbulent hotspot, a goal of this study is to perform a finer analysis of mixing patterns both within and outside of the vortex, in order to determine how patterns in the small-scale turbulent microstructure, as described by $\varepsilon$ and $\chi$, are related to the larger-scale layered structure of the flow.
Figure 1: Large-scale characteristics of the velocity and density fields within the computational domain. a) The vertical average of the dissipation rate $\epsilon$ at gridpoint $(x, y)$, normalized by the domain average. The whole domain is shown, with gridpoints sparsed by a factor of eight in each dimension. The dashed circle highlights a region of elevated $\epsilon$, coinciding with a vortex in the velocity field, as is further examined in Figure 3. A vertical slice of the domain at $y = 200$ is considered in Figure 4. b) The horizontal velocity normal to the plane for a vertical slice at constant $y$ passing through the center of the dashed circle in panel a), revealing a vertically-aligned vortex rotating counterclockwise. The grid has been shifted in $x$ relative to panel a) so as to center the vortex. The buoyancy length $L_B$ and Taylor length $L_T \approx 25L_K$ (where $L_K$ is the Kolmogorov length) are marked for reference, as were the filter sizes used in the segmentation analysis of Portwood et al. (2016). Green contours mark stable interfaces in the density field, as shown in panel d). c) The radially-averaged angular velocity $u_\theta$ and vertical component of vorticity $\omega_z$ as a function of the distance $r$ from the center of the vortex. The dashed line at $r = 80$ corresponds to the dashed circle plotted in panel a). d) The density field corresponding to the vertical slice of velocity plotted in panel b). The green lines in panels b) and d) illustrate contours at the minimum values of the histogram of the density field in panel e), as are marked with vertical green lines, delineating the interfaces between relatively well-mixed density layers in the flow surrounding the vortex.

3. Pointwise statistics conditioned on local density gradient
Motivated by the flow segmentation of Portwood et al. (2016) in terms of the local fraction of overturning $\partial \rho / \partial z > 0$, we first consider how the pointwise distributions of $\epsilon$, $\chi$ and $\Gamma = \chi / \epsilon$ depend on the magnitude of $\partial \rho / \partial z$, for both statically stable and unstable points,
Transport across stable density interfaces

As shown in Figure 2, for illustration, in Figure 2a we split the distribution of $\partial \rho / \partial z$ into three regions: two tails containing 10% by volume of the most stable and unstable points (coloured blue and red, respectively), and the remaining 80% of the intermediate values (green). For such a division, we then consider the distributions of $\epsilon$, $\chi$ and $\Gamma$ within each region, as shown in Figures 2b-d. The bulk of the domain (green) is well characterized by the canonical flux coefficient $\Gamma = 0.2$, but such points contain the lowest $\chi$ and are thus not of primary importance for the total mixing arising within the computational domain. Instead, it is the extreme tails of the $\partial \rho / \partial z$ distribution that must be considered, containing the most significant values of $\chi$. While both the blue and red tails contain elevated but similar distributions of $\epsilon$, they may be distinguished by their asymmetry in $\chi$; the stable tail (blue) contains disproportionately elevated $\chi$ as compared to $\epsilon$, and therefore some of the highest values of $\Gamma$ within the domain.

In Figures 2e-g, we then analyze how the medians of the $\epsilon$, $\chi$ and $\Gamma$ distributions change as a function of the volume contained within the blue and red tails, and additionally plot the relative contributions of these tails to the domain total. Comparing the right panels of Figures 2e and 2f reveals that $\chi$ is far more dominated by extreme events than $\epsilon$, in agreement with the analysis of oceanographic data by Couchman et al. (2021). For instance, when each tail contains 10% volume, the stable (blue) and unstable (red) tails each contain approximately 20% of the total $\epsilon$ in the domain, but 45% and 30% of the total $\chi$, respectively. Furthermore, while the contributions to $\epsilon$ from both tails is roughly equal, the contribution to $\chi$ from the stable tail is always roughly 50% greater than for the unstable tail. While $\Gamma = 0.2$ may thus be a suitable approximation for the bulk of the domain, it may here not be relied upon for capturing the most extreme events in $\chi$, which dominate the bulk mixing statistics.

