Representative Scalar Transport and Vertical Mixing

Ben R. Hodges, Ph.D.

September 23, 2008

Final Report submitted to the Texas Water Development Board

under Research and Planning Fund Contract 0704830660

Contract Manager: Jordan E. Furnans, Ph.D., P.E.

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ABSTRACT

Foundational development and derivations for a Representative-scalar, Gradient-based, Vertical Mixing (RGVM) model are presented in detail. The new model is formulated to address issues of vertical numerical diffusion (i.e. non-physical vertical transport and mixing) in three-dimensional models of environmental flows in lakes, rivers and estuaries. The RGVM approach uses a translation between the average scalar and a representative scalar in a model grid cell along with use of top and bottom grid-cell gradients. The methodology is presented in detail, but full implementation of the model has not yet been achieved. The key difficulty appears to be an instability in a stratified flow when the gradient mixing length is transported.

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TABLE OF CONTENTS

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1 INTRODUCTION

1.1 Goals and achievements

The goal of this research project is development of a new approach to vertical mixing in three-dimensional (3D) models of stratified waters (see Appendix A for contract Statement of Work). The standard approaches for vertical mixing and advective transport in existing models develops excessive numerical diffusion or requires excessively fine vertical grid spacing. We proposed and investigated a new idea that had the potential to overcome numerical diffusion without fine grid resolution. The new approach was founded on the concept of a "representative scalar," which provides an alternative value to the "average scalar" value that is stored in a grid cell. The representative scalar works in conjunction with definition of a linear gradient region at the vertical face between grid cells. We call this a Representative-scalar, Gradient-based, Vertical Mixing (RGVM) model.

There were three interdependent products of this project:

1. Development of the representative to average scalar conversion;
2. Development of gradient-based vertical mixing model;
3. Implementation of 1 and 2 as RGVM model in a 3D hydrostatic model.

Products 1 and 2 have been completed as described in this report. Product 3 was only partially completed due to instabilities that were discovered when testing the transport of gradient mixing regions. Thus, the theory for RGVM is well developed within the project, but implementation was unsuccessful within the scope of the funding. The key roadblock proved to be stability of the transport scheme when the combined representative and average scalar approach was used (see section 1.5.2). As of completion of this contract, it is not clear whether the instabilities are the result of a bug in a fairly complex numerical algorithm, or associated with a fundamental instability that precludes this method from being practical.

1.2 Overview of RGVM model

The key difficulties for 3D numerical models of lakes and estuaries are the relationships between surface thermodynamics, density stratification, and vertical mixing. We unify these three features using an energy balance approach (e.g. Hodges et al 2000) with a subgrid-scale vertical gradient representation. The use of the gradient between vertically adjacent cells required development of the new concept for representative scalars.

The idea that sets the present model apart from standard diffusion-based or transport-based approaches is the definition of a gradient region at the boundary between two vertically-adjacent grid cells. This boundary region is characterized by layer thicknesses. Mixing increases the mixing layer thickness until the center of a grid cell is reached. That is, mixing will transport fluid only into the gradient regions, which does not affect the representative scalar value at the cell center (although it does affect the average scalar value integrated over the cell).

The RGVM model is designed to work in a single step of any existing time-marching 3D model as follows:

1. Compute hydrodynamics from time 'n' to time 'n+1' using the existing 3D model approach.
2. Compute transport of cell-average concentrations for conservative scalars from time 'n' to time 'n+1' using the existing model approach.
3. Compute RGVM
    a. Compute transport of grid-cell top and bottom gradient thicknesses, $h_{T(k)}$ and $h_{B(k)}$, as discussed herein.
    b. Compute the representative scalar fields from the average scalar fields and gradient region thicknesses.
    c. Compute vertical mixing (changing gradient thicknesses and representative scalar fields) integrated with surface thermodynamics.
    d. Compute new average scalar fields.
4. End time step

The above method allows the RGVM to be adapted to any 3D model by including transport of the two gradient thickness variables and solution of the vertical mixing algorithm. Note that the representative scalar values require only temporary storage (i.e. within the time step) as the values are created, used and discarded during the mixing. Thus, the increased computational storage is only two additional scalars over the solution domain.

1.3 Use of representative and mean concentrations

We characterize every conserved scalar volume concentration (generally denoted by ϕ) with both the mean value $\overline{\phi}$ and a representative value, ϕ_R. The representative value allows us to provide a better approximation of gradients between cells to help remove the grid-cell dependence of characterizing mixing by mean value gradients. For each grid cell (k) in a water column, there may be top and bottom mixing layers of thickness $h_{T(k)}$ and $h_{B(k)}$, respectively.

The mixing layer thicknesses must meet the requirement that

$$h_{T(k)} + h_{B(k)} \leq \Delta z_k \tag{1.1}$$

so that there can be considered to exist a region of fluid with ϕ_R in the center of the cell. When the inequality of eq. (1.1) is violated during the mixing process, the entire cell is considered well-mixed and we set

$$h_{T(k)} = h_{B(k)} = 0 \tag{1.2}$$

and

$$\overline{\phi}_{(k)} = \phi_{R(k)} \tag{1.3}$$

In effect, this resetting as well-mixed implies that the processes are being adequately resolved on the model grid scale. Where mixing results in eq. (1.1) being satisfied, an approach referred to as “thin-layer” mixing will be used (i.e. the mixing layer is thin compared to the grid cell). Where conditions of eq. (1.1) are not satisfied, a “thick-layer” mixing approach is used.

1.4 Components of new vertical mixing modeling approach

1.4.1 Mixing energies

The modeling approach quantifies the rates at which different mixing energies are supplied. In general, these are of the form $\partial E / \partial t$ where E is an energy per unit area (w/m^2), so that $\partial E / \partial t$ has the units (kg m^2/s^2) / (m^2 s), which reduces to (kg /s^3). In some derivations, we use the energy per unit volume, which reduces to (kg /s^2 m), so that $\partial e / \partial t$ has the units (kg /s^3 m). The sources of mixing energy are: 1) wind stirring, 2) convective overturns, and 3) shear mixing by Kelvin-Helmholtz (K-H) billows, and 4) boundary mixing. The following general approach is used for mixing in each water column: shear mixing is a separate computation either prior to bottom and surface boundary mixing. Bottom mixing uses a bottom-up sweep and surface mixing in a top-down sweep. Where sweeps overlap, the region of overlap is computed separately.

1.4.2 Integration of surface thermodynamics and mixing

In contrast to the ELCOM approach (Hodges et al 2000), we integrate the surface thermodynamics directly in the mixing rather than developing separate algorithms. That is, in ELCOM the surface thermodynamics creates a new density profile (due to heating, cooling, and evaporation), then the mixing routine mixes energy through the water column. In the new approach, the surface thermodynamics provides the rate of energy supplied to the water column, which may be either stabilizing (increasing temperature so as to provide a larger negative density gradient), or destabilizing through cooling that leads to overturns. Note that this approach allows us to calculate the rate at which destabilizing energy is supplied (which should affect dissipation). That is, we might imagine a case where the heating and cooling are exactly in balance so that the net rate of stabilizing energy exactly equals the net rate of destabilizing energy. In the ELCOM approach, this would be considered a system with zero "available energy" for mixing. Since the ELCOM dissipation rate was based solely on the net available energy for mixing, the parameterization has no ability to distinguish between zero heating/cooling (i.e. quiescence), or an active interplay between heating/cooling that leads to no available energy for mixing, but still engenders turbulence.

1.4.3 Dissipation rates

In Hodges et al (2000), dissipation is simply a function of available mixing energy. We apply three concepts beyond the ELCOM approach: 1) dissipation is a function of the overall thickness of the mixing layer; 2) time-dependency of dissipation is allowed so that higher dissipation rates occur when the wind is just getting started and perhaps lower dissipation rates when it is dropping; and 3) dissipation is a function of the overall level of turbulence, rather than just the available mixing energy. Note that dissipation is considered principally in the surface and bottom boundary mixing layers. For shear regions, the dissipation is built into the mixing efficiency of the K-H billows.

1.4.4 Partial mixing of a cell

Partial mixing in a grid cell is developed for all parts of the mixing scheme to obtain the maximum practical time and grid-spacing independence of the model. The mixing layer thickness (bottom and surface mixing boundaries) is carried as a variable that will influence the dissipation rate and the rate of deepening. This approach allows the mixing scheme to be used with a homogenous fluid, which was a problem for the Hodges et al (2000) approach.

1.4.5 Unstable density gradients

Unstable density gradient are expected to be physically developed in the surface mixing layer, where they will be removed in the mixing process. Where unstable density gradients are developed in other parts of the flow through transport (e.g. where a gravity current flows over a step), the unstable gradient is resolved by flipping the fluid volumes.

1.4.6 Achieving time step and grid size independence

The model is characterized by a model time step Δt_M, grid layers of $\Delta z_{(k)}$ for $k = k_b, k_{b+1} \ldots k_\eta$ being the integers from the bottom layer to the surface in any water column. There is no a priori requirement for a strictly uniform z-layer grid. To make the scheme relatively independent of both Δz and Δt_M we need to invoke sub-time steps. The process of mixing will occur in sub-time steps across a grid face, so we keep track of the time remaining (or the time left) for mixing on the k+1/2 face of a grid cell as $\Delta t_{L(k+1/2)}$. The subtime steps are applied separately in each part of the mixing routine.

1.4.7 Standard notation

In general we will put grid indexes such as (k) in parenthesis so that it is easier to distinguish from a necessary plethora of subscripts. To avoid double subscripts, the 'k' index of the bottom will be represented as a subscript '(D)'. The 'k' index of the free surface will be given as subscript (S). The 'k' index of the partially-mixed cell at the bottom of the surface mixed layer will be subscript (P), while the 'k' index of the partially-mixed cell at the top of the lower layer will be (C). Note that subscripts 'T' 'B' and 'R without parenthesis are not 'k' indexes.

In many places in this paper, it is convenient to represent the difference between the scalar concentrations on the 'k' and 'k+1' grid layers by

$$\Delta\phi_{(k+1/2)} = \phi_{(k+1)} - \phi_{(k)} \tag{1.4}$$

Thus, when ϕ represents the density, a stable density gradient always requires $\Delta\rho \leq 0$.

1.5 Open issues

1.5.1 Large-scale overturns (i.e. fine grid resolution behavior)

An issue that still needs resolution is the relationship between the large-scale overturn time in a mixing layer and the time step. If we follow the ELCOM paradigm, a mixing layer is homogeneous in all properties. However, one can readily imagine a model time step that is smaller than the vertical turbulent transport time through a mixing layer. In such a case, introduction of a tracer at the base of the mixing layer will physically require a finite time to reach the surface, but the model would represent instantaneous mixing. At the larger time and space scales that are typically desired this is unlikely to be a major issue.

1.5.2 Instability of representative density in transport routine.

The RGVM approach requires transport of the top and bottom gradient layer thicknesses (see Section 2) for each grid cell. As our target 3D hydrodynamic models use an Arakawa C grid, the fluxes are defined in each direction only at the grid cell face. We experimented with using simple conservative upwind transport through each face and with using an interpolation method to obtain all velocities co-located on top and bottom grid cell faces for transport. In both cases, the transport of the gradient region thickness led to development of instability in the density field. Within the scope of this project, we were unable to determine the direct cause of the instability or develop a method to address it. Until this issue is solved, the RGVM model is cannot be adequately implemented.

2 RELATIONSHIPS BETWEEN REPRESENTATIVE AND AVERAGE SCALARS

2.1 Introduction

In any finite-volume numerical model, the value of a scalar in a grid cell is taken as the average (arithmetic mean) of the unresolved, subgrid, scalar distribution across the cell. It follows that any numerical diffusion through the bottom of the grid cell becomes available (on the next time step) for numerical diffusion through the top of the grid cell. An approach to counter this problem is in the definition of "representative" scalars and gradient regions as sub-grid scale features of the vertical distribution in a grid cell. Let us consider Figure 1 that represents a density profile in two grid layers wherein the representative density ρ_R is the uniform density in the center of each grid layer. Between the regions of uniform density are linear gradient regions specified thicknesses 'h'. The subscript on h indicates the 'Top' and 'Bottom' gradient region of a grid cell. Subscripts in parentheses indicate the grid cell layer.

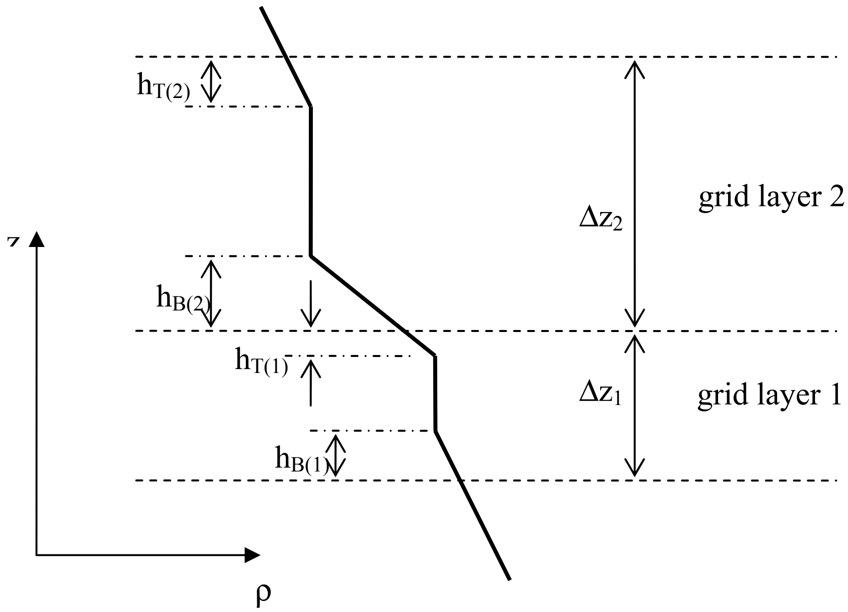


Figure 1. Piecewise linear density profile in two grid layers.

2.2 Average density as a function of representative density

The average density in the ‘k’th cell can be computed by the weighted sum of the average densities in the top and bottom gradient regions and the uniform region as

$$\overline{\rho}_{(k)} = \frac{\left(\Delta z_{(k)} - h_{T(k)} - h_{B(t)}\right)\rho_{R(k)} + h_{T(k)}\overline{\rho}_{T(k)} + h_{B(k)}\overline{\rho}_{B(k)}}{\Delta z} \tag{2.1}$$

The average density in the upper (Top) gradient region is derived in Appendix A, and is given by

$$\overline{\rho}_{T(k)} = \rho_{R(k)} + \frac{h_{T(k)}}{2}\left\{\frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}}\right\} \tag{2.2}$$

Similarly, the average density in the lower (Bottom) gradient region is

$$\overline{\rho}_{B(k)} = \rho_{R(k)} - \frac{h_{B(k)}}{2}\left\{\frac{\rho_{R(k)} - \rho_{R(k-1)}}{h_{B(k)} + h_{T(k-1)}}\right\} \tag{2.3}$$

where eq. (2.3) receives a negative sign instead of the positive in eq. (2.2) to account for the gradient direction. Substituting eqs. (2.2) and (2.3) into (2.1) provides

$$\begin{aligned} \overline{\rho}_{(k)} = {} & \frac{1}{\Delta z_{(k)}}\left(\Delta z_{(k)} - h_{T(k)} - h_{B(t)}\right)\rho_{R(k)} \\ & + \frac{1}{\Delta z_{(k)}} h_{T(k)}\left\{\rho_{R(k)} + \frac{h_{T(k)}}{2}\left\{\frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}}\right\}\right\} \\ & + \frac{1}{\Delta z_{(k)}} h_{B(k)}\left\{\rho_{R(k)} - \frac{h_{B(k)}}{2}\left\{\frac{\rho_{R(k)} - \rho_{R(k-1)}}{h_{B(k)} + h_{T(k-1)}}\right\}\right\} \end{aligned} \tag{2.4}$$

which can be written as (see Appendix B.2)

$$\begin{aligned} \overline{\rho}_{(k)} = {} & \left(1 - \frac{h_{T(k)}^{2}}{2\Delta z_{(k)}\left(h_{T(k)} + h_{B(k+1)}\right)} - \frac{h_{B(k)}^{2}}{2\Delta z_{(k)}\left(h_{B(k)} + h_{T(k-1)}\right)}\right)\rho_{R(k)} \\ & + \frac{h_{T(k)}^{2}}{2\Delta z_{(k)}\left(h_{T(k)} + h_{B(k+1)}\right)}\rho_{R(k+1)} \qquad + \frac{h_{B(k)}^{2}}{2\Delta z_{(k)}\left(h_{B(k)} + h_{T(k-1)}\right)}\rho_{R(k-1)} \end{aligned} \tag{2.5}$$

Define coefficients as:

$$\begin{aligned} \psi_{T(k)} &\equiv \frac{h_{T(k)}^{2}}{2\Delta z_{k}}\left\{\frac{1}{h_{T(k)} + h_{B(k+1)}}\right\} \\ \psi_{B(k)} &\equiv \frac{h_{B(k)}^{2}}{\Delta z_{(k)}}\left\{\frac{1}{h_{B(k)} + h_{T(k-1)}}\right\} \end{aligned} \tag{2.6}$$

Note that $\psi_{T(k)} = 0$ for $h_{T(k)} = 0$ and $h_{B(k+1)} > 0$. However, $\psi_{T(k)} \to 0$ in the limit as $h_{T(k)} \to 0$, even if $h_{B(k+1)} = 0$. Thus, in general $\psi_{T(k)} = 0$ for $h_{T(k)} = 0$ and $\psi_{B(k)} = 0$ for $h_{B(k)} = 0$.

Substituting eqs. (2.6) into eq. (2.5) we obtain the expression for the average density from the representative densities as

$$\bar{\rho}_{(k)} = \left(1 - \psi_{T(k)} - \psi_{B(k)}\right)\rho_{R(k)} + \psi_{T(k)}\rho_{R(k+1)} + \psi_{B(k)}\rho_{R(k-1)} \tag{2.7}$$

2.3 Obtaining representative density from average density

Defining the coefficients

$$\begin{aligned} A_{(k)} &\equiv \psi_{T(k)} \\ B_{(k)} &\equiv 1 - \psi_{T(k)} - \psi_{B(k)} \\ C_{(k)} &\equiv \psi_{B(k)} \end{aligned} \tag{2.8}$$

we can then write the matrix equation linking the grid cells in a water column from eq. (2.7) as

$$\begin{bmatrix} B_{(k\,max)} & C_{(k\,max)} & 0 & 0 & 0 & 0 & 0 \\ A_{(k\,max-1)} & B_{(k\,max-1)} & C_{(k\,max-1)} & 0 & 0 & 0 & 0 \\ 0 & A_{(k\,max-2)} & B_{(k\,max-2)} & C_{(k\,max-2)} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & A_{(3)} & B_{(3)} & C_{(3)} & 0 \\ 0 & 0 & 0 & 0 & A_{(2)} & B_{(2)} & C_{(2)} \\ 0 & 0 & 0 & 0 & 0 & A_{(1)} & B_{(1)} \end{bmatrix} \begin{bmatrix} \rho_{R(k\,max)} \\ \rho_{R(k\,max-1)} \\ \rho_{R(k\,max-2)} \\ \vdots \\ \rho_{R(3)} \\ \rho_{R(2)} \\ \rho_{R(1)} \end{bmatrix} = \begin{bmatrix} \bar{\rho}_{(k\,max)} \\ \bar{\rho}_{(k\,max-1)} \\ \bar{\rho}_{(k\,max-2)} \\ \vdots \\ \bar{\rho}_{(3)} \\ \bar{\rho}_{(2)} \\ \bar{\rho}_{(1)} \end{bmatrix} \tag{2.9}$$

Solution of eq. (2.9) provides reconstruction of the representative density from the mean density field and the thickness of the gradient region.

2.4 Representative and average conservative scalars

The above approach can be extended to any conservative scalar, ϕ as

$$\begin{bmatrix} B_{(k\max)} & C_{(k\max)} & 0 & 0 & 0 & 0 & 0 \\ A_{(k\max-1)} & B_{(k\max-1)} & C_{(k\max-1)} & 0 & 0 & 0 & 0 \\ 0 & A_{(k\max-2)} & B_{(k\max-2)} & C_{(k\max-2)} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & A_{(3)} & B_{(3)} & C_{(3)} & 0 \\ 0 & 0 & 0 & 0 & A_{(2)} & B_{(2)} & C_{(2)} \\ 0 & 0 & 0 & 0 & 0 & A_{(1)} & B_{(1)} \end{bmatrix} \begin{bmatrix} \phi_{R(k\max)} \\ \phi_{R(k\max-1)} \\ \phi_{R(k\max-2)} \\ \vdots \\ \phi_{R(3)} \\ \phi_{R(2)} \\ \phi_{R(1)} \end{bmatrix} = \begin{bmatrix} \overline{\phi}_{(k\max)} \\ \overline{\phi}_{(k\max-1)} \\ \overline{\phi}_{(k\max-2)} \\ \vdots \\ \overline{\phi}_{(3)} \\ \overline{\phi}_{(2)} \\ \overline{\phi}_{(1)} \end{bmatrix} \qquad (2.10)$$

with definitions of eq. (2.8) and (2.6). The computation of the average scalar is similar to eq. (2.7)

$$\overline{\phi}_{(k)} = \left(1 - \psi_{T(k)} - \psi_{B(k)}\right)\phi_{R(k)} + \psi_{T(k)}\phi_{R(k+1)} + \psi_{B(k)}\phi_{R(k-1)} \qquad (2.11)$$

Thus, the transformation from representative scalars and gradient layer thickness to average scalars is given explicitly by eq. (2.11) for each grid cell; whereas the transformation from average scalars and gradient layer thicknesses is given by solution of the tridiagonal eq. (2.10) for each water column.

3 INTERIOR SHEAR MIXING

3.1 Introduction

Away from the boundary layers, we take the principal mixing mechanism in the stratified system to be Kelvin-Helmholtz (KH) billowing driven by vertical velocity shear. As a model process, billows are a means of changing the mixing layer thicknesses across the grid cell interface.

As long as the shear mixing does not take up more than 50% of a grid cell, it does not affect the representative scalar values in the cell (only the mean value is affected). Thus, algorithms for shear mixing that involves more than 50% of a grid cell must be different from algorithms that involve less than 50% of a grid cell. Similarly, a KH billow may either take more than a time step or less than a time step, again implying different algorithms are needed. More details of the derivation are provided in Appendix D. A pseudo-code representation of the interior shear-mixing algorithm is provided in Appendix M

3.2 Time-step and grid-size independent KH mixing

We characterize shear mixing at the 'k+1/2' grid cell face by a billow thickness $\delta_{KH(k+1/2)}$ and a time scale $T_{KH(k+1/2)}$, given as

$$\delta_{KH(k+1/2)} = -\frac{c_\delta \rho_0}{g\,\Delta\rho_{R(k+1/2)}}\left\{\left(\Delta U_{R(k+1/2)}\right)^2 + \left(\Delta V_{R(k+1/2)}\right)^2\right\} \tag{3.1}$$

$$T_{KH(k+1/2)} = -\frac{c_T\,\rho_0}{g\left(\Delta\rho_{R(k+1/2)}\right)}\sqrt{\left(\Delta U_{R(k+1/2)}\right)^2 + \left(\Delta V_{R(k+1/2)}\right)^2} \tag{3.2}$$

where Sherman et al. (1978) recommends $c_\delta = 0.3$, but this could arguably be set in the range as high as 0.6 or as low as 0.2 to represent "at least 70%, and sometimes more than 90% of the kinetic energy given up by the shear flow is simply lost to viscosity."

With a model time step of Δt_M and grid scale of $\Delta z_{(k+1/2)}$, there are four possible conditions:

1. $\Delta t_M \geq T_{KH(k+1/2)}$ and $c_{\Delta z}\Delta z_{(k+1/2)} > \delta_{KH(k+1/2)}$
2. $\Delta t_M < T_{KH(k+1/2)}$ and $c_{\Delta z}\Delta z_{(k+1/2)} > \delta_{m(k+1/2)}$
3. $\Delta t_M \geq T_{KH(k+1/2)}$ and $c_{\Delta z}\Delta z_{(k+1/2)} \leq \delta_{KH(k+1/2)}$

4. $\Delta t_M < T_{KH(k+1/2)}$ and $c_{\Delta z}\Delta z_{(k+1/2)} \leq \delta_{m(k+1/2)}$

where $\delta_{m(k+1/2)}$ is the partial mixing of a KH billow whose time scale is longer than the model time step, and $c_{\Delta z}$ is a fractional coefficient in the range [0,1] to account for non-uniform grid spacing and ensure no more than 50% of the smallest grid cell is involved in a Case 1 or Case 2 mixing event. If the vertical grid spacing is uniform, then $c_{\Delta z} = 1$ is appropriate. However, for a non-uniform grid, we define the grid cell thickness at the cell faces as

$$\Delta z_{(k+1/2)} = \frac{1}{2}\left(\Delta z_{(k)} + \Delta z_{(k+1)}\right) \tag{3.3}$$

To ensure that a Case 1 or Case 2 mixing event does not involve more than 50% of a grid cell, we define

$$c_{\Delta z(k+1/2)} \equiv 1 - \frac{\left|\Delta z_{(k+1)} - \Delta z_{(k)}\right|}{2\Delta z_{(k+1/2)}} \tag{3.4}$$

Using $c_{\Delta z}$ in the above definitions provides the cutoff between multi-step and single step mixing based on the smaller of two vertically-adjacent grid cells.

1. For Case 1, we have a complete KH billow during the time step across the cell boundary that can be represented in only the two cells. This case is the simplest thin-layer mixing as it does not affect the representative values, but only increases the gradient layer. Note that the time used in mixing is less than the time step, so it is possible to have multiple Case 1 billows in a time step through an interaction of processes.

2. For Case 2, only a portion of the KH billow will actually occur during a time step as the billow time is longer than Δt_M. Because this occurs over the entire time step and is defined as a billow that will not move further than 50% of the cells above and below, it may only occur once in a time step.

3. For Case 3, the entire KH billow occurs during the time step, but the result is felt over more than two grid cells, so it must be completed in stages.

4. For Case 4, only a portion of the KH billow occurs during the time step, but the result is still felt over more than two grid cells, so it must be completed in stages, with the mixing layer thickness given as in case 2.

The mixing cases can be simplified by defining the time used for KH mixing as

$$\Delta t_U = \min\left\{\Delta t_M, T_{KH}\right\} \tag{3.5}$$

and the billow mixing height over the mixing time as

$$\delta_{m} = \frac{\Delta t_{U}}{\Delta T_{KH}} \delta_{KH} \tag{3.6}$$

Single-step mixing will occur as long as

$$\Delta z_{(k+1/2)} > \frac{\delta_{m(k+1/2)}}{c_{\Delta z(k+1/2)}} \tag{3.7}$$

whereas multi-step mixing will occur for

$$\Delta z_{(k+1/2)} \leq \frac{\delta_{m(k+1/2)}}{c_{\Delta z(k+1/2)}} \tag{3.8}$$

3.3 Single-step mixing

The single-step mixing is straightforward – the mixing layer thickness is the new gradient region on either side of the cell face, and is split equally between the top and bottom grid cells as

$$h_{T(k)}^{(new)} = \frac{\delta_{m(k+1/2)}}{2} \tag{3.9}$$

$$h_{B(k)}^{(new)} = \frac{\delta_{m(k-1/2)}}{2} \tag{3.10}$$

The mean values of all scalars will be changed based on the mixing as

$$\begin{aligned} \overline{\phi}_{(k)}^{(new)} = \overline{\phi}_{(k)}^{(old)} + \frac{1}{2\Delta z_{(k)}} \Biggl(& \Delta\phi_{R(k+1/2)}^{(old)} \left\{ \frac{\left[h_{T(k)}^{(new)}\right]^2}{h_{T(k)}^{(new)} + h_{B(k+1)}^{(new)}} - \frac{\left[h_{T(k)}^{(old)}\right]^2}{h_{T(k)}^{(old)} + h_{B(k+1)}^{(old)}} \right\} \\ & - \Delta\phi_{R(k-1/2)}^{(old)} \left\{ \frac{\left[h_{T(k-1)}^{(new)}\right]^2}{h_{T(k-1)}^{(new)} + h_{B(k)}^{(new)}} - \frac{\left[h_{T(k-1)}^{(old)}\right]^2}{h_{T(k-1)}^{(old)} + h_{B(k)}^{(old)}} \right\} \Biggr) \end{aligned} \tag{3.11}$$

At the end of single-step mixing, there will be cells that still have some potential mixing time left. These may undergo further single-step mixing after the multi-step mixing.

3.4 Multi-step mixing

Multi-step mixing occurs when the vertical grid resolution is fine compared to the KH mixing heights. As such, the representative velocities used in single-step mixing cannot be used. We recompute the KH billow time scale and mixing layer thicknesses from mean cell values as

$$\delta_{KH(k+1/2)} = -\frac{0.3\rho_0}{g\,\Delta\bar{\rho}_{(k+1/2)}}\left\{\left(\Delta\bar{U}_{(k+1/2)}\right)^2 + \left(\Delta\bar{V}_{(k+1/2)}\right)^2\right\} \tag{3.12}$$

$$T_{KH(k+1/2)} = -\frac{20\rho_0}{g\left(\Delta\bar{\rho}_{(k+1/2)}\right)}\sqrt{\left(\Delta\bar{U}_{(k+1/2)}\right)^2 + \left(\Delta\bar{V}_{(k+1/2)}\right)^2} \tag{3.13}$$

We consider that multi-step shear mixing will only occur if

$$\delta_{KH(k+1/2)} > \Delta z_{(k+1/2)} \tag{3.14}$$

otherwise, the gradient is already at the "collapsed" size of Sherman et al (1978). As multi-step mixing occurs separately from single-step mixing, the time-left billowing value must be defined. Initially this is

$$T_{LKH(k+1/2)} = T_{KH(k+1/2)} \tag{3.15}$$

Similarly, a "thickness left" value is defined as

$$\delta_{LKH(k+1/2)} = \delta_{KH(k+1/2)} \tag{3.16}$$

Finally, a "thickness accumulated" value is initialized as

$$\delta_{c(k+1/2)} = 0 \tag{3.17}$$

It is convenient to define a mixing height anomaly as the difference between the mixing height accumulated and the local grid cell as

$$\delta_{a(k+1/2)} \equiv \delta_{c(k+1/2)} - c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \tag{3.18}$$

We can consider two possible cases:

$$\delta_{a(k+1/2)} \leq c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \tag{3.19}$$

$$\delta_{a(k+1/2)} > c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \tag{3.20}$$

As long as eq. (3.19) is satisfied, the multi-step mixing is working within the two grid cells on either side of the mixing cell face. As soon as eq. (3.20) is satisfied, the mixing would be extending into addition grid cells. Rather than trying to extend the mixing from the k+1/2 face above the k+3/2 face (which causes conceptual problems if the k+3/2 face was already mixing), we instead consider the condition

$$\delta_{a(k+1/2)} = c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \tag{3.21}$$

as a cutoff between an "inner loop" and an "outer loop" multi-step scheme. As long as the mixing is between two grid cells, then $\delta_{a(k+1/2)} \leq c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)}$ and we cycle the inner loop (discussed below). Once $\delta_{a(k+1/2)} = c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)}$, the inner loop is complete and we conduct an "outer loop" that computes new KH billow characteristics at each grid cell face. With these new data, we then conduct additional inner loop mixing between grid cells. Once the outer loop iterations are complete, if there are any grid cell faces with $\Delta t_L > 0$, we continue with another single-step mixing algorithm and additional multi-step mixing until $\Delta t_L = 0$ for all cell faces.

Multi-step mixing is required because the mixing possibly covers more than 50% of the grid cell, such that interaction between an upper mixing layer and and lower mixing layer may affect the same cell (and thus modify the representative values). To allow the upper and lower mixing layers to interact, we use subtime-steps that allow no more than ¼ of the upper grid cell volume to be transported into the lower cell (and vice versa); i.e. ½ of each grid cell is mixed fluid around each cell face. We consider this form of mixing an "inner loop" as we maintain a fixed set of KH billow characteristics (i.e. $T_{KH(k+1/2)}$, $\delta_{KH(k+1/2)}$) and conduct successive fractional mixing steps until the KH mixing time and thickness are exhausted. Each mixing subtime-step will use some mixing time (Δt_U), so that after mixing has occured there is some time left in the KH billow time scale (T_{LKH}) and some time left in the time step (Δt_L). For multi-step mixing, we compute the time required to mix to some height 'h' by a KH billow as

$$-gh^2 \frac{\Delta\bar{\rho}_{(k+1/2)}}{C_C \rho_0} \left\{ \left(\Delta\bar{U}_{(k+1/2)} \right)^2 + \left(\Delta\bar{V}_{(k+1/2)} \right)^2 \right\}^{-3/2}$$

We are interested in an inner-loop step where mixing involves no more than ½ the grid cell, so the maximum mixing height across the 'k+1/2' cell face is $h = c_{\Delta z(k+1/2)} \Delta z_{(k+1/2)}$. It follows that the mixing time required for this height in an inner loop fractional mixing step is

$$\Delta t_{R(k+1/2)} = -g \left(c_{\Delta z(k+1/2)} \Delta z_{(k+1/2)} \right)^2 \frac{\Delta\bar{\rho}_{(k+1/2)}}{C_C \rho_0} \left\{ \left(\Delta\bar{U}_{(k+1/2)} \right)^2 + \left(\Delta\bar{V}_{(k+1/2)} \right)^2 \right\}^{-3/2} \tag{3.22}$$

Thus, multi-step inner loop mixing occurs over mixing sub-time steps defined by the minimum of the time required to mix over ½ the grid cell, the time left in the KH billow time scale, or the time left in the model time step, i.e.

$$\Delta t_{U(k+1/2)} = \min \left\{ \Delta t_{R(k+1/2)}, T_{LKH(k+1/2)}, \Delta t_{L(k+1/2)} \right\} \tag{3.23}$$

The fractional mixing layer thickness, δ_f, over this time interval is computed from

$$\delta_{f(k+1/2)} = \sqrt{ \frac{-C_C \rho_0 \Delta t_{U(k+1/2)}}{g \Delta\bar{\rho}_{(k+1/2)}} \left\{ \left(\Delta\bar{U}_{(k+1/2)} \right)^2 + \left(\Delta\bar{V}_{(k+1/2)} \right)^2 \right\}^{3/2} } \tag{3.24}$$

The mean grid cell values of scalars are updated as

$$\begin{aligned}\overline{\phi}^{(\text{new})}_{(k)} = \overline{\phi}^{(\text{old})}_{(k)} + \frac{1}{2\Delta z_{(k)}}\left(\frac{C_C\rho_0}{g}\right)^{1/2} & \left(\Delta\overline{\phi}^{(\text{old})}_{(k+1/2)}\left\{\frac{\Delta t_{U(k+1/2)}}{-\Delta\overline{\rho}^{(\text{old})}_{(k+1/2)}}\right\}^{1/2}\left\{\left[\Delta\overline{U}^{(\text{old})}_{(k+1/2)}\right]^2+\left[\Delta\overline{V}^{(\text{old})}_{(k+1/2)}\right]^2\right\}^{3/4}\right. \\ & \left. -\Delta\overline{\phi}^{\text{old}}_{k-1/2}\left\{\frac{\Delta t_{U(k-1/2)}}{-\Delta\overline{\rho}^{(\text{old})}_{(k-1/2)}}\right\}^{1/2}\left\{\left[\Delta\overline{U}^{(\text{old})}_{(k-1/2)}\right]^2+\left[\Delta\overline{V}^{(\text{old})}_{(k-1/2)}\right]^2\right\}^{3/4}\right)\end{aligned} \tag{3.25}$$

The times left are updated

$$\Delta t_L^{(\text{new})} = \Delta t_L^{(\text{old})} - \Delta t_U \tag{3.26}$$

$$T_{LKH}^{(\text{new})} = T_{LKH}^{(\text{old})} - \Delta t_U \tag{3.27}$$

The thickness left is updated as

$$\delta^{(\text{new})}_{LKH(k+1/2)} = \delta^{(\text{new})}_{LKH(k+1/2)} - \delta_{f(k+1/2)} \tag{3.28}$$

The accumulated mixing thickness is updated

$$\delta^{(\text{new})}_{c(k+1/2)} = \delta^{(\text{old})}_{c(k+1/2)} + \delta_{f(k+1/2)} \tag{3.29}$$

The mixing thickness anomaly is computed as

$$\delta^{(\text{new})}_{a(k+1/2)} \equiv \delta^{(\text{new})}_{c(k+1/2)} - c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \tag{3.30}$$

The inner loop continues back at eq. (3.22) as long as

$$\begin{aligned} &\Delta t_{L(k+1/2)} > 0 \\ &T_{LKH(k+1/2)} > 0 \\ &\delta_{LKH(k+1/2)} > 0 \\ &\delta_{a(k+1/2)} < c_{\Delta z(k+1/2)}\Delta z_{(k+1/2)} \end{aligned} \tag{3.31}$$

If any one of eq. (3.31) is not satisfied, then the inner loop must end.

If eq. (3.20) is satisfied, then the mixing layer extends into additional grid cells. In this case, it is possible that at the start of the time step a cell only has a mixing layer at the k-1/2 face, but that the multi-step mixing must account for the k+1/2 face becoming involved. In effect, eq. (3.20) implies the grid is small enough that multiple grid cells are involved in a KH billow. To account for this in a simple manner, we provide an "outer loop". Once the inner loop exits, we compute new KH billow characteristics, i.e. eq. (3.12) and (3.13) and proceed back through the inner loop. Note that although the T_{LKH}, δ_{LKH}, and δ_c counters are all reset, the Δt_L counter must not be reset, as mixing must stop when $\Delta t_L = 0$. The outer loop stops when either of the following conditions are met

$$\begin{aligned} &\Delta t_{L(k+1/2)} = 0 \\ &\delta_{KH(k+1/2)} < \Delta z_{(k+1/2)} \end{aligned} \tag{3.32}$$

When a full set of single step and multi-step mixing is completed, we check to see if $\Delta t_{L(k+1/2)} > 0$ anywhere in the system. If mixing time is still available, we conduct another full set of single-step and multi-step mixing until $\Delta t_{L(k+1/2)} = 0$ for all cell faces.

4 SURFACE AND BOTTOM MIXING LAYERS

4.1 Introduction

In contrast to interior shear mixing layers, the surface and bottom mixing layers are considered to have thicknesses (H and G) which typically exceed the model grid cell thickness. The larger-scale coherent motions in these layers are considered to be relatively persistent compared to the time step, so the thickness of the mixing layer must be tracked and changed with the time step. The surface mixing layer is more complex than the bottom mixing layer because it must include the effects of surface thermodynamics and unstable convective mixing.

4.2 Integrating thermodynamics, convective mixing an surface mixed layer

The surface thermodynamics can either stabilize or destabilize the surface mixing layer. The first task of the vertical algorithm is to determine whether the near-surface layers are stabilized or destabilized by thermodynamics. We define a thin layer δ_e such that $\eta - \delta_e \leq z \leq \eta$ where evaporative mass fluxes and sensible/evaporative heat transfer uniformly affect the water column. A second thin layer δ_r is defined where $\eta - \delta_r \leq z \leq \eta$, where penetrative solar radiation is preferentially absorbed in the near surface region. We assume that $\delta_e < \delta_r$. It can be shown, see derivation of eq. **(H.14)** in Appendix H, that the rate that TKE is made available for mixing if the thermodynamics is convectively unstable in the near-surface region $\eta - \delta_r \leq z \leq \eta$ is:

$$\frac{\partial E_{p\delta a}}{\partial t} = \frac{1}{2}\left(\delta_r - \delta_e\right)\left\{ g\beta\rho V_e S_\eta - g\frac{\alpha}{c_p} Q_h \right\} \tag{4.1}$$

where α, β are the thermal and salinity expansion coefficients, V_e is the evaporative flux rate, S_η is the salinity at the free surface and Q_h is the is the net heating/cooling due to sensible/evaporative sources (i.e. without solar radiation). Note that solar radiation does not appear in the above as it is assumed to be linearly absorbed across the entire region $\eta - \delta_r \leq z \leq \eta$.

