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Diascalar flux and the rate of fluid mixing

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We define the rate at which a scalar θ mixes in a fluid flow in terms of the flux of θ across isoscalar surfaces. This flux ϕ_d is purely diffusive and is, in principle, exactly known at all times given the scalar field and the coefficient of molecular diffusivity. In general, the complex geometry of isoscalar surfaces would appear to make the calculation of this flux very difficult. In this paper, we derive an exact expression relating the instantaneous diascalar flux to the average squared scalar gradient on an isoscalar surface which does not require knowledge of the spatial structure of the surface itself. To obtain this result, a time-dependent reference state $\theta(t, z_*)$ is defined. When the scalar is taken to be density, this reference state is that of minimum potential energy. The rate of change of the reference state due to diffusion is shown to equal the divergence of the diffusive flux, i.e. $(\partial/\partial z_*)\phi_d$.

This result provides a mathematical framework that exactly separates diffusive and advective scalar transport in incompressible fluid flows. The relationship between diffusive and advective transport is discussed in relation to the scalar variance equation and the Osborn–Cox model. Estimation of water mass transformation from oceanic microstructure profiles and determination of the time-dependent mixing rate in numerically simulated flows are discussed.

1. Introduction

The rate of mixing is a fundamental property of fluid flows. Mixing influences both the horizontal and vertical dispersion of all conserved quantities which in turn influences the dynamics of the flow at all scales. Furthermore, the rate at which energy is expended in mixing a density-stratified flow can often be a significant fraction of the total energy dissipation rate.

Though mixing is a fundamental process of interest, the rate of mixing is often difficult to measure. Part of the difficulty stems from subtle differences between various definitions of mixing. Intrinsic to many definitions, however, is the notion of a scalar flux. For example, the flux of heat through the fluid is often used to quantify the mixing rate in thermally stratified flows. The flux of heat divided by a suitably defined mean temperature gradient yields the rate of mixing expressed as a diffusivity. Two issues arise immediately: (i) Across what surfaces should the flux be determined? (ii) How should the mean gradient be defined?

The goal of this paper is to clarify these issues and to obtain an unambiguous relationship between mixing, scalar flux and the average squared scalar gradient.

These results bear directly on the estimation of mixing rates, particularly in geophysical flows. Direct measurements of diapycnal mixing rates in oceans and lakes are often obtained from profiling 'microstructure' instruments, which measure one or more components of the temperature gradient. The interpretation of these data relies on the temperature variance equation and a set of simplifying assumptions known as the Osborn–Cox (1972) model (see Gregg 1987). Because the underlying assumptions are often difficult to justify, the accuracy of this technique has been questioned by several authors, in particular by Davis (1994*a,b*, 1996). This paper derives an exact expression which yields the heat flux across isotherms in terms of average squared temperature gradients. The difference between this expression and that derived by Osborn–Cox (1972) rests entirely in using the proper definitions for mean temperature gradient and heat flux.

Our results are derived from the following advection-diffusion equation for an arbitrary scalar θ:

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \nabla \theta = \kappa \nabla^2 \theta \tag{1}$$

where κ is the coefficient of molecular diffusivity and $\nabla \cdot \boldsymbol{u} = 0$. Equation (1) is assumed to hold in a volume V with cross-sectional area A. To simplify the presentation, we assume that A is constant. The volume V is open in the sense that fluid is permitted to enter and leave the domain of analysis. Equation (1) is used extensively to model the evolution of temperature and/or Boussinesq density in geophysical flows. In the discussion that follows, we will frequently refer to a surface on which the arbitrary scalar θ has a constant value as an isoscalar surface. Similarly, we often use the term diascalar for the direction perpendicular to this surface.

2. Scalar flux

2.1. *Diascalar flux*

To define the rate at which scalar flux occurs, one must first define the surface(s) across which the flux is to be measured. A natural choice is to define the flux relative to surfaces of constant θ, or isoscalar surfaces. The appropriate flux is then the diffusive flux $\kappa \nabla \theta$. Note that the flux has dimensions of $[\theta]$ m s^{-1}, where $[\theta]$ denotes the dimensions of the scalar θ. A meaningful average flux ϕ_d can be obtained by integrating over an isoscalar surface S

$$\phi_d = \frac{1}{A} \int_S \kappa \nabla \theta \cdot \hat{n} \, \mathrm{d}S \tag{2}$$

where $\hat{n}$ is the unit vector normal to S in the direction of increasing θ. Strictly speaking, ϕ_d is the total flux of the scalar θ across an isoscalar surface, i.e. the diascalar flux, expressed per unit cross-sectional area, normalized by the area A. In a turbulent flow A_S, the surface area of S, will be much larger than A.

We define the rate of diffusive mixing in terms of ϕ_d, which quantifies the diffusive scalar flux. Its divergence, suitably defined (see §4.1), quantifies the rate of change of scalar concentration, or in an oceanographic context, the rate of water mass modification. The expression (2) provides an unambiguous definition of the mixing rate that does not require any simplifying assumptions about the fluid dynamics. As written however, this expression appears to be difficult to evaluate owing to the geometrical complexity of instantaneously defined isoscalar surfaces.

2.2. *Advective flux*

An alternative approach is based on Reynolds averaging. In this approach, the scalar and velocity fields are decomposed into mean $\langle () \rangle$ and fluctuating $()'$ components as follows:

$$\theta = \langle \theta \rangle + \theta' \quad , \quad \boldsymbol{u} = \langle \boldsymbol{u} \rangle + \boldsymbol{u}'. \tag{3}$$

To provide an explicit contrast to the previous discussion, we take the averaging operator $\langle\rangle$ to be a spatial average over area A. The advective flux across the averaging surface is then

$$\phi_a = \frac{1}{A} \int \theta' \boldsymbol{u}' \cdot \hat{n} \, \mathrm{d}S. \tag{4}$$

Obviously, $\phi_d(t)$ is not generally equal to $\phi_a(t)$. The sign of ϕ_a can be either positive or negative. The sign of ϕ_d is always positive. Diascalar flux ϕ_d results solely from molecular diffusion, while ϕ_a can be produced by motions at any scale. For example, non-diffusive internal waves can produce a time-oscillating ϕ_a with zero mean. Such fluctuations are entirely reversible and contribute nothing to ϕ_d.