Additionally, the statistics in Figure 2 suggest that local instability may not be a sufficient indicator for mixing, given the significance of the blue stable tail. However, we note that such a conclusion cannot definitively be drawn from the pointwise distributions of $\partial \rho / \partial z$, as such a distribution provides no information about the extended spatial environment around each point. For example, in regions of fully-developed turbulence that might emerge after the collapse of a shear-induced billow, there is likely a random mixture of neighbouring unstable and stable points in close proximity (roughly a 50% mixture as identified by Portwood et al. (2016) in their most turbulent patches), and so points within the red and blue tails of Figure 2a could be direct neighbours in space. Therefore, in §4, we extend our pointwise analysis by identifying spatially extended and coherent stable regions, which appear to take the form of ‘interfaces’ with enhanced density gradients. We then assess the significance of these non-overturning structures to the overall mixing statistics.

4. Extended mixing structures

We now consider coherent spatial distributions of the microstructure quantities $\epsilon$ and $\chi$, and their relation to the large-scale flow patterns observed in Figure 1, by focusing on mixing structures arising both within and outside of the vortex. We first perform a closer examination of mixing within the vortex, as shown in Figure 3. Vertical averages of $\epsilon$, $\chi$, $w$ and $\rho'$ are plotted in Figures 3a-d, respectively, highlighting clear differences in the spatial distributions of $\epsilon$ and $\chi$. Such differences are further illustrated in Figures 3e-h, which show the respective radial distributions of the azimuthal velocity $u_\theta$, $\epsilon$, $\chi$ and $\Gamma$ with respect to the vortex core. These radial distributions illustrate that the inner section of the vortex, characterized by roughly rigid-body rotation, is well-mixed and contains the largest values of $\epsilon$ despite having minimal scalar diffusion rates $\chi$. This observation is consistent with the density field shown in Figure 1d, where initially horizontal contours of constant density (green lines) are strongly deflected toward the vertical before reaching the center of the vortex, resulting in...
Figure 2: Pointwise mixing statistics of the DNS data, conditioned by the local vertical density gradient. a) Histogram of the perturbed density gradient $∂ρ′/∂z$ normalized by the magnitude of the imposed uniform background gradient, with values greater than one indicating local overturning. The distribution is split into three regions, by assigning a fixed volume (here 10%) to each tail. Panels b)-d) illustrate the distributions of $\epsilon$, $\chi$ and $\Gamma$, respectively, for the whole domain (black) and the subdomains encompassed by the coloured regions in panel a). Circles mark the median values of each distribution, and the dashed line in panel d) indicates the canonical flux coefficient $\Gamma = 0.2$ for reference. Panels e)-g) illustrate how the medians of the respective distributions in panels b)-d) vary with the tail volume selected in panel a). The circles mark the medians for the segmented distributions shown in panels b)-d) for the case of 10% tail volume. For panels e) and f), the fraction of each quantity ($\epsilon$, $\chi$) contained within each tail relative to the entire domain is also indicated. The dashed diagonal lines mark what would be expected for a uniform distribution of each quantity throughout the domain.

a vertically-extended core of roughly constant density (seen predominantly in the vertical interval $25 \lesssim z \lesssim 175$). Conversely, the majority of $\chi$ is found outside the core at radii where the angular velocity begins to decay, and is distributed in a roughly spiral pattern (Figure 3b). Examination of the vertically-averaged perturbed density field $\rho'$ (Figure 3d) reveals the presence of a strong lateral density gradient, induced by the alternating upwelling of dense fluid and downwelling of lighter fluid within the vortex as a function of $r$. Superimposing the position of this lateral gradient (gray) onto the distribution of $\chi$ in Figure 3b reveals that this gradient is strongly correlated with the spiral distribution of the most intense $\chi$. While...
the vortex was identified by Portwood et al. (2016) to be a patch of vigorous turbulence with elevated $\epsilon$ due to its generation of significant local vertical overturning, our analysis suggests that much of the mixing within the vortex, as quantified by $\chi$, instead results from diffusion across a strong lateral gradient in the perturbed density field.