4.3 Layer definitions

The surface and bottom mixing layers are somewhat more complex than the simple mixing layer shown in Figure 1. In general, these mixing layers will extend over multiple grid cells and then will end in a gradient region where entrainment and billowing may occur. We will denote the surface and bottom mixing layer thicknesses by H_η and H_B respectively. It is also useful to keep track of the number of complete cells in the mixing layers as N and M. We will first look at only the surface mixing layer. For simplicity in notation (and avoiding double superscripting), we define the 'k' index of the partially mixed cell at the base of the surface layer as

$$P = S - N \tag{4.2}$$

From the above definitions, it follows that

$$H_\eta = \delta_{H(P)} + \sum_{q=P+1}^{S} \Delta z_{(q)} \tag{4.3}$$

where $\delta_{H(P)}$ is the well-mixed upper portion of cell $k = P$ that is only partially in the surface mixed layer. Thus, it is required that

$$\delta_{H(P)} \leq \Delta z_{(P)} \tag{4.4}$$

We may then consider the existence of a gradient region below the surface-mixing layer that has a length scale of G_η. There are three possible conditions for this gradient region:

$$\begin{array}{rclcll} & & G_\eta + \delta_{H(P)} & \leq & \Delta z_{(P)} & : \text{ gradient in 1 cell} \\ \Delta z_{(P)} & < & G_\eta + \delta_{H(P)} & \leq & \Delta z_{(P)} + \Delta z_{(P-1)} & : \text{ gradient in 2 cells} \\ \Delta z_{(P)} + \Delta z_{(P-1)} & < & G_\eta + \delta_{H(P)} & & & : \text{ gradient in more than 2 cells} \end{array} \tag{4.5}$$

In the first case provided in eq. (4.5), the gradient region and any entrainment/billowing is entirely within the partial mixed-layer grid cell. In the second case, the gradient region extends into the next grid layer, and so may be characterized by a mixing height regions of $h_{B(P)}$ and $h_{T(P-1)}$. In the third case, the gradient region is considered "resolved" by the grid, resulting in the simplest treatment.

4.4 Surface/bottom mixing layer equations

The surface and bottom mixing layer algorithms provide the means of predicting the increase/decrease in the thicknesses of H and G. At the most basic level, H remains constant when turbulent production is exactly balanced by dissipation. H increases when production is greater than dissipation, and decreases when production is less than dissipation. The thickness of G will depend on whether H is actively entraining, holding steady, or decreasing. In the case of an entraining mixed layer, G will decrease as H increases until the shear is sufficient at the base of the mixed layer to develop KH billows (which increases G). When H is holding steady, KH billows may occasionally form and increase G. When H is decreasing, G will increase and eventually become well-resolved by the model grid.

The approach will be to track the "background" TKE, designated (per unit volume) as e_B. This is the TKE that is sustained in the mixing layer. Using scaling arguments, we derive an equilibrium TKE, (e_E) that represents the background TKE that would be expected if production and dissipation are in balance. The extent to which they are out of balance and the time scale of overturns in the mixing layer leads to a rate at which the background TKE increases or decreases. Using this rate of increase/decrease along with the dissipation rate and the rate of mixing energy supplied, we develop an energy balance that predicts the rate of increase/decrease of the mixing layer thickness.

We define the time used for mixing to equilibrium as

$$\Delta t_U = \min\left\{\Delta t,\, C_T T_H\right\} \tag{4.6}$$

where T_H is the eddy turnover time scale, given by

$$T_H = H\sqrt{\frac{\rho}{2e_B}} \tag{4.7}$$

and C_T is the proportion of eddy turnover time scales required to mix the background TKE to equilibrium TKE. The change in background TKE and depth of the mixing layer are given by

$$e_B^{nM} = e_B^n + \Delta t_U \frac{\partial e_B}{\partial t} \tag{4.8}$$

$$H^{nM} = H^n + \Delta t_U \frac{\partial H}{\partial t} \tag{4.9}$$

where the rate of change of the background TKE is found as

$$\frac{\partial e_B}{\partial t} = \frac{e_E - e_B}{C_T H}\sqrt{\frac{2e_B}{\rho}} \tag{4.10}$$

which is obtained as eq. **(F.39)** in Appendix F.5. The equilibrium TKE is computed from

$$e_E = \frac{1}{2}\left\{\rho^{1/2}\frac{\left(1-C_{\varepsilon 2}\right)}{C_{\varepsilon 1}}\frac{\partial E_s}{\partial t}\right\}^{2/3} \tag{4.11}$$

which is derived as eq. **(F.10)** in Appendix F.2, where $\partial E_S / \partial t$ is the rate of water column production for stirring TKE from all sources. The $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are coefficients relating the dissipation rate due to the existing turbulence level and the dissipation rate due to the supply of mixing energy (respectively), see eq. **(F.3)** in Appendix F.1.

The rate of change of the mixed layer depth is found as

$$\frac{\partial H}{\partial t}=\frac{\sqrt{\frac{2}{\rho}}\left\{2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right]-\frac{\sqrt{e_B}}{C_T}\left(e_E-e_B\right)\right\}}{e_B\left(1+2\hbar C_{\varepsilon 3}\right)+\hbar\frac{\rho}{2}\Delta U^2-\hbar g\Delta\rho\frac{H}{2}} \tag{4.12}$$

which is obtained as eq. **(F.42)** in Appendix F.5. The $\Delta\rho$ is computed as in eq. **(F.28)** in Appendix F.4. The coefficient $C_{\varepsilon 3}$ is introduced for dissipation that occurs in the entrainment process in eq. **(F.24)** in Appendix F.3. In eq. (4.12), $\hbar$ is a Heaviside step function, evaluated as

$$\hbar\equiv\begin{cases}1 & : \quad 2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right] \quad > \quad \frac{\sqrt{e_B}}{C_T}\left(e_E-e_B\right)\\ 0 & : \quad 2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right] \quad \leq \quad \frac{\sqrt{e_B}}{C_T}\left(e_E-e_B\right)\end{cases} \tag{4.13}$$

so that $\hbar=1$ only occurs with a positive value of $\partial H/\partial t$ (i.e. deepening of mixed layer). Thus, eqs. (4.10) and (4.12) provide the prediction of the change in the background TKE and the change in the mixed layer thickness.

The following behaviors may be noted for the coefficients in eqs. (4.10) through (4.12) that will control their values:

1. $C_{\varepsilon 1}$ principally affects the equilibrium TKE level. Increasing $C_{\varepsilon 1}$ will increase the dissipation rate of the background TKE and so reduces the equilibrium level of TKE. The value of this coefficient may be able to be set from prior work and arguments, but unity should be a good starting place.

2. $C_{\varepsilon 2}$ affects the dissipation rate associated with the production rate. Note that if $C_{\varepsilon 2}=1$, then all energy production is dissipated before it can cause any stirring, so it will cause $e_E=0$. In contrast, when $C_{\varepsilon 2}=0$, none of the stirring energy is dissipated, so the dissipation rate is only dependent on the background TKE and not the production rate, which leads to the minimum dissipation and the maximum value for e_E. It is not clear how to best set this coefficient, but 0.5 would probably be a good place to start.

3. $C_{\varepsilon 3}$ may be fairly important in entrainment under neutral stability in reducing the rate of deepening. Increasing $C_{\varepsilon 3}$ will reduce the rate of deepening by increasing the dissipation rate in the entrainment process. It is not clear how to best set this coefficient, but probably should start from unity.

4. C_T will increase the time it takes to mix to equilibrium, so will make more energy available for deepening. Arguably this should be set to unity.

4.5 Surface/bottom mixing layer algorithm

The solution of the surface mixing layer proceeds after solution of the convective mixing algorithm so that the convective mixing energy can be included with wind stirring or bottom shear energy in obtaining the value for production,

5 EVOLUTION OF TURBULENT KINETIC ENERGY

5.1 Introduction

Over long time-scales, turbulence tends to a balance between production and dissipation. However, enforcing this equilibrium over a model time step is generally unrealistic. Instead, we track the increase in the local TKE based on scaling of production and dissipation along with the energy consumed in mixing.

5.2 The basic energy balance

The TKE per unit mass is e_k. The dissipation rate per unit mass is ε. The production rate per unit mass is P. The characteristic TKE at an equilibrium condition is e_c. The increase in background potential energy for mixing of thickness δ into a layer of thickness h is given by de_b / dh. An energy balance is then given by

$$\frac{de_k}{dt} = P - \varepsilon - \frac{de_b}{dh}\frac{dh}{dt} \tag{5.1}$$

The dissipation to scales as

$$\varepsilon = \frac{c_\varepsilon}{2}\frac{e_k^{3/2}}{L_\varepsilon} \tag{5.2}$$

The turbulent velocity scale is given by

$$u' \sim e^{1/2} \tag{5.3}$$

A time scale of the turbulence can be defined by

$$\tau_k \sim \frac{L}{u'} = \frac{L}{e_k^{1/2}} \tag{5.4}$$

However, where turbulence is being produced, we might also consider a time scale of

$$\tau_P \sim \left(\frac{L^2}{P}\right)^{1/3} \tag{5.5}$$

If we consider equilibrium to be where $de_k / dt = 0$, then we have

$$\mathcal{P} - \varepsilon - \frac{de_b}{dh}\frac{dh}{dt} = 0 \tag{5.6}$$

Over some small time interval, the mixing energy available is $e_k + \mathcal{P}\Delta t$ the energy dissipated is $\varepsilon\Delta t$. The increase in the background potential energy is Δe_b and the increase in the TKE is Δe_k. The mixing efficiency is given by the ratio of the change in the BPE and the energy used for mixing:

$$R_f = \frac{\Delta e_b}{\mathcal{P}\Delta t - \Delta e_k} \tag{5.7}$$

or, on a rate basis

$$R_f = \frac{\dfrac{de_b}{dt}}{\mathcal{P} - \dfrac{de_k}{dt}} \tag{5.8}$$

or, as a differential equation:

$$\frac{de_b}{dt} = \left(\mathcal{P} - \frac{de_k}{dt}\right)R_f \tag{5.9}$$

We can also write eq. (5.6) for a discrete change of δ as

$$\mathcal{P} - \varepsilon - \frac{\Delta e_b}{\delta}\frac{\delta}{\Delta t} = 0 \tag{5.10}$$

which could be written as

$$\mathcal{P} - \varepsilon - \frac{de_b}{dt} = 0 \tag{5.11}$$

or, using eq. (5.9)

$$\mathcal{P} - \varepsilon - \left(\mathcal{P} - \frac{de_k}{dt}\right)R_f = 0 \tag{5.12}$$

which is rearranged as

$$\left(1 - R_f\right)\mathcal{P} - \varepsilon + R_f\frac{de_k}{dt} = 0 \tag{5.13}$$

Using eq. (5.2), the basic energy balance then becomes

$$\left(1 - R_f\right)\mathcal{P} - \frac{c_\varepsilon}{2}\frac{e_k^{3/2}}{L_\varepsilon} + R_f\frac{de_k}{dt} = 0 \tag{5.14}$$

The above gives is an equation for the rate of change of turbulent kinetic energy as a function of the stratification and the existing TKE.

5.3 TKE at an equilibrium condition

For equilibrium, we have $de_k / dt = 0$ and $e_k = e_c$ and $R_f = R_{fc}$, which allows eq. (5.14) to be written as

$$e_c^{3/2} = \frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1 - R_{fc}\right)P \tag{5.15}$$

or

$$e_c = \left\{\frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1 - R_{fc}\right)P\right\}^{2/3} \tag{5.16}$$

Writing the equilibrium turbulent time scale, from eq. (5.4) as

$$\tau_c \sim \frac{L_{\varepsilon c}}{e_c^{1/2}} \tag{5.17}$$

We have

$$L_{\varepsilon c} \sim e_c^{1/2}\tau_c \tag{5.18}$$

So eq. (5.15) is also written as

$$\frac{e_c^{3/2}}{e_c^{1/2}} = \frac{2\tau_c}{c_\varepsilon}\left(1 - R_{fc}\right)P \tag{5.19}$$

so that the characteristic TKE scale at equilibrium is given by

$$e_c = \left\{\frac{2\tau_c}{c_\varepsilon}\left(1 - R_{fc}\right)P\right\} \tag{5.20}$$

5.4 Modeling the rate of change of TKE

Our model is based on the idea that TKE is tending toward equilibrium. Thus, the difference between the TKE stored and the characteristic equilibrium TKE affects the rate of change of TKE. We can write this as

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau}\left(e_c - e_k\right) \tag{5.21}$$

where c_τ is an empirical coefficient and τ is the shortest time scale of either production or TKE, defined as

$$\tau = \min\left(\tau_P, \tau_k\right) \quad : \quad L > 0 \tag{5.22}$$

or

$$\tau = \min\left(\left[\frac{L^2}{\mathcal{P}}\right]^{1/3}, \frac{L}{e_k^{1/2}}\right) \quad : \quad L > 0 \tag{5.23}$$

Note that as $\mathcal{P} \to 0$, $\tau_P \to \infty$ and as $e_k \to 0$, $\tau_k \to \infty$, so this formulation ensures a finite time scale. For a layer of thickness 'h', the time scale is

$$\tau = \min\left(\left[\frac{h^2}{\mathcal{P}}\right]^{1/3}, \frac{h}{e_k^{1/2}}\right) \quad : \quad h > 0 \tag{5.24}$$

Substituting eq. (5.20) into eq. (5.21) provides

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau}\left(\frac{2}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\tau_c - e_k\right) \tag{5.25}$$

which can be rearranged as

$$\frac{de_k}{dt} = \frac{2c_\tau}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\frac{\tau_c}{\tau} - c_\tau\frac{e_k}{\tau} \tag{5.26}$$

Using eq. (5.17) for the turbulent time scale provides

$$\frac{de_k}{dt} = \frac{2c_\tau}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\frac{L_{\varepsilon c}}{e_c^{1/2}\tau} - c_\tau\frac{e_k}{\tau} \tag{5.27}$$

Note that eq. (5.15) can be written as

$$e_c^{1/2} = \left\{\frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\right\}^{1/3} \tag{5.28}$$

so substituting eq. (5.28) int eq. (5.27) provides

$$\frac{de_k}{dt} = \frac{2c_\tau}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\frac{1}{\left\{\frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1 - R_{fc}\right)\mathcal{P}\right\}^{1/3}}\frac{L_{\varepsilon c}}{\tau} - \frac{c_\tau e_k}{\tau} \tag{5.29}$$

Rearranging results in

$$\frac{de_k}{dt} = \left[\frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1-R_{fc}\right)\mathcal{P}\right]^{2/3}\frac{c_\tau}{\tau} - \frac{c_\tau e_k}{\tau} \tag{5.30}$$

or

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau}\left\{\left[\frac{2L_{\varepsilon c}}{c_\varepsilon}\left(1-R_{fc}\right)\mathcal{P}\right]^{2/3} - e_k\right\} \tag{5.31}$$

For entrainment into a layer of thickness 'h', we approximate

$$L_{\varepsilon c} \sim h \tag{5.32}$$

In contrast to eq. (5.32), we might actually expect that for initiation of turbulence, $L_{\varepsilon c} > h$, i.e. the equilibrium length scale is larger than the existing layer thickness. In decaying turbulence, we might expect that $L_{\varepsilon c} < h$. However, the subtleties would require developing a model that makes $L_{\varepsilon c} = L_{\varepsilon c}(de_k / dt)$, which would require an unknown coefficient. Thus, we will make the simple approximation in eq. (5.32), and note that performance of the model for initiation and decay of turbulence remains a question for investigation.

From the above, the rate of change of TKE is given by

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau}\left\{\left[\frac{2h}{c_\varepsilon}\left(1-R_{fc}\right)\mathcal{P}\right]^{2/3} - e_k\right\} \tag{5.33}$$

where τ is given by eq. (5.24). Eq. (5.33) provides for both increases in e_k and decreases in e_k, depending on the relationship between the production rate ($\mathcal{P}$) and the stored TKE (e_k). Note that the mixing efficiency is at an equilibrium condition (R_{fc}), so can generally be specified as ~ 0.2. The dissipation coefficient can be set as $c_\varepsilon \sim 1.15$ (Spigel et al. 1986). Thus, given the stored TKE (e_k), layer thickness (h) and production rate ($\mathcal{P}$), we can readily compute the rate of change of TKE.

5.5 Mixing for non-stratified system

5.5.1 TKE at equilibrium for non-stratified system

For a non-stratified system, the energy balance is

$$\frac{de_k}{dt} = \mathcal{P} - \varepsilon \tag{5.34}$$

For an equilibrium condition we have

$$\mathcal{P} = \varepsilon \tag{5.35}$$

using eq. (5.2) with the equilibrium TKE

$$P = \frac{c_\varepsilon}{2L_{\varepsilon c}} e_c^{3/2} \tag{5.36}$$

which is manipulated into

$$e_c^{3/2} = \left(\frac{2L_{\varepsilon c}}{c_\varepsilon} P \right) \tag{5.37}$$

Using eq. (5.18) we find

$$e_c^{3/2} = \frac{2e_c^{1/2}\tau_c}{c_\varepsilon} P \tag{5.38}$$

which becomes

$$e_c = \frac{2\tau_c}{c_\varepsilon} P \tag{5.39}$$

We can compare eq. (5.20) to (5.39) and note the only difference is the factor $1 - R_{fc}$ in the former. Thus, the characteristic TKE for non-stratified is consistent with the stratified system using a mixing efficiency of zero.

5.5.2 Rate of change of TKE for non-stratified system

We use eq. (5.21), so that

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau} \left(\frac{2\tau_c}{c_\varepsilon} P - e_k \right) \tag{5.40}$$

We follow the same pattern as eq. (5.25) through (5.33), but obtain a result without the mixing efficiency

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau} \left\{ \left[\frac{2h}{c_\varepsilon} P \right]^{2/3} - e_k \right\} \tag{5.41}$$

Thus, eq. (5.33), is viable for a non-stratified system by setting $R_{fc} = 0$

6 CONCLUSIONS AND RECOMMENDATIONS

The fundamental difficulty for large-scale modeling of Texas estuaries is in episodically developing, maintaining and destroying the localized vertical stratification that leads to hypoxia. Although this research project was not as successful as envisioned in the Statement of Work (see Appendix A), we have layed the foundations for a new approach that may yet prove valuable in developing 3D models of estuaries and lakes. The underlying idea appears to be viable; i.e. use of representative scalars and energy scaling to prevent unphysical vertical mixing. For completeness, the mathematics in this report are fairly dense; however the actual implementation is not beyond the typical complexity of existing hydrodynamic models (see Appendix M).

The principal roadblock encountered in this project was developing a transport algorithm for the cell gradient thickness that does not destabilize the system (see section 1.5.2). We believe that this is not an insurmountable problem. For follow-on work, we recommend considering a research effort that is focused solely on the relationship between the representative scalar and the gradient transport. Our working hypothesis is that the instability arises from one of three sources: 1) the interpolation of velocities to the cell faces for gradient transport, 2) non-conservative (face-based) transport of gradients, or 3) a bug in the code. We believe that isolating the source of the instability can be done by a careful examination of local changes in the representative scalars during the inversion from the transported gradients and average scalars. It is likely that an inconsistency in the numerical formulation will be apparent upon closer examination of this issue. Once the gradient transport issue is solved, the energy scaling and mixing methods developed herein can be readily applied using the algorithm developed in Appendix M.

Appendix A CONTRACT SCOPE OF WORK

Numerical Implementation of an Advanced Vertical Mixing Model

Project Summary:

As part of work recently funded by TWDB and USACE on desalination brine discharge modeling, Dr. Ben Hodges of UT-CRWR developed a new, theoretical vertical mixing model for distributing energy over water-column depths within 3D-hydrodynamic models. This new mixing model attempts to better represent vertical mixing processes that distribute dissolved oxygen, nutrients, and contaminants throughout the water column. Existing vertical mixing algorithms treat individual grid cells as well mixed units, thereby producing potential "stair-stepped" profiles of scalars (salinity, temperature, etc) in the water column. The new vertical mixing theory attempts to smooth such stair-stepped profiles through the allowance of mixing layers between individual grid cells, while at the same time retains mean-value information required for mass-conservation in the hydrodynamic model solution procedure. Hydrodynamic modeling using this new vertical mixing model should provide the following model improvements:

- More accurate representation of the surface mixed layer and benthic boundary layer, including entrainment processes and Kelvin-Helmholtz billows,
- More accurate distribution of wind energy in the water column, thereby producing a more accurate velocity field and scalar transport pathways than achieved using other vertical mixing models,
- More accurate representation of salinity/temperature stratification that may lead to hypoxia. This is critical to properly model the effects of potential (and existing) desalination brine discharges on the benthos.

The recent modeling work performed by Dr. Hodges indicates that all of these improvements may be obtained using the standard Mellor-Yamada vertical mixing model currently employed within models such as EFDC, TX-ELCIRC, and UTBEST3D. However to achieve such improvements, the vertical grid resolution must be increased to levels impractical for typical modeling applications/computers available to TWDB. The vertical mixing model developed and implemented in this project will allow for these above improvements without the needed high-resolution vertical grid, thereby making the modeling practical for TWDB purposes.

Project Tasks:

Task #1: Vertical Mixing Model Theory Development & Refinement

Dr. Hodges will refine the vertical mixing model theory as included in the final report for TWDB contract 2005-001-059. Refinements will be made for clarity and consistency, and additional theoretical development of "meeting processes" between benthic and surface layer mixing processes will be made. TWDB will review and approve the refined model before numerical algorithm development is completed. Dr. Hodges will also select an appropriate name for the new vertical mixing model.

Task #2: Vertical Mixing Model Implementation

Dr. Hodges will implement the new mixing model into TX-ELCIRC (a version of the ELCIRC model already modified by TWDB staff). The mixing module will be developed as a "portable" module, thus providing the ability of implementing the algorithm into other hydrodynamic models with only slight code revision.

Task #3: Algorithm Testing

Dr. Hodges will conduct extensive initial algorithm tests on model test cases developed in consultation with TWDB. Upon achieving satisfactory algorithm performance on the simple test cases, a final test case will be developed incorporating Corpus Christi Bay and the outflow from Oso Bay, TX where thin-layer density stratification has been observed (see figures below). The model setup will be similar to that used in running the EFDC model of the Corpus Christi Bay/Oso Bay system as discussed in the final report for TWDB contract 2005-001-059. The effectiveness of the vertical mixing model will be assessed in comparing results and code performance when TX-ELCIRC is implemented using the Mellor-Yamada vertical mixing model. Comparisons between model simulations using the Mellor-Yamada and new mixing model will be both quantifiable and qualitative. Time and resource permitting, comparisons with output from the EFDC model of the Corpus Christi Bay/Oso Bay system (as discussed in the final report for TWDB contract 2005-001-059) will also be made.

Task #4: Report Development

Dr. Hodges will provide a detailed report of all activities conducted to satisfy tasks #1-#3 listed above. In consultation with TWDB staff, the report will be formatted per TWDB requirements and for publication in a peer-reviewed journal.

Project Timeframe: 1 year (September 1, 2007-August 31, 2007)

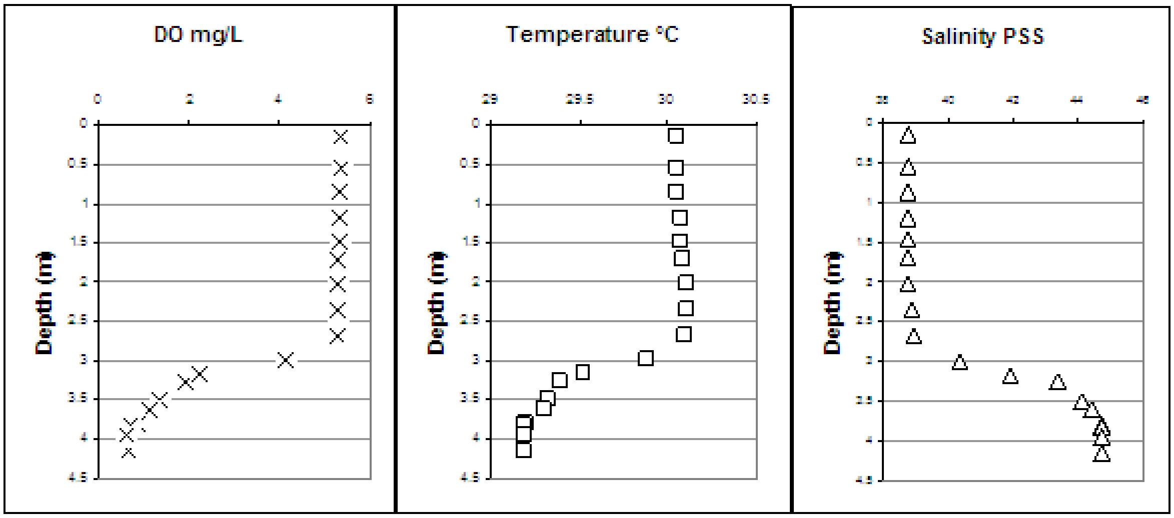


Figure 1 – Field Data from Corpus Christi Bay collected July, 2006. The sharp benthic stratification is not modelable using the Mellor-Yamada vertical mixing model without a prohibitively expensive vertical grid resolution. The vertical mixing model proposed herein should produce better representations of this observed stratification and much coarser (and more practical) vertical grid resolutions. (Figures from Dr. Ben Hodges)

Appendix B VOLUME-BASED DERIVATIONS

B.1 Derivation of the average density in the upper (Top) gradient region of layer k

The average density in an upper (Top) gradient region is analytically defined as

$$\overline{\rho}_{T(k)} = \frac{1}{h_{T(k)}} \int_{h_{T(k)}} \rho_{T(k)} dz \tag{B.1}$$

For a linear gradient, this is

$$\overline{\rho}_{T(k)} = \frac{1}{h_{T(k)}} \int_{0}^{h_{T(k)}} \left\{ \rho_{R(k)} + z \frac{d}{dz} \rho_{T(k)} \right\} dz \tag{B.2}$$

or

$$\overline{\rho}_{T(k)} = \rho_{R(k)} + \frac{1}{h_{T(k)}} \int_{0}^{h_{T(k)}} z \left\{ \frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}} \right\} dz \tag{B.3}$$

or

$$\overline{\rho}_{T(k)} = \rho_{R(k)} + \frac{1}{h_{T(k)}} \left\{ \frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}} \right\} \left\{ \frac{z^2}{2} \right\}_{0}^{h_{T(k)}} \tag{B.4}$$

or

$$\overline{\rho}_{T(k)} = \rho_{R(k)} + \frac{h_{T(k)}}{2} \left\{ \frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}} \right\} \tag{B.5}$$

B.2 Derivation of the average density in a grid cell

Substituting eqs. (2.2) and (2.3) into (2.1) provides

$$\begin{aligned}\overline{\rho}_{(k)} = {} & \frac{1}{\Delta z_{(k)}}\left(\Delta z_{(k)} - h_{T(k)} - h_{B(t)}\right)\rho_{R(k)} \\ & + \frac{1}{\Delta z_{(k)}} h_{T(k)}\left\{\rho_{R(k)} + \frac{h_{T(k)}}{2}\left\{\frac{\rho_{R(k+1)} - \rho_{R(k)}}{h_{T(k)} + h_{B(k+1)}}\right\}\right\} \\ & + \frac{1}{\Delta z_{(k)}} h_{B(k)}\left\{\rho_{R(k)} - \frac{h_{B(k)}}{2}\left\{\frac{\rho_{R(k)} - \rho_{R(k-1)}}{h_{B(k)} + h_{T(k-1)}}\right\}\right\}\end{aligned} \tag{B.6}$$

Regroup the above as

$$\begin{aligned}\Delta z_{(k)}\overline{\rho}_{(k)} = {} & \left(\Delta z_{(k)} - h_{T(k)} - h_{B(t)}\right)\rho_{R(k)} \\ & + h_{T(k)}\rho_{R(k)} + \frac{{h_{T(k)}}^2}{2\left(h_{T(k)} + h_{B(k+1)}\right)}\left\{\rho_{R(k+1)} - \rho_{R(k)}\right\} \\ & + h_{B(k)}\rho_{R(k)} - \frac{{h_{B(k)}}^2}{2\left(h_{B(k)} + h_{T(k-1)}\right)}\left\{\rho_{R(k)} - \rho_{R(k-1)}\right\}\end{aligned} \tag{B.7}$$

Continue regrouping

$$\begin{aligned}\Delta z_{(k)}\overline{\rho}_{(k)} = {} & \left(\Delta z_{(k)} - h_{T(k)} - h_{B(t)}\right)\rho_{R(k)} \\ & + h_{T(k)}\rho_{R(k)} + \frac{{h_{T(k)}}^2}{2\left(h_{T(k)} + h_{B(k+1)}\right)}\rho_{R(k+1)} - \frac{{h_{T(k)}}^2}{2\left(h_{T(k)} + h_{B(k+1)}\right)}\rho_{R(k)} \\ & + h_{B(k)}\rho_{R(k)} - \frac{{h_{B(k)}}^2}{2\left(h_{B(k)} + h_{T(k-1)}\right)}\rho_{R(k)} + \frac{{h_{B(k)}}^2}{2\left(h_{B(k)} + h_{T(k-1)}\right)}\rho_{R(k-1)}\end{aligned} \tag{B.8}$$

or

$$\begin{aligned}\Delta z_{(k)}\overline{\rho}_{(k)} = {} & \left(\Delta z_{(k)} - \cancel{h_{T(k)}} - \cancel{h_{B(t)}} + \cancel{h_{T(k)}} - \frac{{h_{T(k)}}^2}{2\left(h_{T(k)} + h_{B(k+1)}\right)} + \cancel{h_{B(k)}} - \frac{{h_{B(k)}}^2}{2\left(h_{B(k)} + h_{T(k-1)}\right)}\right)\rho_{R(k)} \\ & + \frac{{h_{T(k)}}^2}{2\left(h_{T(k)} + h_{B(k+1)}\right)}\rho_{R(k+1)} \qquad + \frac{{h_{B(k)}}^2}{2\left(h_{B(k)} + h_{T(k-1)}\right)}\rho_{R(k-1)}\end{aligned} \tag{B.9}$$

or

$$\begin{aligned}\overline{\rho}_{(k)} = &\left(1 - \frac{h_{T(k)}{}^{2}}{2\Delta z_{(k)}\left(h_{T(k)} + h_{B(k+1)}\right)} - \frac{h_{B(k)}{}^{2}}{2\Delta z_{(k)}\left(h_{B(k)} + h_{T(k-1)}\right)}\right)\rho_{R(k)} \\ &+ \frac{h_{T(k)}{}^{2}}{2\Delta z_{(k)}\left(h_{T(k)} + h_{B(k+1)}\right)}\rho_{R(k+1)} \qquad + \frac{h_{B(k)}{}^{2}}{2\Delta z_{(k)}\left(h_{B(k)} + h_{T(k-1)}\right)}\rho_{R(k-1)}\end{aligned} \tag{B.10}$$

which is the average density in grid cell 'k' based on the representative densities and layer thicknesses.

B.3 Derivation of entrainment of a lower uniform region into an upper uniform region

We begin with an upper uniform property region of thickness 'h' and an entraining region of uniform properties and thickness δ. The elevation of the bottom of the δ level is $z = b$. The potential energy before mixing is

$$E_{(0)} = g\rho_{\delta(0)} \int_{b}^{b+\delta} z\,dz + g\rho_{h(0)} \int_{b+\delta}^{b+\delta+h} z\,dz \tag{B.11}$$

or

$$E_{(0)} = g\rho_{\delta(0)} \left(\frac{z^2}{2}\right)_{b}^{b+\delta} + g\rho_{h(0)} \left(\frac{z^2}{2}\right)_{b+\delta}^{b+\delta+h} \tag{B.12}$$

or

$$\frac{2E_{(0)}}{g} = \rho_{\delta(0)}\left[\left(b+\delta\right)^2 - b^2\right] + \rho_{h(0)}\left[\left(b+\delta+h\right)^2 - \left(b+\delta\right)^2\right] \tag{B.13}$$

or

$$\frac{2E_{(0)}}{g} = \rho_{\delta(0)}\left[2b\delta + \delta^2\right] + \rho_{h(0)}\left[\cancel{\left(b+\delta\right)^2} + 2\left(b+\delta\right)h + h^2 - \cancel{\left(b+\delta\right)^2}\right] \tag{B.14}$$

or

$$\frac{2E_{(0)}}{g} = \rho_{\delta(0)}\left[2b\delta + \delta^2\right] + \rho_{h(0)}\left[2bh + 2\delta h + h^2\right] \tag{B.15}$$

or

$$\frac{2E_{(0)}}{g} = \rho_{\delta(0)} 2b\delta + \rho_{\delta(0)}\delta^2 + \rho_{h(0)} 2bh + \rho_{h(0)} 2\delta h + \rho_{h(0)} h^2 \tag{B.16}$$

or

$$\frac{2E_{(0)}}{g} = 2b\left(\rho_{\delta(0)}\delta + \rho_{h(0)}h\right) + \rho_{h(0)}h^2 + \rho_{h(0)} 2\delta h + \rho_{\delta(0)}\delta^2 \tag{B.17}$$

Define

$$\Delta\rho \equiv \rho_{h(0)} - \rho_{\delta(0)} \tag{B.18}$$

which provides

$$\rho_{\delta(0)} \equiv \rho_{h(0)} - \Delta\rho \tag{B.19}$$

so that eq. (B.17) can be expanded as

$$\frac{2E_{(0)}}{g} = 2b\left(\left[\rho_{h(0)} - \Delta\rho\right]\delta + \rho_{h(0)}h\right) + \rho_{h(0)}h^2 + \rho_{h(0)} 2\delta h + \left[\rho_{h(0)} - \Delta\rho\right]\delta^2 \tag{B.20}$$

which can be written as

$$\frac{2E_{(0)}}{g} = 2b\left(\rho_{h(0)}\delta + \rho_{h(0)}h\right) + \left(\rho_{h(0)}h^2 + \rho_{h(0)} 2\delta h + \rho_{h(0)}\delta^2\right) - \Delta\rho\delta^2 - 2b\Delta\rho\delta \tag{B.21}$$

or

$$\frac{2E_{(0)}}{g} = 2b\rho_{h(0)}\left(\delta + h\right) + \rho_{h(0)}\left(h^2 + 2\delta h + \delta^2\right) - \Delta\rho\delta\left(\delta + 2b\right) \tag{B.22}$$

or

$$\frac{2E_{(0)}}{g} = 2b\rho_{h(0)}\left(h + \delta\right) + \rho_{h(0)}\left(h + \delta\right)^2 - \Delta\rho\delta\left(\delta + 2b\right) \tag{B.23}$$

The potential energy after mixing is given by

$$E_{(1)} = g\rho_{h(1)} \int_{b}^{b+\delta+h} z\,dz \tag{B.24}$$

or

$$E_{(1)} = g\rho_{h(1)} \left(\frac{z^2}{2}\right)_{b}^{b+\delta+h} \tag{B.25}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(1)}\left[\left(b+\delta+h\right)^2 - \left(b\right)^2\right] \tag{B.26}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(1)}\left[\cancel{b^2} + 2b\left(h+\delta\right) + \left(h+\delta\right)^2 - \cancel{b^2}\right] \tag{B.27}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(1)}\left[2b\left(h+\delta\right) + \left(h+\delta\right)^2\right] \tag{B.28}$$

For conservation, we require

$$\rho_{h(1)}\left(h+\delta\right) = \rho_{h(0)}h + \rho_{\delta(0)}\delta \tag{B.29}$$

or

$$\rho_{h(1)} = \frac{\rho_{h(0)}h + \rho_{\delta(0)}\delta}{\left(h+\delta\right)} \tag{B.30}$$

or

$$\rho_{h(1)} = \frac{\rho_{h(0)}h + \left[\rho_{h(0)} - \Delta\rho\right]\delta}{\left(h+\delta\right)} \tag{B.31}$$

or

$$\rho_{h(1)} = \frac{\rho_{h(0)}h + \rho_{h(0)}\delta - \Delta\rho\delta}{\left(h+\delta\right)} \tag{B.32}$$

or

$$\rho_{h(1)} = \frac{\rho_{h(0)}\left(h+\delta\right) - \Delta\rho\delta}{\left(h+\delta\right)} \tag{B.33}$$

or

$$\rho_{h(1)} = \rho_{h(0)} - \Delta\rho\frac{\delta}{\left(h+\delta\right)} \tag{B.34}$$

So eq. (B.28) is expanded as

$$\frac{2E_{(1)}}{g} = \left[\rho_{h(0)} - \Delta\rho\frac{\delta}{\left(h+\delta\right)}\right]\left[2b\left(h+\delta\right) + \left(h+\delta\right)^2\right] \tag{B.35}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(0)}\left[2b(h+\delta)+(h+\delta)^2\right] - \Delta\rho\frac{\delta}{(h+\delta)}\left[2b(h+\delta)+(h+\delta)^2\right] \tag{B.36}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(0)}2b(h+\delta)+\rho_{h(0)}(h+\delta)^2 - \Delta\rho\frac{\delta}{\cancel{(h+\delta)}}2b\cancel{(h+\delta)} - \Delta\rho\frac{\delta}{\cancel{(h+\delta)}}(h+\delta)^{\cancel{2}} \tag{B.37}$$

or

$$\frac{2E_{(1)}}{g} = \rho_{h(0)}2b(h+\delta)+\rho_{h(0)}(h+\delta)^2 - \Delta\rho 2b\delta - \Delta\rho\delta(h+\delta) \tag{B.38}$$

So the increase in potential energy is given by subtracting eq. (B.38) from eq. (B.28), resulting in

$$\begin{aligned}&\frac{2E_{(1)}}{g}-\frac{2E_{(0)}}{g}\\ &\quad= \cancel{\rho_{h(0)}2b(h+\delta)} + \cancel{\rho_{h(0)}(h+\delta)^2} - \Delta\rho 2b\delta - \Delta\rho\delta(h+\delta)\\ &\quad- \cancel{\rho_{h(0)}2b(h+\delta)} - \cancel{\rho_{h(0)}(h+\delta)^2} + \Delta\rho\delta(\delta+2b)\end{aligned} \tag{B.39}$$

or

$$\frac{2E_{(1)}}{g}-\frac{2E_{(0)}}{g} = -\cancel{\Delta\rho 2b\delta} - \Delta\rho\delta h - \cancel{\Delta\rho\delta^2} + \cancel{\Delta\rho\delta^2} + \cancel{\Delta\rho 2b\delta} \tag{B.40}$$

or

$$\frac{2E_{(1)}}{g}-\frac{2E_{(0)}}{g} = -\Delta\rho\delta h \tag{B.41}$$

or

$$\Delta E_B = -\frac{1}{2}g(\rho_h-\rho_\delta)\delta h \tag{B.42}$$

Units are

$$\Delta E_B = \frac{L}{T^2}\left(\frac{M}{L^3}\right)L^2 = \frac{M}{T^2} \tag{B.43}$$

which is the increase in BPE per unit area (i.e. ML^2T^{-2}/L^2). To get a change per unit mass per unit volume, we divide by the density and the mixing layer thickness

$$\Delta e_B = -\frac{1}{2}g\frac{(\rho_h-\rho_\delta)}{\rho\cancel{h}}\delta\cancel{h} \tag{B.44}$$

where ρ can reasonably be any of the densities. Units are

$$\Delta e_B = \frac{L}{T^2 L} L^2 = \frac{L^2}{T^2} \tag{B.45}$$

which is $\left(ML^2T^{-2}\right)/M$.

