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Available potential energy and mixing in density-stratified fluids

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A conceptual framework for analysing the energetics of density-stratified Boussinesq fluid flows is discussed. The concept of gravitational available potential energy is used to formulate an energy budget in which the evolution of the background potential energy, i.e. the minimum potential energy attainable through adiabatic motions, can be explicitly examined. For closed systems, the background potential energy can change only due to diabatic processes. The rate of change of background potential energy is proportional to the molecular diffusivity. Changes in the background potential energy provide a direct measure of the potential energy changes due to irreversible diapycnal mixing. For open systems, background potential energy can also change due to boundary fluxes, which can be explicitly measured. The analysis is particularly appropriate for evaluation of diabatic mixing rates in numerical simulations of turbulent flows. The energetics of a shear driven mixing layer is used to illustrate the analysis.

1. Introduction

Density-stratified flows are an interesting and dynamically rich class of fluid motion. Because they occur so frequently in nature and in such a wide range of settings, these flows have been extensively studied from a variety of viewpoints. For turbulent flows, it is tempting to think of stratification primarily as a stabilizing force and hence regard density-stratified turbulence as a damped, less-energetic cousin of turbulence in a homogeneous fluid. This viewpoint is overly simplistic, as gravitational forces in an inhomogeneous fluid admit additional modes of motion, e.g. internal gravity waves, adding complexity to the flow dynamics. Fluid displacements result in buoyant restoring forces, providing a pathway for conversion between kinetic and potential energy and the excitation of internal waves. Complicating the dynamics further, internal waves allow energy to be propagated into or away from localized regions of interest. These effects can play significant roles in the energy budgets of these flows. This is especially true in oceanic and atmospheric flows at small scales, where turbulence is often initiated and driven by the breakdown of wave-like flows.

In this paper, we present a conceptual framework that allows the energetics of density-stratified fluid flow to be addressed in a unified and systematic manner. Our discussion is limited to nearly incompressible fluids, in the Boussinesq sense. The analysis presented is based on the simple notion that, for closed fluid systems, only irreversible, diabatic processes can change the probability density function (p.d.f.) of density. We relate changes in the p.d.f. of density to changes in available and background potential energy of the fluid (see e.g. Lorenz 1955) and to the energetics of irreversible diapycnal mixing. Though originally formulated to describe large-scale atmospheric flows, the concept of available potential energy has also been applied in the oceans, both at large scales (Oort *et al.* 1989) and small scales (Dillon & Park, 1987). Oceanographers have long appreciated the intrinsic relationship between available potential energy and turbulent mixing and dissipation. Sorting vertical temperature profiles (Thorpe 1977) and relating the potential energy of overturns to mixing (Dillon & Park 1987) are one-dimensional analogues of the analysis discussed here.

The methodology presented is particularly useful for analysing numerical simulations of density-stratified flows. The analysis is quite general; it can be applied equally well to either direct numerical simulations (DNS) or large-eddy simulations (LES), to spatially homogeneous or localized turbulence, to steady-state or to transient flows. The analysis allows the energetics of density-stratified flows to be partitioned between diabatic and adiabatic processes. A direct consequence of this partitioning is that long time averaging is not required to determine the diabatic flux rates. Our original motivation was to develop an analysis that would allow instantaneous rates of mixing and dissipation to be quantified for a relatively wide class of simulated flows and to correlate the evolution of these rates with the evolution of the easily observable features of the flow.

2. Molecular processes

In order to treat the energetics of density-stratified flow, it is important to utilize the concept of available potential energy discussed by Lorenz (1955). The available potential energy of a fluid is the energy released if the fluid were to be adiabatically rearranged to the state of minimum potential energy. The distinction between adiabatic processes and diabatic processes is central to the analysis. In order to extend the definition to include oceanographic as well as atmospheric flows, we generalize the term adiabatic to describe a process in which there is no heat or molecular mass transfer, and define a diabatic process as one that is not adiabatic. In this discussion, we neglect radiative heat transfer, which could easily be included, and consider only the molecular diffusion of density in Boussinesq fluids. Though our approach can easily be generalized, we make no attempt to distinguish between the differing diffusion rates of, for example, salt and heat, nor do we address issues relating to nonlinearities in the equation of state.

Because dissipation and diffusion rates for turbulent flows are orders of magnitude greater than for laminar flows, it is natural to use kinetic energy dissipation and diapycnal mixing rates to characterize turbulent flows. The kinetic energy dissipation rate is given per unit volume as (see e.g. Landau & Lifshitz 1987)

$$\epsilon' = \tau_{ij}\frac{\partial u_i}{\partial x_j}, \tag{1}$$

where u_i are the components of the velocity vector $\boldsymbol{u}$, τ_{ij} are the elements of the viscous stress tensor $\boldsymbol{\tau}$, and x_j are the spatial coordinates. For density-stratified turbulence, ϵ' gives only a partial description of the molecular processes. Molecular diffusion acts to smooth density gradients, changing the potential energy. Diffusive mixing provides an alternative pathway for energy transfer not available to the flow of homogeneous fluids. In our analysis, we will make a careful distinction between changes in total potential energy and the energy expended in diapycnal mixing. This distinction is motivated in part by the intrinsic importance of molecular mixing for a wide class of turbulent flows. Molecular mixing rates are important in an oceanographic context, for example, because they influence the thermodynamic balance on much larger scales (see e.g. Gregg 1987). Characterization of density-stratified turbulence in terms of the rates at which molecular processes occur, i.e. dissipation and diapycnal mixing, is fundamental and enhances our understanding of the dynamics of these flows.