An estimate of the average mixing rate can, however, often be obtained by sufficiently averaging ϕ_a in space and/or time. Typically, the amount of averaging required depends on aspects of the flow at scales much larger than the largest turbulent scales. Unfortunately, this may average out variability in the mixing rate that is of interest. Clearly, a practical means of estimating ϕ_d without having to average ϕ_a would be useful.

3. A simple derivation of the diascalar flux

We now derive the formal relationship between the diascalar flux per unit area and the average square of the scalar gradient. This derivation is geometrical and does not account for advective effects. An alternative derivation, including advection, is presented in §4.1 and the Appendix. From dimensional considerations, we see immediately that in order to obtain a flux given κ and $|\nabla\theta|^2$, an estimate of the 'mean' scalar gradient is required. Similarly, if one desires to express the scalar flux in terms of a diffusivity the 'mean' gradient is again required. In the development that follows, a precise specification of the 'mean' gradient follows naturally from the analysis.

In deriving these results, we assume only that the scalar θ obeys the advection diffusion equation (1) and that $\nabla \cdot \boldsymbol{u} = 0$. Consider a fixed volume of fluid V with uniform cross-sectional area A. Shown in figure 1 are two isoscalar surfaces S and S_Δ defined by θ and $\theta + \Delta\theta$. These surfaces are drawn schematically; the analysis that follows refers to two arbitrarily convoluted, multivalued surfaces. Regardless of geometrical complexity, the volume of fluid between the surfaces ΔV is well defined.

Suppose that diffusive mixing occurs and there is a net flux of θ across the surfaces S and S_Δ. If the fluxes across the two surfaces do not balance, there is a flux divergence. A flux divergence implies that fluid with scalar value between θ and $\theta + \Delta\theta$ is being created or lost by diffusive mixing and that ΔV changes as a result. Alternatively, we may choose to define the surfaces such that ΔV remains constant. In this case, a flux divergence changes the values of θ associated with the surfaces. We take this approach.

To accomplish this we introduce a new coordinate z_* that satisfies the following two properties: (i) z_* has a single, unique value at all points on an isoscalar surface with $z_*(\theta_2) < z_*(\theta_1)$ whenever $\theta_2 > \theta_1$; (ii) $|\Delta z_*|$, the magnitude of the difference between $z_*(\theta)$ and $z_*(\theta + \Delta\theta)$, is equal to $\Delta V/A$, the volume of fluid within the scalar class spanned by θ and $\theta + \Delta\theta$ divided by the cross-sectional area A.

Note that z_* is an isoscalar coordinate, expressed in units of length, but that the value of θ corresponding to a given value of z_* changes in time.

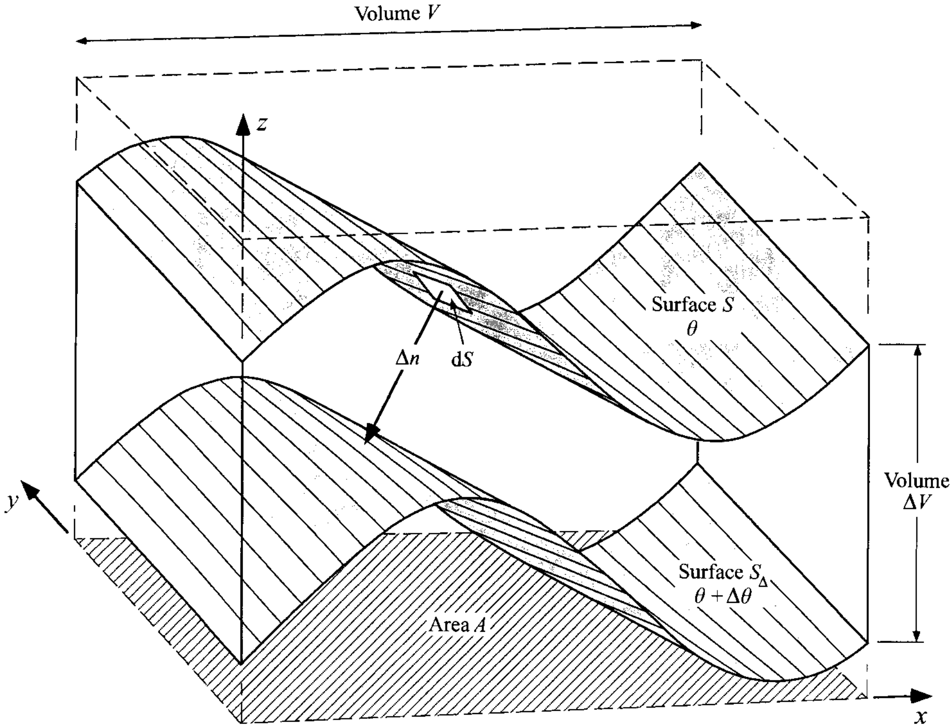

FIGURE 1. Schematic of two isoscalar surfaces in a volume V with cross-sectional area A. Diascalar flux changes ΔV, the volume of fluid between the surfaces S and S_Δ defined by the scalar values θ and $\theta + \Delta\theta$.

Referring again to figure 1, the instantaneous flux of θ across the surface S is given by

$$\kappa \int \nabla\theta \cdot \hat{n} \, \mathrm{d}S \equiv \kappa A_S \langle \nabla\theta \cdot \hat{n} \rangle_{z_*} = A\phi_d \tag{5}$$

where $\langle\rangle_{z_*}$ is the average over the surface S, where z_* maintains a constant value. Note that $\nabla\theta \cdot \hat{n} = |\nabla\theta|$ since the surface normal is everywhere parallel to the scalar gradient and that for nearby isoscalar surfaces $|\nabla\theta| \approx \Delta\theta/\Delta n$ at each point, where Δn is the perpendicular distance between the surfaces (see figure 1).