The rate of change with increasing thickness is given by

$$\frac{de_B}{d\delta} = -\frac{1}{2} g \frac{\left(\rho_h - \rho_\delta\right)}{\rho_h} \frac{d}{d\delta}(\delta) \tag{B.46}$$

In a more general sense, we can write

$$\frac{de_B}{dh} = -\frac{1}{2} g \left(\frac{\rho_h - \rho_\delta}{\rho_h} \right) \tag{B.47}$$

B.4 Derivation of entrainment of a lower gradient region into an upper uniform region

We begin with an upper uniform property region of thickness 'h' and an entraining region of linear gradient properties and thickness δ. The elevation of the bottom of the δ level is $z = b$. The potential energy before mixing is

$$E_{(0)} = g \int_b^{b+\delta} \rho_\delta(z) z dz + g\rho_{h(0)} \int_{b+\delta}^{b+\delta+h} z dz \tag{B.48}$$

Without a loss of generality, we can take b=0 and write

$$E_{(0)} = g \int_0^{\delta} \rho_\delta(z) z dz + g\rho_{h(0)} \int_{\delta}^{\delta+h} z dz \tag{B.49}$$

If the lower gradient region is continuous with the uniform region, then we can write

$$\rho_\delta(z) = \rho_{h(0)} - \left(\delta - z\right) \frac{d\rho_\delta}{dz} \tag{B.50}$$

Thus we have

$$\int_0^\delta \rho_\delta(z) z dz = \int_0^\delta \rho_{h(0)} dz - \int_0^\delta \delta \frac{d\rho_\delta}{dz} z dz + \int_0^\delta \frac{d\rho_\delta}{dz} z^2 dz \tag{B.51}$$

so that eq. (B.49) can be written as

$$E_{(0)} = g\rho_{h(0)} \int_{\delta}^{\delta+h} z dz + g\int_0^{\delta} \rho_{h(0)} dz - g\int_0^{\delta} \delta \frac{d\rho_\delta}{dz} z dz + g\int_0^{\delta} \frac{d\rho_\delta}{dz} z^2 dz \tag{B.52}$$

or

$$E_{(0)} = g\rho_{h(0)} \int_{0}^{\delta+h} z dz - g\delta \frac{d\rho_\delta}{dz} \int_0^{\delta} z dz + g \frac{d\rho_\delta}{dz} \int_0^{\delta} z^2 dz \tag{B.53}$$

or

$$E_{(0)} = g\rho_{h(0)} \left(\frac{z^2}{2}\right)_0^{\delta+h} - g\delta \frac{d\rho_\delta}{dz} \left(\frac{z^2}{2}\right)_0^{\delta} + g \frac{d\rho_\delta}{dz} \left(\frac{z^3}{3}\right)_0^{\delta} \tag{B.54}$$

or

$$E_{(0)} = \frac{1}{2} g\rho_{h(0)} (h+\delta)^2 - \frac{1}{2} g\delta^3 \frac{d\rho_\delta}{dz} + \frac{1}{3} g\delta^3 \frac{d\rho_\delta}{dz} \tag{B.55}$$

or

$$E_{(0)} = \frac{1}{2} g\rho_{h(0)} (h+\delta)^2 - \frac{1}{6} g \frac{d\rho_\delta}{dz} \delta^3 \tag{B.56}$$

The potential energy after mixing is given by

$$E_{(1)} = g\rho_{h(1)} \int^{\delta+h} z dz \tag{B.57}$$

or

$$E_{(1)} = \frac{1}{2} g\rho_{h(1)} (h+\delta)^2 \tag{B.58}$$

The density after mixing is given by

$$\rho_{h(1)} = \left(\frac{1}{h+\delta}\right) \left\{ \rho_{h(0)} h + \int_0^{\delta} \rho_\delta(z) dz \right\} \tag{B.59}$$

using eq. (B.51), we obtain

$$\rho_{h(1)} = \left(\frac{1}{h+\delta}\right) \left\{ \rho_{h(0)} h + \int_0^{\delta} \rho_{h(0)} dz - \int_0^{\delta} \delta \frac{d\rho_\delta}{dz} dz + \int_0^{\delta} z \frac{d\rho_\delta}{dz} dz \right\} \tag{B.60}$$

or

$$\rho_{h(1)} = \left(\frac{1}{h+\delta}\right)\left\{\rho_{h(0)}h + \rho_{h(0)}\delta - \frac{d\rho_\delta}{dz}\delta\int_0^\delta dz + \frac{d\rho_\delta}{dz}\int_0^\delta z dz\right\} \tag{B.61}$$

or

$$\rho_{h(1)} = \left(\frac{1}{h+\delta}\right)\left\{\rho_{h(0)}\left(h+\delta\right) - \frac{d\rho_\delta}{dz}\delta^2 + \frac{d\rho_\delta}{dz}\frac{\delta^2}{2}\right\} \tag{B.62}$$

or

$$\rho_{h(1)} = \left(\frac{1}{h+\delta}\right)\left\{\rho_{h(0)}\left(h+\delta\right) - \frac{1}{2}\frac{d\rho_\delta}{dz}\delta^2\right\} \tag{B.63}$$

or

$$\rho_{h(1)} = \rho_{h(0)} - \frac{\delta^2}{2\left(h+\delta\right)}\frac{d\rho_\delta}{dz} \tag{B.64}$$

Substituting eq. (B.64) into eq. (B.58) provides

$$E_{(1)} = \frac{1}{2}g\left[\rho_{h(0)} - \frac{\delta^2}{2\left(h+\delta\right)}\frac{d\rho_\delta}{dz}\right]\left(h+\delta\right)^2 \tag{B.65}$$

or

$$E_{(1)} = \frac{1}{2}g\rho_{h(0)}\left(h+\delta\right)^2 - \frac{1}{4}g\delta^2\left(h+\delta\right)\frac{d\rho_\delta}{dz} \tag{B.66}$$

To get the change in energy, we subtract the initial from the final, i.e. eq. (B.56) is subtracted from eq. (B.66) to obtain

$$\begin{aligned} E_{(1)} - E_{(0)} = {} & \cancel{\frac{1}{2}g\rho_{h(0)}\left(h+\delta\right)^2} - \frac{1}{4}g\delta^2\left(h+\delta\right)\frac{d\rho_\delta}{dz} \\ & - \cancel{\frac{1}{2}g\rho_{h(0)}\left(h+\delta\right)^2} + \frac{1}{6}g\frac{d\rho_\delta}{dz}\delta^3 \end{aligned} \tag{B.67}$$

or

$$E_{(1)} - E_{(0)} = -\frac{1}{4}g\delta^2 h\frac{d\rho_\delta}{dz} - \frac{1}{4}g\delta^3\frac{d\rho_\delta}{dz} + \frac{1}{6}g\frac{d\rho_\delta}{dz}\delta^3 \tag{B.68}$$

or

$$E_{(1)} - E_{(0)} = -\frac{1}{4}g\delta^2 h\frac{d\rho_\delta}{dz} - \frac{1}{12}g\frac{d\rho_\delta}{dz}\delta^3 \tag{B.69}$$

or

$$\Delta E_B = -\frac{1}{4} g \delta^2 \frac{d\rho_\delta}{dz} \left\{ h + \frac{1}{3}\delta \right\} \tag{B.70}$$

Units are:

$$\Delta E_B = -\frac{L}{T^2} L^2 \frac{\frac{M}{L^3}}{L} L = \frac{M}{T^2} \tag{B.71}$$

On a per unit mass basis, we divide by $\rho(h + \delta / 3)$. Note that we are assuming δ is small compared to h

$$\Delta e_B = -\frac{1}{4\rho\left\{ h + \frac{1}{3}\delta \right\}} g \delta^2 \frac{d\rho_\delta}{dz} \left\{ h + \frac{1}{3}\delta \right\} \tag{B.72}$$

$$\Delta e_B = -\frac{1}{4\rho} g \delta^2 \frac{d\rho_\delta}{dz} \tag{B.73}$$

where ρ can reasonably be any of the densities. Units are

$$\Delta e_B = \frac{L}{T^2 L} L^2 = \frac{L^2}{T^2} \tag{B.74}$$

which is $\left(ML^2T^{-2}\right) / M$.

We can write eq. (B.73) as

$$\frac{de_B}{d\delta} = -\frac{1}{4\rho} g \frac{d\rho_\delta}{dz} (2\delta) \tag{B.75}$$

or

$$\frac{de_B}{d\delta} = -\frac{1}{2\rho} g \frac{d\rho_\delta}{dz} \delta \tag{B.76}$$

B.5 Layer thickness for non-stratified system with boundary production

For a non-stratified system, eq. (L.5) becomes infinite. Thus, we need a simple scaling for the rate in which it can entrain

$$\frac{dh}{dt} \propto {e_k}^{1/2} \tag{B.77}$$

We might otherwise consider

$$\frac{de_{?}}{dh}\frac{dh}{dt} = P - \varepsilon - \frac{de_{k}}{dt} \qquad \text{(B.78)}$$

where $de_{?} / dh$ is the energy loss associated with entraining fluid over the distance dh. This issue requires further investigation.

Appendix C DERIVATION OF ENTRAINMENT ENERGY

C.1 Potential energy required for entrainment

Let us consider the general case of some energy available form mixing ΔE_m per unit area that is entraining fluid of thickness δ with stable density gradient $\partial\rho(z)/\partial z < 0$. The entrained fluid will be completely mixed in a layer of initial thickness h(t) with density $\rho_m(t)$ and will form a layer of thickness $h+\delta$ with density $\rho_m(t+\Delta t)$. Note that much of the following is not used in the method proposed above. The approach below appears to complicated for simple implementation with the surface mixed-layer approach. However, the fundamentals here are useful to document for future development.

How much energy is required to mix this system at 100% efficiency? For this computation, let us consider z=0 is where the mixing stops. It follows that the potential energy before mixing is

$$E_p(t) = g\rho_m(t)\int_{\delta}^{h+\delta} z\,dz + g\int_0^{\delta}\left\{\bar{\rho} - \left(\frac{\delta}{2} - z\right)\frac{\partial\rho}{\partial z}\right\} z\,dz \tag{C.1}$$

where $\bar{\rho}$ is the average density in the linear region. This could be written as

$$E_p(t) = g\rho_m(t)\int_{\delta}^{h+\delta} z\,dz + g\bar{\rho}\int_0^{\delta} z\,dz - g\frac{\delta}{2}\frac{\partial\rho}{\partial z}\int_0^{\delta} z\,dz + g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \tag{C.2}$$

or

$$E_p(t) = g\rho_m(t)\int_{\delta}^{h+\delta} z\,dz + \left\{g\bar{\rho} - g\frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz + g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \tag{C.3}$$

After mixing, the potential energy is

$$E_p(t+\Delta t) = g\rho_m(t+\Delta t)\int_0^{h+\delta} z\,dz \tag{C.4}$$

The density after mixing is found from

$$\rho_m(t+\Delta t) = \frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta} \tag{C.5}$$

So eq. (C.4) becomes

$$E_p(t+\Delta t) = g\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta}\int_0^{h+\delta} z\,dz \tag{C.6}$$

The energy required for mixing is given by

$$\Delta E_m = E_p(t+\Delta t) - E_p(t) \tag{C.7}$$

or

$$\Delta E_m = g\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta}\int_0^{h+\delta} z\,dz - \left[g\rho_m(t)\int_\delta^{h+\delta} z\,dz + g\left\{\bar{\rho} - \frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz + g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \right] \tag{C.8}$$

Which can be written

$$\begin{aligned} \Delta E_m = {} & g\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta}\int_\delta^{h+\delta} z\,dz + g\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta}\int_0^{\delta} z\,dz \\ & - g\rho_m(t)\int_\delta^{h+\delta} z\,dz - g\left\{\bar{\rho} - \frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz - g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \end{aligned} \tag{C.9}$$

combining terms gives

$$\begin{aligned} \Delta E_m = {} & g\left\{\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta} - \rho_m(t)\right\}\int_\delta^{h+\delta} z\,dz + g\left\{\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta} - \bar{\rho} + \frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz \\ & - g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \end{aligned} \tag{C.10}$$

or

$$\begin{aligned} \Delta E_m = {} & g\left\{\frac{\delta\bar{\rho} + \cancel{h\rho_m(t)} - \cancel{h\rho_m(t)} - \delta\rho_m(t)}{h+\delta}\right\}\int_\delta^{h+\delta} z\,dz \\ & + g\left\{\frac{\cancel{\delta\bar{\rho}} + h\rho_m(t) - \cancel{\delta\bar{\rho}} - h\bar{\rho}}{h+\delta} + \frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz \quad - g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \end{aligned} \tag{C.11}$$

or

$$\begin{aligned} \Delta E_m = {} & g\frac{\delta}{h+\delta}\{\bar{\rho} - \rho_m(t)\}\int_\delta^{h+\delta} z\,dz \\ & + g\left\{\frac{h}{h+\delta}[\rho_m(t) - \bar{\rho}] + \frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\int_0^{\delta} z\,dz \quad - g\frac{\partial\rho}{\partial z}\int_0^{\delta} z^2\,dz \end{aligned} \tag{C.12}$$

We evaluate the integrals as

$$\begin{aligned}\Delta E_m &= g\frac{\delta}{h+\delta}\{\bar{\rho}-\rho_m(t)\}\left[\frac{z^2}{2}\right]_{\delta}^{h+\delta} \\ &\quad + g\left\{\frac{h}{h+\delta}[\rho_m(t)-\bar{\rho}]+\frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\left[\frac{z^2}{2}\right]_0^{\delta} \quad - g\frac{\partial\rho}{\partial z}\left[\frac{z^3}{3}\right]_0^{\delta}\end{aligned} \tag{C.13}$$

Using

$$(h+\delta)^2-(\delta)^2 = h^2+2h\delta+\delta^2-\delta^2 = 2h\left(\frac{h}{2}+\delta\right) \tag{C.14}$$

$$\begin{aligned}\Delta E_m &= g\frac{\delta}{h+\delta}\{\bar{\rho}-\rho_m(t)\}h\left(\frac{h}{2}+\delta\right) \\ &\quad + g\left\{\frac{h}{h+\delta}[\rho_m(t)-\bar{\rho}]+\frac{\delta}{2}\frac{\partial\rho}{\partial z}\right\}\frac{\delta^2}{2} \quad - g\frac{\partial\rho}{\partial z}\frac{\delta^3}{3}\end{aligned} \tag{C.15}$$

or

$$\begin{aligned}\Delta E_m &= g\frac{\delta h}{h+\delta}\left(\frac{h}{2}+\delta\right)[\bar{\rho}-\rho_m(t)] \\ &\quad - g\frac{\delta^2}{2}\left(\frac{h}{h+\delta}\right)[\bar{\rho}-\rho_m(t)] \quad + g\frac{\delta^3}{4}\frac{\partial\rho}{\partial z} - g\frac{\partial\rho}{\partial z}\frac{\delta^3}{3}\end{aligned} \tag{C.16}$$

or

$$\begin{aligned}\Delta E_m &= g\left\{\frac{\delta h}{h+\delta}\left(\frac{h}{2}+\delta\right)-\frac{\delta^2}{2}\left(\frac{h}{h+\delta}\right)\right\}[\bar{\rho}-\rho_m(t)] \\ &\quad + g\frac{\partial\rho}{\partial z}\left\{\frac{\delta^3}{4}-\frac{\delta^3}{3}\right\}\end{aligned} \tag{C.17}$$

or

$$\Delta E_m = g\left\{\frac{1}{2}\frac{\delta h^2}{h+\delta}+\frac{\delta^2 h}{h+\delta}-\frac{1}{2}\frac{\delta^2 h}{h+\delta}\right\}[\bar{\rho}-\rho_m(t)] + g\frac{\partial\rho}{\partial z}\left\{\frac{3\delta^3}{12}-\frac{4\delta^3}{12}\right\} \tag{C.18}$$

or

$$\Delta t_{\delta} \tag{C.19}$$

or the mixing energy required to entrain a density gradient into an existing mixing layer is

$$\partial E_A / \partial t \tag{C.20}$$

It follows that mixing energy must be available at the rate

$$\frac{\Delta E_m}{\Delta t} = g\frac{h\delta}{2\Delta t}\left[\bar{\rho} - \rho_m(t)\right] - \frac{g\delta^3}{12\Delta t}\frac{\partial \rho}{\partial z} \tag{C.21}$$

We could write this as the mixing energy rate that will entrain the gradient layer

$$\frac{\partial E_m}{\partial t} = g\frac{h}{2}\left[\bar{\rho} - \rho_m(t)\right]\frac{\partial \delta}{\partial t} - \frac{g\delta^2}{12}\frac{\partial \rho}{\partial z}\frac{\partial \delta}{\partial t} \tag{C.22}$$

Noting that

$$\delta^2\frac{\partial \delta}{\partial t} = \frac{1}{3}\frac{\partial}{\partial t}\left(\delta^3\right) \tag{C.23}$$

We could write

$$\frac{\partial E_m}{\partial t} = g\frac{h}{2}\left[\bar{\rho} - \rho_m(t)\right]\frac{\partial \delta}{\partial t} - \frac{g}{36}\frac{\partial \rho}{\partial z}\frac{\partial}{\partial t}\left(\delta^3\right) \tag{C.24}$$

As a check, let us compare to the energy that would be required if there the entraining region did not have a density gradient. In which case, the potential energy after mixing is the same, but the potential energy before mixing is

$$\frac{\partial}{\partial t}\rho(z) = -\frac{\alpha(1-\gamma)}{c_p}Q_{r0}k\,e^{-k(\eta - z)} \quad : \quad -\infty < z \leq \eta - \delta_r \tag{C.25}$$

or

$$\begin{aligned} E_p(t) &= g\rho_m(t)\left[\frac{z^2}{2}\right]_{\delta}^{h+\delta} + g\bar{\rho}\left[\frac{z^2}{2}\right]_0^{\delta} \\ &= g\rho_m(t)h\left(\frac{h}{2} + \delta\right) + g\bar{\rho}\frac{\delta^2}{2} \end{aligned} \tag{C.26}$$

It follows that the energy required to mix is

$$\Delta E_m = g\left\{\frac{\delta\bar{\rho} + h\rho_m(t)}{h+\delta}\right\}\frac{1}{2}\left(h+\delta\right)^2 - \left[g\rho_m(t)h\left(\frac{h}{2} + \delta\right) + g\bar{\rho}\frac{\delta^2}{2}\right] \tag{C.27}$$

or

$$\Delta E_m = \frac{1}{2}g\left[\delta\bar{\rho} + h\rho_m(t)\right]\left(h+\delta\right) - g\rho_m(t)\frac{h^2}{2} + -g\rho_m(t)\delta h - g\bar{\rho}\frac{\delta^2}{2} \tag{C.28}$$

or

$$\Delta E_m = \frac{1}{2}g\left\{\delta h\bar{\rho} + \delta^2\bar{\rho} + h^2\rho_m(t) + h\delta\rho_m(t) - h^2\rho_m(t) - 2\rho_m(t)\delta h - \bar{\rho}\delta^2\right\} \tag{C.29}$$

or

$$\Delta E_m = \frac{1}{2} g \left\{ \overline{\rho} \left[\delta h + \cancel{\delta^2} - \cancel{\delta^2} \right] + \rho_m(t) \left[\cancel{h^2} \cancel{+h\delta} - \cancel{h^2} - \cancel{2}\delta h \right] \right\} \tag{C.30}$$

or, the energy required to entrain a uniform density layer is

$$\Delta E_m = g \frac{\delta h}{2} \{ \overline{\rho} - \rho_m(t) \} \tag{C.31}$$

which is only different from eq. (C.20) by the δ^3 term. So we have confidence in the derivation for the mixing energy required to entrain a density gradient.

C.2 Entrainment layer thickening

C.2.i Basic theory for entrainment layer thickening

Note that the above requires mixing energy to be supplied at the rate

$$\frac{\partial E_m}{\partial t} = g \frac{h}{2} \{ \overline{\rho} - \rho_m(t) \} \frac{\partial \delta}{\partial t} \tag{C.32}$$

Which can be written as

$$\frac{\partial \delta}{\partial t} = \frac{2}{gh\{ \overline{\rho} - \rho_m(t) \}} \frac{\partial E_m}{\partial t} \tag{C.33}$$

We consider a mixing layer at time (t) with a thickness (h). The deepening of the mixing layer is given by eq. (C.33). Thus we step successively through the grid cells. For example, let us consider a model grid with uniform Δz_k values except for the free surface (which is $\Delta z_{k\max}$). At time 't', the mixing layer thickness is h(t), which puts the entrainment in grid layer 'n', where

$$\sum_{i=n}^{k\max} \Delta z_i < h(t) < \sum_{i=n-1}^{k\max} \Delta z_i \tag{C.34}$$

So the fraction of the entraining grid cell occupied by the mixing layer is

$$\delta_m = h(t) - \sum_{i=n}^{k\max} \Delta z_i \tag{C.35}$$

For mass balance consistency, the average density in the entraining grid cell is given by the $\overline{\rho}_n$ value that is carried as the grid cell density. If we consider the grid cell partially full of the mixed layer fluid, it follows that

$$\overline{\rho}_n = \frac{1}{\Delta z_n} \left\{ \tilde{\rho}_n [\Delta z_n - \delta_m] + \rho_m \delta_m \right\} \tag{C.36}$$

where $\tilde{\rho}_n$ is the fluid in cell 'n' that may still be entrained. Solving for this we have

$$\tilde{\rho}_n = \frac{\overline{\rho}_n \Delta z_n - \rho_m \delta_m}{\Delta z_n - \delta_m} \tag{C.37}$$

We then represent the rate of entrainment as

$$\frac{\partial \delta}{\partial t} = \frac{2}{gh\left\{\tilde{\rho}_n - \rho_m(t)\right\}} \frac{\partial E_m}{\partial t} \tag{C.38}$$

or

$$\frac{\partial \delta}{\partial t} = \frac{2}{gh\left\{\dfrac{\overline{\rho}_n \Delta z_n - \rho_m \delta_m}{\Delta z_n - \delta_m} - \rho_m\right\}} \frac{\partial E_m}{\partial t} \tag{C.39}$$

or

$$\frac{\partial \delta}{\partial t} = \frac{2}{gh\left\{\dfrac{\overline{\rho}_n \Delta z_n - \rho_m \Delta z_n}{\Delta z_n - \delta_m}\right\}} \frac{\partial E_m}{\partial t} \tag{C.40}$$

or

$$\frac{\partial \delta}{\partial t} = \frac{2\left(\Delta z_n - \delta_m\right)}{gh\Delta z_n\left(\overline{\rho}_n - \rho_m\right)} \frac{\partial E_m}{\partial t} \tag{C.41}$$

C.2.ii Application of entrainment layer thickening

As demonstrated above the rate at which a mixing layer (h) that is entraining in grid layer ‘n’, deepens for the grid cell of average density $\overline{\rho}_n$ and a mixing layer density of ρ_m, can be found from the with the rate of supply of mixing energy (per unit area), $\partial E_m / \partial t$ as

$$\frac{\partial \delta}{\partial t} = \frac{2\left(\Delta z_n - \delta_m\right)}{gh\Delta z_n\left(\overline{\rho}_n - \rho_m\right)} \frac{\partial E_m}{\partial t} \tag{C.42}$$

where the mixing layer thickness is h(t), which puts the entrainment in grid layer ‘n’, where

$$\sum_{i=n}^{k\max} \Delta z_i < h(t) < \sum_{i=n-1}^{k\max} \Delta z_i \tag{C.43}$$

So the fraction of the entraining grid cell occupied by the mixing layer is

$$\delta_m = h(t) - \sum_{i=n}^{k\max} \Delta z_i \tag{C.44}$$

The above forms the basis for deepening the surface mixing layer. Assuming that $\partial E_m / \partial t > 0$ we can write

$$\delta = h(t+\Delta t) - h(t) = \frac{2\Delta t\left(\Delta z_n - \delta_m\right)}{gh\Delta z_n\left(\overline{\rho}_n - \rho_m\right)} \frac{\partial E_m}{\partial t} \tag{C.45}$$

It is required that

$$\delta \leq \Delta z_n - \delta_m \tag{C.46}$$

If the above condition is not met, we set

$$\delta = \Delta z_n - \delta_m \tag{C.47}$$

and consider that only a portion of the time step was used in this mixing, Δt_u, so the mixing behavior is obtained by substituting eq. (C.47) into the LHS of (C.45) and recognizing that the Δt is replaced by $\Delta_u t$ when only a portion of the time step is required to mix the grid cell:

$$\Delta z_n - \delta_m = \frac{2\left(\Delta t_u\right)\left(\Delta z_n - \delta_m\right)}{gh\Delta z_n\left(\overline{\rho}_n - \rho_m\right)} \frac{\partial E_m}{\partial t} \tag{C.48}$$

so

$$\Delta t_u = \frac{g}{2} h\Delta z_n\left(\overline{\rho}_n - \rho_m\right)\left(\frac{\partial E_m}{\partial t}\right)^{-1} \tag{C.49}$$

We can then define the time remaining as

$$\Delta t_r = \Delta t - \Delta t_u \tag{C.50}$$

The new density will be

$$\rho_m\left(t+\Delta t_u\right) = \frac{\delta\tilde{\rho} + h\rho_m}{h+\delta} \tag{C.51}$$

where $\tilde{\rho}_n$ is the density of the fluid in cell 'n' that was entrained, and is required to meet the average density of that cell when partitioned with the mixing layer, i.e.

$$\tilde{\rho}_n = \frac{\overline{\rho}_n \Delta z_n - \rho_m \delta_m}{\Delta z_n - \delta_m} \tag{C.52}$$

from which it follows that

$$\rho_m\left(t+\Delta t_u\right) = \frac{\delta\left(\dfrac{\overline{\rho}_n \Delta z_n - \rho_m \delta_m}{\Delta z_n - \delta_m}\right) + h\rho_m}{h+\delta} \tag{C.53}$$

or

$$\rho_m\left(t+\Delta t_u\right)=\frac{1}{h+\delta}\left\{h\rho_m+\frac{\delta\left(\bar{\rho}_n\Delta z_n-\rho_m\delta_m\right)}{\Delta z_n-\delta_m}\right\} \tag{C.54}$$

If the entire grid layer entrains and still has time remaining (i.e. $\Delta t_r > 0$), we then increment to the next grid cell down (n-1) and compute a δ from a modification of eq. (C.45)

$$\delta=\frac{2\left(\Delta t_r\right)\left(\Delta z_{n-1}-\delta'_m\right)}{gh'\Delta z_{n-1}\left(\bar{\rho}_{n-1}-\rho'_m\right)}\frac{\partial E_m}{\partial t} \tag{C.55}$$

where Δt_r is used in place of Δt and the primes indicate that the terms are updated to $t+\Delta t_u$. Using this approach, we can sweep down through the domain until all the time is used.

Appendix D MIXING BY K-H BILLOWS

D.1 Shear mixing by Kelvin-Helmholtz billows using the ELCOM approach

D.1.i Overview

The maximum amount of mixing energy released by shear can be computed by the difference between the kinetic energy of the shear layer before mixing and the kinetic energy of the shear layer after mixing. That is, if you take two layers of different velocities and mix them together, the mixed velocity will have a lower kinetic energy than in the original two layers. This process is generally seen in free shear flows through K-H billows. It is typically argued that only about 20% of the energy available through the mixing of momentum is typically effective at mixing density.

D.1.ii Kinetic energy change for arbitrary thickness layers in 1D

We will derive the shear term based on two arbitrary thickness layers, (1) and (2) with uniform velocities. For simplicity, let us consider only the kinetic energy in the ‘x’ direction. For an unmixed system

$$E_{ku} = \frac{1}{2}\rho_1 h_1 \left(U_1^{\,2}\right) + \frac{1}{2}\rho_2 h_2 \left(U_2^{\,2}\right) \tag{D.1}$$

For the mixed system we have

$$E_{km} = \frac{1}{2}\rho_m h_m \left(U_m^{\,2}\right) \tag{D.2}$$

The change in E_k is

$$E_{km} - E_{ku} = \frac{1}{2}\rho_m h_m \left(U_m^{\,2}\right) - \frac{1}{2}\rho_1 h_1 \left(U_1^{\,2}\right) - \frac{1}{2}\rho_2 h_2 \left(U_2^{\,2}\right) \tag{D.3}$$

We note that conservation of mass between the mixed and the unmixed systems requires

$$\rho_m h_m = \rho_1 h_1 + \rho_2 h_2 \tag{D.4}$$

Furthermore, conservation of momentum requires that

$$\rho_m h_m U_m = \rho_1 h_1 U_1 + \rho_2 h_2 U_2 \tag{D.5}$$

It follows that

$$\rho_m h_m \left(U_m{}^2\right) = \left(\rho_1 h_1 + \rho_2 h_2\right)\left(\frac{\rho_1 h_1 U_1 + \rho_2 h_2 U_2}{\rho_1 h_1 + \rho_2 h_2}\right)^2 = \frac{\left(\rho_1 h_1 U_1 + \rho_2 h_2 U_2\right)^2}{\rho_1 h_1 + \rho_2 h_2} \tag{D.6}$$

So eq. (D.3) could be written over a common denominator as

$$\left(E_{km} - E_{ku}\right) = \frac{\left(\rho_1 h_1 U_1 + \rho_2 h_2 U_2\right)^2 - \left(\rho_1 h_1 + \rho_2 h_2\right)\left\{\rho_1 h_1\left(U_1{}^2\right) + \rho_2 h_2\left(U_2{}^2\right)\right\}}{2\left(\rho_1 h_1 + \rho_2 h_2\right)} \tag{D.7}$$

Expanding the numerator

$$\begin{aligned}
&\left(\rho_1 h_1 U_1 + \rho_2 h_2 U_2\right)^2 - \left(\rho_1 h_1 + \rho_2 h_2\right)\left\{\rho_1 h_1\left(U_1{}^2\right) + \rho_2 h_2\left(U_2{}^2\right)\right\} \\
&= \cancel{\left(\rho_1 h_1 U_1\right)^2} + 2\rho_1 h_1 U_1 \rho_2 h_2 U_2 + \cancel{\left(\rho_2 h_2 U_2\right)^2} - \cancel{\left(\rho_1 h_1 U_1\right)^2} \\
&\qquad - \rho_2 h_2 \rho_1 h_1\left(U_1{}^2\right) - \rho_1 h_1 \rho_2 h_2\left(U_2{}^2\right) - \cancel{\left(\rho_2 h_2 U_2\right)^2} \\
&= +2\rho_1 h_1 \rho_2 h_2 U_1 U_2 - \rho_2 h_2 \rho_1 h_1\left(U_1{}^2\right) - \rho_1 h_1 \rho_2 h_2\left(U_2{}^2\right) \\
&= -\left(\rho_1 \rho_2 h_1 h_2\right)\left\{U_1{}^2 - 2U_1 U_2 + U_2{}^2\right\}
\end{aligned} \tag{D.8}$$

So eq. (D.7) can be written as

$$\left(E_{km} - E_{ku}\right) = \frac{-\left(\rho_1 \rho_2 h_1 h_2\right)\left(U_1 - U_2\right)^2}{2\left(\rho_1 h_1 + \rho_2 h_2\right)} \tag{D.9}$$

D.1.iii Kinetic energy change for arbitrary thickness layers in 2D

Now consider the more general

$$E_{ku} = \frac{1}{2}\rho_1 h_1\left(U_1{}^2 + V_1{}^2\right) + \frac{1}{2}\rho_2 h_2\left(U_2{}^2 + V_2{}^2\right) \tag{D.10}$$

$$E_{km} = \frac{1}{2}\rho_m h_m\left(U_m{}^2 + V_m{}^2\right) \tag{D.11}$$

The change in E_k is

$$E_{km} - E_{k1} = \frac{1}{2}\rho_m h_m\left(U_m{}^2 + V_m{}^2\right) - \frac{1}{2}\rho_1 h_1\left(U_1{}^2 + V_1{}^2\right) - \frac{1}{2}\rho_2 h_2\left(U_2{}^2 + V_2{}^2\right) \tag{D.12}$$

Conservation of mass still requires

$$\rho_m h_m = \rho_1 h_1 + \rho_2 h_2 \tag{D.13}$$

Momentum must be conserved separately in each direction

$$\rho_m h_m U_m = \rho_1 h_1 U_1 + \rho_2 h_2 U_2 \tag{D.14}$$

$$\rho_m h_m V_m = \rho_1 h_1 V_1 + \rho_2 h_2 V_2 \tag{D.15}$$

So we obtain both

$$\rho_m h_m \left(U_m{}^2 \right) = \left(\rho_1 h_1 + \rho_2 h_2 \right) \left(\frac{\rho_1 h_1 U_1 + \rho_2 h_2 U_2}{\rho_1 h_1 + \rho_2 h_2} \right)^2 = \frac{\left(\rho_1 h_1 U_1 + \rho_2 h_2 U_2 \right)^2}{\rho_1 h_1 + \rho_2 h_2} \tag{D.16}$$

$$\rho_m h_m \left(V_m{}^2 \right) = \left(\rho_1 h_1 + \rho_2 h_2 \right) \left(\frac{\rho_1 h_1 V_1 + \rho_2 h_2 V_2}{\rho_1 h_1 + \rho_2 h_2} \right)^2 = \frac{\left(\rho_1 h_1 V_1 + \rho_2 h_2 V_2 \right)^2}{\rho_1 h_1 + \rho_2 h_2} \tag{D.17}$$

So eq. (D.12)

$$\begin{aligned}\left(E_{km} - E_{ku} \right) = \frac{1}{2\left(\rho_1 h_1 + \rho_2 h_2 \right)} \Big[& \left(\rho_1 h_1 U_1 + \rho_2 h_2 U_2 \right)^2 \\ & - \left(\rho_1 h_1 + \rho_2 h_2 \right) \left\{ \rho_1 h_1 \left(U_1{}^2 \right) + \rho_2 h_2 \left(U_2{}^2 \right) \right\} \\ & \left(\rho_1 h_1 V_1 + \rho_2 h_2 V_2 \right)^2 \\ & - \left(\rho_1 h_1 + \rho_2 h_2 \right) \left\{ \rho_1 h_1 \left(V_1{}^2 \right) + \rho_2 h_2 \left(V_2{}^2 \right) \right\} \Big]\end{aligned} \tag{D.18}$$

The pieces must expand just the same, so without further messing around we can simply write

$$\left(E_{km} - E_{ku} \right) = -\frac{\left(\rho_1 \rho_2 h_1 h_2 \right) \left(U_1 - U_2 \right)^2}{2\left(\rho_1 h_1 + \rho_2 h_2 \right)} - \frac{\left(\rho_1 \rho_2 h_1 h_2 \right) \left(V_1 - V_2 \right)^2}{2\left(\rho_1 h_1 + \rho_2 h_2 \right)} \tag{D.19}$$

or

$$\left(E_{km} - E_{ku} \right) = -\frac{\rho_1 \rho_2 h_1 h_2}{2\left(\rho_1 h_1 + \rho_2 h_2 \right)} \left\{ \left(U_1 - U_2 \right)^2 + \left(V_1 - V_2 \right)^2 \right\} \tag{D.20}$$

or, more simply

$$\left(E_{km} - E_{ku} \right) = -\frac{\rho_1 \rho_2 h_1 h_2}{2\left(\rho_1 h_1 + \rho_2 h_2 \right)} \left\{ \Delta U^2 + \Delta V^2 \right\} \tag{D.21}$$

This could be written as

$$\begin{aligned}\frac{\left(\rho_1 h_1+\rho_2 h_2\right)}{\rho_1\rho_2 h_1 h_2} &= \frac{\cancel{\rho_1 h}_1}{\cancel{\rho_1}\rho_2\,\cancel{h_1}h_2}+\frac{\cancel{\rho_2 h_2}}{\rho_1\,\cancel{\rho_2}\,h_1\,\cancel{h_2}}\\ &=\frac{1}{\rho_2 h_2}+\frac{1}{\rho_1 h_1}\\ &=\frac{{}^{1}\!\big/\!{}_{\rho_1 h_2}}{\left(\frac{\rho_1}{\rho_1}+\frac{\Delta\rho}{\rho_1}\right)}+\frac{1}{\rho_1 h_1}\\ &=\frac{1}{\rho_1 h_2}+\frac{1}{\rho_1 h_1}+O\left(\Delta\rho^2\right)\\ &\approx\frac{h_1+h_2}{\rho_1 h_1 h_2}+O\left(\Delta\rho^2\right)\end{aligned} \tag{D.22}$$

So we can write eq. (D.21) as

$$\left(E_{km}-E_{ku}\right)=-\frac{\rho_1 h_1 h_2}{2\left(h_1+h_2\right)}\left\{\Delta U^2+\Delta V^2\right\} \tag{D.23}$$

Note that if $h_1 = h_2 = 2\Delta z$ We arrive at

$$\left(E_{km}-E_{ku}\right)=-\frac{\rho_1\Delta z}{2}\left\{\Delta U^2+\Delta V^2\right\} \tag{D.24}$$

which is the basis of the shear parameterization in Hodges et al (2000) and prior work.