Interestingly, analysis of the evolution equation for potential energy (see §4) does not allow the energetics of reversible processes to be readily distinguished from the energetics of irreversible fluid mixing. The energetics of mixing is most often discussed in terms of the buoyancy flux $-g\overline{\rho w}$ where g is the acceleration due to gravity, ρ is the density, w is the vertical velocity and the overbar represents a spatial and/or temporal averaging operator. The averaging operator is assumed to 'isolate' the turbulent component of the flow. For stratified turbulence in the presence of energetic internal waves, it is very difficult in practice to ensure that the averaging procedure yields an estimate that is free from contamination by adiabatic processes. In general, both spatial and long-time averages are required. Analyses of the energetics of transient mixing events based on this approach are intrinsically problematic. We overcome this difficulty by explicitly separating adiabatic and non-adiabatic changes in potential energy.

3. Partitioning the potential energy

We now address the following question. If we knew the initial state of a fluid flow, as well as its state at some arbitrary later time, how could we measure the energy expended in diabatic mixing that has occurred in the interim? For convenience, we assume that the state of the flow is known within a fixed volume V and that no heat or mass fluxes are allowed at the boundaries. Simply comparing total potential energy of the fluid between the two states is insufficient. As shown in §4, adiabatic processes can change the potential energy of the fluid irrespective of any diffusive mixing. Adiabatic processes transfer energy reversibly between kinetic and potential forms at a rate given by the volume-integrated buoyancy flux. During an arbitrary time interval, adiabatic processes may increase or decrease the total potential energy at a rate that can be either small or large in comparison with the irreversible increase associated with fluid mixing. Allowing the time interval between the two states to become arbitrarily small, we can see that what we really wish to address is the instantaneous rate of change of potential energy due to diapycnal mixing.

To properly quantify the energetics of mixing, we need to be able to explicitly partition the changes in potential energy due to diabatic mixing from changes due to adiabatic processes. This partitioning is possible using Lorenz's concept of available potential energy. The potential energy of a fluid is defined as

$$E_p = g\int_V \rho z \, \mathrm{d}V, \tag{2}$$

where ρ is the density of the fluid and z is the vertical (positive upward) spatial coordinate.

The background potential energy E_b is defined as the minimum potential energy attainable through an adiabatic redistribution of ρ. Denoting the redistributed density field $\rho(z_*)$, where $z_*(\boldsymbol{x}, t)$ gives the vertical position in the reference state of the fluid parcel at position $(\boldsymbol{x}, t)$, we have

$$E_b = g \int_V \rho z_*(\boldsymbol{x}, t) \, \mathrm{d}V. \tag{3}$$

If we think a fluid as an ensemble of macroscopic fluid elements, it is apparent that the background state $\rho(z_*)$ depends only on the p.d.f. of density over the ensemble of elements and is independent of the spatial distribution of the elements.

Since the available potential energy E_a is defined as the potential energy released in an adiabatic transition from $\rho(\boldsymbol{x}, t)$ to $\rho(z_*)$, it follows that

$$E_a = g \int_V \rho(z - z_*) \, \mathrm{d}V \tag{4}$$

and that $E_p = E_a + E_b$. For a closed system, i.e. one in which no heat or mass transfers are allowed at the boundaries, adiabatic processes result in spatial redistribution of the density field ρ and changes in the total potential energy E_p. Adiabatic processes do not change the p.d.f. of density and thus do not alter the background state $\rho(z_*)$. For closed systems, only diabatic mixing can produce changes in the background state $\rho(z_*)$. Furthermore, changes in the potential energy of the background state, E_b, are a direct measure of the energy expended in mixing the fluid. In this paper, we will discuss the energetics associated with changes in reference state induced by diapycnal mixing. In a related paper (Winters & D'Asaro 1995), an evolution equation for the reference state is developed. This leads naturally to an expression for the instantaneous diapycnal flux, which can then be spatially integrated to recover the energetics results discussed here.

The relationship between the reference state of minimum potential energy and diapycnal mixing can be illustrated with a simple example. We consider a density-stratified Boussinesq fluid with prescribed velocity and density profiles that are known to be unstable to Kelvin–Helmholtz (KH) shear instabilities. (The initial profiles and the parameters governing the flow are given in §5.) Figure 1(*a*) shows the initial p.d.f. of density, taken over discrete volume elements within the three-dimensional computational domain V. Also shown is the corresponding reference profile obtained by sorting the volume elements by density.