Outside of the vortex, the vertical homogeneity of the velocity and density fields collapses, forming a vertically layered structure. In Figure 4, we consider a vertical $(x,z)$ slice of the domain at position $y = 200$ in Figure 1a, in order to understand how this large-scale layering pattern gives rise to mixing at the microscale. Motivated by the significance of the stable tail (blue) in the pointwise distribution of $\partial \rho / \partial z$ in Figure 2a, and the observation of horizontally-extended stable filaments of $\partial \rho / \partial z$ in Figure 4a, we examine whether such structures contribute substantially to mixing in the layered flow surrounding the vortex. To isolate these stable filaments, we apply a Gaussian filter to the density field with standard deviation $\sigma \approx 6L_K$ (corresponding to 2 grid points in Figure 4), where $L_K$ denotes the Kolmogorov length scale. The intent of such a filter is to isolate spatially-coherent stable structures from patchy overturning regions that would contain a random assortment of stable and unstable neighbouring points. We note that our filter length is on the order of $10L_K$ as suggested by Kuo & Corrsin (1971) for removing internal intermittency. Further, it is significantly finer than the Taylor length $L_T \approx 25L_K$, which was the smallest filter size considered by Portwood et al. (2016) in their identification of ‘intermittent layers’, allowing us to examine the importance of finer-scale structures within the flow.
Figure 4: Characteristics of the layered flow outside the vortex. Vertical slices at \( y = 200 \) in Figure 1a of a) the density field \( \partial \rho / \partial z \) normalized by the magnitude of the imposed background gradient, b) the result of applying a Gaussian filter with a standard deviation of two gridpoints (\( \approx 6 L_K \)) to the density field in panel a), c) extracted stable filaments from panel b) obtained by retaining points in the bottom (most-stable) 15% of the filtered density distribution, d-e) the \( x \) and \( y \) horizontal components of velocity, and f) the local fraction of unstable overturning computed with a filter size corresponding to the Taylor length (\( L_T \approx 25 L_K \)), following the method of Portwood et al. (2016). The stable filaments from panel c) are overlaid on panels d)-f). The green contours in panels c)-f) correspond to those plotted in Figures 1b,d, marking the stable interfaces separating relatively well-mixed density layers.

Having filtered the density field (Figure 4b), we then extract the most stable density structures by considering points in the bottom (most stable) \( q \) percent of the filtered \( \partial \rho / \partial z \) distribution. For illustration, we here extract structures comprised of the most stable \( q = 15\% \) of points (Figure 4c), and in Appendix A demonstrate the effect of changing this percentage. The green contours from Figures 1b,d are overlaid on Figure 4c, demonstrating that the extracted filaments correspond to segments of the sharp interfaces separating relatively well-mixed layers in the density field. In Figures 4d,e, we again highlight that these stable interfaces are roughly correlated with regions of high vertical shear in the layered velocity field, as are generated by the vortex. Importantly, Figure 4f highlights that the majority of overturning (the segmentation indicator used by Portwood et al. (2016)) occurs in the regions between these stable interfaces. Such an observation thus begs the question as to whether it is the well-mixed overturning layers or their bounding intervening stable interfaces that are most relevant for mixing.

We address this question in Figure 5, by considering the relative contributions of both the vortex and the isolated stable interfaces to the domain totals of \( \epsilon \) and \( \chi \). In agreement with Portwood et al. (2016), despite occupying less than 10% of the domain volume, the vortex contributes approximately a third of the entire domain’s \( \epsilon \) and \( \chi \) (red bars, Figure 5a). Outside of the vortex, however, it is the stable interfaces that play a key role in the overall mixing, contributing

\[
\frac{(\% \text{ in interface}) \cap (\% \text{ outside vortex})}{(\% \text{ outside vortex})} = \frac{26\%}{26\% + 40\%} = 39\%
\]

of the total \( \chi \) outside the vortex, despite appearing unremarkable based on their much smaller contribution to \( \epsilon \) (\( 11\% / (11\% + 55\%) = 17\% \)). Figure 4f thus highlights a key conclusion of this study: while overturning is most prevalent in well-mixed density layers, relatively thin stable interfaces between such relatively deep layers, which are also correlated with high vertical shear, yield a crucial component of the bulk scalar mixing rate \( \chi \). In particular,
Transport across stable density interfaces