D.2 Rate of energy production using the K-H time scale for arbitrary thickness layers

As a total rate of energy production, we can write

$$\frac{\partial E_k}{\partial t}=-\frac{\left(E_{km}-E_{ku}\right)}{T_{kh}}=\frac{\rho_1 h_1 h_2}{2T_{kh}\left(h_1+h_2\right)}\left\{\Delta U^2+\Delta V^2\right\} \tag{D.25}$$

where T_{kh} is the time-scale of shear production and we have applied eq. (D.23) for the energy change based on complete mixing of two layers. We use the time-scale for K-H billows (Thorpe, 1973, as used by Laval et al. 2003).

$$T_{kh}=\frac{20}{g'}\sqrt{\Delta U^2+\Delta V^2} \tag{D.26}$$

where

$$g' = g\frac{\rho_2 - \rho_1}{\rho_1} \tag{D.27}$$

Thus,

$$\frac{\partial E_k}{\partial t} = \frac{g\left(\rho_2 - \rho_1\right)\cancel{\rho_1}\, h_1 h_2}{2(20)\cancel{\rho_1}\left(h_1 + h_2\right)}\sqrt{\Delta U^2 + \Delta V^2} \tag{D.28}$$

Note that we could write this as

$$\frac{\partial E_k}{\partial t} = \frac{1}{2}\left(\frac{g\Delta\rho\, h_1 h_2}{20\left(h_1 + h_2\right)}\right)\sqrt{\Delta U^2 + \Delta V^2} \tag{D.29}$$

If we use a coefficient C_S to represent the efficiency of shear production, we can write the linear rate that energy is made available for mixing through shear associated with two layers over the time $t_0 < t < t_0 + T_{kh}$

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{C_S\, g\Delta\rho\, h_1 h_2}{20\,\left(h_1 + h_2\right)}\right)\sqrt{\Delta U^2 + \Delta V^2} \tag{D.30}$$

Note that if $\Delta t \geq T_{kh}$, then the shear production from a single billow collapse is

$$\Delta t\frac{\partial E_S}{\partial t} = T_{kh}\frac{1}{2}\left(\frac{C_S g\Delta\rho\, h_1 h_2}{20\left(h_1 + h_2\right)}\right)\sqrt{\Delta U^2 + \Delta V^2} \tag{D.31}$$

However, if $\Delta t < T_{kh}$

$$\Delta t\frac{\partial E_S}{\partial t} = \Delta t\frac{1}{2}\left(\frac{C_S g\Delta\rho\, h_1 h_2}{20\left(h_1 + h_2\right)}\right)\sqrt{\Delta U^2 + \Delta V^2} \tag{D.32}$$

D.3 K-H billows using a parameterization from Sherman et al. (1978)

D.3.i Energy production using uniform layers and Sherman et al (1978)

Unfortunately, simple implementation of eq. (D.30) the above makes the mixing fundamentally dependent on the definition of the h_1 and h_2 thicknesses. If we use the grid cells for these, then the mixing will inherently be grid-dependent. Instead, let consider that Sherman et al. (1978) gave a length scale for the interface after billowing of

$$\delta_b = \frac{0.3\Delta U^2}{g'} \tag{D.33}$$

If we let

$$h_1 = h_2 = \frac{\delta_b}{2} \tag{D.34}$$

Then eq. (D.30) becomes

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left[\frac{C_S}{20}\frac{g\Delta\rho\left(\delta_b\right)^2}{4\left(\delta_b\right)}\right]\sqrt{\Delta U^2 + \Delta V^2} \tag{D.35}$$

or

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{C_S}{80}g\Delta\rho\,\delta_b\right)\sqrt{\Delta U^2 + \Delta V^2} \tag{D.36}$$

or

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{C_S}{80}g\Delta\rho\frac{0.3}{g'}\right)\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.37}$$

or

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{C_S}{80}g\Delta\rho\frac{0.3\rho_0}{g\Delta\rho}\right)\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.38}$$

or

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{3C_S}{800}\rho_0\right)\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.39}$$

Note that if $\Delta t \geq T_{kh}$, then the shear production for collapse of a single billow is

$$\Delta t\frac{\partial E_S}{\partial t} = \frac{1}{2}T_{kh}\frac{3C_S}{800}\rho_0\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.40}$$

However, if $\Delta t < T_{kh}$ then a full billow is not collapsed, and linear approximation is

$$\Delta t\frac{\partial E_S}{\partial t} = \frac{1}{2}\Delta t\frac{3C_S}{800}\rho_0\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.41}$$

The above equation could be a basic approximation of the rate that energy is made available for mixing due to shear. To generalize this approach, let us write this as

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} C_T C_S \rho_0 \left(\Delta U^2 + \Delta V^2 \right)^{3/2} \quad : \quad t \leq T_{kh} \tag{D.42}$$

where C_T is the coefficient that results from use of the Thorpe time scale and the Sherman approximation of interface thickness

$$C_T \sim 3.75 \times 10^{-3} \tag{D.43}$$

D.3.ii Energy production based on fully-mixed layer thickness for a given shear

As another approach, let us go back to eq. (D.25), but write for $h_1 = h_2 = h/2$ and then include the mixing efficiency to write

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} C_S \frac{\rho_1 h}{4 T_{kh}} \left\{ \Delta U^2 + \Delta V^2 \right\} \tag{D.44}$$

In notes for CE380S (need to put into appendix), I demonstrate that

$$h \leq \frac{1}{2g'} C_S \Delta U^2 \tag{D.45}$$

This is based upon matching the energy produced by mixing (i.e. the fraction C_S) with the potential energy required to mix when starting from two layers with different velocities and densities and mixing into a single layer of uniform density and viscosity. If we use the maximum possible thickness from eq. (D.45), we can write

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} \frac{\rho_1}{8 g' T_{kh}} {C_S}^2 \left\{ \Delta U^2 + \Delta V^2 \right\}^2 \tag{D.46}$$

Using

$$T_{kh} = \frac{20}{g'} \sqrt{\Delta U^2 + \Delta V^2} \tag{D.47}$$

we obtain

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} \left(\frac{\rho_1}{160} {C_S}^2 \right) \frac{\left\{ \Delta U^2 + \Delta V^2 \right\}^2}{\sqrt{\Delta U^2 + \Delta V^2}} \tag{D.48}$$

or

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} \left(\frac{\rho_1}{160} {C_S}^2 \right) \left\{ \Delta U^2 + \Delta V^2 \right\}^{3/2} \tag{D.49}$$

If we use $C_S \sim 1/5$ we obtain

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{\rho_1}{800} C_S\right)\left\{\Delta U^2 + \Delta V^2\right\}^{3/2} \tag{D.50}$$

which is 1/3 of

$$\frac{\partial E_S}{\partial t} = \frac{1}{2}\left(\frac{3\rho_0}{800} C_S\right)\left(\Delta U^2 + \Delta V^2\right)^{3/2} \tag{D.51}$$

obtained using Sherman's approximation in eq. (D.41). Thus both approaches obtain energy approximations of similar magnitude. It is reasonable that Sherman's approach predicts more energy released because the final state is a linear profile of density rather than a uniform density. Producing the uniform density, i.e. eq. (D.50) requires more mixing energy than producing the linear profile, i.e. eq. (D.51). Thus, it might be reasonable to write the general case as

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} C_T C_S \left\{\Delta U^2 + \Delta V^2\right\}^{3/2} \quad : \quad t < T_{kh} \quad \text{and} \quad 1.25\times10^{-3} \le C_T \le 3.75\times10^{-3} \tag{D.52}$$

Alternatively, we might take eq. (D.49) as the key equation and write

$$\frac{\partial E_S}{\partial t} = \frac{1}{2} C_H C_S{}^2 \rho_0 \left(\Delta U^2 + \Delta V^2\right)^{3/2} \quad : \quad t < T_{kh} \quad \text{and} \quad C_H \sim 6.25\times10^{-3} \tag{D.53}$$

Note that eq. (D.51) may overstate the energy available for mixing since it is based on an E_k that is calculated from complete mixing of momentum to a uniform value across the mixing layer rather than to a gradient. In appendices, sections L.3 and 0, I look at what it requires to parameterize shear mixing from two uniform velocity layers into a linear velocity distribution, but the derivation is a mess and doesn't seem usable. Thus, it would seem like either eq. (D.53) is preferred, or eq. (D.52) with a low value for C_T.

D.4 Thoughts on application of shear mixing for K-H billows

D.4.i General considerations

The basic approach to shear will be to look at the boundary between each layer in a water column and separately compute the energy available, using eq. (D.41) or (D.40), depending on the time scale.

Note that if $\Delta t < T_{kh}$, then we may need to do multiple sweeps. That is, one can imagine the case where there exists multiple K-H billow layers, e.g., a mixing layer at the boundary k-1/2 and another mixing layer between k+3/2. After the mixing across these two boundaries, occurring over time $T_1 = \mathrm{Max}\left(T_{kh(k+1/2)}, T_{kh(k+3/2)}\right)$, there now may be sufficient shear across boundary k+1/2 to cause mixing. We would now need to apply eq. (D.40) to boundary k+1/2 if

$$\Delta t \geq T_1 + T_{2(k+1/2)} \tag{D.54}$$

or we would apply eq. (D.41) if inequality (D.54) is not met. An alternative way of writing this would be to consider

$$\Delta t_{r2(k+1/2)} = \Delta t - T_1 \tag{D.55}$$

and the equivalent criterion is then

$$\Delta t_r \geq T_{2(k+1/2)} \tag{D.56}$$

The sweeps through the domain for K-H billow mixing should be done separately from other mixing routines and should be based upon the T_{kh} at the individual grid cell boundaries. That is, rather than sweeping surface down through the domain, and adding the K-H billow mixing energy to the other mixing energy (as in Hodges et al. 2000, or Laval et al., 2003), we compute the T_{kh} at each grid cell boundary and start mixing from the shortest T_{kh} and move to successively longer T_{kh}. All short T_{kh} (i.e. $\Delta t \geq T_{kh}$) should be done before any long T_{kh} (i.e. $\Delta t < T_{kh}$) is completed.

D.4.ii Is the stuff in sections D.1 to D.3 useful or necessary?

Note the above does seem to have a bit of a circular argument. That is, we compute the kinetic energy released by shear mixing using an approximation developed by Sherman, then we use that energy to vertically mix fluid. Why not simply use the Sherman approach directly? That is, let us begin from two ideas the time scale of billowing

$$T_{kh} = \frac{20}{g'}\sqrt{\Delta U^2 + \Delta V^2} \tag{D.57}$$

and the thickness of the linear layer after collapse.

$$\delta_b = \frac{0.3\Delta U^2}{g'} \tag{D.58}$$

Both T_{kh} and δ_b are directly calculable at the interface between any two grid cells.

We assume that in layer ‘2’ (below) and layer ‘1’ above, the velocity is uniform with values of U_2 and U_1. Similarly, we presume uniform densities of ρ_2 and ρ_1, or for that matter, any species ϕ. If Sherman et al. (1978) is deemed to hold, then the mixing of species over the distance δ_b is required to meet

$$\phi(z) = \frac{\phi_1 + \phi_2}{2} + \left(\phi_1 - \phi_2\right)\frac{\left(z - z_i\right)}{\delta_b} \tag{D.59}$$

where z_i is the z value of the original interface between the layers. Thus, when $z = z_i + \delta_b / 2$ we obtain $\phi(z_i + \delta_b / 2) = \phi_1$. Similarly, when $z = z_i - \delta_b / 2$ we obtain $\phi(z_i - \delta_b / 2) = \phi_2$. For simplicity, let us consider a local coordinate system where $z'(0) = z_i$, so that

$$\phi(z') = \frac{\phi_1 + \phi_2}{2} + \left(\phi_1 - \phi_2\right)\frac{z'}{\delta_b} \tag{D.60}$$

or

$$\phi(z') = \overline{\phi} + \Delta\phi\frac{z'}{\delta_b} \tag{D.61}$$

where

$$\overline{\phi} = \frac{1}{2}\left(\phi_1 + \phi_2\right) \tag{D.62}$$

and

$$\Delta\phi = \left(\phi_1 - \phi_2\right) \tag{D.63}$$

If layer thickness' are given as Δz, and we meet the condition that $\delta_b \leq 2\Delta z$ then the value of ϕ in the upper layer after mixing is

$$\Delta z_1\phi_{1m} = \Delta z_1\phi_1 - \frac{1}{2}\left(\phi_1 - \phi_2\right)\frac{\delta_b}{2} \tag{D.64}$$

or

$$\phi_{1m} = \phi_1 - \frac{\Delta\phi\delta_b}{4\Delta z_1} \tag{D.65}$$

In the same way we find that for the lower layer

$$\begin{aligned} \psi_{Tk} &\equiv \frac{h_{Tk}}{\Delta z_k}\left\{\frac{1}{h_{Tk} + h_{Bk+1}}\right\} \\ \psi_{Bk} &\equiv \frac{h_{Bk}}{\Delta z_k}\left\{\frac{1}{h_{Bk} + h_{Tk-1}}\right\} \end{aligned} \tag{D.66}$$

or

$$\overline{\rho}_k = \rho_{Rk}\left[1 - \left(\frac{h_{Tk}}{\Delta z_k} + \psi_{Tk}\right) - \left(\frac{h_{Bk}}{\Delta z_k} - \psi_{Bk}\right)\right] + \rho_{Rk+1}\psi_{Tk} - \rho_{Rk-1}\psi_{Bk} \tag{D.67}$$

Let us consider what is required when

$$\begin{aligned} A_k &\equiv +\psi_{Tk} \\ B_k &\equiv 1 - \left(\frac{h_{Tk}}{\Delta z_k} + \psi_{Tk} \right) - \left(\frac{h_{Bk}}{\Delta z_k} - \psi_{Bk} \right) \\ C_k &\equiv -\psi_{Bk} \end{aligned}$$

. In such a case, only a fraction of the thickness will mix, which we parameterize as

$$\begin{bmatrix} B_{k\max} & C_{k\max} & 0 & 0 & 0 & 0 & 0 \\ A_{k\max-1} & B_{k\max-1} & C_{k\max-1} & 0 & 0 & 0 & 0 \\ 0 & A_{k\max-2} & B_{k\max-2} & C_{k\max-2} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & A_3 & B_3 & C_3 & 0 \\ 0 & 0 & 0 & 0 & A_2 & B_2 & C_2 \\ 0 & 0 & 0 & 0 & 0 & A_1 & B_1 \end{bmatrix} \begin{bmatrix} \rho_{Rk\max} \\ \rho_{Rk\max-1} \\ \rho_{Rk\max-2} \\ \vdots \\ \rho_{R3} \\ \rho_{R2} \\ \rho_{R1} \end{bmatrix} = \begin{bmatrix} \overline{\rho}_{k\max} \\ \overline{\rho}_{k\max-1} \\ \overline{\rho}_{k\max-2} \\ \vdots \\ \overline{\rho}_3 \\ \overline{\rho}_2 \\ \overline{\rho}_1 \end{bmatrix} \tag{D.68}$$

Thus, for any scalar we have

$$\delta_{KH} = \frac{0.3 \Delta U^2}{g'} \tag{D.69}$$

where the above is only correct for $\delta_{KHk+1/2} = \frac{0.3\rho_0}{g\left(\rho_{Rk} - \rho_{Rk+1}\right)} \left\{ \left(U_{Rk+1} - U_{Rk} \right)^2 + \left(V_{Rk+1} - V_{Rk} \right)^2 \right\}$.

Thus, the above approach provides direct estimation of the mixing caused by K-H billows using the approach of Sherman et al. (1978) and the K-H time scales of Thorpe (1973).

D.4.iii Problems for shear mixing

The principle problem for shear mixing is that we are actually mixing a small region (assuming $\Delta U_{Rk+1/2} \equiv U_{Rk+1} - U_{Rk}$) near the grid boundary to a linear profile. However, this affects the overall density (or other species) throughout the cell. We might consider what happens if we try to store a value 'h' on each cell interface that characterizes the mixing between the cells. This mixing 'h' could be considered a transportable variable (but is not cell-centered, which could cause problems). It might be possible to consider a cell to have a "representative" density as ρ_r. At the start, let us consider a simple layered system where ρ_r is the actual density throughout the cell, i.e. $\rho(z)$, as well as the average density $\overline{\rho}$ in the cell. We then have K-H billows on both the upper and lower faces of the cell, such that mass is transferred upwards in both cases. Across the upper face, we have loss mass such that there is a mass deficit (per unit area) of

$$\Delta m_{k+1/2} = -\frac{\Delta \rho_{k+1/2} \delta_{b(k+1/2)}}{4} \tag{D.70}$$

where δ_b is given by eq. (D.68) and

$$\Delta\rho_{k+1/2} = \rho_{r(k)} - \rho_{r(k+1)} \tag{D.71}$$

In the same way, we have a mass gain through the lower boundary as

$$\Delta m_{k-1/2} = +\frac{\Delta\rho_{k-1/2}\delta_{b(k-1/2)}}{4} \tag{D.72}$$

Thus, the average density is given by

$$\overline{\rho}_k = \frac{\Delta z_k \rho_r + \Delta m_{k+1/2} + \Delta m_{k-1/2}}{\Delta z_k} \tag{D.73}$$

or

$$\overline{\rho}_k = \rho_r - \frac{\Delta\rho_{k+1/2}\delta_{b(k+1/2)}}{4\Delta z_k} + \frac{\Delta\rho_{k-1/2}\delta_{b(k-1/2)}}{4\Delta z_k} \tag{D.74}$$

If we use a more general mixing height 'h' to represent the gradient, we have

$$h_{Tk}^{n+1} = \begin{cases} h_{Tk}^{n} + \dfrac{\Delta t}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \ \Delta t \le T_{KHk+1/2} \\ h_{Tk}^{n} + \dfrac{T_{KHk+1/2}}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \ \Delta t > T_{KHk+1/2} \end{cases} \tag{D.75}$$

As long as we meet the requirement

$$h_{Bk+1}^{n+1} = \begin{cases} h_{Bk+1}^{n} + \dfrac{\Delta t}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \ \Delta t \le T_{KHk+1/2} \\ h_{Bk+1}^{n} + \dfrac{T_{KHk+1/2}}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \ \Delta t > T_{KHk+1/2} \end{cases} \tag{D.76}$$

it can be argued that $h_{Tk}^{n+1} = \begin{cases} h_{Tk}^{n} + \dfrac{\Delta t}{2}\left[\dfrac{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)}{T_{KHk+1/2}}\right] & : \ \Delta t \le T_{KHk+1/2} \\ h_{Tk}^{n} + \dfrac{T_{KHk+1/2}}{2}\left[\dfrac{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)}{T_{KHk+1/2}}\right] & : \ \Delta t > T_{KHk+1/2} \end{cases}$ is a better representative of the density at the center of the cell than is the average density $\overline{\rho}_k$. This concept can be extended to other scalars as well. However, transport of scalars must use the average value rather than the representative value to maintain conservation. If we apply eq. (D.71) in eq. (D.74) we obtain

$$\bar{\rho}_k = \rho_{r(k)} - \frac{h_{k+1/2}}{4\Delta z_k}\left(\rho_{r(k)} - \rho_{r(k+1)}\right) + \frac{h_{k-1/2}}{4\Delta z_k}\rho_{r(k-1)} - \rho_{r(k)} \tag{D.77}$$

which could be written as

$$+\left\{\frac{h_{k+1/2}}{4\Delta z_k}\right\}\rho_{r(k+1)} + \left\{1 - \frac{h_{k+1/2}}{4\Delta z_k} - \frac{h_{k-1/2}}{4\Delta z_k}\right\}\rho_{r(k)} + \left\{\frac{h_{k-1/2}}{4\Delta z_k}\right\}\rho_{r(k-1)} = \bar{\rho}_k \tag{D.78}$$

or

$$+A_k\rho_{r(k+1)} + B_k\rho_{r(k)} + C_k\rho_{r(k-1)} = \bar{\rho}_k \tag{D.79}$$

so that we have the matrix equation

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 \\ 0 & \cdots & \cdots & 0 \\ 0 & 0 & A_{k\max} & B_{k\max} \end{bmatrix} \begin{bmatrix} \rho_{r(1)} \\ \rho_{r(2)} \\ \vdots \\ \rho_{r(k\max)} \end{bmatrix} = \begin{bmatrix} \bar{\rho}_1 \\ \bar{\rho}_2 \\ \\ \bar{\rho}_{k\max} \end{bmatrix} \tag{D.80}$$

which can be solved by a tridiagonal inversion. The above can be extended to any scalar.

If we use this approach, we consider 'h' initially to be zero at all cell faces at time t=0. As such all variables satisfy $\phi_r = \bar{\phi}$ at any grid cell. We then conduct shear mixing to compute 'h' at each interface as $\delta_{KHk+1/2} = -\frac{0.3\rho_0}{g\,\Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\}$ according to eq. (D.58). The new average densities are computed using eq. (D.77) and the mixing layer thickness. We then check for mixing layers that are large compared to the local grid cell thickness. That is, where

$$T_{KHk+1/2} = -\frac{20\rho_0}{g\,\Delta\rho_{Rk+1/2}}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2} \tag{D.81}$$

we set a new value for the representative density on either side of the interface using

$$\rho_{r(k)} = \rho_{r(k)} - \frac{\Delta\rho_{k+1/2}h_{k+1/2}}{4\Delta z_k} \tag{D.82}$$

$$\rho_{r(k+1)} = \rho_{r(k+1)} + \frac{\Delta\rho_{k+1/2}h_{k+1/2}}{4\Delta z_{k+1}} \tag{D.83}$$

and then set $h_{k+1/2} = 0$. Note that if both the upper and lower mixing layers of a grid cell have large 'h', then the density will satisfy $\rho_{r(k)} = \bar{\rho}_k$. For the moment, let us ignore other parts of the mixing routine. Using the above scheme we have mixing that produces the average density (which is conservative) and a representative density, which is not conservative but provides a better characterization of the gradients. We then transport all scalars and 'h'. Note that only the average density is transportable, since the representative density is not conservative. Once transport is finished, we use solution of eq. (D.80) to update the reference densities. We use a similar solution to update reference values for all the scalars. We then begin a new time step where we have a field that has average and reference values for all scalars. We now consider the computation of the K-H billow thickness that scales as

$$\delta_b = \frac{0.3\Delta U^2}{g'} \tag{D.84}$$

can be computed for each cell interface as

$$\delta_{b(k+1/2)} = 0.3\frac{\rho_0}{g\left(\rho_{r(k)} - \rho_{r(k+1)}\right)}\left\{\left(U_{r(k)} - U_{r(k+1)}\right)^2 + \left(V_{r(k)} - V_{r(k+1)}\right)^2\right\} \tag{D.85}$$

We then check if

$$\delta_{b(k+1/2)} \le h_{k+1/2} \tag{D.86}$$

then no further billowing will occur at that time step. Where

$$\delta_{b(k+1/2)} > h_{k+1/2} \tag{D.87}$$

we consider billowing to occur so that there is an increase in the mixing layer thickness by an upward transport of mass. We model this process as changing the gradient between the representative densities.

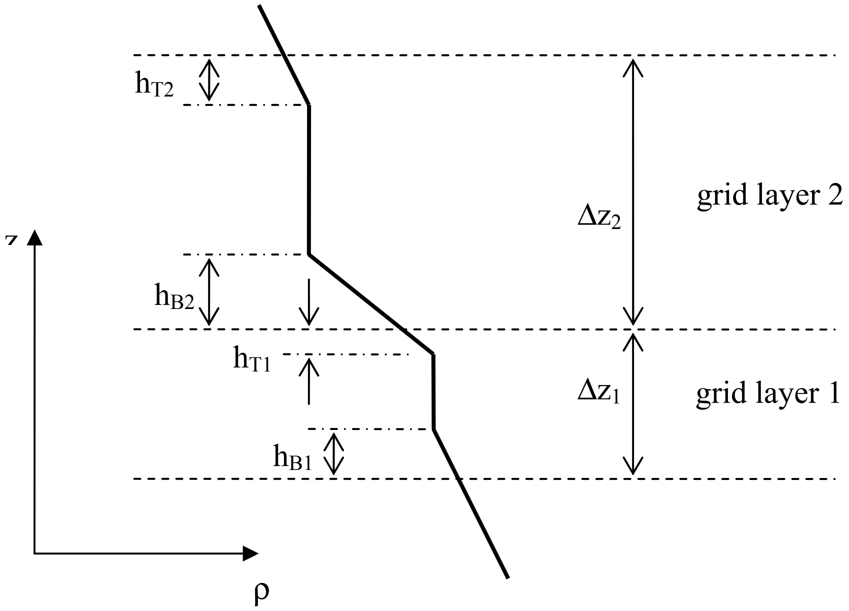
D.5 K-H billows using a separately defined gradient regions at top and bottom of each grid cell

Let us consider the diagram shown below. Note that the nomenclature is somewhat different than above to try to keep the derivation as simple as possible. Let ρ_R be the representative density of each layer, which corresponds to the uniform density in the middle of the layer. It follows that the average density, $\overline{\rho}$ is given by

$$\overline{\rho}_k = \frac{\left(\Delta z_k - h_{Tk} - h_{Bk}\right)}{\Delta z_k}\rho_{Rk} + \left(\frac{\rho_{Rk+1} - \rho_{Rk}}{h_{Tk} + h_{Bk+1}}\right)\frac{h_{Tk}}{\Delta z_k} + \left(\frac{\rho_{Rk} - \rho_{Rk-1}}{h_{Bk} + h_{Tk-1}}\right)\frac{h_{Bk}}{\Delta z_k} \tag{D.88}$$

The average density along with h_{Tk} and h_{Bk} will be transported scalars, so we will need an equation that can reconstruct the representative densities from the layer thicknesses and the average densities. We can write the above as

$$\Delta z_k \overline{\rho}_k = \left(\Delta z_k - h_{Tk} - h_{Bk}\right)\rho_{Rk} + \left(\rho_{Rk+1} - \rho_{Rk}\right)\left(\frac{h_{Tk}}{h_{Tk} + h_{Bk+1}}\right) + \left(\rho_{Rk} - \rho_{Rk-1}\right)\frac{h_{Bk}}{h_{Bk} + h_{Tk-1}} \tag{D.89}$$



which regroups as

$$\begin{aligned}\Delta z_k \overline{\rho}_k = \rho_{Rk}&\left[\Delta z_k - h_{Tk} - h_{Bk} - \left(\frac{h_{Tk}}{h_{Tk}+h_{Bk+1}}\right) + \left(\frac{h_{Bk}}{h_{Bk}+h_{Tk-1}}\right)\right] \\ &+ \rho_{Rk+1}\left(\frac{h_{Tk}}{h_{Tk}+h_{Bk+1}}\right) - \rho_{Rk-1}\left(\frac{h_{Bk}}{h_{Bk}+h_{Tk-1}}\right)\end{aligned} \qquad (D.90)$$

or

$$\begin{aligned}\overline{\rho}_k = \rho_{Rk}&\left[1 - \left(\frac{h_{Tk}}{\Delta z_k} + \frac{h_{Tk}}{\Delta z_k}\left\{\frac{1}{h_{Tk}+h_{Bk+1}}\right\}\right) - \left(\frac{h_{Bk}}{\Delta z_k} - \frac{h_{Bk}}{\Delta z_k}\left\{\frac{1}{h_{Bk}+h_{Tk-1}}\right\}\right)\right] \\ &+ \rho_{Rk+1}\frac{h_{Tk}}{\Delta z_k}\left(\frac{1}{h_{Tk}+h_{Bk+1}}\right) - \rho_{Rk-1}\frac{h_{Bk}}{\Delta z_k}\left(\frac{1}{h_{Bk}+h_{Tk-1}}\right)\end{aligned} \qquad (D.91)$$

Let

$$\begin{aligned}\psi_{Tk} &\equiv \frac{h_{Tk}}{\Delta z_k}\left\{\frac{1}{h_{Tk}+h_{Bk+1}}\right\}\\ \psi_{Bk} &\equiv \frac{h_{Bk}}{\Delta z_k}\left\{\frac{1}{h_{Bk}+h_{Tk-1}}\right\}\end{aligned} \tag{D.92}$$

then we have

$$\overline{\rho}_k = \rho_{Rk}\left[1-\left(\frac{h_{Tk}}{\Delta z_k}+\psi_{Tk}\right)-\left(\frac{h_{Bk}}{\Delta z_k}-\psi_{Bk}\right)\right]+\rho_{Rk+1}\psi_{Tk}-\rho_{Rk-1}\psi_{Bk} \tag{D.93}$$

Define

$$\begin{aligned}A_k &\equiv +\psi_{Tk}\\ B_k &\equiv 1-\left(\frac{h_{Tk}}{\Delta z_k}+\psi_{Tk}\right)-\left(\frac{h_{Bk}}{\Delta z_k}-\psi_{Bk}\right)\\ C_k &\equiv -\psi_{Bk}\end{aligned} \tag{D.94}$$

We can then write the matrix equation

$$\begin{bmatrix} B_{k\max} & C_{k\max} & 0 & 0 & 0 & 0 & 0 \\ A_{k\max-1} & B_{k\max-1} & C_{k\max-1} & 0 & 0 & 0 & 0 \\ 0 & A_{k\max-2} & B_{k\max-2} & C_{k\max-2} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & A_3 & B_3 & C_3 & 0 \\ 0 & 0 & 0 & 0 & A_2 & B_2 & C_2 \\ 0 & 0 & 0 & 0 & 0 & A_1 & B_1 \end{bmatrix}\begin{bmatrix} \rho_{Rk\max} \\ \rho_{Rk\max-1} \\ \rho_{Rk\max-2} \\ \vdots \\ \rho_{R3} \\ \rho_{R2} \\ \rho_{R1} \end{bmatrix} = \begin{bmatrix} \overline{\rho}_{k\max} \\ \overline{\rho}_{k\max-1} \\ \overline{\rho}_{k\max-2} \\ \vdots \\ \overline{\rho}_3 \\ \overline{\rho}_2 \\ \overline{\rho}_1 \end{bmatrix} \tag{D.95}$$

which allows us to reconstruct the representative density from the mean density field and the thickness of the gradient region.

Let us examine how the figure above will provide for a K-H billow mixing scheme. We go back to the Sherman et al (1978) approximation for the thickness of the layer after billowing:

$$\delta_{KH} = \frac{0.3\Delta U^2}{g'} \tag{D.96}$$

Which we will model in 3D as

$$\delta_{KHk+1/2} = \frac{0.3\rho_0}{g\left(\rho_{Rk}-\rho_{Rk+1}\right)}\left\{\left(U_{Rk+1}-U_{Rk}\right)^2+\left(V_{Rk+1}-V_{Rk}\right)^2\right\} \tag{D.97}$$

So that we will always define differences such as

$$\Delta U_{Rk+1/2} \equiv U_{Rk+1} - U_{Rk} \tag{D.98}$$

it follows that eq. (D.97) should be written as

$$\delta_{KHk+1/2} = -\frac{0.3\rho_0}{g\,\Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\} \tag{D.99}$$

Billowing will not occur at interface $k+1/2$ if

$$\delta_{KHk+1/2} \le h_{Tk} + h_{Bk+1} \tag{D.100}$$

In the case that $\delta_{KHk+1/2} > h_{Tk} + h_{Bk+1}$, it follows that billowing should occur. If the billowing continues to completion, we would then require

$$h_{Tk}^{n+1} + h_{Bk+1}^{n+1} = \delta_{KHk+1/2} \tag{D.101}$$

it follows that

$$\frac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) = \frac{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)}{T_{KHk+1/2}} \quad : \quad 0 \le t \le T_{KHk+1/2} \tag{D.102}$$

where the limitation is that the rate of change only applies for times less that T_{KH}, where

$$T_{KH} = \frac{20}{g'}\sqrt{\Delta U^2 + \Delta V^2} \tag{D.103}$$

so that

$$T_{KHk+1/2} = -\frac{20\rho_0}{g\,\Delta\rho_{Rk+1/2}}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2} \tag{D.104}$$

We will assume that the thickening of the interface occurs symmetrically, so that at time n+1, the new interface thicknesses are

$$h_{Tk}^{n+1} = \begin{cases} h_{Tk}^{n} + \dfrac{\Delta t}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \quad \Delta t \le T_{KHk+1/2} \\ h_{Tk}^{n} + \dfrac{T_{KHk+1/2}}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.105}$$

$$h_{Bk+1}^{n+1} = \begin{cases} h_{Bk+1}^{n} + \dfrac{\Delta t}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \quad \Delta t \le T_{KHk+1/2} \\ h_{Bk+1}^{n} + \dfrac{T_{KHk+1/2}}{2}\dfrac{\partial}{\partial t}\left(h_{Tk} + h_{Bk+1}\right) & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.106}$$

Thus, using eq. (D.102) and eq. (D.105) we have

$$h_{Tk}^{n+1} = \begin{cases} h_{Tk}^{n} + \dfrac{\Delta t}{2}\left[\dfrac{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)}{T_{KHk+1/2}}\right] & : \quad \Delta t \le T_{KHk+1/2} \\ h_{Tk}^{n} + \dfrac{T_{KHk+1/2}}{2}\left[\dfrac{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)}{T_{KHk+1/2}}\right] & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.107}$$

or

$$h_{Tk}^{n+1} = \begin{cases} h_{Tk}^{n} + \dfrac{\Delta t}{2T_{KHk+1/2}}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t \le T_{KHk+1/2} \\ h_{Tk}^{n} + \dfrac{1}{2}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.108}$$

or

$$h_{Tk}^{n+1} = \begin{cases} \dfrac{1}{2}\left\{\dfrac{\Delta t\delta_{KHk+1/2}}{T_{KHk+1/2}} - \dfrac{\Delta t h_{Tk}^{n}}{T_{KHk+1/2}} - \dfrac{\Delta t h_{Bk+1}^{n}}{T_{KHk+1/2}} + 2h_{Tk}^{n}\right\} & : \quad \Delta t \le T_{KHk+1/2} \\ \dfrac{1}{2}\left\{\delta_{KHk+1/2} + h_{Tk}^{n} - h_{Bk+1}^{n}\right\} & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.109}$$

or

$$h_{Tk}^{n+1} = \begin{cases} \dfrac{1}{2}\left[\dfrac{\Delta t\delta_{KHk+1/2}}{T_{KHk+1/2}} - h_{Bk+1}^{n}\dfrac{\Delta t}{T_{KHk+1/2}} + h_{Tk}^{n}\left(2 - \dfrac{\Delta t}{T_{KHk+1/2}}\right)\right] & : \quad \Delta t \le T_{KHk+1/2} \\ \dfrac{1}{2}\left[\delta_{KHk+1/2} + h_{Tk}^{n} - h_{Bk+1}^{n}\right] & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.110}$$

or

$$h_{Tk}^{n+1} = \begin{cases} \dfrac{1}{2}\left[\dfrac{\Delta t \dfrac{0.3\cancel{\rho_0}}{\cancel{g}\ \cancel{\Delta\rho_{Rk+1/2}}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\}}{\dfrac{20\cancel{\rho_0}}{\cancel{g}\ \cancel{\Delta\rho_{Rk+1/2}}}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2}} - h_{Bk+1}^{n}\dfrac{\Delta t}{T_{KHk+1/2}} + h_{Tk}^{n}\left(2 - \dfrac{\Delta t}{T_{KHk+1/2}}\right)\right] & : \quad \Delta t \le T_{KHk+1/2} \\ \dfrac{1}{2}\left[-\dfrac{0.3\rho_0}{g\ \Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\} + h_{Tk}^{n} - h_{Bk+1}^{n}\right] & : \quad \Delta t > T_{KHk+1/2} \end{cases}$$

(D.111)

$$h_{Tk}^{n+1} = \begin{cases} \dfrac{1}{2}\left[\dfrac{0.3\Delta t}{20}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2} - h_{Bk+1}^{n}\dfrac{\Delta t}{T_{KHk+1/2}} + h_{Tk}^{n}\left(2 - \dfrac{\Delta t}{T_{KHk+1/2}}\right)\right] & : \quad \Delta t \le T_{KHk+1/2} \\ \dfrac{1}{2}\left[-\dfrac{0.3\rho_0}{g\ \Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\} + h_{Tk}^{n} - h_{Bk+1}^{n}\right] & : \quad \Delta t > T_{KHk+1/2} \end{cases}$$

(D.112)

Note that the above is not substantially easier to deal with, so it seems best to stick with eq. (D.99), (D.104) and (D.108) defining the change in the thickness. It will be convenient to repeat these here as

$$\delta_{KHk+1/2} = -\frac{0.3\rho_0}{g\ \Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\} \tag{D.113}$$

$$T_{KHk+1/2} = -\frac{20\rho_0}{g\,\Delta\rho_{Rk+1/2}}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2} \tag{D.114}$$

$$\Delta h_{k+1/2}^{n\rightarrow n+1} \equiv h_{Tk}^{n+1} - h_{Tk}^{n} = \begin{cases} \dfrac{\Delta t}{2T_{KHk+1/2}}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t \leq T_{KHk+1/2} \\ \dfrac{1}{2}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n} + h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.115}$$

where it is convenient to write the latter in terms of the change in the thickness. We note that the assumption of symmetry in the mixing allows only one value of $\Delta h_{k+1/2}$, so it follows that

$$h_{Tk}^{n+1} - h_{Tk}^{n} = h_{Bk+1}^{n+1} - h_{Bk+1}^{n} \tag{D.116}$$

and there it is not necessary to solve eq. (D.106).