The initial state was allowed to evolve, resulting in the formation of finite-amplitude KH billows at the interface. Figure 1(*b*) shows the density contours obtained from a single vertical-streamwise plane after three buoyancy periods. Examining the density contours, it is clear that the shear instability acts to produce fluid with more uniform properties, i.e. a mixed layer. The extent to which this process has occurred is evident in the corresponding p.d.f. shown in figure 1(*c*). The excess of intermediate density values, coupled with deficits of both heavier and lighter values is an unambiguous signature of diabatic mixing. Changes in the p.d.f. of density indicate changes in the reference state $\rho(z_*)$, as shown in figure 1(*c*), and the background potential energy E_b.

For closed systems, only molecular mixing can alter the density p.d.f., the background state $\rho(z_*)$, and the background potential energy. For these flows, E_b is a robust indicator of the energetics associated with diabatic mixing. Open systems, i.e. those in which boundary fluxes are permitted, are more difficult to analyse. In open systems, changes in the background state can also result from advective surface fluxes

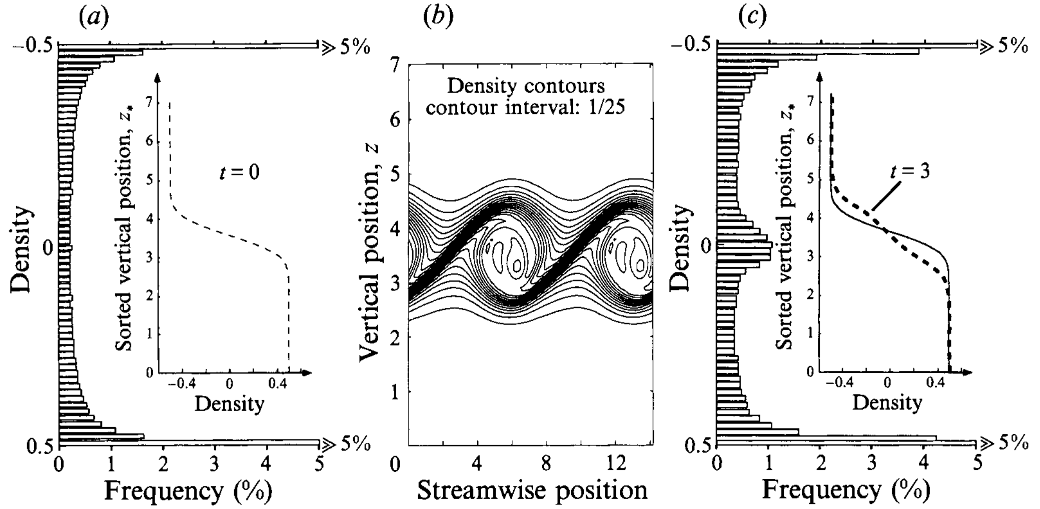

FIGURE 1. (*a*) The initial p.d.f. of density and the corresponding reference profile. (*b*) Density contours from a direct numerical simulation of a stably stratified mixing layer. (*c*) The p.d.f. of density and the reference profile after the fluid has become partially mixed.

even in the absence of molecular mixing. In general, these fluxes alter both available and background potential energy. For example, one can imagine mass-conserving horizontal fluxes that change E_a without changing E_b. A vertical mass flux across a horizontal surface, however, can produce changes in E_b without altering E_a if the fluid is statically stable near the surface.

4. Evolution of the potential energy

These ideas can be made more precise by defining the energetic quantities of interest and deriving the corresponding evolution equations. The development is generalized to allow treatment of open systems in which heat and mass are advected and/or diffused across bounding surfaces. The equations of motion for a Boussinesq fluid (see e.g. Drazin & Reid 1981; Pedlosky 1979) are

$$\rho_0\left[\frac{\partial}{\partial t}\boldsymbol{u}+\boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\right] = -\boldsymbol{\nabla}p+\rho\boldsymbol{g}+\boldsymbol{\nabla}\cdot\boldsymbol{\tau}, \tag{5}$$

$$\frac{\partial}{\partial t}\rho+\boldsymbol{u}\cdot\boldsymbol{\nabla}\rho = \kappa\nabla^2\rho, \tag{6}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0, \tag{7}$$

where ρ is the Boussinesq density, ρ_0 is a constant reference density, p is the pressure, t represents time, and $\boldsymbol{\nabla}\cdot\boldsymbol{\tau}$ is the divergence of the viscous stress tensor τ_{ij}.

Within a fixed volume V, the potential energy E_p is given in (2) and the kinetic energy E_k is defined as

$$E_k = \frac{\rho_0}{2}\int_V (u^2+v^2+w^2)\,\mathrm{d}V. \tag{8}$$

In the following development, we consider only cylindrical domains V, with cross-sectional area A, and horizontal upper and lower bounding surfaces.