As long as z_* satisfies the two properties stated, (2) can be rewritten as

$$\phi_d = \lim_{\Delta\theta\to 0} \frac{1}{A\Delta z_*} \int \kappa |\nabla\theta| \frac{\Delta\theta}{\Delta n} \frac{\Delta z_*}{\Delta\theta} \Delta n \, \mathrm{d}S \, . \tag{6}$$

Since $A\Delta z_* = -\Delta V$ by definition, this expression can be recognized as the volume average of $-\kappa|\nabla\theta|(\Delta\theta/\Delta n)(\Delta z_*/\Delta\theta)$. Taking the limit, i.e. as the nearby surfaces are brought arbitrarily close together, we find that

$$\phi_d = -\kappa \frac{\mathrm{d}z_*}{\mathrm{d}\theta} \langle |\nabla\theta|^2 \rangle_{z_*} \, . \tag{7}$$

Equation (7) is the main result of this paper. It states that the instantaneous diascalar flux across a given isoscalar surface is proportional to the square of the scalar gradient averaged over the given isoscalar surface, times the inverse of the scalar gradient with respect to the z_*-coordinate. Several features of this equation are worth noting. The first is that $\nabla\theta$ is the physical gradient defined with respect to spatial position. Second, (7) provides a definition of the mean gradient required to infer diffusive flux. The appropriate mean gradient is the derivative of θ with respect to the z_*-coordinate. Lastly, we note this result is valid for any scalar satisfying (1) with $\nabla \cdot \boldsymbol{u} = 0$. No dynamical assumptions are required.

The effective diffusivity in turbulent flows is very much larger than molecular. This results from the large strains which increase the surface area S, the gradients $|\nabla\theta|$ and thus ϕ_d. Our result can be interpreted in terms of these effects. Combining (2), (7) and (5) gives the magnification of isoscalar surface area in a turbulent flow:

$$\frac{A_S}{A} = -\frac{\mathrm{d}z_*}{\mathrm{d}\theta} \frac{\langle|\nabla\theta|^2\rangle_{z_*}}{\langle|\nabla\theta|\rangle_{z_*}} . \tag{8}$$

We see from figure 1 that

$$\frac{1}{\langle|\nabla\theta|\rangle_{z_*}} = \lim_{\Delta\theta\to 0} \frac{\langle\Delta n\rangle_{z_*}}{\Delta\theta} . \tag{9}$$

Since $\Delta V = -A\Delta z_* = A_S\langle\Delta n\rangle_{z_*}$, it follows that $\langle\Delta n\rangle_{z_*} = -(A/A_S)\Delta z_*$. Therefore,

$$\frac{1}{\langle|\nabla\theta|\rangle_{z_*}} = \lim_{\Delta\theta\to 0} -\frac{A}{A_S}\frac{\Delta z_*}{\Delta\theta} = -\frac{A}{A_S}\frac{\mathrm{d}z_*}{\mathrm{d}\theta}, \tag{10}$$

showing the average increase in scalar gradient resulting from the increase in isoscalar surface area. Substituting this into (8) yields

$$\left(\frac{A_S}{A}\right)^2 = \left(\frac{\mathrm{d}z_*}{\mathrm{d}\theta}\right)^2 \langle|\nabla\theta|^2\rangle_{z_*}. \tag{11}$$

The turbulent eddy diffusivity

$$K_\theta \equiv -\phi_d \frac{\mathrm{d}z_*}{\mathrm{d}\theta} = \kappa \left(\frac{A_S}{A}\right)^2 \tag{12}$$

is greatly increased relative to the molecular diffusivity when the isoscalar surface area A_S increases relative to A. This is a simple, geometrical interpretation of (7).

4. The z_*-coordinate and the reference state

In deriving (7) and (12) we made use of two properties of the coordinate z_*. In this section we display a mathematical definition of z_*, demonstrate that the two required properties are indeed satisfied and give a physical interpretation of the reference state $\theta(z_*)$.

The field $z_*(\boldsymbol{x}, t)$ is defined by

$$z_*(\boldsymbol{x}, t) = \frac{1}{A}\int H(\theta(\boldsymbol{x}', t) - \theta(\boldsymbol{x}, t))\, \mathrm{d}V' \tag{13}$$

where H is the Heaviside step function satisfying

$$H(x) = \begin{cases} 0, & x < 0 \\ 1/2, & x = 0 \\ 1, & x > 0 . \end{cases}$$

Equation (13) is a non-local coordinate transformation from three-dimensional space $\boldsymbol{x}$ to the one-dimensional space z_*. It is easily seen that (i) $z_*(\boldsymbol{x}_1, t) = z_*(\boldsymbol{x}_2, t)$ for all points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ on the same isoscalar surface; z_* is thus a unique function of the scalar θ. (ii) $Az_*(\boldsymbol{x},t)$ is the volume of fluid in V with θ greater than or equal to $\theta(\boldsymbol{x},t)$. $A|z_*(\boldsymbol{x}_2,t)-z_*(\boldsymbol{x}_1,t)|$ is equal to the volume of fluid with θ between the values $\theta(\boldsymbol{x}_1,t)$ and $\theta(\boldsymbol{x}_2,t)$. Thus z_* satisfies the two required properties. Though z_* is constant on an isoscalar surface, it is a normalized volume coordinate rather than an isoscalar coordinate. Diffusive mixing changes both the range of θ spanned by two z_*-surfaces as well as the volume of fluid enclosed by two isoscalar surfaces.

The variable z_* has dimensions of length and can be interpreted as an ordering of the fluid elements, with $z_*(\boldsymbol{x}_1,t) < z_*(\boldsymbol{x}_2,t)$ when $\theta(\boldsymbol{x}_1,t) > \theta(\boldsymbol{x}_2,t)$. When θ is taken to be fluid density ρ, $\rho(z_*)$ is the statically stable reference density profile obtained by repeatedly exchanging light parcels with heavier ones below. In this case z_* can be thought of as the vertical coordinate (increasing upward) after the restratification process has been completed. When θ is taken to be potential temperature, $\theta(z_*)$ is the reference temperature profile with z_* increasing downward. When θ is independent of density, the direction of increasing z_* has no physical significance. For randomly selected fluid parcels in V, $z_*(\theta)$ is proportional to the cumulative probability distribution function for θ.