D.5.i Obtaining the volume transfer for a change in the interface thickness

We consider the change in the gradient region $\Delta h_{k+1/2}$ as shown in the figure below for k=1. We are interested in the mass exchange between the cells. We assume a conservation of volume such that the volume of fluid of density ρ_{R1} that moves into grid layer 2 is exactly the same as the volume of fluid of density ρ_{R2} that moves into layer 1. If we consider only the upper half of grid layer 1, we can say that before mixing it has the average density $\overline{\rho}_{T1}$ so that the total mass can be written by the average density in the upper half or by the gradients of the representative density:

$$\frac{\Delta z_1}{2}\overline{\rho}_{T1} = \rho_{R1}\left(\frac{\Delta z_1}{2} - h_{T1}^{n}\right) + \underbrace{\frac{1}{2}\left\{\rho_{R1} + \underbrace{\left[\rho_{R1} - \left(\frac{\rho_{R1} - \rho_{R2}}{h_{T1}^{n} + h_{B2}^{n}}\right)h_{T1}^{n}\right]}_{\text{density at } 1/2}\right\}}_{\text{average density in top gradient region of 1}}\left(h_{T1}^{n}\right) \tag{D.117}$$

which can be written as

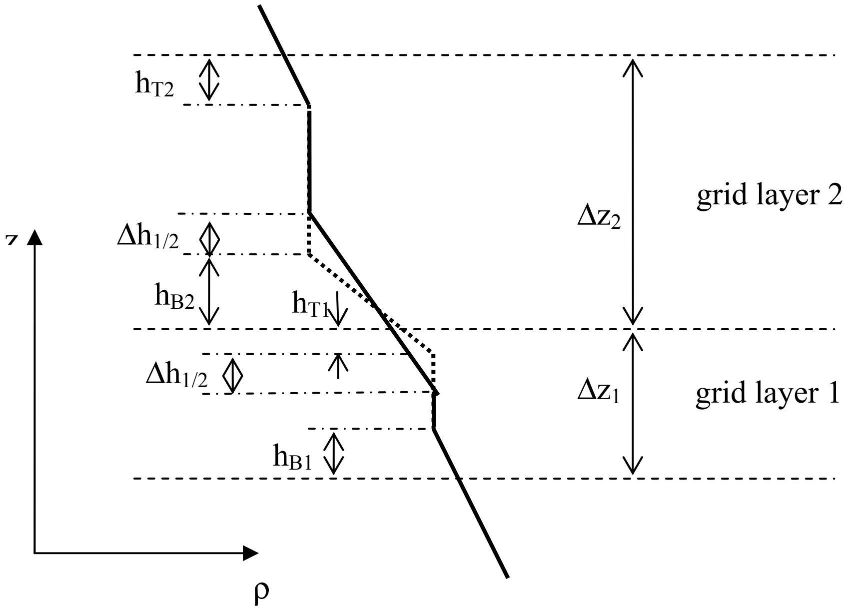
$$\frac{\Delta z_1}{2}\overline{\rho}_{T1} = \rho_{R1}\left(\frac{\Delta z_1}{2} - h_{T1}^{n}\right) + \rho_{R1}h_{T1}^{n} + \frac{\left(h_{T1}^{n}\right)^2}{2\left(h_{T1}^{n} + h_{B2}^{n}\right)}\Delta\rho_{R1/2} \tag{D.118}$$

where the form of eq. (D.98) is used to define $\Delta\rho_{R1/2}$. Further simplification provides

$$\frac{\Delta z_1}{2}\overline{\rho}_{T1} = \rho_{R1}\left(\frac{\Delta z_1}{2} - \cancel{h_{T1}^{n}} + \cancel{h_{T1}^{n}}\right) + \frac{\left(h_{T1}^{n}\right)^2}{2\left(h_{T1}^{n} + h_{B2}^{n}\right)}\Delta\rho_{R1/2} \tag{D.119}$$

so that we have

$$\overline{\rho}_{T1}^{n} = \rho_{R1}^{n} + \frac{\left(h_{T1}^{n}\right)^2}{\Delta z_1\left(h_{T1}^{n} + h_{B2}^{n}\right)}\Delta\rho_{R1/2}^{n} \tag{D.120}$$



In a similar fashion, after mixing we would have

$$\overline{\rho}_{T1}^{n+1} = \rho_{R1}^{n+1} + \frac{\left(h_{T1}^{n+1}\right)^2}{\Delta z_1\left(h_{T1}^{n+1} + h_{B2}^{n+1}\right)}\Delta\rho_{R1/2}^{n+1} \tag{D.121}$$

As long as

$$h_{T1}^{n+1} \le \frac{\Delta z_1}{2} \quad \text{and} \quad h_{B2}^{n+1} \le \frac{\Delta z_2}{2} \tag{D.122}$$

the representative density does not change, so that

$$\rho_{R1}^{n+1} = \rho_{R1}^{n} \quad \text{and} \quad \rho_{R2}^{n+1} = \rho_{R2}^{n} \quad \text{and} \quad \Delta\rho_{R1/2}^{n+1} = \Delta\rho_{R1/2}^{n} \tag{D.123}$$

It follows that the average density in the upper half of the layer 1 is given by

$$\overline{\rho}_{T1}^{n+1} - \overline{\rho}_{T1}^{n} = \frac{\Delta\rho_{R1/2}^{n}}{\Delta z_1}\left\{\frac{\left(h_{T1}^{n+1}\right)^2}{\left(h_{T1}^{n+1} + h_{B2}^{n+1}\right)} - \frac{\left(h_{T1}^{n}\right)^2}{\left(h_{T1}^{n} + h_{B2}^{n}\right)}\right\} \tag{D.124}$$

In a similar manner to eq. (D.117), the average density in the lower half of layer 2 is given by

$$\frac{\Delta z_2}{2}\overline{\rho}_{B2} = \rho_{R2}\left(\frac{\Delta z_2}{2} - h^n_{B2}\right) + \underbrace{\frac{1}{2}\left\{\rho_{R2} + \underbrace{\left[\rho_{R2} + \left(\frac{\rho_{R1}-\rho_{R2}}{h^n_{T1}+h^n_{B2}}\right)h^n_{B2}\right]}_{\text{density at } 1/2}\right\}}_{\text{average density in bottom gradient region of 2}}\left(h^n_{B2}\right) \tag{D.125}$$

which becomes

$$\frac{\Delta z_2}{2}\overline{\rho}_{B2} = \rho_{R2}\left(\frac{\Delta z_1}{2} - h^n_{B2}\right) + \rho_{R2}h^n_{B2} + \frac{\left(h^n_{B2}\right)^2}{2\left(h^n_{T1}+h^n_{B2}\right)}\Delta\rho_{R1/2} \tag{D.126}$$

or

$$\frac{\Delta z_2}{2}\overline{\rho}_{B2} = \rho_{R2}\left(\frac{\Delta z_1}{2} - \cancel{h^n_{B2}} + \cancel{h^n_{TB2}}\right) + \frac{\left(h^n_{B2}\right)^2}{2\left(h^n_{T1}+h^n_{B2}\right)}\Delta\rho_{R1/2} \tag{D.127}$$

or, at time ‘n’

$$\overline{\rho}^n_{B2} = \rho^n_{B2} + \frac{\left(h^n_{B2}\right)^2}{\Delta z_2\left(h^n_{T1}+h^n_{B2}\right)}\Delta\rho^n_{R1/2} \tag{D.128}$$

The change due to mixing is then

$$\overline{\rho}^{n+1}_{B2} - \overline{\rho}^n_{B2} = \frac{\Delta\rho^n_{R1/2}}{\Delta z_2}\left\{\frac{\left(h^{n+1}_{B2}\right)^2}{\left(h^{n+1}_{T1}+h^{n+1}_{B2}\right)} - \frac{\left(h^n_{B2}\right)^2}{\left(h^n_{T1}+h^n_{B2}\right)}\right\} \tag{D.129}$$

The net mass transfer (per unit area) upward out of grid cell 1 is given based on the layer 1 cell as

$$\frac{\Delta m_1}{\Delta x\,\Delta y} = \frac{\Delta z_1}{2}\left(\overline{\rho}^{n+1}_{T1} - \overline{\rho}^n_{T1}\right) \tag{D.130}$$

which will be negative since the average density will decrease. Similarly, the net mass transfer (per unit area) downward out of grid cell 2 is given based on the layer 2 cell as

$$\frac{\Delta m_2}{\Delta x\,\Delta y} = \frac{\Delta z_2}{2}\left(\overline{\rho}^{n+1}_{B2} - \overline{\rho}^n_{B2}\right) \tag{D.131}$$

which will be positive since the average density is increasing in layer 2, so we have $\Delta m_1 = -\Delta m_2$

We assume that the above mass transfer is accomplished by the exchange of equal volumes of fluids of density ρ_{R1} and ρ_{R2}, which can be represented by a volume V Thus we require that the net mass into layer 2 be given by the mass arriving from layer 1 and the mass leaving layer 2,

$$\Delta m_2 = V_{1/2}\rho_{R1} - V_{1/2}\rho_{R2} \tag{D.132}$$

Similarly, the change in mass in layer 1 is given by

$$\Delta m_1 = -V_{1/2}\rho_{R1} + V_{1/2}\rho_{R2} \tag{D.133}$$

so that $\Delta m_1 = -\Delta m_2$, and mass is exactly conserved.

Using eq. (D.130) and eq. (D.133) we find

$$\frac{\Delta z_1}{2}\left(\overline{\rho}_{T1}^{n+1} - \overline{\rho}_{T1}^{n}\right) = \frac{-V_{1/2}\rho_{R1}^{n} + V_{1/2}\rho_{R2}^{n}}{\Delta x\,\Delta y} \tag{D.134}$$

So we can solve for the volume exchange as

$$-V_{1/2} = \Delta x\,\Delta y\frac{\Delta z_1}{2}\frac{\left(\overline{\rho}_{T1}^{n+1} - \overline{\rho}_{T1}^{n}\right)}{\left(\rho_{R1}^{n} - \rho_{R2}^{n}\right)} = \tag{D.135}$$

which can be written as the volume exchange due to mixing.

$$V_{1/2} = \Delta x\,\Delta y\frac{\Delta z_1}{2}\frac{\left(\overline{\rho}_{T1}^{n+1} - \overline{\rho}_{T1}^{n}\right)}{\Delta\rho_{R1/2}^{n}} \tag{D.136}$$

Applying eq. (D.124), we end up with

$$V_{1/2} = \Delta x\,\Delta y\frac{\cancel{\Delta z_1}}{2}\frac{1}{\cancel{\Delta\rho_{R1/2}^{n}}}\frac{\cancel{\Delta\rho_{R1/2}^{n}}}{\cancel{\Delta z_1}}\left\{\frac{\left(h_{T1}^{n+1}\right)^2}{\left(h_{T1}^{n+1} + h_{B2}^{n+1}\right)} - \frac{\left(h_{T1}^{n}\right)^2}{\left(h_{T1}^{n} + h_{B2}^{n}\right)}\right\} \tag{D.137}$$

or

$$V_{1/2} = \frac{\Delta x\,\Delta y}{2}\left\{\frac{\left(h_{T1}^{n+1}\right)^2}{\left(h_{T1}^{n+1} + h_{B2}^{n+1}\right)} - \frac{\left(h_{T1}^{n}\right)^2}{\left(h_{T1}^{n} + h_{B2}^{n}\right)}\right\} \tag{D.138}$$

Similar to eq. (D.134), if we use eq. (D.131) and (D.132), we obtain

$$\frac{\Delta z_2}{2}\left(\overline{\rho}_{B2}^{n+1} - \overline{\rho}_{B2}^{n}\right) = \frac{V_{1/2}\rho_{R1}^{n} - V_{1/2}\rho_{R2}^{n}}{\Delta x\,\Delta y} \tag{D.139}$$

From which it follows that

$$V_{1/2} = \Delta x\,\Delta y \frac{\Delta z_2}{2} \frac{\left(\bar{\rho}^{n+1}_{B2} - \bar{\rho}^{n}_{B2}\right)}{\rho^{n}_{R1} - \rho^{n}_{R2}} \tag{D.140}$$

or

$$V_{1/2} = -\Delta x\,\Delta y \frac{\Delta z_2}{2} \frac{\left(\bar{\rho}^{n+1}_{B2} - \bar{\rho}^{n}_{B2}\right)}{\Delta\rho^{n}_{R1/2}} \tag{D.141}$$

Applying eq. (D.129)

$$V_{1/2} = -\Delta x\,\Delta y \frac{\cancel{\Delta z_2}}{2} \frac{\cancel{\Delta\rho^{n}_{R1/2}}}{\cancel{\Delta z_2}\ \cancel{\Delta\rho^{n}_{R1/2}}} \left\{ \frac{\left(h^{n+1}_{B2}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{B2}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} \right\} \tag{D.142}$$

or

$$V_{1/2} = -\frac{\Delta x\,\Delta y}{2} \left\{ \frac{\left(h^{n+1}_{B2}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{B2}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} \right\} \tag{D.143}$$

Since the volume flux upward must be identical to the volume flux downward, eq. (D.138) and (D.143) can be equated and

$$\frac{\left(h^{n+1}_{T1}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{T1}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} = -\left\{ \frac{\left(h^{n+1}_{B2}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{B2}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} \right\} \tag{D.144}$$

To generalize the above, it follows that the change in the average volume concentration of any conserved scalar, ϕ, in the upper half of layer 1 due to mixing by K-H billows is given by a the volume fluxes and the representative scalar concentrations as

$$\Delta x \Delta y \frac{\Delta z_1}{2} \bar{\phi}^{n+1}_{T1} = \Delta x \Delta y \frac{\Delta z_1}{2} \bar{\phi}^{n}_{T1} - V_{1/2}\phi^{n}_{R1} + V_{1/2}\phi^{n}_{R2} \tag{D.145}$$

or

$$\cancel{\Delta x \Delta y} \frac{\Delta z_1}{2} \bar{\phi}^{n+1}_{T1} = \cancel{\Delta x \Delta y} \frac{\Delta z_1}{2} \bar{\phi}^{n}_{T1} + \left(\phi^{n}_{R2} - \phi^{n}_{R1}\right) \frac{\cancel{\Delta x \Delta y}}{2} \left\{ \frac{\left(h^{n+1}_{T1}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{T1}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} \right\} \tag{D.146}$$

or

$$\bar{\phi}^{n+1}_{T1} = \bar{\phi}^{n}_{T1} + \frac{\Delta\phi^{n}_{R1/2}}{\Delta z_1} \left\{ \frac{\left(h^{n+1}_{T1}\right)^2}{\left(h^{n+1}_{T1} + h^{n+1}_{B2}\right)} - \frac{\left(h^{n}_{T1}\right)^2}{\left(h^{n}_{T1} + h^{n}_{B2}\right)} \right\} \tag{D.147}$$

which is (not surprisingly) the same as eq. (D.124) with the density replaced by the general scalar volume concentration ϕ.

In the same way, for the lower half of the layer 2 grid cell we obtain

$$\Delta x\Delta y\frac{\Delta z_2}{2}\overline{\phi}_{B2}^{n+1} = \Delta x\Delta y\frac{\Delta z_2}{2}\overline{\phi}_{B2}^{n} + V_{1/2}\phi_{R1}^{n} - V_{1/2}\phi_{R2}^{n} \tag{D.148}$$

or, using eq. (D.143)

$$\cancel{\Delta x\Delta y}\frac{\Delta z_2}{\cancel{2}}\overline{\phi}_{B2}^{n+1} = \cancel{\Delta x\Delta y}\frac{\Delta z_2}{\cancel{2}}\overline{\phi}_{B2}^{n} - \left(\phi_{R1}^{n} - \phi_{R2}^{n}\right)\cancel{\frac{\Delta x\,\Delta y}{2}}\left\{\frac{\left(h_{B2}^{n+1}\right)^2}{\left(h_{T1}^{n+1}+h_{B2}^{n+1}\right)} - \frac{\left(h_{B2}^{n}\right)^2}{\left(h_{T1}^{n}+h_{B2}^{n}\right)}\right\} \tag{D.149}$$

which provides

$$\overline{\phi}_{B2}^{n+1} = \overline{\phi}_{B2}^{n} + \frac{\Delta\phi_{R1/2}^{n}}{\Delta z_2}\left\{\frac{\left(h_{B2}^{n+1}\right)^2}{\left(h_{T1}^{n+1}+h_{B2}^{n+1}\right)} - \frac{\left(h_{B2}^{n}\right)^2}{\left(h_{T1}^{n}+h_{B2}^{n}\right)}\right\} \tag{D.150}$$

Noting eq. (D.144), eq. (D.150) can be written as

$$\overline{\phi}_{B2}^{n+1} = \overline{\phi}_{B2}^{n} - \frac{\Delta\phi_{R1/2}^{n}}{\Delta z_2}\left\{\frac{\left(h_{T1}^{n+1}\right)^2}{\left(h_{T1}^{n+1}+h_{B2}^{n+1}\right)} - \frac{\left(h_{T1}^{n}\right)^2}{\left(h_{T1}^{n}+h_{B2}^{n}\right)}\right\} \tag{D.151}$$

Thus, for a general grid cell ‘k’, eq. (D.147) is written as

$$\overline{\phi}_{Tk}^{n+1} = \overline{\phi}_{Tk}^{n} + \frac{\Delta\phi_{Rk+1/2}^{n}}{\Delta z_k}\left\{\frac{\left(h_{Tk}^{n+1}\right)^2}{\left(h_{Tk}^{n+1}+h_{Bk+1}^{n+1}\right)} - \frac{\left(h_{Tk}^{n}\right)^2}{\left(h_{Tk}^{n}+h_{Bk+1}^{n}\right)}\right\} \tag{D.152}$$

and eq. (D.151) is

$$\overline{\phi}_{Bk}^{n+1} = \overline{\phi}_{Bk}^{n} - \frac{\Delta\phi_{Rk-1/2}^{n}}{\Delta z_k}\left\{\frac{\left(h_{Tk-1}^{n+1}\right)^2}{\left(h_{Tk-1}^{n+1}+h_{Bk}^{n+1}\right)} - \frac{\left(h_{Tk-1}^{n}\right)^2}{\left(h_{Tk-1}^{n}+h_{Bk}^{n}\right)}\right\} \tag{D.153}$$

Considering a general cell at grid level ‘k’ which may have changes at both top and bottom interfaces, we can write

$$\Delta z_k\overline{\phi}_{k}^{n+1} = \frac{\Delta z_k}{2}\left(\overline{\phi}_{Tk}^{n+1} + \overline{\phi}_{Bk}^{n+1}\right) \tag{D.154}$$

So substituting eq. (D.152) and (D.153) we obtain

$$\begin{aligned}\overline{\phi}_{k}^{n+1} = \frac{1}{2}\Bigg[& \overline{\phi}_{Tk}^{n} + \frac{\Delta\phi_{Rk+1/2}^{n}}{\Delta z_k}\left\{\frac{\left(h_{Tk}^{n+1}\right)^2}{\left(h_{Tk}^{n+1}+h_{Bk+1}^{n+1}\right)} - \frac{\left(h_{Tk}^{n}\right)^2}{\left(h_{Tk}^{n}+h_{Bk+1}^{n}\right)}\right\} \\ & + \overline{\phi}_{Bk}^{n} - \frac{\Delta\phi_{Rk-1/2}^{n}}{\Delta z_k}\left\{\frac{\left(h_{Tk-1}^{n+1}\right)^2}{\left(h_{Tk-1}^{n+1}+h_{Bk}^{n+1}\right)} - \frac{\left(h_{Tk-1}^{n}\right)^2}{\left(h_{Tk-1}^{n}+h_{Bk}^{n}\right)}\right\}\Bigg]\end{aligned} \tag{D.155}$$

We note that

$$\overline{\phi}_{k}^{n} = \frac{1}{2}\left(\overline{\phi}_{Tk}^{n} + \overline{\phi}_{Bk}^{n}\right) \tag{D.156}$$

so that we obtain

$$\begin{aligned}\overline{\phi}_{k}^{n+1} = \overline{\phi}_{k}^{n} + \frac{1}{2\Delta z_k}\Bigg[& \Delta\phi_{Rk+1/2}^{n}\left\{\frac{\left(h_{Tk}^{n+1}\right)^2}{\left(h_{Tk}^{n+1}+h_{Bk+1}^{n+1}\right)} - \frac{\left(h_{Tk}^{n}\right)^2}{\left(h_{Tk}^{n}+h_{Bk+1}^{n}\right)}\right\} \\ & - \Delta\phi_{Rk-1/2}^{n}\left\{\frac{\left(h_{Tk-1}^{n+1}\right)^2}{\left(h_{Tk-1}^{n+1}+h_{Bk}^{n+1}\right)} - \frac{\left(h_{Tk-1}^{n}\right)^2}{\left(h_{Tk-1}^{n}+h_{Bk}^{n}\right)}\right\}\Bigg]\end{aligned} \tag{D.157}$$

Thus, eq. (D.157) provides the K-H billow mixing of the average volume concentration of any conserved scalar (including components of momentum).

D.5.ii Summary of the K-H billow where the billow thickness is small compared to the grid cell

The K-H billow thickness is predicted from eq. (D.99), (D.104) and (D.108), rewritten here as:

$$\delta_{KHk+1/2} = -\frac{0.3\rho_0}{g\,\Delta\rho_{Rk+1/2}}\left\{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2\right\} \tag{D.158}$$

$$T_{KHk+1/2} = -\frac{20\rho_0}{g\,\Delta\rho_{Rk+1/2}}\sqrt{\left(\Delta U_{Rk+1/2}\right)^2 + \left(\Delta V_{Rk+1/2}\right)^2} \tag{D.159}$$

$$h_{Tk}^{n+1} = h_{Tk}^{n} + \begin{cases} \dfrac{\Delta t}{2T_{KHk+1/2}}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n}+h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t \le T_{KHk+1/2} \\ \dfrac{1}{2}\left\{\delta_{KHk+1/2} - \left(h_{Tk}^{n}+h_{Bk+1}^{n}\right)\right\} & : \quad \Delta t > T_{KHk+1/2} \end{cases} \tag{D.160}$$

along with the definition that

$$\Delta h_{Tk}^{n\rightarrow n+1} \equiv h_{Tk}^{n+1} - h_{Tk}^{n} \tag{D.161}$$

and the requirement of symmetry in the interface growth

$$\Delta h_{Bk+1}^{n\rightarrow n+1} = \Delta h_{Tk}^{n\rightarrow n+1} \tag{D.162}$$

The change in the average volume concentration of any scalar is then found from eq. (D.157), rewritten here as:

$$\begin{aligned} \overline{\phi}_k^{n+1} = \overline{\phi}_k^{n} + \frac{1}{2\Delta z_k}\Bigg[& \Delta\phi_{Rk+1/2}^{n}\left\{\frac{\left(h_{Tk}^{n+1}\right)^2}{h_{Tk}^{n+1}+h_{Bk+1}^{n+1}} - \frac{\left(h_{Tk}^{n}\right)^2}{h_{Tk}^{n}+h_{Bk+1}^{n}}\right\} \\ & - \Delta\phi_{Rk-1/2}^{n}\left\{\frac{\left(h_{Tk-1}^{n+1}\right)^2}{h_{Tk-1}^{n+1}+h_{Bk}^{n+1}} - \frac{\left(h_{Tk-1}^{n}\right)^2}{h_{Tk-1}^{n}+h_{Bk}^{n}}\right\}\Bigg] \end{aligned} \tag{D.163}$$

Once the mixing of the average volume concentrations and the interface thicknesses have been calculated as above, the hydrodynamic code is used to transport all values of $\overline{\phi}, h_T, h_B$. Thus, in addition to the mixing algorithm above, we need to compute the transport of two additional scalars. Note that the algorithm for transporting h's remains to be carefully derived. After the transport, we need to reconstruct the values of the representative concentrations, ϕ_R. Generalizing from the derivation for density in eqs. (D.92), (D.93), (2.8) and (2.9), we need to solve a tridiagonal for each scalar as

$$\overline{\phi}_k = \phi_{Rk}\left[1 - \left(\frac{h_{Tk}}{\Delta z_k} + \psi_{Tk}\right) - \left(\frac{h_{Bk}}{\Delta z_k} - \psi_{Bk}\right)\right] + \phi_{Rk+1}\psi_{Tk} - \phi_{Rk-1}\psi_{Bk} \tag{D.164}$$

where

$$\begin{aligned} \psi_{Tk} &\equiv \frac{h_{Tk}}{\Delta z_k}\left\{\frac{1}{h_{Tk}+h_{Bk+1}}\right\} \\ \psi_{Bk} &\equiv \frac{h_{Bk}}{\Delta z_k}\left\{\frac{1}{h_{Bk}+h_{Tk-1}}\right\} \end{aligned} \tag{D.165}$$

Using

$$\begin{aligned} A_k &\equiv +\psi_{Tk} \\ B_k &\equiv 1 - \left(\frac{h_{Tk}}{\Delta z_k} + \psi_{Tk}\right) - \left(\frac{h_{Bk}}{\Delta z_k} - \psi_{Bk}\right) \\ C_k &\equiv -\psi_{Bk} \end{aligned} \tag{D.166}$$

We can write the matrix equation

$$\begin{bmatrix} B_{k\max} & C_{k\max} & 0 & 0 & 0 & 0 & 0 \\ A_{k\max-1} & B_{k\max-1} & C_{k\max-1} & 0 & 0 & 0 & 0 \\ 0 & A_{k\max-2} & B_{k\max-2} & C_{k\max-2} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & A_3 & B_3 & C_3 & 0 \\ 0 & 0 & 0 & 0 & A_2 & B_2 & C_2 \\ 0 & 0 & 0 & 0 & 0 & A_1 & B_1 \end{bmatrix} \begin{bmatrix} \phi_{Rk\max} \\ \phi_{Rk\max-1} \\ \phi_{Rk\max-2} \\ \vdots \\ \phi_{R3} \\ \phi_{R2} \\ \phi_{R1} \end{bmatrix} = \begin{bmatrix} \overline{\phi}_{k\max} \\ \overline{\phi}_{k\max-1} \\ \overline{\phi}_{k\max-2} \\ \vdots \\ \overline{\phi}_3 \\ \overline{\phi}_2 \\ \overline{\phi}_1 \end{bmatrix} \quad \text{(D.167)}$$

which is inverted to provide the representative values in the cells.

D.6 K-H billows for small grid cells

A difficulty arises with the approach in D.5 when $h_T > \Delta z / 2$ or $h_B > \Delta z / 2$. In such cases, the method fails because there is a possible interaction between the T and B layers. As shown in the sketch below, if we were to keep with the idea of two gradient regions and a center region, a large increase in the thickness of the two gradient regions leads to inconsistency at the center of the grid cell. Arguably, the method might actually be considered to provide correct results as long as

$$h_{Tk}^{n+1} + h_{Bk}^{n+1} \le \Delta z_k \quad \text{(D.168)}$$

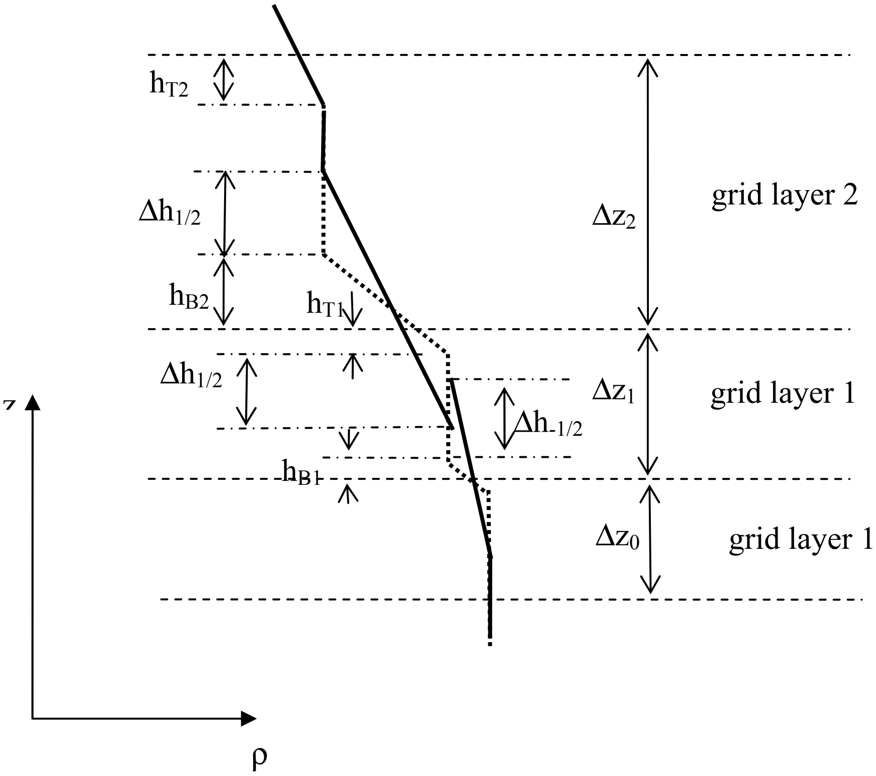
The simplest fix might be to consider that for any cell wherein eq. (D.168) is violated, the cell has mixing layers from both the bottom to the top. The gradient layer thicknesses would be set to zero, i.e.

$$h_{Tk}^{n+1} = h_{Bk}^{n+1} = h_{Tk-1}^{n+1} = h_{Bk+1}^{n+1} = 0 \quad \text{where} \quad h_{Tk}^{n+1} + h_{Bk}^{n+1} > \Delta z_k \quad \text{(D.169)}$$

Note that because we define a continuous gradient across the cell faces, the adjacent gradient heights in the adjacent cells are also zero. The above definitions will then require that

$$\overline{\phi}_k^{n+1} = \phi_{Rk}^{n+1} \quad \text{where} \quad h_{Tk}^{n+1} + h_{Bk}^{n+1} > \Delta z_k \quad \text{(D.170)}$$

It does not appear that eq. (D.163) could be correctly used to compute the updated $\bar{\phi}$. We need to re-derive a method for computing the flux across the k+1/2 boundary where the mixing thickness connects across the grid cell. We may want to go back to the approach derived as eq.**(D.53)**, namely, across the k+1/2 boundary we have



$$\frac{\partial E_{Sk+1/2}}{\partial t} = \frac{1}{2} C_H C_S{}^2 \rho_0 \left\{ \left(\Delta \bar{U}_{k+1/2}\right)^2 + \left(\Delta \bar{V}_{k+1/2}\right)^2 \right\}^{3/2} \quad : \quad t \le T_{kh} \tag{D.171}$$

And we can calculate a similar supply of energy across the k-1/2 boundary. To keep things general, let us write eq. (D.171) as

$$\frac{\partial E_{Sk+1/2}}{\partial t} = \frac{1}{2} C_C \rho_0 \left\{ \left(\Delta \bar{U}_{k+1/2}\right)^2 + \left(\Delta \bar{V}_{k+1/2}\right)^2 \right\}^{3/2} \quad : \quad t \le T_{kh} \tag{D.172}$$

where $C_C = C_H C_S{}^2$ returns eq. (D.171) and $C_C = C_T C_S$ returns eq. **(D.52)**. Thus, the choice of form does not affect the following results.

Where $h_{Tk}^{n+1} + h_{Bk}^{n+1} > \Delta z_k$, the top and bottom mixing layers are deemed to have met in the middle of the grid cell, so the representative density, ρ_{Rk} is no longer a reasonable approximation of the cell density for use in mixing computations. Instead, we will use the average density in the cell as our baseline for mixing. With mixing possible at both the top and bottom boundaries of a cell, the volume flux exchanged through each boundary should be limited to no more than half the grid cell volume. If a volume flux greater than half the volume is implied, then the mixing should be done in stages.

If we use eq. (D.172) for the rate at which mixing energy is supplied, we can compute the rate at which mixing occurs between based on potential energy arguments. We argue that mixing occurs at the rate

$$\frac{\partial E_S}{\partial t} = \frac{\partial E_P}{\partial t} \tag{D.173}$$

The potential energy per unit area in two layers of arbitrary thickness h_1 and h_2 on either side of an interface at elevation z_I is obtained as

$$E_{Pu} = \bar{\rho}_1 g \int_{z_I - h_1}^{z_I} z\,dz + \bar{\rho}_2 g \int_{z_I}^{z_I + h_2} z\,dz \tag{D.174}$$

or (dropping the overbar for simplicity)

$$E_{Pu} = \rho_1 g \left(\frac{z^2}{2} \right)_{z_I - h_1}^{z_I} + \rho_2 g \left(\frac{z^2}{2} \right)_{z_I}^{z_I + h_2} \tag{D.175}$$

or

$$E_{Pu} = \frac{g}{2} \left\{ \rho_1 \left(z_I^2 - [z_I - h_1]^2 \right) + \rho_2 \left([z_I + h_2]^2 - z_I^2 \right) \right\} \tag{D.176}$$

or

$$E_{Pu} = \frac{g}{2} \left\{ \rho_1 \left(\cancel{z_I^2} - \cancel{z_I^2} + 2 z_I h_1 - h_1^2 \right) + \rho_2 \left(\cancel{z_I^2} - 2 z_I h_2 + h_2^2 - \cancel{z_I^2} \right) \right\} \tag{D.177}$$

or

$$E_{Pu} = \frac{g}{2} \left\{ \rho_1 h_1 \left(2 z_I - h_1 \right) + \rho_2 h_2 \left(2 z_I + h_2 \right) \right\} \tag{D.178}$$

After mixing, the potential energy is

$$E_{Pm} = \rho_m g \int_{z_I - h_1}^{z_I + h_2} z\,dz \tag{D.179}$$

or

$$E_{Pm} = \frac{g}{2}\rho_m\left(\left[z_I + h_2\right]^2 - \left[z_I - h_1\right]^2\right) \tag{D.180}$$

or

$$E_{Pm} = \frac{g}{2}\rho_m\left(\cancel{z_I^2} + 2z_I h_2 + h_2^2 - \cancel{z_I^2} + 2z_I h_1 - h_1^2\right) \tag{D.181}$$

or

$$E_{Pm} = \frac{g}{2}\rho_m\left\{h_2\left(2z_I + h_2\right) + h_1\left(2z_I - h_1\right)\right\} \tag{D.182}$$

We require that mass should be conserved during mixing, so

$$\rho_m = \frac{\rho_1 h_1 + \rho_2 h_2}{h_1 + h_2} \tag{D.183}$$

Thus, eq. (D.182) becomes

$$E_{Pm} = \frac{g}{2}\left(\frac{\rho_1 h_1 + \rho_2 h_2}{h_1 + h_2}\right)\left\{h_2\left(2z_I + h_2\right) + h_1\left(2z_I - h_1\right)\right\} \tag{D.184}$$

The change in PE over the course of mixing is found by subtracting eq. (D.178) from (D.184)

$$\begin{aligned} E_{Pm} - E_{Pu} = {} & \frac{g}{2}\left(\frac{\rho_1 h_1 + \rho_2 h_2}{h_1 + h_2}\right)\left\{h_2\left(2z_I + h_2\right) + h_1\left(2z_I - h_1\right)\right\} \\ & -\frac{g}{2}\left\{\rho_1 h_1\left(2z_I - h_1\right) + \rho_2 h_2\left(2z_I + h_2\right)\right\} \end{aligned} \tag{D.185}$$

which expands to

$$\begin{aligned} \frac{2}{g}\left(E_{Pm} - E_{Pu}\right) = {} & \left(\frac{1}{h_1 + h_2}\right)\left\{2\rho_1 h_1 h_2 z_I + \rho_1 h_1 h_2^2 + 2\rho_1 h_1^2 z_I - \rho_1 h_1^3\right\} \\ & + \left(\frac{1}{h_1 + h_2}\right)\left\{2\rho_2 h_2 h_2 z_I + \rho_2 h_2 h_2^2 + 2\rho_2 h_2 h_1 z_I - \rho_2 h_2 h_1^2\right\} \\ & - 2\rho_1 h_1 z_I + \rho_1 h_1^2 - 2\rho_2 h_2 z_I - \rho_2 h_2^2 \end{aligned} \tag{D.186}$$

or

$$
\begin{aligned}
\frac{2}{g}\left(E_{Pm}-E_{Pu}\right) &= \left(\frac{1}{h_1+h_2}\right)\left\{\bcancel{2\rho_1 h_1 h_2 z_I}+\rho_1 h_1 h_2^2+\bcancel{2\rho_1 h_1^2 z_I}-\cancel{\rho_1 h_1^3}\right\} \\
&+\left(\frac{1}{h_1+h_2}\right)\left\{\xcancel{2\rho_2 h_2^2 z_I}+\bcancel{\rho_2 h_2^3}+\cancel{2\rho_2 h_1 h_2 z_I}-\rho_2 h_1^2 h_2\right\} \\
&+\left(\frac{1}{h_1+h_2}\right)\left\{-\bcancel{2\rho_1 h_1^2 z_I}-\bcancel{2\rho_1 h_1 h_2 z_I}+\cancel{\rho_1 h_1^3}+\rho_1 h_1^2 h_2\right\} \\
&+\left(\frac{1}{h_1+h_2}\right)\left\{-\cancel{2\rho_2 h_1 h_2 z_I}-\xcancel{2\rho_2 h_2^2 z_I}-\rho_2 h_1 h_2^2-\underleftrightarrow{\rho_2 h_2}^3\right\}
\end{aligned}
\qquad \text{(D.187)}
$$

or

$$\frac{2}{g}\left(E_{Pm}-E_{Pu}\right)\left(h_1+h_2\right)=h_1 h_2^2\left(\rho_1-\rho_2\right)+h_1^2 h_2\left(\rho_1-\rho_2\right) \qquad \text{(D.188)}$$

or

$$E_{Pm}-E_{Pu}=\frac{2gh_1 h_2^2}{2\left(h_1+h_2\right)}\left(\rho_1-\rho_2\right) \qquad \text{(D.189)}$$

or

$$E_{Pm}-E_{Pu}=\frac{gh_1 h_2^2}{\left(h_1+h_2\right)}\left(\rho_1-\rho_2\right) \qquad \text{(D.190)}$$

Note that if $h_1=h_2=h$ we obtain

$$E_{Pm}-E_{Pu}=\frac{1}{2}gh^2\left(\rho_1-\rho_2\right) \qquad \text{(D.191)}$$

We will model the mixing as an exchange of equal volumes across the grid cell interface, so the rate of increase of potential energy is given by

$$\frac{\partial}{\partial t}\left(E_{Pm}-E_{Pu}\right)=\frac{1}{2}g\left(\rho_1-\rho_2\right)\frac{\partial}{\partial t}\left\{h^2\right\} \qquad \text{(D.192)}$$

or

$$\frac{\partial E_P}{\partial t}=g\left(\rho_1-\rho_2\right)h\frac{\partial h}{\partial t} \qquad \text{(D.193)}$$

In terms of some general grid cell at level ‘k’

$$\frac{\partial E_{Pk+1/2}}{\partial t}=g\left(\rho_k-\rho_{k+1}\right)h\frac{\partial h}{\partial t} \qquad \text{(D.194)}$$

Setting eq. (D.194) and (D.172)

$$\frac{1}{2}C_C\rho_0\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2+\left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2}=g\left(\rho_k-\rho_{k+1}\right)h\frac{\partial h}{\partial t} \quad : \quad t\le T_{kh} \qquad \text{(D.195)}$$

However, it will probably work better to proceed with a discrete version of (D.191) over some increment of time as

$$\Delta t\frac{\partial E_{Pk+1/2}}{\partial t}=\frac{1}{2}gh^2\left(\bar{\rho}_k-\bar{\rho}_{k+1}\right) \qquad \text{(D.196)}$$

Now we consider eq. (D.172) as

$$\Delta t\frac{\partial E_{Sk+1/2}}{\partial t}=\frac{\Delta t}{2}C_C\rho_0\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2+\left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2} \quad : \quad \Delta t\le T_{kh} \qquad \text{(D.197)}$$

so that equating (D.196) and (D.197) provides

$$\frac{\Delta t}{2}C_C\rho_0\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2+\left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2}=\frac{1}{2}gh^2\left(\bar{\rho}_k-\bar{\rho}_{k+1}\right) \quad : \quad \Delta t\le T_{kh} \qquad \text{(D.198)}$$

Thus, the thickness of the mixing region on either side of the grid cell interface is given by

$$h=\sqrt{\frac{\Delta t C_C\rho_0}{g\left(\bar{\rho}_k-\bar{\rho}_{k+1}\right)}\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2+\left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2}} \quad : \quad \Delta t\le T_{kh} \qquad \text{(D.199)}$$

Which can be written as a time interval to mix to a given height as

$$\Delta t_R=gh^2\frac{\left(\bar{\rho}_k-\bar{\rho}_{k+1}\right)}{C_C\rho_0}\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2+\left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{-3/2} \quad : \quad \Delta t_R\le T_{kh} \qquad \text{(D.200)}$$

Since ‘h’ is the height on either side of the interface and is identical on both sides, it follows that the volume flux transported upward from grid cell ‘k’ into grid cell k+1 is exactly equal to the volume flux transported downward from grid cell ‘k+1’ into ‘k’ and must be exactly equal to

$$V=\frac{h}{2}\Delta x\,\Delta y \qquad \text{(D.201)}$$

Thus, the volume flux rate of the mixing exchange is given by

$$\frac{V}{\Delta t}=\frac{h}{2\Delta t}\Delta x\,\Delta y \qquad \text{(D.202)}$$

It follows that the volume exchanged is 25% of the grid cell thickness when

$$V=\frac{\Delta z}{4}\Delta x\,\Delta y \qquad \text{(D.203)}$$

or

$$h = \frac{\Delta z}{2} \tag{D.204}$$

The time at which ¼ of the volume of the cell has been exchanged is found by solving eq. (D.200) using (D.204), or

$$\Delta t_R = \frac{-g\left(\Delta z_k\right)^2 \Delta\bar{\rho}_{k+1/2}}{4C_C\rho_0}\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2 + \left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{-3/2} \tag{D.205}$$

If $T_{kh} \leq \Delta t_R$ then the KH mixing is conducted in a single step such that the mixing thickness in a single cell is

$$h_{k+1/2} = \sqrt{\frac{T_{kh}C_C\rho_0}{g\left(\bar{\rho}_k - \bar{\rho}_{k+1}\right)}\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2 + \left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2}} \tag{D.206}$$

and the volume flux (per unit area) is given by

$$\frac{\mathcal{V}}{\Delta x\,\Delta y} = \frac{1}{2}\sqrt{\frac{T_{kh}C_C\rho_0}{g\left(\bar{\rho}_k - \bar{\rho}_{k+1}\right)}\left\{\left(\Delta\bar{U}_{k+1/2}\right)^2 + \left(\Delta\bar{V}_{k+1/2}\right)^2\right\}^{3/2}} \tag{D.207}$$

It follows that the change of any conservative scalar average volume concentration, $\bar{\phi}$, is given by

$$\bar{\phi}_k^{n+1}\Delta z = \bar{\phi}_k^n\Delta z - \frac{V_{k+1/2}}{\Delta x\,\Delta y}\bar{\phi}_k^n + \frac{V_{k+1/2}}{\Delta x\,\Delta y}\bar{\phi}_{k+1}^n - \frac{V_{k-1/2}}{\Delta x\,\Delta y}\bar{\phi}_k^n + \frac{V_{k-1/2}}{\Delta x\,\Delta y}\bar{\phi}_{k-1}^n \tag{D.208}$$

or

$$\bar{\phi}_k^{n+1}\Delta z = \bar{\phi}_k^n\Delta z + \frac{V_{k+1/2}}{\Delta x\,\Delta y}\left(\bar{\phi}_{k+1}^n - \bar{\phi}_k^n\right) - \frac{V_{k-1/2}}{\Delta x\,\Delta y}\left(\bar{\phi}_k^n - \bar{\phi}_{k-1}^n\right) \tag{D.209}$$

Substituting eq. (D.207) when both $T_{KHk+1/2} \leq \Delta t_{Rk+1/2}$ and $T_{KHk-1/2} \leq \Delta t_{Rk-1/2}$ we obtain

$$\begin{aligned}\bar{\phi}_k^{n+1}\Delta z = \bar{\phi}_k^n\Delta z + \frac{1}{2}\left(\frac{C_C\rho_0}{g}\right)^{1/2} & \left\{\Delta\bar{\phi}_{k+1/2}^n\left(\frac{T_{KHk+1/2}}{-\Delta\bar{\rho}_{k+1/2}}\right)^{1/2}\left[\left(\Delta\bar{U}_{k+1/2}\right)^2 + \left(\Delta\bar{V}_{k+1/2}\right)^2\right]^{3/4}\right. \\ & \left. -\Delta\bar{\phi}_{k-1/2}^n\left(\frac{T_{KHk-1/2}}{-\Delta\bar{\rho}_{k-1/2}}\right)^{1/2}\left[\left(\Delta\bar{U}_{k-1/2}\right)^2 + \left(\Delta\bar{V}_{k-1/2}\right)^2\right]^{3/4}\right\}\end{aligned} \tag{D.210}$$

However, in the case where $T_{KHk+1/2} \geq \Delta t_{Rk+1/2}$ or $T_{KHk-1/2} \geq \Delta t_R$, then we must proceed in several steps. That is, as defined in eq. (D.205), Δt_R is the time required for fully ½ of the grid cell volume to be involved in mixing. At this point, it is reasonable to assume that similar mixing at the k-1/2 boundary may affect the mixing at the k+1/2 boundary. Thus, where $T_{KHk+1/2} \geq \Delta t_R$ or $T_{KHk-1/2} \geq \Delta t_R$ we will slightly modify eq. (D.210) as

$$\begin{aligned} \overline{\phi}_k^{S1}\Delta z = \overline{\phi}_k^{n}\Delta z + \frac{1}{2}\left(\frac{C_C\rho_0}{g}\right)^{1/2} \Bigg\{ & \Delta\overline{\phi}^n_{k+1/2}\left(\frac{\Delta t^{S0}}{-\Delta\overline{\rho}_{k+1/2}}\right)^{1/2}\left[\left(\Delta\overline{U}_{k+1/2}\right)^2 + \left(\Delta\overline{V}_{k+1/2}\right)^2\right]^{3/4} \\ & -\Delta\overline{\phi}^n_{k-1/2}\left(\frac{\Delta t^{S0}}{-\Delta\overline{\rho}_{k-1/2}}\right)^{1/2}\left[\left(\Delta\overline{U}_{k-1/2}\right)^2 + \left(\Delta\overline{V}_{k-1/2}\right)^2\right]^{3/4}\Bigg\} \end{aligned} \tag{D.211}$$

where $\Delta t^{S0} = \min\left[\Delta t_{Rk+1/2}, \Delta t_{Rk-1/2}\right]$ and ϕ^{S1} is the new value of ϕ after a single step of Δt_{S1}. Once we have computed new values for the set $\left[\overline{U}^{S1}, \overline{V}^{S1}, \overline{\rho}^{S1}, \overline{\phi}^{S1}\right]$ we can compute a new value of Δt_R^{S1} for both the k+1/2 and k-1/2 faces from (for example)

$$\Delta t^{S1}_{Rk+1/2} = \frac{-g\left(\Delta z_k\right)^2 \Delta\overline{\rho}^{S1}_{k+1/2}}{4C_C\rho_0}\left\{\left(\Delta\overline{U}^{S1}_{k+1/2}\right)^2 + \left(\Delta\overline{V}^{S1}_{k+1/2}\right)^2\right\}^{-3/2} \tag{D.212}$$

We then define $\Delta t^{S1} = \min\left[\Delta t^{S1}_{Rk+1/2}, \Delta t^{S1}_{Rk-1/2}\right]$. If $T_{KHk+1/2} \geq \Delta t^{S0} + \Delta t^{S1}$ or $T_{KHk-1/2} \geq \Delta t^{S0} + \Delta t^{S1}$, then it will be necessary to perform both a second step similar to eq. (D.211) and a third step as well. To write this in a more general form, we will have to take note that the last step will need to be limited by $\Delta t^{last} = T_{KH} - \sum_{i=1,n} \Delta t^{Si}$.