An equation for the time rate of change of kinetic energy can be derived from (8) using (5) (see e.g. Gill 1982; Landau & Lifshitz 1987; Bird, Stewart & Lightfoot 1960):

$$\frac{\mathrm{d}}{\mathrm{d}t}E_k = -\oint_S [p\boldsymbol{u}+\rho_0\boldsymbol{u}\tfrac{1}{2}(u^2+v^2+w^2)-\boldsymbol{u}\cdot\boldsymbol{\tau}]\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S-\int_V g\rho w\,\mathrm{d}V-\epsilon. \tag{9}$$

Here $\boldsymbol{u}\cdot\boldsymbol{\tau}$ is the vector with components $u_i\tau_{ij}$, $\hat{\boldsymbol{n}}$ denotes the unit vector normal to the surface S enclosing V, and ϵ is the volume integral of ϵ' defined in (1). An evolution equation for potential energy can also be developed using (2), (6) and (7):

$$\frac{\mathrm{d}}{\mathrm{d}t}E_p = -\oint_S gz\rho\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S+\int_V g\rho w\,\mathrm{d}V+\kappa g\oint_S z\nabla\rho\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S-\kappa gA(\bar{\rho}_{top}-\bar{\rho}_{bottom}). \tag{10}$$

The first term on the right-hand side of (9) gives the rate change of kinetic energy resulting from pressure work, advection, and viscous diffusion of energy across the bounding surface S. The second term gives the reversible rate of exchange with potential energy (due to buoyancy flux), while the third term gives the irreversible rate of conversion from mechanical to internal energy through viscous dissipation. Similarly, the first two terms on the right-hand side of (10) show that reversible changes in potential energy result from advective fluxes across S or through exchange with kinetic energy via the buoyancy flux. The third term gives the rate of change due to diffusive mass fluxes across S while the fourth term is the Boussinesq form of the conversion rate from internal to potential energy. The overbars indicate spatial averaging over the fixed horizontal area A.

We would like to explicitly partition those changes in potential energy resulting from diabatic processes from those due to adiabatic processes. To accomplish this, we develop separate evolution equations for the background and available potential energies. Let $z_*(\boldsymbol{x},t)$ be the reference position (in the state of minimum gravitational potential energy) of the infinitesimal element at $(\boldsymbol{x},t)$ with density $\rho(\boldsymbol{x},t)$. Since Boussinesq fluid elements retain their density under adiabatic rearrangement, we can write

$$z_*(\boldsymbol{x},t) = \frac{1}{A}\int H(\rho(\boldsymbol{x}',t)-\rho(\boldsymbol{x},t))\,\mathrm{d}V', \tag{11}$$

where H is the Heaviside step function satisfying

$$H(\rho(\boldsymbol{x},t)-\rho(\boldsymbol{x}_0,t)) = \begin{cases} 0, & \rho(\boldsymbol{x},t) < \rho(\boldsymbol{x}_0,t) \\ \frac{1}{2}, & \rho(\boldsymbol{x},t) = \rho(\boldsymbol{x}_0,t) \\ 1, & \rho(\boldsymbol{x},t) > \rho(\boldsymbol{x}_0,t). \end{cases}$$

The variable z_* has dimensions of length and can be interpreted as a statically stable ordering of the fluid elements, with $z_*(\boldsymbol{x}_1,t) < z_*(\boldsymbol{x}_2,t)$ when $\rho(\boldsymbol{x}_1,t) > \rho(\boldsymbol{x}_2,t)$. The function $z_*(\boldsymbol{x},t)$ has the same value at all points on a given isopycnal surface and so z_* can be considered a unique function of density ρ.

The time rate of change of background potential energy can then be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \frac{\mathrm{d}}{\mathrm{d}t}\int_V gz_*(\boldsymbol{x},t)\rho(\boldsymbol{x},t)\,\mathrm{d}V. \tag{12}$$

Differentiating, noting that the integration volume is fixed in time, gives

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \int_V g\left[z_*\frac{\partial\rho}{\partial t}+\rho\frac{\partial z_*}{\partial t}\right]\mathrm{d}V. \tag{13}$$

Using (11), the second term in (13) can be shown to be equal to zero when integrated over V. Substituting for $\partial\rho/\partial t$ using (6), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \int_V g z_*\{-\boldsymbol{u}\cdot\nabla\rho+\kappa\nabla^2\rho\}\,\mathrm{d}V. \tag{14}$$

Because the spatial dependence of z_* is determined implicitly through $\rho(\boldsymbol{x}, t)$, we can write

$$z_*\nabla\rho = \nabla\psi \quad \text{where} \quad \psi = \int^{\rho} z_*(\hat{\rho})\,\mathrm{d}\hat{\rho}. \tag{15}$$

Using (15) and integrating by parts, the time rate of change of E_b can be expressed in terms of surface and volume integrals:

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = -g\oint \psi\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S+\kappa g\int_V z_*\nabla^2\rho\,\mathrm{d}V. \tag{16}$$

Noting that $\nabla z_* = (\mathrm{d}z_*/\mathrm{d}\rho)\nabla\rho$, the divergence operator in (16) can be distributed as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \underbrace{-g\oint\psi\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S}_{S_{adv}}\ \underbrace{+\kappa g\oint_S z_*\nabla\rho\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S}_{S_{diff}}+\underbrace{\kappa g\int_V -\frac{\mathrm{d}z_*}{\mathrm{d}\rho}|\nabla\rho|^2\,\mathrm{d}V}_{\Phi_d}. \tag{17}$$

Here S_{adv} and S_{diff}, respectively, are the rates of change of E_b due to advective and diffusive transfers of heat or mass across the bounding surface S. For closed systems, S_{adv} and S_{diff} are both zero. Φ_d gives the rate of change of E_b due to material changes in density within V, or equivalently, due to diapycnal mixing. Since the reference profile is statically stable by construction, $\mathrm{d}z_*/\mathrm{d}\rho < 0$ and so $\Phi_d \geqslant 0$. Thus, background potential energy E_b always increases as a result of diapycnal mixing.