Figure 5: Mixing contributions of the vortex and stable interfaces. a) Fractional contributions to the domain total of the dissipation rates of kinetic energy $\epsilon$ and scalar variance $\chi$, from within the vortex (red), stable interfaces outside the vortex (dark blue), and the rest of the domain outside both the vortex and interfaces (light blue). Histograms of b) $\epsilon$, c) $\chi$ and d) $\Gamma$ outside the vortex (black), further split according to whether points are contained within a stable interface (dark blue) or not (light blue). Dashed lines indicate median values of the respective distributions.

Figures 5b,c highlight that while these interfaces may be strongly distinguished by their distributions of $\chi$, they are virtually indistinguishable based on $\epsilon$. This mismatch between the spatial distributions of $\epsilon$ and $\chi$ results in significantly elevated $\Gamma$ within the interfaces, well above the canonical value $\Gamma = 0.2$ (Figure 5d). It thus appears crucial to consider the independent information provided by the distributions of $\epsilon$ and $\chi$ within a domain when quantifying mixing, particularly for identifying the locations of the most extreme events.

5. Discussion

We have considered local correlations between the vertical density gradient $\partial \rho / \partial z$ and the dissipation rates of kinetic energy $\epsilon$ and scalar variance $\chi$ in order to characterize the spatial distributions of mixing within a forced direct numerical simulation of density-stratified turbulence. The forcing scheme is found to generate a vertically-aligned vortex within the domain, largely explaining the concentrated ‘patch’ region of vigorous turbulence reported by Portwood et al. (2016). Outside of the vortex, the flow is characterized by a layered density profile, with thin, highly stable interfaces separating relatively well-mixed layers. While a mixing analysis based solely on the identification of overturning would deem the well-mixed layers to be of primary importance, as in the identification of ‘intermittent layers’ with elevated $\epsilon$ by Portwood et al. (2016), we have demonstrated that a significant fraction of $\chi$ is localized to the edges of such layers, within the stable intervening interfaces. Notably, these interfaces appear unremarkable if looking at $\epsilon$ alone (see Figure 5b), emphasizing the importance of $\chi$ as an independent indicator of mixing. As the flux coefficient $\Gamma = \chi / \epsilon$ has been found to strongly depend on the time history of a turbulent event (Mashayek et al. 2021), it would be instructive to now consider the time evolution and formation of these interfaces, characterized by strongly elevated $\Gamma$. For instance, as the density interfaces are correlated with regions of high vertical shear, it is conceivable that they might be remnants of the previous collapse of shear-induced billows that are now only visible in signals of $\chi$ but not $\epsilon$, as coined ‘fossil turbulence’ by Nasmyth (1970).

Our findings have two potential implications for the parameterization of ocean mixing. Firstly, our analysis highlights the importance of adequately sampling rare, yet extreme mixing events in a turbulent flow, as was also recently discussed by Cael & Mashayek (2021). In agreement with the analysis of oceanographic data by Couchman et al. (2021), Figure 2d
demonstrates that although the majority of the domain indeed appears to be well characterized by the canonical flux coefficient $\Gamma = 0.2$, significantly elevated $\Gamma$ is associated with the most extreme events in $\chi$, events that are not reflected by a corresponding local increase in $\epsilon$. Given the current relative sparsity of measurements within the ocean, mixing parameterizations may thus be biased toward the most commonly measured events, which are not necessarily the most significant. Secondly, even with perfect sampling, different proxies for mixing are likely to yield contrasting predictions for the amount and spatial distribution of mixing within the highly-anisotropic layered flow considered here. For example, if measurements of $\chi$ were not available, the stable filaments at the edges of the overturning layers (Figure 4f) would appear unremarkable, as they appear locally quiescent based on their density gradient and are not correlated with any discernible increase in $\epsilon$. Further, given the strong spatial variability of $\Gamma$ within the vertically-layered flow (see Figure 5d), it is unclear what value of $\Gamma$ should be used in the method of Osborn (1980) if trying to infer a flux from values of $\epsilon$ measured directly by a microstructure profiler or derived from a Thorpe overturning analysis.