Appendix E DERIVATION OF GRADIENT MIXING

E.1 Introduction

We are interested in determining the change in kinetic energy and the change in potential energy when a gradient region increases in thickness. Let us consider a simple system that begins with two uniform density (and velocity) regions separated by a linearly-varying region. We will call the initial state α. After some mixing, the gradient region is now thicker, but still provides a linear gradient between unchanged uniform density and velocity regions (i.e. the mixing does not affect properties outside the gradient region. The final state after mixing is β. The initial linear region has thickness h_α and the final state linear region has thickness h_β. We require

$$0 \leq h_\alpha \leq h_\beta \tag{E.1}$$

and define the thickness difference as

$$\delta_h \equiv h_\beta - h_\alpha \tag{E.2}$$

Let $z_0 = 0$ be the base of the linear gradient region in the final state. Let ρ_1, U_1 represent the lower layer characteristics and ρ_2, U_2 represent the upper layer.

E.2 Summary of the derivation

The following sections show that the inital potential energy (before mixing) is given by eq. (E.58). The final potential energy (after mixing) is given by eq. (E.10). The initial kinetic energy is given by eq. (E.103). The final kinetic energy is given by eq. (E.20). The change in potential energy is given by eq. (E.62), and the change in kinetic energy is given by eq. (E.128).

E.3 Potential energy in final state

The potential energy in the final state is

$$E_{p\beta} = \int_0^{h_\beta} g\rho_\beta(z) z dz \tag{E.3}$$

The density in the linear region at the final state is given by

$$\rho_\beta(z) = \rho_1 - \frac{z}{h_\beta}(\rho_1 - \rho_2) \tag{E.4}$$

To be consistent with taking differences from the upper to the lower level we define

$$\Delta\rho \equiv \rho_2 - \rho_1 \tag{E.5}$$

such that $\Delta\rho < 0$. We then have

$$\rho_\beta(z) = \rho_1 + \frac{z}{h_\beta}\Delta\rho \tag{E.6}$$

So the potential energy is

$$E_{p\beta} = g\int_0^{h_\beta}\left(\rho_1 + \frac{z}{h_\beta}\Delta\rho\right)zdz \tag{E.7}$$

or

$$E_{p\beta} = g\rho_1\int_0^{h_\beta} zdz + g\frac{\Delta\rho}{h_\beta}\int_0^{h_\beta} z^2dz \tag{E.8}$$

or

$$E_{p\beta} = \frac{1}{2}g\rho_1 {h_\beta}^2 + \frac{1}{3}g\frac{\Delta\rho}{h_\beta}{h_\beta}^3 \tag{E.9}$$

or

$$E_{p\beta} = g{h_\beta}^2\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) \tag{E.10}$$

E.4 Kinetic energy in final state

The kinetic energy in the final state is given by

$$E_{k\beta} = \int_0^{h_\beta}\frac{1}{2}\rho(z)\left\{U_\beta(z)\right\}^2 dz \tag{E.11}$$

We have

$$U_\beta(z) = U_1 + \frac{z}{h_\beta}\Delta U \tag{E.12}$$

where

$$\Delta U \equiv U_2 - U_1 \tag{E.13}$$

so we obtain

$$E_{k\beta} = \int_0^{h_\beta} \frac{1}{2}\left\{\rho_1 + \frac{z}{h_\beta}\Delta\rho\right\}\left\{U_1 + \frac{z}{h_\beta}\Delta U\right\}^2 dz \tag{E.14}$$

expanding

$$E_{k\beta} = \int_0^{h_\beta} \frac{1}{2}\left\{\rho_1 + \frac{z}{h_\beta}\Delta\rho\right\}\left\{U_1^{\,2} + 2\frac{z}{h_\beta}\Delta U U_1 + \frac{z^2}{h_\beta^{\,2}}\Delta U^2\right\}dz \tag{E.15}$$

more expanding

$$E_{k\beta} = \frac{1}{2}\rho_1 \int_0^{h_\beta}\left\{U_1^{\,2} + 2\frac{z}{h_\beta}\Delta U U_1 + \frac{z^2}{h_\beta^{\,2}}\Delta U^2\right\}dz + \frac{1}{2}\frac{\Delta\rho}{h_\beta}\int_0^{h_\beta}\left\{U_1^{\,2}z + 2\frac{z^2}{h_\beta}\Delta U U_1 + \frac{z^3}{h_\beta^{\,2}}\Delta U^2\right\}dz \tag{E.16}$$

more expanding

$$\begin{aligned} E_{k\beta} = {} & \frac{1}{2}\rho_1 U_1^{\,2}\int_0^{h_\beta} dz + \frac{1}{h_\beta}\rho_1 \Delta U U_1 \int_0^{h_\beta} z dz + \frac{1}{2h_\beta^{\,2}}\rho_1 \Delta U^2 \int_0^{h_\beta} z^2 dz \\ & + \frac{1}{2h_\beta}\Delta\rho U_1^{\,2}\int_0^{h_\beta} z dz + \frac{1}{h_\beta^{\,2}}\Delta\rho\Delta U U_1 \int_0^{h_\beta} z^2 dz + \frac{1}{2h_\beta^{\,3}}\Delta\rho\Delta U^2 \int_0^{h_\beta} z^3 dz \end{aligned} \tag{E.17}$$

integrating

$$\begin{aligned} E_{k\beta} = {} & \frac{1}{2}\rho_1 U_1^{\,2}\left(h_\beta\right) + \frac{1}{h_\beta}\rho_1 \Delta U U_1\left(\frac{h_\beta^{\,2}}{2}\right) + \frac{1}{2h_\beta^{\,2}}\rho_1 \Delta U^2\left(\frac{h_\beta^{\,3}}{3}\right) \\ & + \frac{1}{2h_\beta}\Delta\rho U_1^{\,2}\left(\frac{h_\beta^{\,2}}{2}\right) + \frac{1}{h_\beta^{\,2}}\Delta\rho\Delta U U_1\left(\frac{h_\beta^{\,3}}{3}\right) + \frac{1}{2h_\beta^{\,3}}\Delta\rho\Delta U^2\left(\frac{h_\beta^{\,4}}{4}\right) \end{aligned} \tag{E.18}$$

canceling

$$\begin{aligned} E_{k\beta} = {} & \frac{1}{2}\rho_1 U_1^{\,2} h_\beta + \frac{1}{2}\rho_1 \Delta U U_1 h_\beta + \frac{1}{6}\rho_1 \Delta U^2 h_\beta \\ & + \frac{1}{4}\Delta\rho U_1^{\,2} h_\beta + \frac{1}{3}\Delta\rho\Delta U U_1 h_\beta + \frac{1}{8}\Delta\rho\Delta U^2 h_\beta \end{aligned} \tag{E.19}$$

combining

$$E_{k\beta} = U_1{}^2 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right) + \Delta U U_1 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) + \Delta U^2 h_\beta\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) \tag{E.20}$$

So eq. (E.10) and (E.20) provide the potential and kinetic energy of the section of fluid in state β.

E.5 Potential energy in initial state

Now let us consider the potential energy in state α, which is more complex due to the need to treat the uniform sections above and below the linear section of thickness h_α

$$E_{p\alpha} = \int_0^{\delta_h/2} g\rho_1 z dz + \int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\rho_\alpha(z) z dz + \int_{h_\beta-\delta_h/2}^{h_\beta} g\rho_2 z dz \tag{E.21}$$

where

$$\rho_\alpha(z) = \rho_1 + \frac{z - \frac{1}{2}\delta_h}{h_\alpha}\Delta\rho \tag{E.22}$$

The first term of eq. (E.21) is

$$\int_0^{\delta_h/2} g\rho_1 z dz = \frac{1}{2} g\rho_1\left(\frac{\delta_h}{2}\right)^2 \tag{E.23}$$

or

$$\int_0^{\delta_h/2} g\rho_1 z dz = \frac{1}{8} g\rho_1 \delta_h{}^2 \tag{E.24}$$

The third term of eq. (E.21) is

$$\int_{h_\beta-\delta_h/2}^{h_\beta} g\rho_2 z dz = \frac{1}{2} g\rho_2\left\{h_\beta{}^2 - \left[h_\beta - \frac{1}{2}\delta_h\right]^2\right\} \tag{E.25}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} g\rho_2 z dz = \frac{1}{2} g\rho_2\left\{h_\beta{}^2 - \left[h_\beta{}^2 - \delta_h h_\beta + \frac{1}{4}\delta_h{}^2\right]\right\} \tag{E.26}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} g\rho_2 z dz = \frac{1}{2} g\rho_2 \left(\delta_h h_\beta - \frac{1}{4}\delta_h{}^2 \right) \tag{E.27}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} g\rho_2 z dz = \frac{1}{2} g\rho_2 \delta_h h_\beta - \frac{1}{8} g\rho_2 \delta_h{}^2 \tag{E.28}$$

The second term of eq. (E.21) is

$$\int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\{\rho_\alpha(z)\} z dz = \int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\left\{ \rho_1 + \frac{z-\frac{1}{2}\delta_h}{h_\alpha}\Delta\rho \right\} z dz \tag{E.29}$$

or

$$\int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\{\rho_\alpha(z)\} z dz = g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz + \frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} \left\{ z - \frac{1}{2}\delta_h \right\} z dz \tag{E.30}$$

or

$$\int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\{\rho_\alpha(z)\} z dz = g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz + \frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz - \frac{1}{2h_\alpha} g\Delta\rho\delta_h \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz \tag{E.31}$$

or

$$\int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\{\rho_\alpha(z)\} z dz = \left(g\rho_1 - \frac{1}{2h_\alpha} g\Delta\rho\delta_h \right) \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz + \frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz \tag{E.32}$$

The first term of eq. (E.32) is

$$g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz = \frac{1}{2}\left(g\rho_1 - \frac{1}{2h_\alpha} g\Delta\rho\delta_h \right) \left\{ \left[h_\alpha + \frac{1}{2}\delta_h \right]^2 - \frac{1}{4}\delta_h{}^2 \right\} \tag{E.33}$$

or

$$g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z dz = \frac{1}{2}\left(g\rho_1 - \frac{1}{2h_\alpha} g\Delta\rho\delta_h \right) \left\{ \left[h_\alpha{}^2 + \delta_h h_\alpha + \frac{1}{4}\delta_h{}^2 \right] - \frac{1}{4}\delta_h{}^2 \right\} \tag{E.34}$$

or

$$g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z\,dz = \frac{1}{2}\left(g\rho_1 - \frac{1}{2h_\alpha} g\Delta\rho\delta_h \right) h_\alpha \left\{ h_\alpha + \delta_h \right\} \tag{E.35}$$

or

$$g\rho_1 \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z\,dz = \frac{1}{2} g\rho_1 h_\alpha h_\beta - \frac{1}{4} g\Delta\rho\delta_h h_\beta \tag{E.36}$$

The second term of eq. (E.32) is

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3h_\alpha} g\Delta\rho \left\{ \left[h_\alpha + \frac{1}{2}\delta_h \right]^3 - \frac{1}{8}\delta_h{}^3 \right\} \tag{E.37}$$

or

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3h_\alpha} g\Delta\rho \left\{ \left[h_\alpha{}^2 + \delta_h h_\alpha + \frac{1}{4}\delta_h{}^2 \right]\left[h_\alpha + \frac{1}{2}\delta_h \right] - \frac{1}{8}\delta_h{}^3 \right\} \tag{E.38}$$

or

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3h_\alpha} g\Delta\rho \left\{ h_\alpha{}^3 + \delta_h h_\alpha{}^2 + \frac{1}{4}\delta_h{}^2 h_\alpha + \frac{1}{2}\delta_h h_\alpha{}^2 + \frac{1}{2}\delta_h{}^2 h_\alpha + \frac{1}{8}\delta_h{}^3 - \frac{1}{8}\delta_h{}^3 \right\} \tag{E.39}$$

or

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3h_\alpha} g\Delta\rho \left\{ h_\alpha{}^3 + \frac{3}{2}\delta_h h_\alpha{}^2 + \frac{3}{4}\delta_h{}^2 h_\alpha \right\} \tag{E.40}$$

or

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3} g\Delta\rho \left\{ h_\alpha{}^2 + \frac{3}{2}\delta_h h_\alpha + \frac{3}{4}\delta_h{}^2 \right\} \tag{E.41}$$

or

$$\frac{1}{h_\alpha} g\Delta\rho \int_{\delta_h/2}^{h_\alpha+\delta_h/2} z^2 dz = \frac{1}{3} g\Delta\rho h_\alpha{}^2 + \frac{1}{2} g\Delta\rho\delta_h h_\alpha + \frac{1}{4} g\Delta\rho\delta_h{}^2 \tag{E.42}$$

Putting together eq. (E.36), and (E.42), we have eq. (E.32), which is the second term in eq. (E.21) as

$$\int_{\delta_h/2}^{h_\alpha+\delta_h/2} g\{\rho_\alpha(z)\} z dz = \frac{1}{2} g\rho_1 h_\alpha h_\beta - \frac{1}{4} g\Delta\rho\delta_h h_\beta + \frac{1}{3} g\Delta\rho h_\alpha{}^2 + \frac{1}{2} g\Delta\rho\delta_h h_\alpha + \frac{1}{4} g\Delta\rho\delta_h{}^2 \quad \text{(E.43)}$$

Putting together eq. (E.24), (E.28) and (E.43) to provide eq. (E.21), as

$$\begin{aligned} E_{p\alpha} = &\left\{\frac{1}{8} g\rho_1\delta_h{}^2\right\} + \left\{\frac{1}{2} g\rho_1 h_\alpha h_\beta - \frac{1}{4} g\Delta\rho\delta_h h_\beta + \frac{1}{3} g\Delta\rho h_\alpha{}^2 + \frac{1}{2} g\Delta\rho\delta_h h_\alpha + \frac{1}{4} g\Delta\rho\delta_h{}^2\right\} \\ &+ \left\{\frac{1}{2} g\rho_2\delta_h h_\beta - \frac{1}{8} g\rho_2\delta_h{}^2\right\} \end{aligned} \quad \text{(E.44)}$$

or

$$E_{p\alpha} = g\rho_1\left(\frac{1}{8}\delta_h{}^2 + \frac{1}{2} h_\alpha h_\beta\right) + g\Delta\rho\left\{\frac{1}{3} h_\alpha{}^2 + \frac{1}{2}\delta_h h_\alpha + \frac{1}{4}\delta_h{}^2 - \frac{1}{4}\delta_h h_\beta\right\} + g\rho_2\left(\frac{1}{2}\delta_h h_\beta - \frac{1}{8}\delta_h{}^2\right) \text{(E.45)}$$

using eq. (E.5), the last term of eq. (E.45) is

$$g\rho_2\left(\frac{1}{2}\delta_h h_\beta - \frac{1}{8}\delta_h{}^2\right) = g(\rho_1 + \Delta\rho)\left(\frac{1}{2}\delta_h h_\beta - \frac{1}{8}\delta_h{}^2\right) \quad \text{(E.46)}$$

or

$$g\rho_2\left(\frac{1}{2}\delta_h h_\beta - \frac{1}{8}\delta_h{}^2\right) = \frac{1}{2} g\rho_1\delta_h h_\beta - \frac{1}{8} g\rho_1\delta_h{}^2 + \frac{1}{2} g\Delta\rho\delta_h h_\beta - \frac{1}{8} g\Delta\rho\delta_h{}^2 \quad \text{(E.47)}$$

so that eq. (E.45) is now

$$\begin{aligned} E_{p\alpha} = &g\rho_1\left(\frac{1}{8}\delta_h{}^2 + \frac{1}{2} h_\alpha h_\beta\right) + g\Delta\rho\left\{\frac{1}{3} h_\alpha{}^2 + \frac{1}{2}\delta_h h_\alpha + \frac{1}{4}\delta_h{}^2 - \frac{1}{4}\delta_h h_\beta\right\} \\ &+ g\rho_1\frac{1}{2}\delta_h h_\beta - g\rho_1\frac{1}{8}\delta_h{}^2 + g\Delta\rho\frac{1}{2}\delta_h h_\beta - g\Delta\rho\frac{1}{8}\delta_h{}^2 \end{aligned} \quad \text{(E.48)}$$

combining terms provides:

$$\begin{aligned} E_{p\alpha} = &g\rho_1\left(\cancel{\frac{1}{8}\delta_h{}^2} + \frac{1}{2} h_\alpha h_\beta + \frac{1}{2}\delta_h h_\beta - \cancel{\frac{1}{8}\delta_h{}^2}\right) \\ &+ g\Delta\rho\left\{\frac{1}{3} h_\alpha{}^2 + \frac{1}{2}\delta_h h_\alpha + \frac{1}{4}\delta_h{}^2 - \frac{1}{4}\delta_h h_\beta + \frac{1}{2}\delta_h h_\beta - \frac{1}{8}\delta_h{}^2\right\} \end{aligned} \quad \text{(E.49)}$$

or

$$\begin{aligned} E_{p\alpha} &= g\rho_1\left(\frac{1}{2}h_\alpha h_\beta + \frac{1}{2}\delta_h h_\beta\right) \\ &\quad + g\Delta\rho\left\{\frac{1}{3}{h_\alpha}^2 + \frac{1}{2}\delta_h h_\alpha + \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \end{aligned} \tag{E.50}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 h_\beta\left(h_\alpha + \delta_h\right) + g\Delta\rho\left\{\frac{1}{3}{h_\alpha}^2 + \frac{1}{2}\delta_h h_\alpha + \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \tag{E.51}$$

using the definitions implied by eq. (E.2)

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}\left(h_\beta - \delta_h\right)^2 + \frac{1}{2}\delta_h\left(h_\beta - \delta_h\right) + \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \tag{E.52}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}\left({h_\beta}^2 - 2\delta_h h_\beta + {\delta_h}^2\right) + \frac{1}{2}\left(\delta_h h_\beta - {\delta_h}^2\right) + \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \tag{E.53}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}{h_\beta}^2 - \frac{2}{3}\delta_h h_\beta + \frac{1}{3}{\delta_h}^2 + \frac{1}{2}\delta_h h_\beta - \frac{1}{2}{\delta_h}^2 + \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \tag{E.54}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}{h_\beta}^2 + {\delta_h}^2\left(\frac{1}{3} - \frac{1}{2} + \frac{1}{8}\right) + \delta_h h_\beta\left(\frac{1}{2} - \frac{2}{3} + \frac{1}{4}\right)\right\} \tag{E.55}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}{h_\beta}^2 + {\delta_h}^2\left(\frac{8}{24} - \frac{12}{24} + \frac{3}{24}\right) + \delta_h h_\beta\left(\frac{6}{12} - \frac{8}{12} + \frac{3}{12}\right)\right\} \tag{E.56}$$

or

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + g\Delta\rho\left\{\frac{1}{3}{h_\beta}^2 - \frac{1}{24}{\delta_h}^2 + \frac{1}{12}\delta_h h_\beta\right\} \tag{E.57}$$

So the potential energy at the initial state is

$$E_{p\alpha} = \frac{1}{2}g\rho_1 {h_\beta}^2 + \frac{1}{3}g\Delta\rho\left\{{h_\beta}^2 - \frac{1}{8}{\delta_h}^2 + \frac{1}{4}\delta_h h_\beta\right\} \tag{E.58}$$

E.6 Change in potential energy

So the change in the potential energy from state α to β is obtained by subtracting eq. (E.58) from eq. (E.10)

$$E_{p\beta} - E_{p\alpha} = g h_\beta^2 \left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho \right) - \frac{1}{2} g \rho_1 h_\beta^2 - \frac{1}{3} g \Delta\rho \left(h_\beta^2 - \frac{1}{8}\delta_h^2 + \frac{1}{4}\delta_h h_\beta \right) \tag{E.59}$$

or

$$E_{p\beta} - E_{p\alpha} = g h_\beta^2 \left(\xcancel{\frac{1}{2}\rho_1 - \frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho - \frac{1}{3}\Delta\rho} \right) - \frac{1}{3} g \Delta\rho \left(-\frac{1}{8}\delta_h^2 + \frac{1}{4}\delta_h h_\beta \right) \tag{E.60}$$

or

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{3} g \Delta\rho \delta_h \left(\frac{1}{4} h_\beta - \frac{1}{8}\delta_h \right) \tag{E.61}$$

or, the increase in PE due to gradient mixing is:

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{12} g \Delta\rho \delta_h \left(h_\beta - \frac{1}{2}\delta_h \right) \tag{E.62}$$

or

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{24} g \Delta\rho \delta_h \left(h_\beta + h_\alpha \right) \tag{E.63}$$

or

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{24} g \Delta\rho \left(h_\beta - h_\alpha \right)\left(h_\beta + h_\alpha \right) \tag{E.64}$$

or

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{24} g \Delta\rho \left(h_\beta^2 - h_\alpha^2 \right) \tag{E.65}$$

or

$$E_{p\beta} - E_{p\alpha} = \frac{1}{24} \rho_0 g' \left(h_\beta^2 - h_\alpha^2 \right) \tag{E.66}$$

write this as either

$$E_P = \frac{1}{2} c_{S\rho} \rho_{avg} g' \left(h_\beta^2 - h_\alpha^2 \right) \tag{E.67}$$

or, using eq. (E.63)

$$E_P = c_{S\rho}\rho_{avg}g'\delta_h h_{avg} \quad : \quad \frac{M}{L^3}\frac{L}{T^2}LL = \frac{M}{T^2} = \frac{\text{energy}}{\text{unit area}} \tag{E.68}$$

where we use

$$g' \equiv -g\frac{\Delta\rho}{\rho_0} \tag{E.69}$$

To check eq. (E.62), let us consider the case where $h_\alpha = 0$ so that $\delta_h = h_\beta$. We obtain

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{12}g\Delta\rho h_\beta\left(h_\beta - \frac{1}{2}h_\beta\right) \tag{E.70}$$

or

$$E_{p\beta} - E_{p\alpha} = -\frac{1}{24}g\Delta\rho {h_\beta}^2 \tag{E.71}$$

The above is identical to that of Sherman et al. (1978), attributed to Turner (1973, pp. 322,323). For $h_\alpha = 0$, we have the potential energy in state α as

$$E_{p\alpha(0)} = \int_0^{h_\beta/2} g\rho_1 z dz + \int_{h_\beta/2}^{h_\beta} g\rho_2 z dz \tag{E.72}$$

or

$$E_{p\alpha(0)} = \frac{1}{2}g\rho_1\left(\frac{h_\beta}{2}\right)^2 + \frac{1}{2}g\rho_2\left\{{h_\beta}^2 - \left(\frac{h_\beta}{2}\right)^2\right\} \tag{E.73}$$

or

$$E_{p\alpha(0)} = \frac{1}{8}g\rho_1{h_\beta}^2 + \frac{3}{8}g\rho_2{h_\beta}^2 \tag{E.74}$$

or

$$E_{p\alpha(0)} = \frac{1}{8}g\rho_1{h_\beta}^2 + \frac{3}{8}g\rho_1{h_\beta}^2 + \frac{3}{8}g\Delta\rho{h_\beta}^2 \tag{E.75}$$

or

$$E_{p\alpha(0)} = \frac{1}{2}g\rho_1{h_\beta}^2 + \frac{3}{8}g\Delta\rho{h_\beta}^2 \tag{E.76}$$

So the subtracting eq. (E.76) from eq, (E.10) provides

$$E_{p\beta} - E_{p\alpha(0)} = gh_\beta{}^2\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) - \frac{1}{2}g\rho_1 h_\beta{}^2 - \frac{3}{8}g\Delta\rho h_\beta{}^2 \tag{E.77}$$

or

$$E_{p\beta} - E_{p\alpha(0)} = gh_\beta{}^2\left(\cancel{\frac{1}{2}\rho_1 - \frac{1}{2}\rho_1} + \frac{1}{3}\Delta\rho - \frac{3}{8}\Delta\rho\right) \tag{E.78}$$

or

$$E_{p\beta} - E_{p\alpha(0)} = gh_\beta{}^2\Delta\rho\left(\frac{8}{24} - \frac{9}{24}\right) \tag{E.79}$$

or

$$E_{p\beta} - E_{p\alpha(0)} = -gh_\beta{}^2\Delta\rho\left(\frac{1}{24}\right) \tag{E.80}$$

or

$$E_{p\beta} - E_{p\alpha(0)} = -\frac{1}{24}g\Delta\rho h_\beta{}^2 \tag{E.81}$$

As eq. (E.81) matches eq. (E.71), we have some confidence that eq. (E.62) is correctly derived.

Also, as a further check, let us consider the change in PE derived in class note for CE380S which considers only uniform layers. We there obtain

$$\Delta E_p = -\frac{1}{2}g\Delta\rho\left(\frac{h}{2}\right)^2 \tag{E.82}$$

where h is the mixing layer thickness. We then obtain

$$\Delta E_p = -\frac{1}{8}g\Delta\rho h^2 \tag{E.83}$$

Note that eq. (E.81) is significantly smaller change in PE than eq. (E.83), which is as expected as the latter implies mixing into a uniform layer.

E.7 Kinetic energy at initial state

Next let us consider the kinetic energy in the case of the α state

$$E_{k\alpha} = \int_0^{\delta_h/2}\frac{1}{2}\rho_1 U_1{}^2 dz + \int_{\delta_h/2}^{h_\beta-\delta_h/2}\frac{1}{2}\rho_\alpha(z)\{U_\alpha(z)\}^2 dz + \int_{h_\beta-\delta_h/2}^{h_\beta}\frac{1}{2}\rho_2 U_2{}^2 dz \tag{E.84}$$

Considering the first term in eq. (E.84)

$$\int_0^{\delta_h/2} \frac{1}{2}\rho_1 U_1{}^2 dz = \frac{1}{2}\rho_1 U_1{}^2 \left(\frac{\delta_h}{2}\right) \tag{E.85}$$

or

$$\int_0^{\delta_h/2} \frac{1}{2}\rho_1 U_1{}^2 dz = \frac{1}{4}\rho_1 U_1{}^2 \delta_h \tag{E.86}$$

The third term in eq. (E.84) is

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{2}\rho_2 U_2{}^2 \left\{h_\beta - \left[h_\beta - \frac{\delta_h}{2}\right]\right\} \tag{E.87}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{4}\rho_2 U_2{}^2 \delta_h \tag{E.88}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{4}\rho_1 U_2{}^2 \delta_h + \frac{1}{4}\Delta\rho U_2{}^2 \delta_h \tag{E.89}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{4}\rho_1 \left(U_1 + \Delta U\right)^2 \delta_h + \frac{1}{4}\Delta\rho\left(U_1 + \Delta U\right)^2 \delta_h \tag{E.90}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{4}\rho_1 \left(U_1{}^2 + 2\Delta U U_1 + \Delta U^2\right)\delta_h + \frac{1}{4}\Delta\rho\left(U_1{}^2 + 2\Delta U U_1 + \Delta U^2\right)\delta_h \tag{E.91}$$

or

$$\int_{h_\beta-\delta_h/2}^{h_\beta} \frac{1}{2}\rho_2 U_2{}^2 dz = \frac{1}{4}U_1{}^2\delta_h\left\{\rho_1 + \Delta\rho\right\} + \frac{1}{2}\Delta U U_1 \delta_h\left\{\rho_1 + \Delta\rho\right\} + \frac{1}{4}\Delta U^2 \delta_h\left\{\rho_1 + \Delta\rho\right\} \tag{E.92}$$

The second term in eq. (E.84) could be re-written as

$$\int_0^{h_\alpha} \frac{1}{2}\rho_\gamma(z)\left\{U_\lambda(z)\right\}^2 dz \tag{E.93}$$

where

$$\rho_\gamma(z) = \rho_1 + \frac{z}{h_\alpha}\Delta\rho \quad : \quad 0 \le z \le h_\alpha \tag{E.94}$$

and

$$U_\gamma(z) = U_1 + \frac{z}{h_\alpha}\Delta U \quad : \quad 0 \le z \le h_\alpha \tag{E.95}$$

so that we have

$$\int_0^{h_\alpha} \frac{1}{2}\rho_\gamma(z)\left\{U_\lambda(z)\right\}^2 dz = \frac{1}{2}\int_0^{h_\alpha} \left(\rho_1 + \frac{z}{h_\alpha}\Delta\rho\right)\left\{U_1 + \frac{z}{h_\alpha}\Delta U\right\}^2 dz \tag{E.96}$$

which is of the same form as eq. (E.14), repeated here for convenience, except that h_α everywhere replaces h_β

$$E_{k\beta} = \int_0^{h_\beta} \frac{1}{2}\left\{\rho_1 + \frac{z}{h_\beta}\Delta\rho\right\}\left\{U_1 + \frac{z}{h_\beta}\Delta U\right\}^2 dz \tag{E.97}$$

Thus, without further derivation, the integration of eq. (E.96) can be based on the integration of eq. (E.97), which is given as eq. (E.20) – the result is

$$\int_0^{h_\alpha} \frac{1}{2}\rho_\gamma(z)\left\{U_\lambda(z)\right\}^2 dz = U_1{}^2 h_\alpha\left(\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right) + \Delta U U_1 h_\alpha\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) + \Delta U^2 h_\alpha\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) \tag{E.98}$$

Putting together eq. (E.86), (E.92) and (E.98) to provide the integration of eq. (E.84)

$$\begin{aligned} E_{k\alpha} &= \frac{1}{4}\rho_1 U_1{}^2 \delta_h \\ &+ U_1{}^2 h_\alpha\left(\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right) + \Delta U U_1 h_\alpha\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) + \Delta U^2 h_\alpha\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) \\ &+ \frac{1}{4}U_1{}^2\delta_h\left\{\rho_1 + \Delta\rho\right\} + \frac{1}{2}\Delta U U_1 \delta_h\left\{\rho_1 + \Delta\rho\right\} + \frac{1}{4}\Delta U^2 \delta_h\left\{\rho_1 + \Delta\rho\right\} \end{aligned} \tag{E.99}$$

or

$$\begin{aligned}
E_{k\alpha} &= U_1{}^2\delta_h\left(\frac{1}{4}\rho_1\right) \\
&+U_1{}^2\left(h_\beta-\delta_h\right)\left\{\frac{1}{2}\rho_1+\frac{1}{4}\Delta\rho\right\}+\Delta UU_1\left(h_\beta-\delta_h\right)\left(\frac{1}{2}\rho_1+\frac{1}{3}\Delta\rho\right)+\Delta U^2\left(h_\beta-\delta_h\right)\left(\frac{1}{6}\rho_1+\frac{1}{8}\Delta\rho\right) \\
&+U_1{}^2\delta_h\left(\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho\right)+\Delta UU_1\delta_h\left(\frac{1}{2}\rho_1+\frac{1}{2}\Delta\rho\right)+\Delta U^2\delta_h\left(\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho\right)
\end{aligned} \tag{E.100}$$

or

$$\begin{aligned}
E_{k\alpha} &= U_1{}^2\delta_h\left(\frac{1}{4}\rho_1\right) \\
&+U_1{}^2h_\beta\left\{\frac{1}{2}\rho_1+\frac{1}{4}\Delta\rho\right\}-U_1{}^2\delta_h\left\{\frac{1}{2}\rho_1+\frac{1}{4}\Delta\rho\right\}+\Delta UU_1h_\beta\left(\frac{1}{2}\rho_1+\frac{1}{3}\Delta\rho\right)-\Delta UU_1\delta_h\left(\frac{1}{2}\rho_1+\frac{1}{3}\Delta\rho\right) \\
&+\Delta U^2h_\beta\left(\frac{1}{6}\rho_1+\frac{1}{8}\Delta\rho\right)-\Delta U^2\delta_h\left(\frac{1}{6}\rho_1+\frac{1}{8}\Delta\rho\right) \\
&+U_1{}^2\delta_h\left(\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho\right)+\Delta UU_1\delta_h\left(\frac{1}{2}\rho_1+\frac{1}{2}\Delta\rho\right)+\Delta U^2\delta_h\left(\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho\right)
\end{aligned} \tag{E.101}$$

or

$$\begin{aligned}
E_{k\alpha} &= U_1{}^2\delta_h\left(\frac{1}{4}\rho_1-\frac{1}{2}\rho_1-\frac{1}{4}\Delta\rho+\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho\right) \\
&+U_1{}^2h_\beta\left\{\frac{1}{2}\rho_1+\frac{1}{4}\Delta\rho\right\}+\Delta UU_1h_\beta\left(\frac{1}{2}\rho_1+\frac{1}{3}\Delta\rho\right) \\
&+\Delta U^2h_\beta\left(\frac{1}{6}\rho_1+\frac{1}{8}\Delta\rho\right) \\
&+\Delta UU_1\delta_h\left(\frac{1}{2}\rho_1+\frac{1}{2}\Delta\rho-\frac{1}{2}\rho_1-\frac{1}{3}\Delta\rho\right)+\Delta U^2\delta_h\left(\frac{1}{4}\rho_1+\frac{1}{4}\Delta\rho-\frac{1}{6}\rho_1-\frac{1}{8}\Delta\rho\right)
\end{aligned} \tag{E.102}$$

so the kinetic energy in the initial state can be written in terms of the final state as

$$\begin{aligned}
E_{k\alpha} &= +U_1{}^2h_\beta\left\{\frac{1}{2}\rho_1+\frac{1}{4}\Delta\rho\right\}+\Delta UU_1h_\beta\left(\frac{1}{2}\rho_1+\frac{1}{3}\Delta\rho\right) \\
&+\Delta UU_1\delta_h\left(\frac{1}{6}\Delta\rho\right)+\Delta U^2h_\beta\left(\frac{1}{6}\rho_1+\frac{1}{8}\Delta\rho\right)+\Delta U^2\delta_h\left(\frac{1}{12}\rho_1+\frac{1}{8}\Delta\rho\right)
\end{aligned} \tag{E.103}$$

As a check, let us consider the case of $h_\alpha = 0$ such that $h_\beta = \delta_h$, so that eq. (E.103) should reduce to

$$\int_{\delta_h/2}\frac{1}{2}\rho_1U_1{}^2dz+\int_{\delta_h/2}\frac{1}{2}\rho_2U_2{}^2dz=\frac{1}{4}\rho_1U_1{}^2\delta_h+\frac{1}{4}\rho_2U_2{}^2\delta_h \tag{E.104}$$

To demonstrate, substituting $h_\beta = \delta_h$ in eq. (E.103) provides

$$\begin{aligned} E_{k\alpha} &= +U_1{}^2\delta_h\left\{\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right\} + \Delta U U_1\delta_h\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) \\ &+ \Delta U U_1\delta_h\left(\frac{1}{6}\Delta\rho\right) + \Delta U^2\delta_h\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) + \Delta U^2\delta_h\left(\frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \end{aligned} \tag{E.105}$$

or

$$\begin{aligned} E_{k\alpha} &= +U_1{}^2\delta_h\left\{\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right\} + \Delta U U_1\delta_h\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho + \frac{1}{6}\Delta\rho\right) \\ &+ \Delta U^2\delta_h\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho + \frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \end{aligned} \tag{E.106}$$

or

$$E_{k\alpha} = +U_1{}^2\delta_h\left\{\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right\} + \Delta U U_1\delta_h\left(\frac{1}{2}\rho_1 + \frac{1}{2}\Delta\rho\right) + \Delta U^2\delta_h\left(\frac{1}{4}\rho_1 + \frac{1}{4}\Delta\rho\right) \tag{E.107}$$

or

$$E_{k\alpha} = \frac{1}{4}U_1{}^2\delta_h + \frac{1}{4}U_1{}^2\delta_h\left\{\rho_1 + \Delta\rho\right\} + \frac{1}{2}\Delta U U_1\delta_h\left(\rho_1 + \Delta\rho\right) + \frac{1}{4}\Delta U^2\delta_h\left(\rho_1 + \Delta\rho\right) \tag{E.108}$$

or

$$E_{k\alpha} = \frac{1}{4}\delta_h\left\{U_1{}^2\rho_1 + U_1{}^2\left\{\rho_1 + \Delta\rho\right\} + 2\Delta U U_1\left(\rho_1 + \Delta\rho\right) + \Delta U^2\left(\rho_1 + \Delta\rho\right)\right\} \tag{E.109}$$

or

$$E_{k\alpha} = \frac{1}{4}\delta_h\left\{U_1{}^2\rho_1 + \left(\rho_1 + \Delta\rho\right)\left(U_1{}^2 + 2\Delta U U_1 + \Delta U^2\right)\right\} \tag{E.110}$$

or

$$E_{k\alpha} = \frac{1}{4}\delta_h\left\{U_1{}^2\rho_1 + \left(\rho_1 + \Delta\rho\right)\left(U_1 + \Delta U\right)^2\right\} \tag{E.111}$$

or

$$E_{k\alpha} = \frac{1}{4}\delta_h\left\{U_1{}^2\rho_1 + \left(\rho_2\right)\left(U_2\right)^2\right\} \tag{E.112}$$

or

$$E_{k\alpha} = \frac{1}{4}\rho_1 U_1{}^2\delta_h + \frac{1}{4}\rho_2 U_2{}^2\delta_h \tag{E.113}$$

which is the same as eq. (E.104), so eq. (E.103) appears to be the correct initial kinetic energy state.