For closed systems, (17) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \kappa\rho_0\int_V\left[\frac{|\nabla\rho|}{|\mathrm{d}z_*/\mathrm{d}\rho|^{-1}}\right]^2 N_*^2\,\mathrm{d}V, \tag{18}$$

where $N_*^2 = (g/\rho_0)\,|\mathrm{d}z_*/\mathrm{d}\rho|^{-1}$ and ρ_0 is the characteristic density. The function N_*^2 is simply the buoyancy frequency obtained from the reference state of minimum potential energy. The term in brackets is closely related to the Cox number (see Gregg 1987), as discussed in Winters & D'Asaro (1995).

Since $E_p = E_a+E_b$, (17) implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}E_a = \Phi_z-g\oint_S(z\rho-\psi)\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S-\Phi_d+\Phi_i+\kappa g\oint_S(z-z_*)\nabla\rho\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S, \tag{19}$$

where Φ_z is the reversible vertical buoyancy flux $\int_V g\rho w\,\mathrm{d}V$ and $\Phi_i = -\kappa g A(\bar{\rho}_{top}-\bar{\rho}_{bottom})$, the rate of conversion from internal to potential energy (see (10)). Equations (17) and (19) are generalizations of those given by Lombard (1989). The surface integrals in (19) give the rate of change of available potential energy resulting from advective and diffusive heat and mass transfer across bounding the surface. These terms vanish for closed systems.

The energetics analysis can be summarized in the energy diagram shown in figure 2. We have found a time-dependent analysis based upon the energy diagram, i.e. an

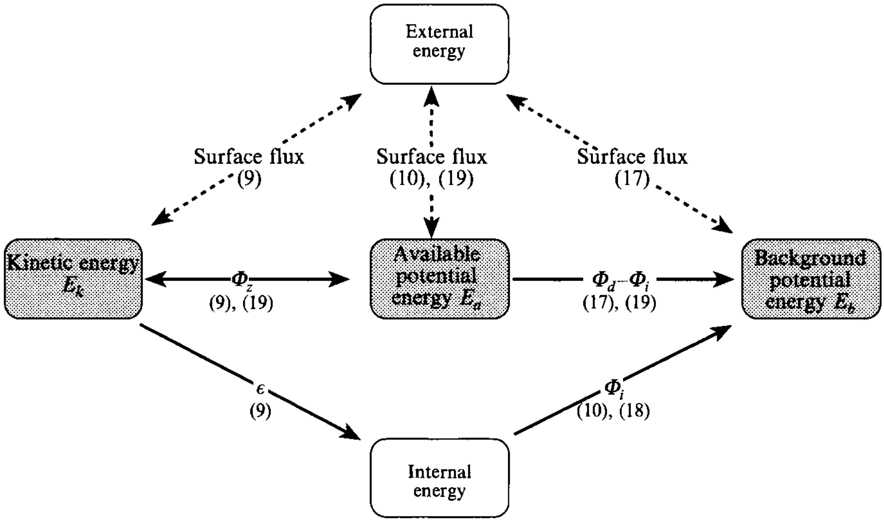

FIGURE 2. Energy diagram for density-stratified Boussinesq flow. The energy within a fixed volume can be stored as kinetic, available potential, background potential, or internal energy. Energy is input to the flow through surface fluxes. Energy exchanges occur through buoyancy flux, diabatic mixing or viscous dissipation. The equation numbers giving the energy exchange rates are listed for each pathway. Φ_z is the reversible buoyancy flux, Φ_d the irreversible diapycnal mixing, ϵ the irreversible kinetic energy dissipation and Φ_i the irreversible conversion of internal to potential energy.

instantaneous evaluation of the energy content of each component, along with the associated exchange rates, to be an extremely valuable tool for studying the dynamics of numerically simulated flows. The evolution equations for the various energy components can be obtained directly from the diagram. The time derivative of each component is equal to the sum of the rates corresponding to the arrows associated with that component.

5. Energetics of a stably stratified mixing layer

We now illustrate these ideas by examining the energetics of a shear instability in a density-stratified Boussinesq flow. A three-dimensional direct numerical simulation, very similar to the simulation of a stably stratified mixing layer studied by Staquet & Riley (1989), was performed and analysed in terms of available, background and total potential energy. A brief description of the numerical simulation is included here; a more detailed discussion is given in Staquet & Riley (1989).