4.1. *The evolution of* $\theta(z_*)$

The function $\theta(t,z_*)$ is monotonic in z_* at all times t. Given the advection-diffusion equation (1) and $\nabla\cdot\boldsymbol{u}=0$, an expression for the time rate of change of $\theta(t,z_*)$ can be developed. The result gives the rate at which water mass transformations occur in V. The time derivative is

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta(t,z_*) = \left\langle \frac{\mathrm{d}\theta}{\mathrm{d}t} \right\rangle_{z_*} + \frac{\mathrm{d}\theta}{\mathrm{d}z_*}\left\langle \frac{\mathrm{d}z_*}{\mathrm{d}t} \right\rangle_{z_*} \tag{14}$$

where the average $\langle\rangle_{z_*}$ is taken over the set of points $\boldsymbol{x}$ comprising an isoscalar surface at time t. It is shown in the Appendix that

$$\left\langle \frac{\mathrm{d}\theta}{\mathrm{d}t} \right\rangle_{z_*} = \kappa\langle\nabla^2\theta\rangle_{z_*} = -\frac{\partial}{\partial z_*}\phi_d(t,z_*) \tag{15}$$

and

$$\left\langle \frac{\mathrm{d}z_*}{\mathrm{d}t} \right\rangle_{z_*} = -\frac{1}{A}\oint_S H(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S \tag{16}$$

where $\boldsymbol{x}'$ is any point on the isoscalar surface corresponding to z_*. Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta(t,z_*) = -\frac{\partial}{\partial z_*}\phi_d(t,z_*) - \frac{\mathrm{d}\theta}{\mathrm{d}z_*}\frac{1}{A}\oint_S H(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S\ . \tag{17}$$

This second result extends (7) by relating the diascalar flux ϕ_d to the time rate of change of the reference state in open systems. Equation (17) shows that the reference state $\theta(t,z_*)$ evolves in time due to both diffusion across isoscalar surfaces and to advection of fluid into V and/or ΔV (see figure 1). For closed systems $\boldsymbol{u}\cdot\hat{\boldsymbol{n}}=0$ and $\theta(t,z_*)$ changes only due to diffusion or diascalar mixing. The coordinate z_* provides a reference frame in which the scalar fluxes associated with irreversible diascalar mixing are particularly simple.

4.2. *Available potential energy*

For $\theta=\rho$ the reference state $\rho(z_*)$ is closely related to the concept of available potential energy. As discussed in Winters *et al.* (1995) (hereafter referred to as

WLRD95), the potential energy associated with $\rho(t, z_*)$,

$$E_b = gA \int \rho(t, z_*) z_* \, \mathrm{d}z_* = g \int z_*(\boldsymbol{x}, t) \rho(\boldsymbol{x}, t) \, \mathrm{d}V \, , \tag{18}$$

is the minimum potential energy attainable through adiabatic restratification of the fluid. Here g is the gravitational acceleration. We call this the background potential energy E_b. The difference between the total potential energy

$$E_p = g \int z \rho(\boldsymbol{x}, t) \, \mathrm{d}V \tag{19}$$

and the background potential energy is the amount of energy released if complete adiabatic restratification were to occur. This is known as the available potential energy E_a. WLRD95 show that the transfer rate between kinetic energy and E_a is measured by the advective flux $g \int_V w\rho \mathrm{d}V$. This exchange is reversible and motions at all scales may contribute. WLRD95 also show that the rate at which diffusive mixing increases the background potential energy is $g \int \phi_d \, \mathrm{d}V$. This transfer is irreversible; mixing always increases E_b.

5. Diascalar mixing in the ocean thermocline

The theoretical basis for microstructure measurements of mixing in the stably stratified ocean thermocline is the Osborn–Cox (1972) model. This model is based on an analysis of the evolution equation for scalar variance. Our presentation of the Osborn–Cox (1972) model follows that of Gregg (1987).

The analysis begins by decomposing the scalar and velocity fields into mean $\langle () \rangle$ and fluctuating $()'$ components as in (3) and assuming that $\langle \theta' \rangle = \langle \boldsymbol{u}' \rangle = 0$. Using this decomposition, an equation for the temporal evolution of scalar variance can be obtained from (1):

$$\tfrac{1}{2}(\partial_t + \langle \boldsymbol{u} \rangle \cdot \nabla)\langle \theta'^2 \rangle + \langle \boldsymbol{u}'\theta' \rangle \cdot \nabla \langle \theta \rangle + \tfrac{1}{2}\nabla \cdot \langle \boldsymbol{u}'\theta'^2 \rangle = \kappa \langle \theta' \nabla^2 \theta' \rangle. \tag{20}$$

The physical interpretation of this equation and the numerical balance between terms depends not only on the underlying fluid dynamics but also on the averaging or filtering scheme $\langle \rangle$ used to separate the mean from the fluctuating fields.

To assess the rate of turbulent mixing in the ocean thermocline, Osborn & Cox (1972) took $\langle \rangle$ as a volume average and argued that the principal balance in (20) was between downgradient transport and variance dissipation as given by

$$\langle w'\theta' \rangle = -\kappa \left[\frac{\mathrm{d}}{\mathrm{d}z} \langle \theta \rangle \right]^{-1} \langle |\nabla \theta'|^2 \rangle \, . \tag{21}$$

Equation (21) relates scalar gradients, which can be measured using microstructure profilers, to an average advective flux. The relationship is approximate (see Gregg 1987; Davis 1994*b*; Holloway 1989).

While the right-hand sides of (21) and (7) are similar in form, they are not identical. Equation (7) is formulated on isoscalar surfaces while (21) is formulated in spatial coordinates. In (7), the quantity $|\nabla \theta|^2$ is averaged over isoscalar surfaces and the mean gradient is obtained from $\theta(z_*)$. This ensures that the right-hand side of (7) is always positive. In contrast, (21) requires that $|\nabla \theta|^2$ and the mean gradient be averaged at fixed depths. Note that (21) can be of either sign since $\mathrm{d}\theta/\mathrm{d}z$ is not, in general, of known sign.