E.8 Change in kinetic energy

Now let us consider what happens when we subtract eq. (E.103) from eq. (E.20)

$$\begin{aligned} E_{k\beta} - E_{k\alpha} = {} & U_1{}^2 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right) + \Delta U U_1 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) + \Delta U^2 h_\beta\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) \\ & - U_1{}^2 h_\beta\left\{\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho\right\} - \Delta U U_1 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho\right) \\ & - \Delta U U_1 \delta_h\left(\frac{1}{6}\Delta\rho\right) - \Delta U^2 h_\beta\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho\right) - \Delta U^2 \delta_h\left(\frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \end{aligned} \tag{E.114}$$

or

$$\begin{aligned} E_{k\beta} - E_{k\alpha} = {} & U_1{}^2 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{4}\Delta\rho - \frac{1}{2}\rho_1 - \frac{1}{4}\Delta\rho\right) \\ & + \Delta U U_1 h_\beta\left(\frac{1}{2}\rho_1 + \frac{1}{3}\Delta\rho - \frac{1}{2}\rho_1 - \frac{1}{3}\Delta\rho\right) + \Delta U^2 h_\beta\left(\frac{1}{6}\rho_1 + \frac{1}{8}\Delta\rho - \frac{1}{6}\rho_1 - \frac{1}{8}\Delta\rho\right) \\ & - \Delta U U_1 \delta_h\left(\frac{1}{6}\Delta\rho\right) - \Delta U^2 \delta_h\left(\frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \end{aligned} \tag{E.115}$$

or

$$E_{k\beta} - E_{k\alpha} = -\Delta U U_1 \delta_h\left(\frac{1}{6}\Delta\rho\right) - \Delta U^2 \delta_h\left(\frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \tag{E.116}$$

so the change in kinetic energy is

$$E_{k\beta} - E_{k\alpha} = -\Delta U U_1 \delta_h\left(\frac{1}{6}\Delta\rho\right) - \Delta U^2 \delta_h\left(\frac{1}{12}\rho_1 + \frac{1}{8}\Delta\rho\right) \tag{E.117}$$

or

$$E_{k\beta} - E_{k\alpha} = \Delta U \delta_h\left\{-U_1\frac{4}{24}\Delta\rho - \Delta U\frac{2}{24}\rho_1 - \Delta U\frac{3}{24}\Delta\rho\right\} \tag{E.118}$$

$$E_{k\beta} - E_{k\alpha} = \Delta U \delta_h\left\{-U_1\Delta\rho\frac{2}{24} - U_1\Delta\rho\frac{2}{24} - \Delta U\rho_1\frac{1}{24} - \Delta U\rho_1\frac{1}{24} - \Delta U\Delta\rho\frac{2}{24} - \Delta U\Delta\rho\frac{1}{24}\right\} \tag{E.119}$$

or

$$E_{k\beta} - E_{k\alpha} = -\Delta U \delta_h \left\{ \Delta\rho \frac{2}{24}\left(U_1 + \Delta U\right) + U_1 \Delta\rho \frac{2}{24} + \Delta U \rho_1 \frac{1}{24} + \Delta U \frac{1}{24}\left(\rho_1 + \Delta\rho\right) \right\} \tag{E.120}$$

or

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{24} \Delta U \delta_h \left\{ 2\Delta\rho\left(U_1 + \Delta U\right) + 2U_1 \Delta\rho + \Delta U \rho_1 + \Delta U\left(\rho_1 + \Delta\rho\right) \right\} \tag{E.121}$$

or

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{24} \Delta U \delta_h \left\{ 2\Delta\rho U_2 + 2\Delta\rho U_1 + \rho_1 \Delta U + \rho_2 \Delta U \right\} \tag{E.122}$$

or

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \Delta\rho U_2 \Delta U + \Delta\rho U_1 \Delta U + \frac{1}{2}\rho_1 \Delta U^2 + \frac{1}{2}\rho_2 \Delta U^2 \right\} \tag{E.123}$$

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \Delta\rho U_2\left(U_2 - U_1\right) + \Delta\rho U_1\left(U_2 - U_1\right) + \frac{1}{2}\rho_1\left(U_2 - U_1\right)^2 + \frac{1}{2}\rho_2\left(U_2 - U_1\right)^2 \right\} \tag{E.124}$$

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \Delta\rho\left(U_2^2 - U_1 U_2\right) + \Delta\rho\left(U_1 U_2 - U_1^2\right) + \frac{1}{2}\rho_1\left(U_2 - U_1\right)^2 + \frac{1}{2}\rho_2\left(U_2 - U_1\right)^2 \right\} \tag{E.125}$$

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \Delta\rho\left(U_2^2 - U_1 U_2 + U_1 U_2 - U_1^2\right) + \frac{1}{2}\left(\rho_1 + \rho_2\right)\left(U_2 - U_1\right)^2 \right\} \tag{E.126}$$

or

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \Delta\rho\left(U_2^2 - U_1^2\right) + \frac{1}{2}\left(\rho_1 + \rho_2\right)\left(U_2 - U_1\right)^2 \right\} \tag{E.127}$$

So the change in kinetic energy can be written as

$$E_{k\beta} - E_{k\alpha} = -\frac{1}{12} \delta_h \left\{ \frac{1}{2}\left(\rho_1 + \rho_2\right)\Delta U^2 + \Delta\rho\left(U_2^2 - U_1^2\right) \right\} \tag{E.128}$$

Note that if the density difference is small, the change in KE can be written as

$$E_{k\beta} - E_{k\alpha} \sim -\frac{1}{12} \delta_h \rho_0 \Delta U^2 \tag{E.129}$$

Which is identical to that gviven in Sherman et al (1978) and attributed to Turner (1973, pp. 322, 323).

However, let us write the above as

$$\Delta E_S = -\left(E_{S\beta} - E_{S\alpha}\right) = c_S \delta_h \left\{ \rho_{avg} \Delta U^2 + \Delta\rho\left(U_2^2 - U_1^2\right) \right\} \tag{E.130}$$

where

$$\delta_h = h_\beta - h_\alpha \tag{E.131}$$

and

$$\rho_{avg} \equiv \frac{1}{2}(\rho_1 + \rho_2) \tag{E.132}$$

and

$$\Delta\rho = \rho_2 - \rho_1 \tag{E.133}$$

which is negative for a stably-stratified fluid (index 2 is above index 1). The c_S coefficient represents the bulk energy relationship between the velocity shear and the change in kinetic energy for mixing over the thickness mixing. Using $c_{sk} = 1/12$ is the theoretical value for mixing from a linear shear layer of thickness h_α to a linear shear layer of thickness h_β. Eq. (E.128) can be written as

$$\Delta E_S = c_{sk}\delta_h\rho_{avg}\Delta U^2\left\{1 + \frac{\Delta\rho}{\rho_{avg}}\frac{\left(U_2{}^2 - U_1{}^2\right)}{\Delta U^2}\right\} \tag{E.134}$$

Noting further that

$$\frac{\left(U_2{}^2 - U_1{}^2\right)}{\Delta U^2} = \frac{(U_2 - U_1)(U_2 + U_1)}{(U_2 - U_1)^2} = \frac{(U_2 + U_1)}{(U_2 - U_1)} = \frac{(U_2 + U_1)}{\Delta U} = \frac{2U_{avg}}{\Delta U} \tag{E.135}$$

Thus, eq. (E.134) becomes

$$\Delta E_S = c_{sk}\delta_h\rho_{avg}\Delta U^2\left\{1 + \frac{\Delta\rho}{\rho_{avg}}\frac{2U_{avg}}{\Delta U}\right\} \quad : \quad L\frac{M}{L^3}\frac{L^2}{T^2} = \frac{M}{T^2} = \frac{\text{Energy}}{\text{unit area}} \tag{E.136}$$

Note that we cannot, in general, neglect the second term as small!

The above compares to the value of

$$E_{k\beta} - E_{k\alpha} \sim -\frac{1}{2}\frac{h_1 h_2}{h_1 + h_2}\rho_0\Delta U^2 \tag{E.137}$$

derived in the CE380S class notes for two uniform layers of different thicknesses that are mixed into a single layer of uniform thickness. If we let $h_1 = h_2 = \delta_h / 2$, the above becomes

$$E_{k\beta} - E_{k\alpha} \sim -\frac{1}{2}\frac{\frac{\delta_h}{2}\frac{\delta_h}{2}}{\delta_h}\rho_0\Delta U^2 \tag{E.138}$$

or

$$E_{k\beta} - E_{k\alpha} \sim -\frac{1}{8}\delta_h \rho_0 \Delta U^2 \qquad \text{(E.139)}$$

which is reasonably close (but slightly larger) than eq. (E.129). Thus, we have some confidence that the derivation is correct.

Appendix F SURFACE/BOTTOM MIXING LAYER ENTRAINMENT

F.1 Equilibrium TKE

We take any mixing layer to provide a source of stirring energy (per unit surface area) that can be represented as E_S, with units of J/m^2 The rate at which this energy is supplied is given as $\partial E_S / \partial t$. There is a background level of turbulence in the mixed layer that is given as an energy per unit volume of e_B. We can define an "equilibrium" of background TKE, again per unit volume, that we will define as e_E. The mixed layer is characterized by large-scale eddies of a length scale H. A mixing layer where $\partial H / \partial t = 0$ will be one in which the dissipation and supply of TKE are exactly balanced, i.e. for a uniformly distributed dissipation rate over H, we can write

$$\frac{\partial E_S}{\partial t} = H\rho\varepsilon_E \tag{F.1}$$

Checking the units here we have

$$\frac{J}{m^2 s} = \frac{Nm}{m^2 s} = \frac{kg\,m^2}{m^2 s^3} = m\frac{kg}{m^3}\frac{m^2}{s^3} \tag{F.2}$$

which matches.

We consider the equilibrium dissipation rate (per unit mass) to scale on the background turbulence in the layer, the thickness of the layer, and the rate of energy supply, thus

$$\varepsilon_E = C_{\varepsilon 1}\frac{{u_E}^3}{H} + \frac{C_{\varepsilon 2}}{\rho H}\frac{\partial E_S}{\partial t} \tag{F.3}$$

where u_E is the equilibrium TKE velocity scale. Checking units

$$\frac{m^2}{s^3} \sim \frac{m^3}{s^3 m} + \frac{\dfrac{N\,m}{m^2}}{m\dfrac{kg}{m^3}s} = \frac{\dfrac{\cancel{kg}\,\cancel{m}}{s^2}\dfrac{\cancel{m}}{\cancel{m^2}}}{m\dfrac{\cancel{kg}}{m^3}s} = \frac{m^2}{s^3} \tag{F.4}$$

The relationship between the equilibrium TKE and velocity scale is given by

$$e_E = \frac{1}{2}\rho {u_E}^2 \quad \Rightarrow \quad u_E = \sqrt{\frac{2e_E}{\rho}} \tag{F.5}$$

so that eq. (F.3) becomes

$$\varepsilon_E = \frac{C_{\varepsilon 1}}{H}\left(\frac{2e_E}{\rho}\right)^{3/2} + \frac{C_{\varepsilon 2}}{\rho H}\frac{\partial E_S}{\partial t} \tag{F.6}$$

Thus, a balance of production and dissipation for a constant thickness layer, eq. (F.1) requires

$$\frac{\partial E_S}{\partial t} = H\rho\left[\frac{C_{\varepsilon 1}}{H}\left(\frac{2e_E}{\rho}\right)^{3/2} + \frac{C_{\varepsilon 2}}{\rho H}\frac{\partial E_S}{\partial t}\right] \tag{F.7}$$

or

$$\frac{\partial E_s}{\partial t} = \frac{C_{\varepsilon 1}}{\rho^{1/2}}\left(2e_E\right)^{3/2} + C_{\varepsilon 2}\frac{\partial E_S}{\partial t} \tag{F.8}$$

or, the equilibrium TKE is modeled as

$$\left(2e_E\right)^{3/2} = \rho^{1/2}\frac{\left(1-C_{\varepsilon 2}\right)}{C_{\varepsilon 1}}\frac{\partial E_s}{\partial t} \tag{F.9}$$

which is also

$$e_E = \frac{1}{2}\left\{\rho^{1/2}\frac{\left(1-C_{\varepsilon 2}\right)}{C_{\varepsilon 1}}\frac{\partial E_s}{\partial t}\right\}^{2/3} \tag{F.10}$$

Eq. (F.10) will be used to determine the equilibrium TKE in a mixed layer. Note that as the forcing changes, the equilibrium TKE changes, which will force the background to respond.

F.2 Neutral stability conditions

An energy balance requires the rate at which the energy in the mixing layer per unit area (He_B) increases must be equal to the rate of energy supply minus the dissipation in the mixing layer (ε_H) minus the rate of work required to entrain the fluid below the mixing layer into the mixing layer ($\dot{W}_e$). In neutral stratification, we take this work as composed of 1) the work required to accelerate the fluid to the velocity of the mixed layer plus 2) the work required to overcome increased dissipation associated with the entraining layer. Note that increase in TKE required for the entraining layer will be directly included in the differential equation through the $\partial\left(He_B\right)/\partial t$ term. Also note that the work term is positive definite and applies only we entraining; i.e. there is no work gain by detrainment.

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(He_B\right)=\frac{\partial E_S}{\partial t}-\rho H\varepsilon_H-\dot{W}_e \quad : \quad \dot{W}_e\geq 0\\
&\frac{LML^2}{TL^3T^2}=\frac{ML^2}{TL^2T^2}-\frac{MLL^2}{L^3T^3}-\frac{1}{T}\left(\frac{M}{L^3}\right)\frac{L^2}{T^2}L\\
&\frac{M}{T^3}=\frac{M}{T^3}-\frac{M}{T^3}
\end{aligned} \qquad \text{(F.11)}$$

It would seem that the appropriate to make the entrainment work

$$\dot{W}_e=\hbar\frac{1}{2}\rho\Delta U^2\frac{\partial H}{\partial t}+\hbar\rho H\Delta\varepsilon_e \qquad \text{(F.12)}$$

where $\hbar$ is a Heaviside step function

$$\hbar\equiv\begin{cases}1 \quad : & \dfrac{\partial H}{\partial t}>0\\ 0 & \dfrac{\partial H}{\partial t}\leq 0\end{cases} \qquad \text{(F.13)}$$

and where ΔU^2 represents the change in the mean kinetic energy of the entraining fluid for simplicity in exposition, but we recognize that the full term is $\Delta U^2+\Delta V^2$. The dissipation term, $\Delta\varepsilon_e$ is the additional dissipation rate that results from the entrainment process, whose scaling is still to be determined.

Eq. (F.11) with eq. (F.12) provides

$$\frac{\partial}{\partial t}\left(He_B\right)=\frac{\partial E_S}{\partial t}-\rho H\left(\varepsilon_H+\hbar\Delta\varepsilon_e\right)-\hbar\frac{\rho}{2}\Delta U^2\frac{\partial H}{\partial t} \qquad \text{(F.14)}$$

or

$$H\frac{\partial e_B}{\partial t}+e_B\frac{\partial H}{\partial t}=\frac{\partial E_S}{\partial t}-\rho H\left(\varepsilon_H+\hbar\Delta\varepsilon_e\right)-\hbar\frac{\rho}{2}\Delta U^2\frac{\partial H}{\partial t} \qquad \text{(F.15)}$$

or

$$\left(e_B+\hbar\frac{\rho}{2}\Delta U^2\right)\frac{\partial H}{\partial t}=\frac{\partial E_S}{\partial t}-\rho H\left(\varepsilon_H+\hbar\Delta\varepsilon_e\right)-H\frac{\partial e_B}{\partial t} \qquad \text{(F.16)}$$

which provides the basic balance between entrainment, mixing energy supply, dissipation and background TKE.

F.3 Scaling dissipation

Similar to eq. (F.6) for the equilibrium dissipation, we argue that the actual dissipation rate over the mixed layer scales as

$$\varepsilon_H = \frac{C_{\varepsilon 1}}{H}\left(\frac{2e_B}{\rho}\right)^{3/2} + \frac{C_{\varepsilon 2}}{\rho H}\frac{\partial E_S}{\partial t} \tag{F.17}$$

so eq. (F.16) is

$$\left(e_B + \hbar\frac{\rho}{2}\Delta U^2\right)\frac{\partial H}{\partial t} = \frac{\partial E_S}{\partial t} - \rho H\left\{\frac{C_{\varepsilon 1}}{H}\left(\frac{2e_B}{\rho}\right)^{3/2} + \frac{C_{\varepsilon 2}}{\rho H}\frac{\partial E_S}{\partial t} + \hbar\Delta\varepsilon_e\right\} - H\frac{\partial e_B}{\partial t} \tag{F.18}$$

or

$$\left(e_B + \hbar\frac{\rho}{2}\Delta U^2\right)\frac{\partial H}{\partial t} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_S}{\partial t} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - \hbar\rho H\Delta\varepsilon_e - H\frac{\partial e_B}{\partial t} \tag{F.19}$$

We model the additional dissipation rate associated with entrainment based on the rate of deepening, the velocity scale u_B and overturn time scale, T_H, as

$$\Delta\varepsilon_e \sim \frac{\partial H}{\partial t}\frac{u_B}{T_H} \tag{F.20}$$

where

$$u_B = \sqrt{\frac{2e_B}{\rho}} \tag{F.21}$$

and

$$T_H = \frac{H}{u_B} \tag{F.22}$$

It follows that

$$\Delta\varepsilon_e = C_{\varepsilon 3}\frac{\partial H}{\partial t}\frac{u_B}{H/u_B} \quad = \frac{C_{\varepsilon 3}}{H}{u_B}^2\frac{\partial H}{\partial t} \quad = \frac{C_{\varepsilon 3}}{H}\frac{2e_B}{\rho}\frac{\partial H}{\partial t} \tag{F.23}$$

or

$$\Delta\varepsilon_e = 2\frac{C_{\varepsilon 3}}{\rho H}e_B\frac{\partial H}{\partial t} \tag{F.24}$$

so that eq. (F.19) becomes

$$\left(e_B + \hbar\frac{\rho}{2}\Delta U^2\right)\frac{\partial H}{\partial t} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_S}{\partial t} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - 2\hbar C_{\varepsilon 3} e_B \frac{\partial H}{\partial t} - H\frac{\partial e_B}{\partial t} \qquad \text{(F.25)}$$

or

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2\right\}\frac{\partial H}{\partial t} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_S}{\partial t} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - H\frac{\partial e_B}{\partial t} \qquad \text{(F.26)}$$

F.4 Mixed-layer under stratification conditions

The energy required for mixing the density can be obtained, see eq. **(C.31)** , as

$$\frac{\partial E_{mix}}{\partial t} = -g\Delta\rho\frac{H}{2}\frac{\partial H}{\partial t} \qquad \text{(F.27)}$$

where

$$\Delta\rho = \overline{\rho}_{(S)} - \overline{\rho}_E \qquad \text{(F.28)}$$

with $\overline{\rho}_{(S)}$ as the mean density in the surface cell (k=S), which is also the density throughout the mixed layer. The $\overline{\rho}_G$ is the mean density of the entrained fluid, is approximated by the density of the fluid in the grid cell below the mixed layer and the lower portion of the grid cell that partially contains the mixed layer.

$$\overline{\rho}_E = \frac{\overline{\rho}_{B(P)} h_{B(P)} + \overline{\rho}_{(P-1)}\Delta z_{(P-1)}}{h_{B(P)} + \Delta z_{(P-1)}} \qquad \text{(F.29)}$$

Note that eq. (F.27) is based on mixing of two uniform density layers rather than a uniform density layer and a gradient layer. Thus, eq. (F.27) combined with eq. (F.29) may somewhat overestimate the mixing energy required for gradient layers that only progress to the next grid cell. However, $\overline{\rho}_E$ is taken from the density in the partially mixed layer and the density in the first complete cell below the mixed layer, so in the case of a rapidly deepening layer (compared to the grid scale), this will underestimate the density that is lifted. This approach therefore includes a grid and time step dependency. While it is possible to improve this estimate somewhat by considering a linear gradient in the entraining region, it would then require $\Delta\rho$ as a function of $\partial H / \partial t$, which would then create a quadratic in the $\partial H / \partial t$ equation developed below as eq. (F.42). Such an approach would still fail when the entrainment is large and moves beyond a simple gradient region. Arguably, a more correct approach would be to use the above as an approach to get an estimated $\partial H / \partial t$, then use this value to find the entrainment region upper (P) and lower (Q) bounds and obtain a better approximation of $\overline{\rho}_E$ as

$$\bar{\rho}_E = \frac{1}{H^{nM} - H^n}\left\{\bar{\rho}^n_{(P)}\delta^n_{B(P)} + \bar{\rho}^n_{(Q)}\delta^{nM}_{T(Q)} + \sum_{r=Q+1}^{P-1}\bar{\rho}_{(r)}\Delta z_{(r)}\right\} \tag{F.30}$$

which can be better interpreted by consulting section F.6. This approach would require at least two computations of $\partial H / \partial t$ when entraining in a stably-stratified region.

The energy overall energy equation starts from eq. (F.26) with an additional term for the RHS,

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2\right\}\frac{\partial H}{\partial t} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_S}{\partial t} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2}{}_e - H\frac{\partial e_B}{\partial t} + \hbar g\Delta\rho\frac{H}{2}\frac{\partial H}{\partial t} \tag{F.31}$$

where the last term is added to the RHS since $\Delta\rho$ is negative. This equation becomes

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2 - \hbar g\Delta\rho\frac{H}{2}\right\}\frac{\partial H}{\partial t} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_S}{\partial t} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - H\frac{\partial e_B}{\partial t} \tag{F.32}$$

The above provides the basic relationship between deepening, energy supply, dissipation and TKE background levels. Note that we identify the meaning of each term as:

$$\begin{array}{lll}
e_B\dfrac{\partial H}{\partial t} & \rightarrow & \text{power to entrain fluid to mixed-layer turbulence level} \\
2C_{\varepsilon 3}\dfrac{\partial H}{\partial t} & \rightarrow & \text{rate of dissipation for entrained fluid} \\
\dfrac{\rho}{1}\Delta U^2\dfrac{\partial H}{\partial t} & \rightarrow & \text{power required to accelerate entrained fluid to mean velocity} \\
-g\Delta\rho\dfrac{H}{2}\dfrac{\partial H}{\partial t} & \rightarrow & \text{power required for mixing stable density profile} \\
\left(1 - C_{\varepsilon 2}\right)\dfrac{\partial E_S}{\partial t} & \rightarrow & \text{net rate of mixing energy supply (after dissipation)} \\
\dfrac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} & \rightarrow & \text{dissipation rate of background TKE} \\
H\dfrac{\partial e_B}{\partial t} & \rightarrow & \text{rate of TKE increase in mixed layer}
\end{array} \tag{F.33}$$

F.5 Change in e_B and H

Let us note that eq. (F.9) provides

$$\left(2e_E\right)^{3/2} = \rho^{1/2}\frac{\left(1 - C_{\varepsilon 2}\right)}{C_{\varepsilon 1}}\frac{\partial E_s}{\partial t} \tag{F.34}$$

or

$$\frac{C_{\varepsilon 1}}{\rho^{1/2}}\left(2e_E\right)^{3/2} = \left(1 - C_{\varepsilon 2}\right)\frac{\partial E_s}{\partial t} \tag{F.35}$$

so that eq. (F.32)is

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2 - \hbar g\Delta\rho\frac{H}{2}\right\}\frac{\partial H}{\partial t} = \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_E\right)^{3/2} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - H\frac{\partial e_B}{\partial t} \tag{F.36}$$

The TKE either increases or decreases towards equilibrium at a rate that may be modeled as

$$\frac{\partial e_B}{\partial t} = \frac{e_E - e_B}{T_B} \tag{F.37}$$

where T_B is the time scale for mixing the background TKE. Let us model this time scale using the overturn time scale, eq. (F.22)

$$T_B \sim C_T T_H = C_T\frac{H}{u_B} \tag{F.38}$$

where C_T is a coefficient that sets the proportion of the overturn time scale required for mixing to TKE equilibrium. Using eq. (F.21), we obtain eq. (F.37) is

$$\frac{\partial e_B}{\partial t} = \frac{e_E - e_B}{C_T H}\sqrt{\frac{2e_B}{\rho}} \tag{F.39}$$

It follows that eq. (F.36) is

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2 - \hbar g\Delta\rho\frac{H}{2}\right\}\frac{\partial H}{\partial t} = \frac{C_{\varepsilon 1}}{\rho^{1/2}}\left(2e_E\right)^{3/2} - \frac{C_{\varepsilon 1}}{\sqrt{\rho}}\left(2e_B\right)^{3/2} - \frac{e_E - e_B}{C_T}\sqrt{\frac{2e_B}{\rho}} \tag{F.40}$$

or, resorting the first two terms on RHS

$$\left\{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\frac{\rho}{2}\Delta U^2 - \hbar g\Delta\rho\frac{H}{2}\right\}\frac{\partial H}{\partial t} = 2C_{\varepsilon 1}\sqrt{\frac{2}{\rho}}\left\{\left(e_E\right)^{3/2} - \left(e_B\right)^{3/2}\right\} - \frac{e_E - e_B}{C_T}\sqrt{\frac{2e_B}{\rho}} \tag{F.41}$$

We can solve for the rate of change of the mixing layer as

$$\frac{\partial H}{\partial t} = \frac{\sqrt{\dfrac{2}{\rho}}\left\{2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2} - \left(e_B\right)^{3/2}\right] - \dfrac{\sqrt{e_B}}{C_T}\left(e_E - e_B\right)\right\}}{e_B\left(1 + 2\hbar C_{\varepsilon 3}\right) + \hbar\dfrac{\rho}{2}\Delta U^2 - \hbar g\Delta\rho\dfrac{H}{2}} \tag{F.42}$$

The above should be correct for all conditions. Note that the denominator is positive for any stable density gradient (i.e. $\Delta\rho < 0$), so the Heaviside step function can be evaluated from the sign of the bracketed portion in the numerator

$$2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right] \;\geq\; \frac{\sqrt{e_B}}{C_T}\left(e_E-e_B\right) \;\Rightarrow\; \hbar=1 \tag{F.43}$$

$$2C_{\varepsilon 1}\left[\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right] \;<\; \frac{\sqrt{e_B}}{C_T}\left(e_E-e_B\right) \;\Rightarrow\; \hbar=0 \tag{F.44}$$

Note that if $\hbar = 1$ the additional terms in the denominator can only serve to reduce the rate of increase of H, but cannot cause a change in sign.

F.6 Implementation of changing mixed layer thickness

We have arrived at eq. (F.42), in concert with (F.43) and (F.44) that can be used to find $\partial H / \partial t$, and eq. (F.39) that can be used to find $\partial e_B / \partial t$ To implement over a time step of Δt, we must apply the limitation that the background TKE may only increase or decrease towards the equilibrium value, but cannot move across it. Thus,

$$e_B + \Delta t \frac{\partial e_B}{\partial t} \leq e_E \tag{F.45}$$

or

$$\frac{\partial e_B}{\partial t} \leq \frac{e_E - e_B}{\Delta t} \tag{F.46}$$

It follows that there are three possible conditions: $\Delta t < C_T T_B$; $\Delta t = C_T T_B$; $\Delta t > C_T T_B$. In the first and second cases, eqs. (F.39) and (F.42) may be applied over the entire time step as

$$e_B^{nM} = e_B^n + \Delta t \frac{\partial e_B}{\partial t} \tag{F.47}$$

$$H^{nM} = H^n + \Delta t \frac{\partial H}{\partial t} \tag{F.48}$$

However, for the case where $\Delta t > C_T T_B$, then use of eq. (F.47) and (F.48) would move the energy past equilibrium. Thus, we require the definition of a time used for mixing to equilibrium as

$$\Delta t_U = \min\left\{\Delta t,\, C_T T_H\right\} \tag{F.49}$$

where the change in background TKE and depth of the mixing layer are given by

$$e_B^{nM} = e_B^n + \Delta t_U \frac{\partial e_B}{\partial t} \tag{F.50}$$

$$H^{nM} = H^{n} + \Delta t_{U} \frac{\partial H}{\partial t} \qquad \text{(F.51)}$$

Once we have established the new mixed-layer depth (H^{nM}), it is necessary to find the new value for any scalar in the mixed layer. The number of full grid cells in the surface layer before mixing is noted as N^{n}, while the number of full grid cells after mixing is N^{nM}. The 'k' index of the partially-mixed cell in the surface layer before mixing is (P), while the index after mixing will be given as (Q). Determining the new cells in the surface mixed layer for a grid with nonuniform Δz grid requires a sweep, whose iteration step is indicated by a superscript in parentheses. The mixed-layer height remaining to be allocated is ΔH_{L} so that at the start of the sweep

$$\Delta H_{L}^{(0)} = H^{nM} - H^{n} \qquad \text{(F.52)}$$

For simplicity in exposition, we will consider the case where the surface mixed layer is deepening, such that $H^{nM} > H^{n}$. We then have

$$\Delta H_{L}^{(1)} = \max\left\{0, \Delta H_{L}^{(0)} - \delta_{B(P)}\right\} \qquad \text{(F.53)}$$

where $\delta_{B(P)}$ is the thickness of the region below the mixed layer in the partially-mixed grid cell k=P. Eq. (F.53) is followed by a decision algorithm.

Let i=1, then

```
if $\Delta H_{L}^{(1)} = 0$ then    (mixing does not move to next grid cell)
    $Q = P$
    $N^{nM} = N^{n}$
    $\delta_{H(Q)}^{nM} = \delta_{H(P)}^{n} + \Delta H_{L}^{(0)}$
    $\delta_{B(Q)}^{nM} = \Delta z_{H(Q)} - \delta_{H(Q)}^{nM}$
    stop                                                          (F.54)
else    (mixing moves to next grid cell)
    $\delta_{H(P)}^{nM} = 0$
    $\delta_{B(P)}^{nM} = 0$
    $i = i + 1$
endif
```

Once the first step is taken, the remaining of the sweep proceeds as

$$\Delta H_{L}^{(i)} = \max\left\{0, \Delta H_{L}^{(n-1)} - \Delta z_{(Q)}\right\} \qquad \text{(F.55)}$$

followed by the decision algorithm that is iterated for $i > 1$

```
if $\Delta H_L^{(i)} = 0$ then    (mixing does not move to next grid cell)
    $Q = P - (i-1)$
    $\delta_{H(Q)}^{nM} = \Delta H_L^{(i-1)}$
    $\delta_{B(Q)}^{nM} = \Delta z_{H(Q)} - \Delta H_L^{(i-1)}$
    $N^{nM} = N^n + i - 1$
    stop                                                    (F.56)
else    (mixing moves to next grid cell)
    $\delta_{H(Q)}^{nM} = 0$
    $\delta_{B(Q)}^{nM} = 0$
    $i = i + 1$
endif
```

Once the cycle is completed, we have P as the 'k' index of the original partially-mixed cell at the bottom of the surface mixed layer, and Q as the 'k' index of the new bottom of the partially-mixed layer. The above algorithm is only correct for the case where $Q \leq P$. Once Q and P are identified, the new mixed layer concentration of any scalar is given by

$$\phi_{(S \geq k \geq Q)}^{nM} = \frac{1}{H^{nM}} \left\{ \overline{\phi}_{(Q)}^{n} \delta_{H(Q)}^{nM} + \sum_{r=Q+1}^{S} \overline{\phi}_{(r)} \Delta z_{(r)} \right\} \tag{F.57}$$

Appendix G CONVECTIVE MIXING BASICS

G.1 Introduction

The surface mixed layer can be treated as a control volume that may expand or contract with time. At some time (t), the mixed layer is characterized by H(t), dH/dt, and a single density $\rho_m(t)$.

G.2 Solar radiation

We introduce solar radiation $Q_r > 0$. That is, let Q_r represent the solar radiation flux (watts/m^2) with Q_{r0} as the solar radiation that penetrates the free surface of elevation η. Based on TVA, the solar radiation profile below the free surface can be given as

$$Q_r(z) = Q_{r0}\left(1-\gamma\right)e^{-k(\eta - z)} \quad : \quad -\infty < z \leq \eta - \delta_r \tag{G.1}$$

where δ_r is some small thickness of an upper layer in which γQ_{r0} solar radiation is rapidly absorbed. While no data appears to be available, it will be convenient to assume that the solar radiation is absorbed linearly over the thickness so that

$$Q_r(z) = Q_{r0}\left(1-\gamma\frac{\eta - z}{\delta_r}\right) \quad : \quad \eta - \delta_r < z \leq \eta \tag{G.2}$$

We will represent the solar radiation energy per unit volume as e_r, where the rate at which it is absorbed in a layer of thickness Δz is found from

$$\frac{\partial}{\partial t}e_r\left(\frac{z_a + z_b}{2}\right) = \frac{Q_r\left(z_a\right) - Q_r\left(z_b\right)}{\Delta z} \tag{G.3}$$

where $z_a = z_b + \Delta z$. In the limit as $\Delta z \rightarrow 0$ we can write this as

$$\frac{\partial}{\partial t}e_r(z) = \frac{\partial}{\partial z}Q_r(z) \tag{G.4}$$

It follows that

$$\frac{\partial}{\partial t} e_r(z) = \begin{cases} \dfrac{\gamma}{\delta_r} Q_{r0} & : \quad \eta - \delta_r < z \leq \eta \\ Q_{r0}(1-\gamma) k e^{-k(\eta - z)} & : \quad -\infty < z \leq \eta - \delta_r \end{cases} \tag{G.5}$$

Following this thread, let us consider the effect this energy has on temperature, which we will represent as θ.

$$\frac{\partial e}{\partial t} = \rho c_p \frac{\partial \theta}{\partial t} \tag{G.6}$$

so it follows that

$$\frac{\partial}{\partial t} \theta(z) = \begin{cases} \dfrac{\gamma}{\delta_r \rho c_p} Q_{r0} & : \quad \eta - \delta_r < z \leq \eta \\ \dfrac{(1-\gamma)}{\rho c_p} Q_{r0} k e^{-k(\eta - z)} & : \quad -\infty < z \leq \eta - \delta_r \end{cases} \tag{G.7}$$

Relating temperature to density by

$$\frac{\partial \rho}{\partial t} = -\alpha \rho \frac{\partial \theta}{\partial t} \tag{G.8}$$

We then arrive at

$$\frac{\partial}{\partial t} \rho_r(z) = \begin{cases} -\dfrac{\alpha \gamma}{\delta_r c_p} Q_{r0} & : \quad \eta - \delta_r < z \leq \eta \\ -\dfrac{\alpha(1-\gamma)}{c_p} Q_{r0} k e^{-k(\eta - z)} & : \quad -\infty < z \leq \eta - \delta_r \end{cases} \tag{G.9}$$

G.3 Evaporative mass loss

Next, let us consider the effect of mass removal by evaporation, which is given by a velocity V_e that represents the rate at which pure water is evaporated. We will consider there is some thin layer, δ_e, over which the evaporation leaves behind higher salinity water (generally we expect that $\delta_e < \delta_r$). We will assume that in the layer $-\delta_e < z \leq 0$, the salt is uniformly mixed. It follows that the rate of increase of salinity in the thin layer is given by

$$\frac{\partial S}{\partial t} = \frac{V_e}{\delta_e} S_\eta \tag{G.10}$$

where S_η is the salinity at the free surface. Thus, using

$$\frac{\partial \rho}{\partial t} = \beta \rho \frac{\partial S}{\partial t} \tag{G.11}$$

the density relationship due to evaporation is given by

$$\frac{\partial}{\partial t} \rho_e(z) = \frac{\beta \rho V_e}{\delta_e} S_\eta \quad : \quad \eta - \delta_e < z \le \eta \tag{G.12}$$

G.4 Effects of precipitation

Not completed. This should require both mass gain due to precipitation volume and possibly stabilizing/destabilizing thermal effects depending on precipitation temperature.

G.5 Surface heat fluxes

Next, we consider the addition of longwave, sensible and latent heating and cooling. The net will be given by Q_h where $Q_h > 0$ is heating and $Q_h < 0$ is cooling. For convenience, we consider this heating/cooling to occur over the same small layer as the evaporation, so that the rate of change of thermal energy due to the heating/cooling is given by

$$\frac{\partial e_h}{\partial t} = \frac{Q_h}{\delta_e} \tag{G.13}$$

it follows that

$$\frac{\partial e_h}{\partial t} = \rho c_p \frac{\partial \theta_h}{\partial t} \tag{G.14}$$

It is useful (for later) to note that eq. (G.14) and (G.13) can be combined to write

$$\frac{\partial \theta_h}{\partial t} = \frac{Q_h}{\rho c_p \delta_e} \quad : \quad \eta - \delta_e < z \le \eta \tag{G.15}$$

The density change due to the heating/cooling is

$$\frac{\partial \rho_h}{\partial t} = -\alpha \rho \frac{\partial \theta_h}{\partial t} = -\frac{\alpha}{c_p} \frac{\partial e_h}{\partial t} \tag{G.16}$$

so that

$$\frac{\partial}{\partial t}\rho_h(z) = -\frac{\alpha}{\delta_e c_p} Q_h \quad : \quad \eta - \delta_e < z \le \eta \tag{G.17}$$

G.6 Handling grid sizes in the near-surface region

The equations used for mixing in the near surface regions will result in one of several possibilities:

1. The system is well-mixed from η down to δ_r
2. The system is well-mixed down to $\delta_e < h < \delta_r$, and has a different (but modeled as uniform value over the interval $\eta - \delta_r \le z \le \eta - h$.
3. The system has a uniform value over $\delta_e \le z \le \eta$ and a different uniform value over the interval $\eta - \delta_r \le z \le \eta - \delta_e$.