An initial value problem for a stably stratified mixing layer was solved numerically using a three-dimensional, pseudo-spectral model. The equations of motion (5)–(7) were non-dimensionalized using the initial vorticity thickness of the flow, δ, and the initial velocity and density differences across the mixing layer, ΔU and $\Delta\rho$, as the length, velocity and density scales respectively. The initial state was specified by prescribing the following velocity and density profiles:

$$\bar{u}(z) = \tfrac{1}{2}\mathrm{erf}(\pi^{1/2}(z-z_{1/2})), \quad \bar{\rho}(z) = -\tfrac{1}{2}\mathrm{erf}(\pi^{1/2}(z-z_{1/2})), \tag{20}$$

where $z_{1/2}$ is the vertical midpoint. The Richardson number of the initial state is defined as $Ri = N^2\delta^2/\Delta U^2$, where $N^2 = (g/\rho_0)\,\Delta\rho/\delta$ and was set to 0.167. The initial state is thus unstable to KH shear instabilities (Drazin & Reid 1981; Thorpe 1987). The Reynolds number $\delta\Delta U/\nu$ and the Prandtl number ν/κ were given values of 600 and 1 respectively.

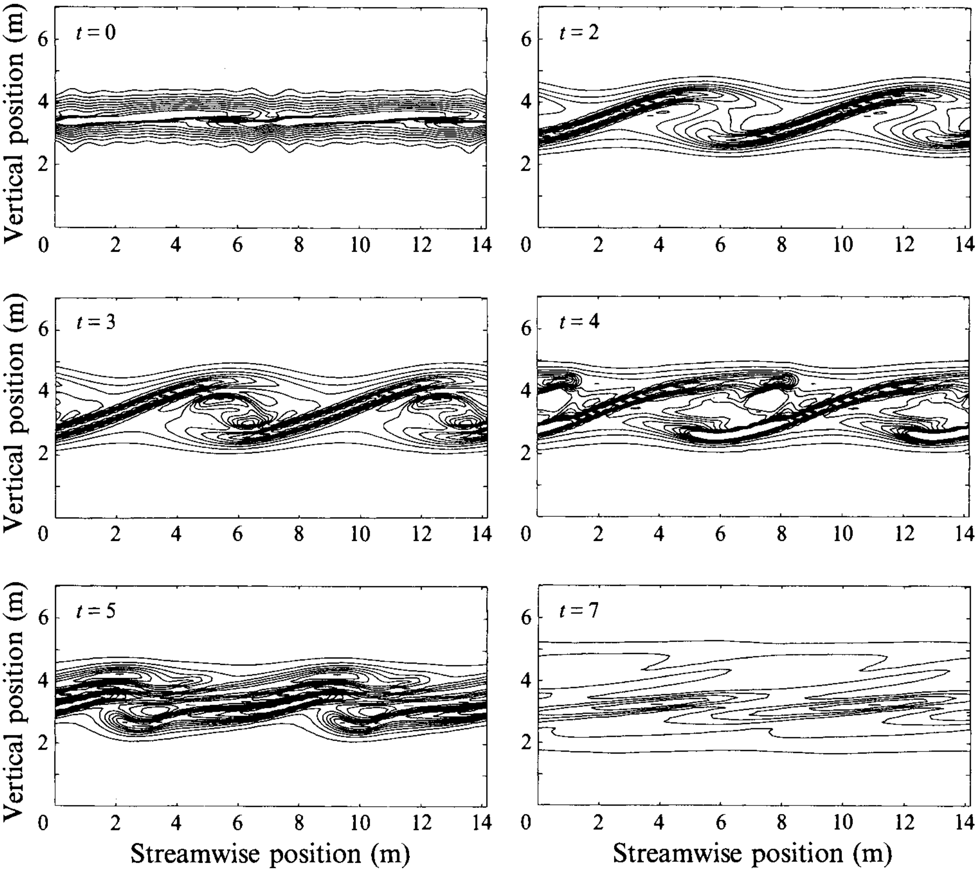

FIGURE 3. Temporal evolution of the spanwise vorticity for a stably stratified mixing layer. Times are given in buoyancy periods.

A two-dimensional velocity perturbation, obtained by solving the Taylor–Goldstein equation for the most unstable mode for the profiles (20), was added to the initial conditions at low amplitude. In addition, a broad-banded spectrum of three-dimensional 'noise' was prescribed. The equations of motion were then solved numerically in a cubic domain with sides of length $2\pi/k$, where k is the horizontal wavenumber of the most unstable KH mode. The solution was required to satisfy free-slip conditions at the upper and lower boundaries and periodicity conditions in both horizontal directions and was obtained on a $64 \times 64 \times 65$ numerical grid. The calculation discussed here differs slightly from that of Staquet & Riley (1989) in that the Prandtl number is unity rather than 0.7, the Reynolds number is increased from 440 to 600 and a broad-banded rather than a narrow-banded three-dimensional noise field was initialized.

Figure 3 shows the time evolution of the y-component of vorticity $\zeta = w_x - u_y$, where subscripts indicate differentiation, in the $y = \pi/k$ streamwise-vertical plane. The KH mode of instability is well developed by $t = 2$. Smaller scales of motion are clearly evident by $t = 4$. The initial vorticity is much reduced and exists over a significantly expanded vertical extent by $t = 7$. The corresponding isopycnals, as well as contours of kinetic energy and density variance dissipation rates are shown in Winters & D'Asaro (1995).