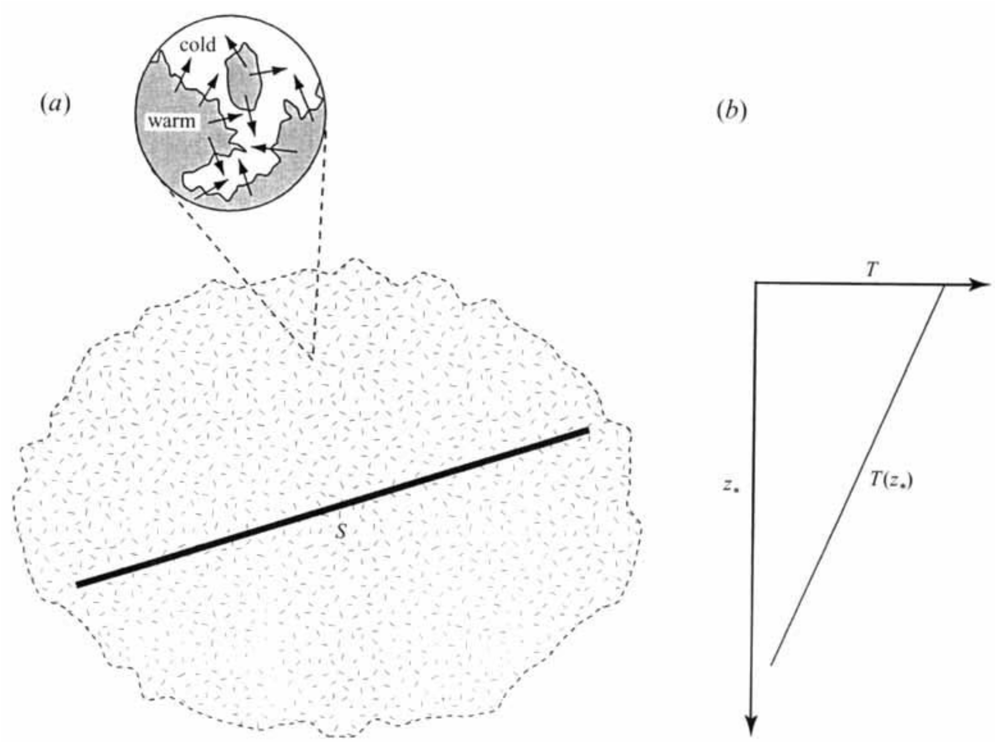

FIGURE 2. (*a*) Schematic of an isotropic, spatially homogeneous turbulent flow. Inset depicts the heat flux from warm to cold fluid at small scale. The advective flux across an arbitrarily oriented plane S and spatially defined mean gradients are equal to zero. (*b*) The reference temperature $T(z_*)$ increases monotonically and has a well-defined gradient.

The Osborn–Cox (1972) model is an approximate balance between advective and diffusive terms. This model has recently been re-examined by Davis (1994*b*) who argues on the basis of scaling arguments that it is difficult to justify the use of (21) for deducing fluxes appropriate for the oceanic general circulation. Taking $\theta = \rho$, WLRD95 showed that for closed systems, advective and diffusive fluxes balance, i.e.

$$\int \rho w \, \mathrm{d}V = \int \phi_d \, \mathrm{d}V, \tag{22}$$

if and only if the time rate of change of available potential energy E_a is equal to zero. A similar result without an energetic interpretation holds for arbitrary scalars θ. In this special case (21) and (7) give the same volume-integrated result.

6. Isotropic turbulence

In some circumstances ϕ_d and ϕ_a measure very different quantities. We now consider a flow in which the rate of fluid mixing is given by ϕ_d but not by ϕ_a. Consider a volume of fluid with uniformly distributed temperature fluctuations T'. Let the motion be specified by a spatially homogeneous, isotropic velocity field $\boldsymbol{u}'$. Figure 2*a* is a schematic of such a flow.

Let S denote an arbitrarily oriented plane with area A. There is no preferred direction to the flow, so the advective heat flux vanishes, i.e.

$$\int T'\boldsymbol{u}' \cdot \hat{n}\, \mathrm{d}S = 0. \tag{23}$$

Similarly, the mean temperature gradient in any direction is zero because the average temperature on S is equal to that on all nearby surfaces. The Osborn–Cox flux (see (21)) is not defined. For this flow, the temperature variance equation is not well approximated by (21). Rather, the primary balance is the decay of temperature fluctuations by diffusion:

$$\partial_t \langle T'^2 \rangle = -2\kappa \langle |\nabla T'|^2 \rangle \,. \tag{24}$$

Of course, this does not imply that no mixing occurs. Regions of hot and cold fluid exist at small scale and heat flows from the hot regions to the cold ones, warming the cold fluid and cooling the hot fluid. ϕ_d is the normalized integral of these fluxes over the highly convoluted and multiply connected isotherms. The reference profile $T(z_*)$ is well defined as shown schematically in figure 2*b*. Recall that $z_*(T_2) - z_*(T_1)$ is proportional to the volume of fluid with $T_1 \leqslant T \leqslant T_2$. The reference profile is linear if the temperature fluctuations are uniformly distributed. The squared gradient $|\nabla T|^2$ is strictly positive whereas the inverse gradient of the reference state $\mathrm{d}z_*/\mathrm{d}T$ is strictly negative as long as there are temperature fluctuations in the fluid. Thus, ϕ_d is always positive and measures the rate at which hot and cold fluid mix to form warm fluid.

7. A recipe for estimating ϕ_d from profile data

As written, (7) and (21) require total knowledge of the θ-field. Although this is fine for direct numerical simulations, microstructure data are often obtained in oceans and lakes along vertical profiles. We now give a recipe for processing such data, which converges to ϕ_d as the number of profiles increases. We assume that N profiles are obtained from throughout the volume V. As N becomes large, we assume that V becomes well sampled. We do not explicitly address sampling or instrumental issues here.

Let each profile be measured at equally spaced depths z^j, spanning the range z_0 to z_1, for $j = 1, 2, ...M$ with $z^m > z^n$ for $m > n$. Let $\theta_i(z^j)$ and $|\nabla\theta|^2_i(z^j)$ for $i = 1, 2, ...N$ be the measurements at these depths. The N-profile estimate $\phi_d{}^N(\theta)$ of the diascalar flux across the isoscalar surface θ is obtained as follows.

(i) Sort each profile in descending θ order. Both θ and $|\nabla\theta|^2$ are to be sorted together. This step converts the set of profiles $\theta_i(z^j)$ and $|\nabla\theta|^2_i(z^j)$ to $\theta_i(z_T{}^j)$ and $|\nabla\theta|^2_i(z_T{}^j)$ where $z_T{}^j$ is the set of equally spaced sorted depths. The profiles $\theta_i(z_T{}^j)$ increase monotonically with depth. The procedure here is commonly known as 'Thorpe sorting' after Thorpe (1977).

(ii) The uniformly sampled profiles $\theta_i(z_T{}^j)$ and $|\nabla\theta|^2_i(z_T{}^j)$ can also be thought of as non-uniformly sampled profiles $z_{T\,i}(\theta^j)$ and $|\nabla\theta|^2_i(\theta^j)$. Interpolate these data onto a set of equally spaced scalar values.