As discussed by Caulfield (2021), an accurate parameterization of the flux coefficient $\Gamma$ is likely to depend on multiple dimensionless groups characterizing the underlying flow, such as the buoyancy Reynolds number $Re_b$, Froude number $Fr$, and Prandtl number $Pr$. For instance, DNS studies have demonstrated that bulk-averages of $\Gamma$ decrease with increasing $Pr$ (Salehipour et al. 2015) and decreasing $Fr$ (Maffioli et al. 2016). A promising future direction of inquiry would be to try and rationalize such variations in $\Gamma$ in terms of differences in the prevalence and structure of smaller-scale extreme events within the flow, such as analyzing changes in the morphology of the stable filaments considered here. It would also be instructive to extend our analysis to simulations of decaying turbulence which also develop layered structures (de Bruyn Kops & Riley 2019), in order to establish whether the spatial distribution of mixing events observed here changes significantly in forced versus unforced scenarios.

Finally, following Portwood et al. (2016) and typical oceanographic measurements, we have here primarily relied upon the local density gradient $\partial \rho / \partial z$ to inform our analysis of spatial mixing patterns. However, there are likely more optimal flow variables, or linear combinations thereof, that could lead to a more robust segmentation of the turbulent domain into distinct regimes. For example, one could imagine constructing more insightful indicator functions of mixing from components of the velocity gradient tensor $\partial u_i / \partial x_j$, as suggested by de Bruyn Kops et al. (2019). Applying data-driven techniques, such as unsupervised clustering or dimensionality reduction, to the wealth of observational, experimental and numerical stratified turbulence data currently available has the potential to discover automatically optimal mixing indicators free of human bias. Such an analysis would hopefully further our understanding of the dominant mixing mechanisms present in different flow regimes, along with their prevalence, guiding the search for a more universal and accurate mixing parameterization.

**Acknowledgements.** This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. SdeBK was supported under U.S. Office of Naval Research Grant number N00014-19-1-2152. For the purpose of open access, the authors have applied a Creative Commons Attribution (CC BY) licence to any Author Accepted Manuscript version arising from this submission.

**Declaration of interests.** The authors report no conflict of interest.
Appendix A. Thresholding of stable filaments

The stable filaments (black) plotted in Figure 4c were extracted by identifying points within the bottom (most stable) $q = 15\%$, by volume, of the Gaussian-filtered distribution of the density gradient $\partial \rho / \partial z$ (Figure 4b). We here briefly consider how changing this thresholding percentage $q$ influences the characteristics of the extracted stable structures.

In Figure 6, we plot the stable structures that are identified by varying the percentage $q$ from 5\% to 30\%. As $q$ is increased, meaning that more points in the stable tail of the filtered $\partial \rho / \partial z$ distribution are considered, the identified stable structures are found to grow primarily in the horizontal direction, tracing out more of the stable interfaces identified by the green contours from Figures 1b,d. Figure 6 thus highlights that the magnitude of the vertical density gradient along such stable contours is not uniform, with certain segments having stronger gradients (as identified by using a smaller $q$) and thus being characterized by a larger local $\chi$.