We now examine the changes in potential energy of the flow as it evolves in time. Since the flow under consideration comprises a closed system, the following simplified energy equations hold:

$$\frac{\mathrm{d}}{\mathrm{d}t}E_p = \Phi_z + \Phi_i, \tag{21}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E_b = \Phi_d, \tag{22}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E_a = \Phi_z - (\Phi_d - \Phi_i). \tag{23}$$

Before analysing the simulated flow, it is instructive to consider a related simpler problem. Suppose that the initial state were to consist of the initial density and velocity profiles (20), but with no perturbations. For this case, $E_p = E_b$ and $E_a = 0$ initially. Because no vertical motions develop, the buoyancy flux Φ_z remains identically equal to zero. The initial density profile diffuses, increasing the potential energy E_p at the rate Φ_i. The increase in potential energy occurs at the expense of the internal energy of the fluid. Provided the upper and lower boundaries are sufficiently far away, the rate of increase of E_p remains constant. Because the slowly evolving density profile maintains its static stability as it diffuses, the flow is always in its reference state of minimum potential energy. No available potential energy is created and hence $\Phi_d = \Phi_i$. (Note that for this one-dimensional flow, $\nabla\rho = \mathrm{d}\rho/\mathrm{d}z$ and $\mathrm{d}z_*/\mathrm{d}\rho = (\mathrm{d}\rho/\mathrm{d}z)^{-1}$. Thus, Φ_d can be formally reduced to Φ_i.)

If we now consider perturbed initial conditions, such that a shear instability is allowed to develop, we expect the rate of mixing, i.e. Φ_d, to increase substantially in relation to the unperturbed flow, especially if the mixing layer becomes turbulent. Figure 4(*a*) shows the time evolution of the potential energies of the simulated, perturbed flow relative to their initial values. Note that the cumulative energy change associated with the uniform rate of laminar diffusion has been subtracted from the total and background potential energies, thus emphasizing the energetics associated with the shear instability. The resulting energies are denoted E_p' and E_b'. The energy transfer rates are shown in figure 4(*b*).

Early in the flow evolution, between about $t = 0$ and 2, the potential energy increases owing to the positive vertical buoyancy flux Φ_z. The increase in potential energy results from the adiabatic displacement of fluid parcels away from their equilibrium positions and is stored almost exclusively as available potential energy. This process occurs at lengthscales that are large in comparison to the diffusive scales. During this time interval, the background potential energy does not change appreciably.

The production of background potential energy E_b', which occurs primarily between about $t = 2$ and 5, is the result of small-scale diffusive mixing. Note that the irreversible rate of production Φ_d is maximal during this time interval and that the available potential energy decreases despite a gradient ($\Phi_z > 0$) buoyancy flux.

After about $t = 5$, the buoyancy flux is nearly zero though often slightly counter-gradient. During this period of (weak) restratification, $\Phi_d > 0$ and the background potential energy E_b' continues to increase via diffusive mixing. This example illustrates one of the difficulties inherent in diagnosing mixing via the buoyancy flux. Even prolonged periods of zero or counter-gradient buoyancy flux do not necessarily imply the absence of diapycnal mixing. That irreversible diffusive mixing can take place in a restratifying flow is more clearly shown in the large-eddy simulation of wave instability

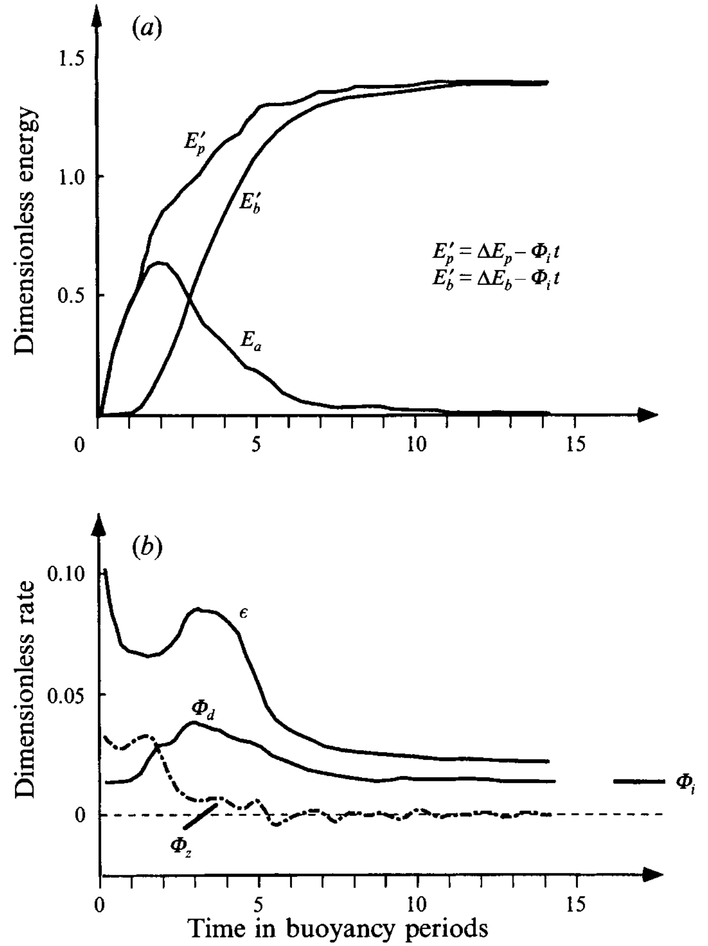

FIGURE 4. (*a*) Time evolution of total, available and background potential energies. (*b*) Instantaneous rates of energy exchange.

near a critical level discussed in Winters & D'Asaro (1994) (see figure 14 of that paper). In that simulation, nearly all the observed mixing occurred during the collapse of the wave packet while the buoyancy flux was counter-gradient.