(iii) Form isoscalar averages:

$$\langle|\nabla\theta|^2\rangle^N(\theta^j) = \frac{1}{N}\sum_{i=1}^{N} |\nabla\theta|^2_i(\theta^j),$$

$$\langle z_T \rangle^N(\theta^j) = \frac{1}{N}\sum_{i=1}^{N} z_{Ti}(\theta^j).$$

Note that in the limit $N \to \infty$, $\langle z_T \rangle^N(\theta) \to z_*(\theta)$ and $\langle |\nabla\theta|^2 \rangle^N$ converges to the isoscalar average of $|\nabla\theta|^2$.

(iv) Compute the N-profile estimate of the reference state gradient $(\mathrm{d}z_*/\mathrm{d}\theta)^N$ by computing the discrete derivative of $\langle z_T \rangle^N(\theta)$.

(v) The N-profile estimate of the diascalar flux across the isoscalar surface θ^j is given by

$$\phi_d{}^N(\theta^j) = \kappa\left(\frac{\mathrm{d}z_*}{\mathrm{d}\theta}\right)^N(\theta^j)\langle |\nabla\theta|^2 \rangle^N(\theta^j).$$

In the limit that N profiles densely sample the fluid at a fixed time, this procedure yields the exact result (7) for each isoscalar surface sampled. The analysis presented here provides a formal justification of the common practice of Thorpe-sorting scalar profiles to obtain stable mean gradients (Thorpe 1977; Dillon & Park 1987) with the additional steps (ii) and (iii) of isoscalar averaging.

Of course in practice, one can sample neither densely nor synoptically. Estimation errors resulting from sampling will depend on instrument response and resolution, the degree of isotropy of small-scale gradients, the spatial distribution of turbulent mixing, and the interpolation and differentiation schemes employed. An analysis of sampling and instrumentation errors is beyond the intended scope of this paper. However, the problems are common to both our procedure and that of Osborn–Cox (1972). Often, isoscalar averages converge faster than depth averages as they filter out variability due to internal waves and other adiabatic motions. We therefore expect that (7) will converge more rapidly than (21).

8. Direct numerical simulations

We now illustrate the application of these ideas to calculating mixing rates in direct numerical simulations. Using (7), (13) and (14), the time history and the instantaneous rate of change of the reference state can be determined. This procedure is easily carried out using standard sorting algorithms and can be performed independent of the magnitude and/or sign of reversible advective fluxes. We calculate the diapycnal flux ϕ_d associated with a low-Reynolds-number, shear-driven mixing layer. Based on the initial vorticity thickness of the layer, the Reynolds, Prandtl and Richardson numbers of the simulation are 600, 1, and 0.167 respectively. The details of numerical simulation and a discussion of the energetics, emphasizing the evolution of available and background potential energy, are given in WLRD95.

Figure 3 shows a time sequence of isopycnals in a fixed vertical plane for a shear layer initially located at mid-depth. By $t = 2$ (all times in buoyancy periods) a shear instability has reached finite amplitude. The classic core and braid structures associated with stratified shear instabilities (see Koop & Browand 1979) are readily apparent in the figure. The finite-amplitude billows are significantly distorted by $t = 4$ and by $t = 7$ the perturbed flow is nearly quiescent. The cumulative effect of diapycnal mixing results in a substantially reduced density gradient.

Figure 4 shows the evolution of $\rho(t, z_*)$, the reference state. Transformation of the density field from $\boldsymbol{x}$ to z_* converts a complicated three-dimensional field to a simple one-dimensional profile at each time. There is a clear physical interpretation of this

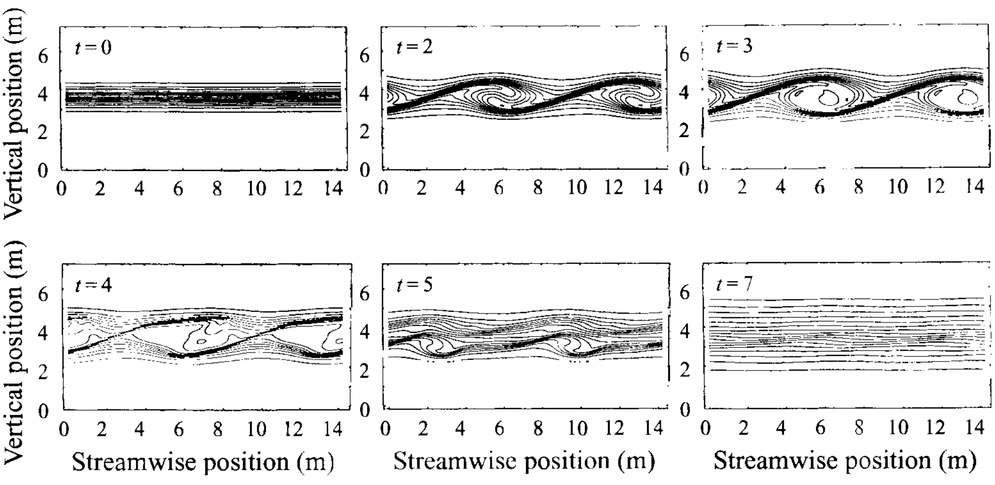

FIGURE 3. Dimensionless density contours in a single vertical plane from the numerical simulation of WLRD95. The density field evolves from an initially undisturbed state. A finite-amplitude shear instability distorts the isopycnals, enhancing diffusive mixing. By $t = 7$ buoyancy periods, vertical displacements of the isopycnals are slight and diapycnal mixing has substantially reduced the vertical density gradient of the layer.

state. Because boundary fluxes are zero in this simulation, changes in $\rho(t, z_*)$ arise solely from diapycnal mixing as given by (17). In the absence of mixing, isopycnals would remain flat. As the flow evolves in time, and mixes, these isopycnals spread and the volume of fluid between two given isopycnals changes. This change is given by the z_*-gradient of ϕ_d. The flux ϕ_d can be calculated directly via (7) or from the rate of spreading of the isopycnals. Shaded contours of ϕ_d are shown in the figure. They show the mixing rate as a function of time. In this flow, the most rapid mixing occurs at about $t = 3$ after the cores of the Kelvin–Helmholtz billows have become well developed but before they collapse. WLRD95 (their figure 4*b*) show that volume averages of ϕ_d and ϕ_a, denoted by Φ_d and Φ_z respectively in WLRD95, become equal when averaged over the lifetime of the mixing event, but have very different time histories. At times, the volume-averaged ϕ_a is negative, i.e. the buoyancy flux is countergradient. Regardless, ϕ_d, and thus the mixing rate, is always positive. Winters & D'Asaro (1994) analyse a simulation of internal wave breaking at a critical level and show that, for this flow, nearly all the mixing occurs while ϕ_a is countergradient.