It is also natural to consider how the mixing statistics presented in Figure 5a depend on the thresholding percentage $q$. In Figure 7, considering only the computational domain outside of the vortex, we plot the percent contribution of the extracted interfaces to $\epsilon$ and $\chi$, as a function of $q$. The points at $q = 15\%$ correspond to the statistics presented in Figure 5a, noting that in Figure 7 the percent contributions are normalized by the domain total outside the vortex, and not the entire domain including the vortex as in Figure 5a. Figure 7 demonstrates that over a wide range of threshold percentages $q$, the identified stable filaments always contribute over twice the amount of $\chi$ as compared to $\epsilon$. 


Figure 6: Extracted stable filaments as a function of the thresholding percentage $q$. Filaments (black) are identified as the union of points within the bottom (most stable) $q\%$ of the filtered density distribution (see discussion in §4). The filaments detected using values of $q$ between 5% and 30% are shown in panels a)-f), respectively. Panel c) corresponds to Figure 4c.

Figure 7: The percent contributions of $\epsilon$ and $\chi$ contained within the stable interfaces identified in Figure 6, normalized by the domain totals outside of the vortex, as a function of the thresholding percentage $q$. The statistics at $q = 15\%$ correspond to those presented in Figure 5a, noting that in Figure 5a the contributions are normalized by the total domain including the vortex.

REFERENCES

Almalkie, S. & de Bruyn Kops, S.M. 2012 Kinetic energy dynamics in forced, homogeneous, and axisymmetric stably stratified turbulence. *Journal of Turbulence* 13 (29).

Billant, P. & Chomaz, J.-M. 2001 Self-similarity of strongly stratified inviscid flows. *Physics of Fluids* 13 (6), 1645–1651.

de Bruyn Kops, S.M. & Riley, J.J. 2019 The effects of stable stratification on the decay of initially isotropic homogeneous turbulence. *Journal of Fluid Mechanics* 860, 787–821.

Cael, B.B. & Mashayek, A. 2021 Log-skew-normality of ocean turbulence. *Physical Review Letters* 126 (22), 224502.

Caulfield, C.P. 2020 Open questions in turbulent stratified mixing: Do we even know what we do not know? *Physical Review Fluids* 5 (11), 110518.

Caulfield, C.P. 2021 Layering, instabilities, and mixing in turbulent stratified flows. *Annual Review of Fluid Mechanics* 53, 113–145.

Couchman, M.M.P., Wynne-Cattanach, B., Alford, M.H., Caulfield, C.P., Kerswell, R.R., MacKinnon, J.A. & Voet, G. 2021 Data-driven identification of turbulent oceanic mixing from observational microstructure data. *Geophysical Research Letters* 48 (23), e2021GL094978.

de Bruyn Kops, S.M. 2015 Classical turbulence scaling and intermittency in stably stratified Boussinesq turbulence. *Journal of Fluid Mechanics* 775, 436–463.
Transport across stable density interfaces

de Bruyn Kops, S.M., Saunders, D.J., Rieman, E.A. & Portwood, G.D. 2019 Unsupervised machine learning to teach fluid dynamicists to think in 15 dimensions. arXiv:1907.10035

Fernando, H.J.S. 1991 Turbulent mixing in stratified fluids. Annual Review of Fluid Mechanics 23, 455–493.

Garanaik, A. & Venayagamoorthy, S.K. 2019 On the inference of the state of turbulence and mixing efficiency in stably stratified flows. Journal of Fluid Mechanics 867, 323–333.

Gregg, M.C., D’Asaro, E.A., Riley, J.J. & Kunze, E. 2018 Mixing efficiency in the ocean. Annual Review of Marine Science 10, 443–473.

Howland, C.J., Taylor, J.R. & Caulfield, C.P. 2021 Quantifying mixing and available potential energy in vertically periodic simulations of stratified flows. Journal of Fluid Mechanics 914.

Iuchi, T., St. Laurent, L., Polzin, K.L. & Toole, J.M. 2020 How variable is mixing efficiency in the abyss? Geophysical Research Letters 47 (7), e2019GL086813.

Ivey, G.N., Bluteau, C.E. & Jones, N.L. 2018 Quantifying diapycnal mixing in an energetic ocean. Journal of Geophysical Research: Oceans 123 (1), 346–357.