Figure 4(*b*) also shows that the maximum value of Φ_d is only about three times the laminar rate Φ_i. For truly turbulent flows, the ratio of these rates will be much higher, even by orders of magnitude. The low ratio observed here indicates that the simulated flow is hardly turbulent at all, a consequence of the low Reynolds number. It is interesting to note that the instantaneous mixing efficiency, i.e. the ratio of the rate of irreversible increase of background potential energy due to mixing Φ_d to the rate of irreversible kinetic energy dissipation ϵ, is quite high compared to the values typically observed in laboratory grid turbulence (see e.g. Ivey & Imberger 1989). The mixing efficiency ranges from about 0.38 at $t \approx 4$ to 0.65 by about $t = 14$. These high values may also be a consequence of the low Reynolds number of the simulation. Further discussion of the mixing efficiency of this flow can be found in Winters & D'Asaro (1995).

6. Numerical implementation

As we have seen in §4, the partitioning of potential energy into available and background components depends on being able to determine the reference profile $\rho(z_*)$ associated with the minimum potential energy state. This state is obtained in principle by allowing the fluid to restratify adiabatically. It can be obtained mathematically via (11). Alternatively, a three-dimensional sorting of discrete fluid elements can be used to yield a useful approximation. If we let the fluid elments correspond to volume elements of a numerical grid, then standard sorting algorithms can be used to produce a one-dimensional array of monotonically increasing density values. These density values can then be distributed through the original grid with the heaviest elements on the bottom and lighter elements above. A three-dimensional, sorted density field is obtained that is everywhere statically stable and approximately uniform over each horizontal plane. This state can then be used as a numerical approximation the reference state.

The computed background density is only an approximation of the density distribution with minimum potential energy. This is because each horizontal layer of fluid elements in the sorted field generally consists of different density values. In a physical system, fluid elements that are represented numerically as being side by side in a layer could change their shape, producing separate layers of continuously varying density. In other words, a physical system can adjust to create a density gradient exactly parallel to gravity, while that is not possible in our approximate numerical representation. By interpolating the density field between each level, the available potential energy that remains in the sorted density distribution can be calculated and used as an error estimate. For a flow in which the displacements are small in comparison with the vertical grid spacing, the remaining potential energy is a significant fraction of the available potential energy. We have found generally that when the r.m.s. displacement exceeds the vertical grid spacing, the error in the computed available potential energy is insignificant. In one case we studied, the displacements were always small with respect to the grid spacing and interpolation of the density field was required before the sorting procedure converged to the background profile.

Once the reference density distribution has been found, the total and background potential energies can be easily computed by numerically integrating over the volume of interest. The available potential energy is then found by simply taking the difference between the total potential energy of the fluid and the potential energy of the numerically approximated reference profile. Further discussion and an estimate of approximation errors can be found in Lombard (1989).

7. Discussion

We have outlined an approach for analysing the energetics of density-stratified turbulence. To a large degree, our approach depends on an explicit distinction between diabatic and adiabatic processes made possible by exploiting the concept of available potential energy. We believe that this approach, summarized in the energy diagram of figure 2, provides a useful framework for analysing density-stratified turbulence. Because of the intrinsic importance of turbulent mixing in geophysical flows, our discussion has emphasized the energetics of mixing in stratified flows. There appears to be a lack of consensus in the literature with respect to the interpretation of buoyancy flux, particularly counter-gradient buoyancy flux, and its relationship to diabatic mixing. As this relationship depends critically on available potential energy dynamics, we hope that this conceptual framework will help to clarify this issue.

It is important to realize that changes in potential energy produced by a buoyancy flux occur adiabatically, at the expense of kinetic energy, as fluid elements are advected away from their equilibrium positions. This process is distinct from diabatic mixing and occurs even in non-diffusive fluids. The relationship between buoyancy flux and mixing is unambiguously defined by the balance equation for available potential energy. If there are no surface fluxes and E_a remains constant, then the diabatic mixing rate Φ_a is balanced by the buoyancy flux Φ_z. Buoyancy flux is an indirect rather than a direct measure of diapycnal mixing. Because a direct relationship between rates of buoyancy flux and diapycnal mixing does not hold generally, inferring mixing rates using only the buoyancy flux is not a robust procedure and often leads to confusion.

Simplified energetics balances are often used to interpret bulk averages of instantaneous microstructure measurements in the ocean (Gregg 1987). These balances do not necessarily describe the energetics of isolated transient events that may characterize oceanic turbulence. For these and other unsteady flows, at least in numerical simulations, a more precise accounting of the energy exchanges is possible. A better understanding of the transient dynamics of representative turbulent flows may in fact lead to a better understanding of the statistics of oceanic microstructure data.

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