9. Discussion

We believe that the analyses presented here and in WLRD95 provide a framework for diagnosing mixing rates and for separating diffusive and advective processes for a broad range of fluid flows. By not defining mixing in terms of a Reynolds-averaged flux, it is readily apparent that mixing can occur even if these fluxes are countergradient. By not requiring specific balances in the scalar variance equation, these techniques can be used to infer mixing rates for flows which are unsteady, inhomogeneous and/or strongly advective. For example, in an oceanographic context the rate of water mass transformation in unsteady intrusions or nearly well-mixed layers can be estimated from microstructure measurements. For density-

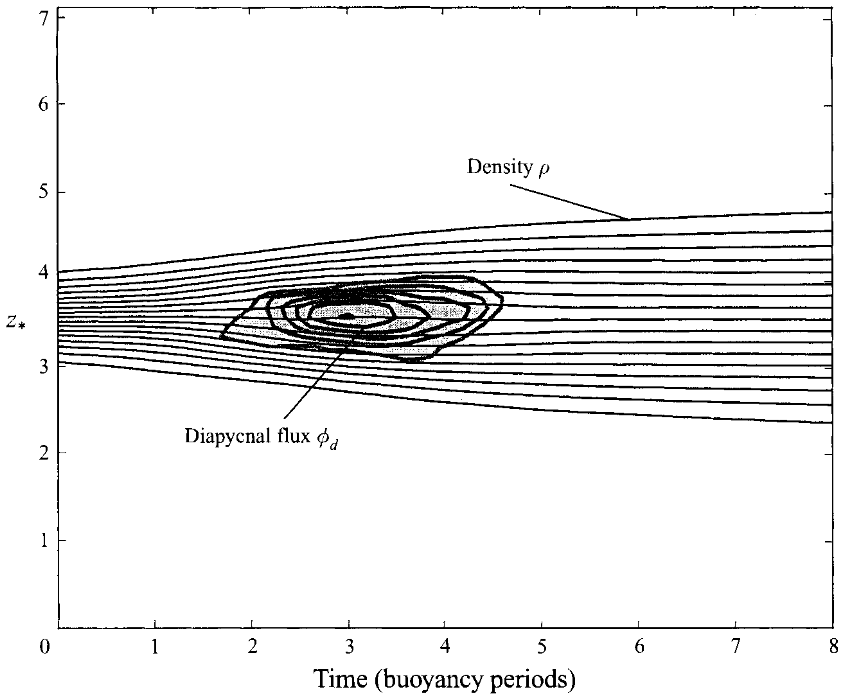

FIGURE 4. Contours of the reference state $\rho(t, z_*)$, the state of minimal potential energy attainable through adiabatic redistribution of fluid elements. The time rate of change of the reference state is completely determined by the diapycnal flux ϕ_d, shown in shaded contours.

stratified flows, this analysis extends the concept of available potential energy to open systems.

Our analysis assumes incompressible or Boussinesq flow. Thus, volume is conserved in the transformation defining the reference state $\theta(t, z_*)$. To extend this framework to compressible fluids, a new transformation that conserves mass rather than volume is needed. Since the ocean and atmosphere are only approximately Boussinesq, such an extension is probably necessary to make this analysis exact for large-scale flows in the ocean and atmosphere.

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Appendix A

It remains to be shown that

$$\kappa \langle \nabla^2 \theta \rangle_{z_*} = -\frac{\partial}{\partial z_*} \phi_d(t, z_*) \qquad \text{(A 1)}$$

and that

$$\left\langle \frac{\mathrm{d}z_*}{\mathrm{d}t} \right\rangle_{z_*} = -\frac{1}{A}\oint_S H(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\boldsymbol{u}\cdot\hat{n}\,\mathrm{d}S \qquad \text{(A 2)}$$

where $\langle\rangle_{z_*}$ indicates averaging over the isoscalar surface $\theta(z_*)$.

A.1.

To show (A 1), we let $\kappa\langle\nabla^2\theta\rangle_{z_*} = -(\partial/\partial z_*)\mathscr{F}$ and show that $\mathscr{F}(t,z_*) = \phi_d$. From (A 1)

$$\mathscr{F}(t,z_*) = -\kappa\int_0^{z_*}\langle\nabla^2\theta\rangle_{z_*}(t,z_*')\,\mathrm{d}z_*'. \qquad \text{(A 3)}$$

Let z_0 and z_1 be the z_* values corresponding to two isoscalar surfaces and let ΔV be the volume of fluid between these two surfaces. Define $\bar{\mathscr{F}}$ as the volume average of $\mathscr{F}$ in ΔV:

$$\bar{\mathscr{F}} = \frac{A}{\Delta V}\int_{z_0}^{z_1}\mathscr{F}\,\mathrm{d}z_*\,. \qquad \text{(A 4)}$$

Noting that $\nabla z_* = (\mathrm{d}z_*/\mathrm{d}\theta)\nabla\theta$ and integrating by parts, we find that

$$\bar{\mathscr{F}} = \frac{A}{\Delta V}(z_1\mathscr{F}(t,z_1) - z_0\mathscr{F}(t,z_0)) + \frac{A}{\Delta V}\kappa\int_{z_0}^{z_1}\nabla\cdot z_*\nabla\theta\,\mathrm{d}z_*$$
$$-\frac{A}{\Delta V}\kappa\int_{z_0}^{z_1}\frac{\mathrm{d}z_*}{\mathrm{d}\theta}|\nabla\theta|^2\,\mathrm{d}z_*\,. \qquad \text{(A 5)}$$

As the two surfaces are brought together, i.e. in the limit that z_0 and z_1 approach the same value z_*, the first two terms on the right of (A5) vanish. The third term survives and takes the value $-(\mathrm{d}z_*/\mathrm{d}\theta)\langle|\nabla\theta|^2\rangle_{z_*}$. Thus

$$\lim_{z_0,z_1\to z_*}\bar{\mathscr{F}} = \mathscr{F}(t,z_*) = -\kappa\frac{\mathrm{d}z_*}{\mathrm{d}\theta}\langle|\nabla\theta|^2\rangle_{z_*} = \phi_d(t,z_*) \qquad \text{(A 6)}$$

and (A 1) is established.