Kuo, A.Y.S. & Corrsin, S. 1971 Experiments on internal intermittency and fine-structure distribution functions in fully turbulent fluid. Journal of Fluid Mechanics 50 (2), 285–319.

Lilly, D.K. 1983 Stratified turbulence and the mesoscale variability of the atmosphere. Journal of Atmospheric Sciences 40 (3), 749–761.

Lorenz, E.N. 1955 Available potential energy and the maintenance of the general circulation. Tellus 7 (2), 157–167.

MacKinnon, J.A., Zhao, Z., Whalen, C.B. & Others 2017 Climate process team on internal wave–driven ocean mixing. Bulletin of the American Meteorological Society 98 (11), 2429–2454.

Maffioli, A., Brethouwer, G. & Lindborg, E. 2016 Mixing efficiency in stratified turbulence. Journal of Fluid Mechanics 794.

Mashayek, A., Caulfield, C.P. & Alford, M.H. 2021 Goldilocks mixing in oceanic shear-induced turbulent overturns. Journal of Fluid Mechanics 928, A1.

Nasmyth, P.W. 1970 Oceanic turbulence. PhD thesis, University of British Columbia.

Osborn, T.R. 1980 Estimates of the local rate of vertical diffusion from dissipation measurements. Journal of Physical Oceanography 10 (1), 83–89.

Osborn, T.R. & Cox, C.S. 1972 Oceanic fine structure. Geophysical Fluid Dynamics 3 (4), 321–345.

Portwood, G.D., de Bruyn Kops, S.M. & Caulfield, C.P. 2019 Asymptotic dynamics of high dynamic range stratified turbulence. Physical Review Letters 122 (19), 194504.

Portwood, G.D., de Bruyn Kops, S.M., Taylor, J.R., Salehipour, H. & Caulfield, C.P. 2016 Robust identification of dynamically distinct regions in stratified turbulence. Journal of Fluid Mechanics 807.

Rao, K.J. & de Bruyn Kops, S.M. 2011 A mathematical framework for forcing turbulence applied to horizontally homogeneous stratified flow. Physics of Fluids 23 (6), 065110.

Salehipour, H., Peltier, W.R. & Mashayek, A. 2015 Turbulent diapycnal mixing in stratified shear flows: the influence of Prandtl number on mixing efficiency and transition at high Reynolds number. Journal of Fluid Mechanics 773, 178–223.

Shih, L.H., Koseff, J.R., Ivey, G.N. & Ferziger, J.H. 2005 Parameterization of turbulent fluxes and scales using homogeneous sheared stably stratified turbulence simulations. Journal of Fluid Mechanics 525, 193–214.

Tailleux, R. 2009 On the energetics of stratified turbulent mixing, irreversible thermodynamics, Boussinesq models and the ocean heat engine controversy. Journal of Fluid Mechanics 638, 339–382.

Taylor, J.R., de Bruyn Kops, S.M., Caulfield, C.P. & Linden, P.F. 2019 Testing the assumptions underlying ocean mixing methodologies using direct numerical simulations. Journal of Physical Oceanography 49 (11), 2761–2779.

Thorpe, S.A. 1977 Turbulence and mixing in a Scottish loch. Philosophical Transactions of the Royal Society of London A 286 (1334), 125–181.

Villermaux, E. 2019 Mixing versus stirring. Annual Review of Fluid Mechanics 51 (1), 245–273.

Whalen, C.B., de Laverge, C., Garabato, A.C.N., Klymak, J.M., Mackinnon, J.A. & Sheen, K.L. 2020 Internal wave-driven mixing: governing processes and consequences for climate. Nature Reviews Earth & Environment 1 (11), 606–621.

Winters, K.B., Lombard, P.N., Riley, J.J. & D’Asaro, E.A. 1995 Available potential energy and mixing in density-stratified fluids. Journal of Fluid Mechanics 289, 115–128.

Wunsch, C. & Ferrari, R. 2004 Vertical mixing, energy, and the general circulation of the oceans. Annual Review of Fluid Mechanics 36, 281–314.