A.2.

We now show (A 2). Let $\boldsymbol{x}'$ be a Lagrangian label that uniquely specifies a single fluid element. Here we take $\boldsymbol{x}'$ to be the position of a given element at some time t. Let θ' be the scalar value associated with the $\boldsymbol{x}'$ element at time t. The time rate of change of $z_*(\boldsymbol{x}',t)$ can be obtained by differentiating (13). We obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}z_*(\boldsymbol{x}',t) = \frac{1}{A}\int_V \delta(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\left\{-\boldsymbol{u}\cdot\nabla\theta + \kappa\nabla^2\theta(\boldsymbol{x},t) - \kappa\nabla^2\theta(\boldsymbol{x}',t)\right\}\mathrm{d}V, \quad \text{(A 7)}$$

where $\delta(x-a)$ is the Dirac delta function. For convenience, we rewrite this expression as the sum of two integrals, I_1 and I_2, where

$$I_1(\boldsymbol{x}',t) = \frac{\kappa}{A}\int_V \delta(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\left\{\nabla^2\theta(\boldsymbol{x},t) - \nabla^2\theta(\boldsymbol{x}',t)\right\}\mathrm{d}V \qquad \text{(A 8)}$$

and

$$I_2(\boldsymbol{x}',t) = -\frac{1}{A}\int_V \delta(\,\theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\,)\{\boldsymbol{u}\cdot\nabla\theta\}\,\mathrm{d}V. \qquad \text{(A 9)}$$

A.2.1. $\langle I_1\rangle_{z_*}$

We now show that the isopycnal average of I_1, i.e. the average over the set of labels corresponding to the fluid elements defining an isoscalar surface at time t, is equal to zero. Let $J = (\partial(x,y,z))/(\partial(\theta,p,q))$ be the Jacobian of the transformation from (x,y,z) to (θ,p,q). I_1 can be written as

$$I_1 = \frac{\kappa}{A}\int\int\int \delta(\ \theta-\theta'\ )\left\{\nabla^2\theta(\theta,p,q)-\nabla^2\theta(\theta',p',q')\right\}J(\theta,p,q)\,\mathrm{d}\theta\,\mathrm{d}p\,\mathrm{d}q. \qquad \text{(A 10)}$$

Integrating with respect to θ gives

$$I_1 = \int\int \nabla^2\theta(\theta',p,q)J(\theta',p,q)\ \mathrm{d}p\,\mathrm{d}q - \nabla^2\theta(\theta',p',q')\int\int J(\theta',p,q)\ \mathrm{d}p\,\mathrm{d}q\ . \qquad \text{(A 11)}$$

The sum of contributions from all points $\boldsymbol{x}'$ on the θ' isoscalar surface is obtained by integrating the expression

$$\int I_1 J(\theta',p',q')\ \mathrm{d}p'\mathrm{d}q'\ . \qquad \text{(A 12)}$$

This gives

$$\begin{aligned}\int I_1 J(\theta',p',q')\ \mathrm{d}p'\mathrm{d}q' &= \int\int\int\int \nabla^2\theta(\theta',p,q)J(\theta',p,q)J(\theta',p',q')\ \mathrm{d}p\,\mathrm{d}q\,\mathrm{d}p'\,\mathrm{d}q' \\ &\quad - \int\int\int\int \nabla^2\theta(\theta',p',q')J(\theta',p,q)J(\theta',p',q')\ \mathrm{d}p\,\mathrm{d}q\,\mathrm{d}p'\,\mathrm{d}q' \qquad \text{(A 13)}\end{aligned}$$

which can be reduced to

$$\begin{aligned}&\int\int I_1 J(\theta',p',q')\ \mathrm{d}p'\mathrm{d}q' \\ &= \left(\int\int \nabla^2\theta(\theta',p,q)J(\theta',p,q)\ \mathrm{d}p\,\mathrm{d}q\right)\int\int J(\theta',p',q')\ \mathrm{d}p'\mathrm{d}q' \\ &\quad - \left(\int\int \nabla^2\theta(\theta',p',q')J(\theta',p',q')\ \mathrm{d}p'\mathrm{d}q'\right)\int\int J(\theta',p,q)\ \mathrm{d}p\,\mathrm{d}q \\ &= 0. \qquad \text{(A 14)}\end{aligned}$$

Thus, $\langle I_1\rangle_{z_*} = 0$.

A.2.2. $\langle I_2\rangle_{z_*}$

Now consider I_2. Since

$$\nabla H(\ \theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\ ) = \delta(\ \theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\ )\nabla\theta, \qquad \text{(A 15)}$$

(A 9) can be written as

$$I_2(\boldsymbol{x}',t) = -\frac{1}{A}\int_V \boldsymbol{u}\cdot\nabla H(\ \theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\ )\mathrm{d}V. \qquad \text{(A 16)}$$

For incompressible flows $\nabla\cdot\boldsymbol{u}=0$ and so $\boldsymbol{u}\cdot\nabla H = \nabla\cdot H\boldsymbol{u}$. Equation (A 16) can thus be rewritten as a surface integral,

$$I_2(\boldsymbol{x}',t) = -\frac{1}{A}\oint_S H(\ \theta(\boldsymbol{x},t)-\theta(\boldsymbol{x}',t)\ )\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\ \mathrm{d}S, \qquad \text{(A 17)}$$

where S is the surface enclosing the volume V and $\hat{\boldsymbol{n}}$ is the outward facing unit vector normal to S. Note that $I_2(\boldsymbol{x}_i',t) = I_2(\boldsymbol{x}_j',t)$ as long as the labels $\boldsymbol{x}_i'$ and $\boldsymbol{x}_j'$ correspond to elements on the same isoscalar surface. Thus, $I_2(\boldsymbol{x}',t)$ is equal to the isopycnally averaged value. The value of I_2 at time t is thus uniquely determined by specifying a scalar value θ or the corresponding value $z_*(\theta)$. Since $\langle \mathrm{d}z_*/\mathrm{d}t\rangle_{z_*} = \langle I_1\rangle_{z_*} + \langle I_2\rangle_{z_*}$ and $\langle I_1\rangle_{z_*} = 0$, (A 2) is established.

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