Thus, we imagine the near surface layer having up to two steps whose thickness varies with the surface forcing. For convenience, we will define these as

$$\Delta\delta_e \equiv \eta - \delta_e \tag{G.18}$$

$$\Delta\delta_r \equiv \delta_r - \delta_e \tag{G.19}$$

There are the following possibilities for the relationship between the upper layer thicknesses and the model grid cell at the surface (k = S)

1. $\Delta\delta_e > \Delta z_{(S)}$
2. $\Delta\delta_e = \Delta z_{(S)}$
3. $\Delta\delta_e < \Delta z_{(S)}$

We will consider $\Delta\delta_e$ and $\Delta\delta_r$ to be constant, whose values need to be set after further research. That is, these layer thicknesses represent the region over which sensible heating/cooling and relatively uniform absorption of solar radiation take place. As starting points, we can use $\Delta\delta_e \sim 0.5\text{m}$ and $\Delta\delta_r = 0.5\text{m}$. Note that we are arguing that $\delta_e \le \delta_r$; that is, the uniform region of solar radiation penetration is always at least as deep as the uniform penetration of sensible heating/cooling.

Let us consider the case where $\Delta\delta_e + \Delta\delta_r < \Delta z_{(S)}$, so that both thin layers are in the uppermost cell of the model grid. Let us define the region in cell (S) that is outside the near-surface layers as

$$\Delta\delta_{B(S)} = \Delta z_{(S)} - \Delta\delta_e - \Delta\delta_r \tag{G.20}$$

At the beginning of the mixing routine in time step ‘n’, we will have stored the mean concentrations of all transported variables (i.e. $\overline{\phi}^n$) along with the values of the concentrations in the $\Delta\delta_e^n$ and $\Delta\delta_r^n$ regions after transport, Thus, we will need to perform separate transport algorithms for the scalars in the near-surface regions. Having a dual transport algorithm applying to scalars in a single grid cell will require a method to adjust the scalar values in the $\Delta\delta_e$ and $\Delta\delta_r$ to satisfy the 3D transported scalar mean.

In a more general sense, we will always have one of four types of cells in the near surface region

1. A cell that is entirely either $\Delta\delta_e$ or $\Delta\delta_r$
2. A cell that contains only $\Delta\delta_e$ and $\Delta\delta_r$
3. A cell that contains only $\Delta\delta_r$ and $\Delta\delta_{B(k)}$
4. A cell that contains $\Delta\delta_e$, $\Delta\delta_r$ and $\Delta\delta_{B(k)}$

For the first case, after transport we require that a cell that is entirely $\Delta\delta_e$ at the ‘k’ level must satisfy

$$\phi_{e(k)} = \overline{\phi}_{(k)} \tag{G.21}$$

where the RHS represents the (mean) scalar value from the 3D transport for the cell (k). Similarly, a cell that is entirely $\Delta\delta_r$ at the ‘k’ level must satisfy

$$\phi_{r(k)} = \overline{\phi}_{(k)} \tag{G.22}$$

That is, we ignore the independent 2D transport results of the ϕ_r and ϕ_e when the layers are resolved by the grid.

For a cell that contains only $\Delta\delta_e$ *and* $\Delta\delta_r$, we define the portion of the ‘k’ level grid cell in the $\Delta\delta_e$ region as

$$\Delta z_{e(k)} = \Delta\delta_e - \sum_{q=k+1}^{S} \Delta z_{(q)} \tag{G.23}$$

It follows that the portion of the ‘k’ level grid in the ‘r’ region is

$$\Delta z_{r(k)} = \Delta z_{(k)} - \Delta z_{e(k)} \tag{G.24}$$

we have an estimated mean that satisfies

$$\overline{\phi}^*_{(k)} = \frac{\phi^*_{e(k)}\Delta z_{e(k)} + \phi^*_{r(k)}\Delta z_{r(k)}}{\Delta z_{(k)}} \tag{G.25}$$

However, we need to make the mean of the layers equal the mean obtained in the 3D transport. The scalar difference is defined as

$$\Delta\phi_{(k)} \equiv \overline{\phi}_{(k)} - \overline{\phi}^*_{(k)} \tag{G.26}$$

The scalar adjustments are defined as

$$\phi^n_{e(k)} \equiv \phi^*_{e(k)} + \Delta\phi_{(k)} \tag{G.27}$$

$$\phi^n_{r(k)} \equiv \phi^*_{r(k)} + \Delta\phi_{(k)} \tag{G.28}$$

If the above works, then the mean should be satisfied by the scalar values in the two portions of the near surface region as

$$\overline{\phi}_{(k)} = \frac{\Delta z_{e(k)}\phi^n_{e(k)} + \Delta z_{r(k)}\phi^n_{r(k)}}{\Delta z_{(k)}} \tag{G.29}$$

To check, substitute eq. (G.27) and (G.28) into (G.29)

$$\Delta z_{(k)}\overline{\phi}_{(k)} = \Delta z_{e(k)}\phi^*_{e(k)} + \Delta z_{e(k)}\Delta\phi + \Delta z_{r(k)}\phi^*_{r(k)} + \Delta z_{r(k)}\Delta\phi \tag{G.30}$$

Using eq. (G.25) as

$$\Delta z_{(k)}\overline{\phi}^*_{(k)} = \phi^*_{e(k)}\Delta z_{e(k)} + \phi^*_{r(k)}\Delta z_{r(k)} \tag{G.31}$$

we obtain eq. (G.30) as

$$\Delta z_{(k)}\overline{\phi}_{(k)} = \Delta z_{(k)}\overline{\phi}^*_{(k)} + \left\{\Delta z_{e(k)} + \Delta z_{r(k)}\right\}\Delta\phi \tag{G.32}$$

which is simply eq. (G.26)

$$\overline{\phi}_{(k)} - \overline{\phi}^*_{(k)} = \Delta\phi \tag{G.33}$$

so the approach is mass conservative.

We could have looked in this in a more general way, we still require eq. (G.29) as

$$\Delta z_{(k)}\overline{\phi}_{(k)} = \Delta z_{e(k)}\phi^n_{e(k)} + \Delta z_{r(k)}\phi^n_{r(k)} \tag{G.34}$$

We then define a general form as

$$\phi^n_{e(k)} \equiv \phi^*_{e(k)} + F_e\Delta\phi_{(k)} \tag{G.35}$$

$$\phi^n_{r(k)} \equiv \phi^*_{r(k)} + F_r\Delta\phi_{(k)} \tag{G.36}$$

so that

$$\Delta z_{(k)}\overline{\phi}_{(k)} = \Delta z_{e(k)}\left(\phi^{*}_{e(k)} + F_e\Delta\phi_{(k)}\right) + \Delta z_{r(k)}\left(\phi^{*}_{r(k)} + F_r\Delta\phi_{(k)}\right) \tag{G.37}$$

Using eq. (G.25) as

$$\Delta z_{(k)}\overline{\phi}^{*}_{(k)} = \phi^{*}_{e(k)}\Delta z_{e(k)} + \phi^{*}_{r(k)}\Delta z_{r(k)} \tag{G.38}$$

then eq. (G.37) becomes

$$\Delta z_{(k)}\overline{\phi}_{(k)} = \Delta z_{(k)}\overline{\phi}^{*}_{(k)} + \Delta z_{e(k)}F_e\Delta\phi_{(k)} + \Delta z_{r(k)}F_r\Delta\phi_{(k)} \tag{G.39}$$

So we obtain

$$\Delta z_{(k)}\left\{\overline{\phi}_{(k)} - \overline{\phi}^{*}_{(k)}\right\} = +\left\{\Delta z_{e(k)}F_e + \Delta z_{r(k)}F_r\right\}\Delta\phi_{(k)} \tag{G.40}$$

Noting eq. (G.26) , this requires

$$\Delta z_{(k)} = \Delta z_{e(k)}F_e + \Delta z_{r(k)}F_r \tag{G.41}$$

Thus, we can use $F_e = F_r = 1$, and obtain

$$\Delta z_{(k)} = \Delta z_{e(k)}(1) + \Delta z_{r(k)}(1) \tag{G.42}$$

Which is what we used for eq. (G.27) and (G.28). However, the above could be used to obtain some different apportionments of the scalar difference. For now, we will stick with the simplest.

Next we consider the case of a cell that has only $\Delta\delta_r$ and $\Delta\delta_{B(k)}$. Again, we have a transported scalar in the 'r' layer given as $\phi^{*}_{r(k)}$, and we have a transported mean value of the scalar given as $\overline{\phi}_{(k)}$. We also have a value of the scalar in the layer below as $\overline{\phi}_{(k-1)}$. We require values for $\phi^{n}_{r(k)}$ and $\phi^{n}_{B(k)}$ such that

$$\overline{\phi}_{(k)} = \frac{\Delta z_{r(k)}\phi^{n}_{r(k)} + \Delta z_{B(k)}\phi^{n}_{B(k)}}{\Delta z_{(k)}} \tag{G.43}$$

and the value for $\phi^{n}_{B(k)}$ must be bounded by the surroundings, such that either

$$\overline{\phi}_{(k-1)} \le \phi^{n}_{B(k)} \le \phi^{n}_{r(k)} \tag{G.44}$$

or

$$\overline{\phi}_{(k-1)} \ge \phi^{n}_{B(k)} \ge \phi^{n}_{r(k)} \tag{G.45}$$

is satisfied

Let us consider the possibility that $\phi^n_{r(k)} = \phi^*_{r(k)}$ will satisfy the conditions. It follows from eq. (G.43) that

$$\phi^*_{B(k)} = \frac{\Delta z_{(k)}\overline{\phi}_{(k)} - \Delta z_{r(k)}\phi^*_{r(k)}}{\Delta z_{B(k)}} \tag{G.46}$$

If the result satisfies either eq. (G.44) or (G.45), it follows that

$$\begin{aligned} \phi^n_{r(k)} &= \phi^*_{r(k)} \\ \phi^n_{B(k)} &= \phi^*_{B(k)} \end{aligned} \tag{G.47}$$

However, if the result of eq. (G.46) fails to satisfy eq. (G.44) or (G.45), then we require

$$\phi^n_{B(k)} = \overline{\phi}_{(k-1)} \tag{G.48}$$

and

$$\phi^n_{r(k)} = \frac{\Delta z_{(k)}\overline{\phi}_{(k)} - \Delta z_{B(k)}\phi^n_{B(k)}}{\Delta z_{r(k)}} \tag{G.49}$$

Next, for the case where a cell that contains $\Delta\delta_e$, $\Delta\delta_r$ and $\Delta\delta_{B(k)}$. We have a transported scalar in the 'r' layer given as $\phi^*_{r(k)}$, a transported scalar in the 'e' layer given as $\phi^*_{e(k)}$ and we have a transported mean value of the scalar given as $\overline{\phi}_{(k)}$. We require

$$\overline{\phi}_{(k)} = \frac{\Delta z_{e(k)}\phi^n_{e(k)} + \Delta z_{r(k)}\phi^n_{r(k)} + \Delta z_{B(k)}\phi^n_{B(k)}}{\Delta z_{(k)}} \tag{G.50}$$

Again, we require the value for $\phi^n_{B(k)}$ must be bounded by the surroundings, such that either

$$\overline{\phi}_{(k-1)} \le \phi^n_{B(k)} \le \phi^n_{r(k)} \tag{G.51}$$

or

$$\overline{\phi}_{(k-1)} \ge \phi^n_{B(k)} \ge \phi^n_{r(k)} \tag{G.52}$$

is satisfied. There are two possibilities for a cell such as this: 1) if this is the surface cell, then there is no cell above it; 2) if this is not the surface cell, then the cell above it must be entirely within the δ_e layer. Let us require the first case meets the condition $\phi^n_{e(S)} = \phi^*_{e(S)}$, and the second case meets the condition $\phi^n_{e(k)} = \phi^*_{e(S)}$. It follows that

$$\overline{\phi}_{(k)} = \frac{\Delta z_{e(k)} \phi^{*}_{e(S)} + \Delta z_{r(k)} \phi^{n}_{r(k)} + \Delta z_{B(k)} \phi^{n}_{B(k)}}{\Delta z_{(k)}} \tag{G.53}$$

or

$$\Delta z_{r(k)} \phi^{n}_{r(k)} + \Delta z_{B(k)} \phi^{n}_{B(k)} = \Delta z_{(k)} \overline{\phi}_{(k)} - \Delta z_{e(k)} \phi^{*}_{e(S)} \tag{G.54}$$

G.7 Mixing of scalars in the near-surface region

Scalars other than temperature, salinity and density in the region $\eta - \delta_r \le z \le \eta$ are computed from

$$\phi^{M}_{\delta} = \frac{1}{h} \left\{ \phi_e \delta_e + \phi_r \left(h - \delta_e \right) \right\} \tag{G.55}$$

However, for the temperature and salinity we must consider both starting values in regions 'e' and 'r' and the change do to thermodynamics.

For temperature (θ), we note that eq. (G.7) models the solar radiation in the near surface region providing a uniform temperature change

$$\frac{\partial \theta_r}{\partial t} = \frac{\gamma}{\delta_r \rho c_p} Q_{r0} \quad : \quad \eta - \delta_r < z \le \eta \tag{G.56}$$

Similarly, the surface heating/cooling is considered uniform and is given by eq. (G.15) as

$$\phi^{n}_{r(k)} \equiv \phi^{*}_{r(k)} + \Delta \phi_{(k)} \tag{G.57}$$

It follows that the temperature in the near-surface mixed region is given by

$$\overline{\phi}_{(k)} = \frac{\Delta z_{e(k)} \phi^{n}_{e(k)} + \Delta z_{r(k)} \phi^{n}_{r(k)}}{\Delta z_{(k)}} \tag{G.58}$$

Using eq. (G.56) and (G.57) this becomes

$$\theta^{M}_{\delta} = \frac{1}{h} \left\{ \left(\theta_e + \frac{\Delta t Q_h}{\rho c_p \delta_e} \right) \delta_e + \theta_r \left(h - \delta_e \right) + \frac{h \Delta t \gamma}{\delta_r \rho c_p} Q_{r0} \right\} \tag{G.59}$$

For salinity, we have effective gain in concentration in the upper layer by

$$S^{M}_{\delta} = \frac{1}{h} \left\{ \left(S_e + \Delta t \frac{\partial S}{\partial t} \right) \delta_e + S_r \left(h - \delta_e \right) \right\} \tag{G.60}$$

Using eq. (G.10), we obtain

$$S_{\delta}^{M} = \frac{1}{h}\left\{\left(S_e + \Delta t \frac{V_e}{\delta_e} S_e\right)\delta_e + S_r\left(h - \delta_e\right)\right\} \tag{G.61}$$

or

$$S_{\delta}^{M} = \frac{1}{h}\left\{\left(1 + \Delta t V_e\right) S_e \delta_e + S_r\left(h - \delta_e\right)\right\} \tag{G.62}$$

Appendix H ENERGY IN THE NEAR-SURFACE REGION

H.1 An energy rate approach

The rate of change of density due to the surface forcing is given by

$$\frac{\partial}{\partial t}\rho(z) = \frac{\partial}{\partial t}\rho_r(z) + \frac{\partial}{\partial t}\rho_e(z) + \frac{\partial}{\partial t}\rho_h(z) \tag{H.1}$$

which is given by

$$\frac{\partial}{\partial t}\rho(z) = \begin{cases} -\dfrac{\alpha\gamma}{\delta_r c_p}Q_{r0} + \dfrac{\beta\rho V_e}{\delta_e}S_\eta - \dfrac{\alpha}{\delta_e c_p}Q_h & : \ \eta - \delta_e < z \leq \eta \\ -\dfrac{\alpha\gamma}{\delta_r c_p}Q_{r0} & : \ \eta - \delta_r < z \leq \eta - \delta_e \\ -\dfrac{\alpha(1-\gamma)}{c_p}Q_{r0} k\, e^{-k(\eta - z)} & : \ -\infty < z \leq \eta - \delta_r \end{cases} \tag{H.2}$$

Let us consider only the two regions from $\eta - \delta_r < z \leq \eta$. Note that in both the upper region $\eta - \delta_e < z \leq \eta$ and the lower region $\eta - \delta_r < z \leq \eta - \delta_e$ the density will change uniformly over each layer. Let us define

$$\overline{\rho}_r \equiv \overline{\rho}(\eta - h < z < \eta - \delta_e) \quad \text{and} \quad \overline{\rho}_e \equiv \overline{\rho}(\delta_e \leq z \leq \eta) \tag{H.3}$$

and

$$\Delta\rho_{er} = \overline{\rho}_e - \overline{\rho}_r \tag{H.4}$$

If we do not allow large-scale advection to create unstable density gradients, then at the beginning of the mixing algorithm, the density field will meet the condition

$$\Delta\rho_{er}(t) \leq 0 \tag{H.5}$$

From eq. (H.2) we can write the rate of change of the difference between the densities will be

$$\frac{\partial}{\partial t}\left(\overline{\rho}_e - \overline{\rho}_r\right) = \frac{\partial}{\partial t}\left(\Delta\rho_{er}\right) = \frac{\beta\rho V_e}{\delta_e}S_\eta - \frac{\alpha}{\delta_e c_p}Q_h \tag{H.6}$$

Thus, the density gradient at any point in time is found as

$$\Delta\rho_{er}(t+\Delta t) = \Delta\rho_{er}(t) + \Delta t \frac{\partial}{\partial t}\left(\Delta\rho_{er}\right) \tag{H.7}$$

Since $\Delta\rho_{er} > 0$ is unstable, we are interested in the time to instability, Δt_I when $\Delta\rho_{er}(t+\Delta t_I) > 0$

$$\Delta\rho_{er}(t) + \Delta t_I \frac{\partial}{\partial t}\left(\Delta\rho_{er}\right) > 0 \tag{H.8}$$

or

$$\Delta t_I \frac{\partial}{\partial t}\left(\Delta\rho_{er}\right) > -\Delta\rho_{er}(t) \tag{H.9}$$

or

$$\Delta t_I \left\{ \frac{\beta\rho V_e}{\delta_e} S_\eta - \frac{\alpha}{\delta_e c_p} Q_h \right\} > -\Delta\rho_{er}(t) \tag{H.10}$$

Note that if the term in the brackets is negative, then $\Delta t_I = \infty$, since eq. (H.5) requires a neutral or negative density gradient at the start of mixing and a negative term in the brackets would indicate stabilization by thermodynamics. If the initial density gradient is neutral and the bracketed term is positive, then $\Delta t_I = 0$ and instability immediately occurs. Thus

$$\Delta t_I = \begin{cases} \text{undefined} & : \ \Delta\rho_{er}(t) > 0 \\ 0 & : \ \Delta\rho_{er}(t) = 0 \\ -\Delta\rho_{er}(t)\left\{ \dfrac{\beta\rho V_e}{\delta_e} S_\eta - \dfrac{\alpha}{\delta_e c_p} Q_h \right\}^{-1} & : \ \dfrac{\beta\rho V_e}{\delta_e} S_\eta - \dfrac{\alpha}{\delta_e c_p} Q_h > 0 \quad \text{and} \quad \Delta\rho_{er}(t) < 0 \\ \infty & : \ \dfrac{\beta\rho V_e}{\delta_e} S_\eta - \dfrac{\alpha}{\delta_e c_p} Q_h < 0 \quad \text{and} \quad \Delta\rho_{er}(t) < 0 \end{cases} \tag{H.11}$$

If $\Delta t_I < \Delta t$, then unstable mixing will occur. That is, the surface thermodynamics can force the density profile to neutral over time Δt_I, and then further surface thermodynamics lead to instability. It can be shown that the energy made available by unstable mixing of the two layers over time Δt is found as in eq. (H.61) below, repeated here in slightly modified form as

$$\Delta E_{A\max}(t+\Delta t) = \frac{1}{2} g \delta_e \left(\delta_r - \delta_e\right)\left(\Delta\rho_{er}(t) + \frac{\Delta t \beta\rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right) \tag{H.12}$$

where $\rho_{er}(t)$ is the density gradient at the start of mixing and $\Delta E_{A\max}$ indicates the maximum energy that can be made available due to unstable mixing (i.e. it does not include dissipation). Once time Δt_I is reached, we have $\rho_{er}(t+\Delta t_I) = 0$, so we can write

$$\Delta E_{A\max}(\Delta t-\Delta t_I)=\frac{1}{2}g\delta_e\left(\delta_r-\delta_e\right)\left(\frac{\Delta t_I\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t_I\alpha}{\delta_e c_p}Q_h\right) \tag{H.13}$$

Thus, if the thickness of the layers and the forcing is considered constant, the rate at which energy is provided by the surface thermodynamics over the time $t_0+\Delta t_I \le t \le t_0+\Delta t$ is

$$\frac{\partial E_{A\max}}{\partial t}=\frac{1}{2}g\left(\delta_r-\delta_e\right)\left(\beta\rho V_e S_\eta-\frac{\alpha}{c_p}Q_h\right) \quad : \quad t_0+\Delta t_I \le t \le t_0+\Delta t \tag{H.14}$$

So, to handle the two thin layers, we start by computing Δt_I from eq. (H.11). If $0\le\Delta t_I\le\Delta t$ then unstable mixing occurs and provides the maximum mixing energy at the rate from eq. (H.14).

However, we should reduce the unstable mixing energy to account for dissipation that occurs during the mixing of the initial stable density gradient $\Delta\rho_{er}(t)<0$. We note that the energy required to mix $\Delta\rho_{er}(t)<0$ (i.e. without any thermodynamics) is

$$\Delta E_M(t+\Delta t)=-\frac{1}{2}g\delta_e\left(\delta_r-\delta_e\right)\Delta\rho_{er}(t) \tag{H.15}$$

This mixing occurs over time Δt_I, so the rate that mixing energy is consumed is

$$\frac{\partial E_M}{\partial t}=-\frac{1}{2\Delta t_I}g\delta_e\left(\delta_r-\delta_e\right)\Delta\rho_{er}(t) \tag{H.16}$$

Similar to eq. **(F.17)**, we scale dissipation as

$$\varepsilon_\delta=\frac{C_{\varepsilon 1}}{\delta}\left(\frac{2e_B}{\rho}\right)^{3/2}+\frac{C_{\varepsilon 2}}{\rho\delta}\frac{\partial E_M}{\partial t} \tag{H.17}$$

The energy that is available at the end of Δt_I is then

$$\Delta E_A=\Delta E_{A\max}-\Delta t_I\rho\delta\varepsilon_\delta \tag{H.18}$$

which is required to be non-negative. Substituting eq.(H.13), (H.16) and (H.17) into (H.18)

$$\begin{aligned}\Delta E_A=&\frac{1}{2}g\delta_e\left(\delta_r-\delta_e\right)\left(\frac{\Delta t_I\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t_I\alpha}{\delta_e c_p}Q_h\right)\\&-\Delta t_I\rho\delta\left\{\frac{C_{\varepsilon 1}}{\delta}\left(\frac{2e_B}{\rho}\right)^{3/2}-\frac{C_{\varepsilon 2}}{\rho\delta}\left[\frac{1}{2\Delta t_I}g\delta_e\left(\delta_r-\delta_e\right)\Delta\rho_{er}(t)\right]\right\}\end{aligned} \tag{H.19}$$

which must be non-negative. If the value is computed as negative, it must be set to zero as it implies that all the energy that would have been available for convective mixing was instead used up in dissipation. Eq. (H.19) can be written as

$$\begin{aligned}\Delta E_A = {} & \frac{\Delta t_I}{2} g\left(\delta_r - \delta_e\right)\left(\beta\rho V_e S_\eta - \frac{\alpha}{c_p} Q_h\right) \\ & - \Delta t_I 2 C_{\varepsilon 1}\left(e_B\right)^{3/2}\sqrt{\frac{2}{\rho}} + \frac{1}{2} C_{\varepsilon 2} g \delta_e \left(\delta_r - \delta_e\right)\Delta\rho_{er}(t) \quad : \quad \Delta E_A \geq 0\end{aligned} \tag{H.20}$$

Thus, the rate at which mixing energy is made available from $t_0 + \Delta t_I \leq t \leq t_0 + \Delta t$ is

$$\begin{aligned}\frac{\partial E_A}{\partial t} = {} & \frac{1}{2} g\left(\delta_r - \delta_e\right)\left(\beta\rho V_e S_\eta - \frac{\alpha}{c_p} Q_h\right) \\ & - 2 C_{\varepsilon 1}\left(e_B\right)^{3/2}\sqrt{\frac{2}{\rho}} + \frac{1}{2\Delta t_I} C_{\varepsilon 2} g \delta_e \left(\delta_r - \delta_e\right)\Delta\rho_{er}(t) \quad : \quad \frac{\partial E_A}{\partial t} \geq 0 \quad \text{and} \quad \Delta t_I > 0\end{aligned} \tag{H.21}$$

Note that $\Delta t_I = 0$, if and only if $\Delta\rho_{er} = 0$, in which case the last term has the form 0/0. In effect if the initial gradient is neutral, then we can consider the available mixing energy is supplied at the maximum rate, i.e.

$$\frac{\partial E_A}{\partial t} = \frac{1}{2} g\left(\delta_r - \delta_e\right)\left(\beta\rho V_e S_\eta - \frac{\alpha}{c_p} Q_h\right) \quad : \quad \frac{\partial E_A}{\partial t} \geq 0 \quad \text{and} \quad \Delta t_I = 0 \tag{H.22}$$

and all dissipation is handled in the surface mixing algorithm

H.2 Energy released/required for mixing in the near surface region

Let’s look at some small time step Δt . The change in the density profile is given by

$$\rho(z, t + \Delta t) = \rho(z, t) + \Delta t \frac{\partial \rho}{\partial t} \tag{H.23}$$

So we have

$$\rho(z, t + \Delta t) = \rho(z, t) + \Delta t \frac{\partial}{\partial t}\rho(z) = \begin{cases} -\dfrac{\alpha\gamma}{\delta_r c_p} Q_{r0} + \dfrac{\beta\rho V_e}{\delta_e} S_\eta - \dfrac{\alpha}{\delta_e c_p} Q_h & : \quad \eta - \delta_e < z \leq \eta \\ -\dfrac{\alpha\gamma}{\delta_r c_p} Q_{r0} & : \quad \eta - \delta_r < z \leq \eta - \delta_e \\ -\dfrac{\alpha\left(1 - \gamma\right)}{c_p} Q_{r0} k \, e^{-k(\eta - z)} & : \quad -\infty < z \leq \eta - \delta_r \end{cases} \tag{H.24}$$

Thus, we obtain

$$\rho(z,t+\Delta t)=\rho(z,t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}+\frac{\Delta t\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t\alpha}{\delta_e c_p}Q_h \quad : \quad \eta-\delta_e<z\le\eta \tag{H.25}$$

$$\rho(z,t+\Delta t)=\rho(z,t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0} \quad : \quad \eta-\delta_r<z\le\eta-\delta_e \tag{H.26}$$

$$\rho(z,t+\Delta t)=\rho(z,t)-\frac{\Delta t\alpha(1-\gamma)}{c_p}Q_{r0}k\,e^{-k(\eta-z)} \quad : \quad -\infty<z\le\eta-\delta_r \tag{H.27}$$

Note that eq. (H.25) and (H.26) have uniform density profiles, so it is convenient to introduce the notation

$$\overline{\rho}_r(t)\equiv\overline{\rho}(\eta-h<z<\eta-\delta_e,t) \quad \text{and} \quad \overline{\rho}_e(t)\equiv\overline{\rho}(\delta_e\le z\le\eta,t) \tag{H.28}$$

so we have

$$\overline{\rho}_e(t+\Delta t)=\overline{\rho}_e(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}+\frac{\Delta t\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t\alpha}{\delta_e c_p}Q_h \tag{H.29}$$

$$\overline{\rho}_r(t+\Delta t)=\overline{\rho}_r(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0} \tag{H.30}$$

$$\rho(z,t+\Delta t)=\rho(z,t)-\frac{\Delta t\alpha(1-\gamma)}{c_p}Q_{r0}k\,e^{-k(\eta-z)} \quad : \quad -\infty<z\le\eta-\delta_r \tag{H.31}$$

The unmixed potential energy from some point ‘h’ where $\delta_e<h\le\delta_r$

$$E_U(t+\Delta t)=g\overline{\rho}_e\int_{\eta-\delta_e}^{\eta}zdz+g\overline{\rho}_r\int_{\eta-h}^{\eta-\delta_e}zdz \tag{H.32}$$

which is

$$E_U=g\left\{\overline{\rho}_e(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}+\frac{\Delta t\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t\alpha}{\delta_e c_p}Q_h\right\}\int_{\eta-\delta_e}^{\eta}zdz+g\left\{\overline{\rho}_r(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}\right\}\int_{\eta-h}^{\eta-\delta_e}zdz \tag{H.33}$$

or

$$\begin{aligned}E_U&=g\left\{\overline{\rho}_e(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}+\frac{\Delta t\beta\rho V_e}{\delta_e}S_\eta-\frac{\Delta t\alpha}{\delta_e c_p}Q_h\right\}\left\{\frac{z^2}{2}\right\}_{\eta-\delta_e}^{\eta}\\&+g\left\{\overline{\rho}_r(t)-\frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}\right\}\left\{\frac{z^2}{2}\right\}_{\eta-h}^{\eta-\delta_e}\end{aligned} \tag{H.34}$$

or

$$\begin{aligned} E_U = & \frac{1}{2} g \left\{ \bar{\rho}_e(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right\} \left\{ \eta^2 - (\eta - \delta_e)^2 \right\} \\ & + \frac{1}{2} g \left\{ \bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \right\} \left\{ (\eta - \delta_e)^2 - (\eta - h)^2 \right\} \end{aligned} \tag{H.35}$$

We could write this as

$$E_U = \frac{1}{2} g \{A\} \left\{ \eta^2 - (\eta - \delta_e)^2 \right\} + \frac{1}{2} g \{B\} \left\{ (\eta - \delta_e)^2 - (\eta - h)^2 \right\} \tag{H.36}$$

where

$$A = \bar{\rho}_3(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \tag{H.37}$$

$$B = \bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \tag{H.38}$$

If we consider the mixed density

$$\rho_M(t + \Delta t) = \frac{1}{h} \left\{ \bar{\rho}_r(t + \Delta t) \int_{\eta - \delta_e}^{\eta} dz + \bar{\rho}_e(t + \Delta t) \int_{\eta - h}^{\eta - \delta_e} dz \right\} \tag{H.39}$$

or

$$\begin{aligned} \rho_M = & \frac{1}{h} \left\{ \bar{\rho}_e(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right\} \int_{\eta - \delta_e}^{\eta} dz \\ & + \frac{1}{h} \left\{ \bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \right\} \int_{\eta - h}^{\eta - \delta_e} dz \end{aligned} \tag{H.40}$$

or

$$\begin{aligned} \rho_M(t + \Delta t) = & \frac{1}{h} \left\{ \bar{\rho}_e(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right\} \{z\}_{\eta - \delta_e}^{\eta} \\ & + \frac{1}{h} \left\{ \bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \right\} \{z\}_{\eta - h}^{\eta - \delta_e} \end{aligned} \tag{H.41}$$

or

$$\rho_M = \left(\frac{\delta_e}{h} \right) \left\{ \bar{\rho}_e(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right\} + \left(\frac{h - \delta_e}{h} \right) \left\{ \bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \right\} \tag{H.42}$$

The potential energy after mixing is

$$E_M(t+\Delta t) = g\rho_M(t+\Delta t)\int_{\eta-h}^{\eta} z dz \tag{H.43}$$

So that we get

$$E_M = \frac{1}{2} g\rho_M \left\{\eta^2 - (\eta - h)^2\right\} \tag{H.44}$$

or

$$\begin{aligned} E_M = &\frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{\delta_e}{h}\right)\left\{\bar{\rho}_e(t) - \frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0} + \frac{\Delta t\beta\rho V_e}{\delta_e}S_\eta - \frac{\Delta t\alpha}{\delta_e c_p}Q_h\right\} \\ &+\frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{h-\delta_e}{h}\right)\left\{\bar{\rho}_r(t) - \frac{\Delta t\alpha\gamma}{\delta_r c_p}Q_{r0}\right\} \end{aligned} \tag{H.45}$$

or

$$\begin{aligned} E_M = &\frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{\delta_e}{h}\right)\{A\} \\ &+\frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{h-\delta_e}{h}\right)\{B\} \end{aligned} \tag{H.46}$$

where A and B are defined as eq. (H.37) and (H.38). Using eq. (H.46) and (H.36), so that we can write

$$\begin{aligned} E_M - E_U = &\frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{\delta_e}{h}\right)\{A\} + \frac{1}{2} g\left\{\eta^2 - (\eta-h)^2\right\}\left(\frac{h-\delta_e}{h}\right)\{B\} \\ &-\frac{1}{2} g\{A\}\left\{\eta^2 - (\eta-\delta_e)^2\right\} - \frac{1}{2} g\{B\}\left\{(\eta-\delta_e)^2 - (\eta-h)^2\right\} \end{aligned} \tag{H.47}$$

Grouping some terms, we obtain

$$\begin{aligned} E_M - E_U = &\frac{1}{2} gA\left[\left(\frac{\delta_e}{h}\right)\left\{\eta^2 - (\eta-h)^2\right\} - \eta^2 + (\eta-\delta_e)^2\right] \\ &+\frac{1}{2} gB\left[\left\{\eta^2 - (\eta-h)^2\right\}\frac{(h-\delta_e)}{h} - (\eta-\delta_e)^2 + (\eta-h)^2\right] \end{aligned} \tag{H.48}$$

Expanding terms, we obtain

$$\begin{aligned}E_M - E_U = \frac{1}{2} gA\left[\left(\frac{\delta_e}{h}\right)\left\{\cancel{\eta^2} - \cancel{\eta^2} + 2\eta h - h^2\right\} - \cancel{\eta^2} + \cancel{\eta^2} - 2\eta\delta_e + \delta_e^{\,2}\right] \\ + \frac{1}{2} gB\left[\left\{\cancel{\eta^2} - \cancel{\eta^2} + 2\eta h - h^2\right\}\frac{(h-\delta_e)}{h} - \cancel{\eta^2} + 2\eta\delta_e - \delta_e^{\,2} + \cancel{\eta^2} - 2\eta h + h^2\right]\end{aligned} \tag{H.49}$$

or

$$\begin{aligned}E_M - E_U = \frac{1}{2} gA\left[\left(\frac{\delta_e}{h}\right)\left\{2\eta h - h^2\right\} - 2\eta\delta_e + \delta_e^{\,2}\right] \\ + \frac{1}{2} gB\left[\left\{2\eta h - h^2\right\}\frac{(h-\delta_e)}{h} + 2\eta\delta_e - \delta_e^{\,2} - 2\eta h + h^2\right]\end{aligned} \tag{H.50}$$

or

$$\begin{aligned}E_M - E_U = \frac{1}{2} gA\left[2\eta \cancel{h}\frac{\delta_e}{\cancel{h}} - \frac{\delta_e}{\cancel{h}} h^{\cancel{2}} - 2\eta\delta_e + \delta_e^{\,2}\right] \\ + \frac{1}{2} gB\left[2\eta \cancel{h}\frac{(h-\delta_e)}{\cancel{h}} - h^{\cancel{2}}\frac{(h-\delta_e)}{\cancel{h}} + 2\eta\delta_e - \delta_e^{\,2} - 2\eta h + h^2\right]\end{aligned} \tag{H.51}$$

or

$$\begin{aligned}E_M - E_U = \frac{1}{2} gA\left[\cancel{2\eta\delta_e} - \delta_e h - \cancel{2\eta\delta_e} + \delta_e^{\,2}\right] \\ + \frac{1}{2} gB\left[\cancel{2\eta h} - \cancel{2\eta\delta_e} - \cancel{h^2} + h\delta_e + \cancel{2\eta\delta_e} - \delta_e^{\,2} - \cancel{2\eta h} + \cancel{h^2}\right]\end{aligned} \tag{H.52}$$

or

$$E_M - E_U = \frac{1}{2} gA\delta_e\left[\delta_e - h\right] + \frac{1}{2} gB\delta_e\left[h - \delta_e\right] \tag{H.53}$$

or

$$E_M - E_U = \frac{1}{2} g\delta_e\left\{B\left[h - \delta_e\right] - A\left[h - \delta_e\right]\right\} \tag{H.54}$$

or

$$E_M - E_U = \frac{1}{2} g\delta_e\left\{\left[B - A\right]\left[h - \delta_e\right]\right\} \tag{H.55}$$

Note that

$$\begin{aligned} B - A = &+\bar{\rho}_r(t) - \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} \\ &- \bar{\rho}_e(t) + \frac{\Delta t \alpha \gamma}{\delta_r c_p} Q_{r0} - \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta + \frac{\Delta t \alpha}{\delta_e c_p} Q_h \end{aligned} \tag{H.56}$$

or

$$B - A = +\bar{\rho}_r(t) - \bar{\rho}_e(t) - \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta + \frac{\Delta t \alpha}{\delta_e c_p} Q_h \tag{H.57}$$

It is convenient to define

$$\Delta\rho_{er} = \bar{\rho}_e - \bar{\rho}_r \tag{H.58}$$

so that

$$B - A = -\Delta\rho_{er} - \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta + \frac{\Delta t \alpha}{\delta_e c_p} Q_h \tag{H.59}$$

we then obtain the change in potential energy due to mixing as

$$E_M - E_U = \frac{1}{2} g \delta_e \left\{ \left[-\Delta\rho_{er} - \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta + \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right] \left[h - \delta_e \right] \right\} \tag{H.60}$$

or

$$E_M - E_U = -\frac{1}{2} g \delta_e \left(h - \delta_e \right) \left(\Delta\rho_{er} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right) \tag{H.61}$$

If $E_M - E_U \geq 0$ then it requires energy to mix the two upper layers down to depth h. If η, for δ_r, then energy is made available by the mixing down to the depth h.

We can solve for h as

$$\delta_e < h < \delta_r \tag{H.62}$$

which can be interpreted as the h that is reached when some mixing energy $\eta - \delta_r \leq z \leq \eta - h$ is applied. Note that since the layer $\delta_e \leq z \leq \eta$ is of uniform density, it must all mix (i.e. $\eta - \delta_r \leq z \leq \eta - \delta_e$) if $\Delta\delta_e \equiv \eta - \delta_e$.

We note that the maximum value for h is $\Delta\delta_r \equiv \delta_r - \delta_e$, so going back to eq. (H.61) we obtain the energy made available (or required) for mixing the surface layers as

$$E_M - E_U = -\frac{1}{2} g \delta_e \left(\delta_r - \delta_e \right) \left(\Delta\rho_{er} + \frac{\Delta t \beta \rho V_e}{\delta_e} S_\eta - \frac{\Delta t \alpha}{\delta_e c_p} Q_h \right) \tag{H.63}$$

Appendix I MIXING IN THE SOLAR PENETRATION REGION

The thermodynamic analysis of the near surface region either produces either 1) stabilizing change in the density field, 2) destabilizing change in the density field, or 3) neutral change in the density field. In contrast, the thermodynamics below the near-surface region are entirely stabilizing due to the penetration only of stabilizing solar radiation. Thus, any destabilizing forcing in this region must be propagating down from the near-surface region.

After mixing the near surface region, we find that one of two cases will exist: 1) all the wind stirring energy will have been depleted in mixing to a depth of $H \le \delta_r$ and unstable mixing energy will not exist or 2) there will be some remaining wind-stirring energy and/or some unstable mixing energy for application in mixing below the near-surface region.

Let us deal with the second case, i.e. where wind-stirring production or unstable production exists after mixing to δ_r. The mixing energy remaining in the time step after near-surface mixing is either

$$\left(\Delta t\right)\frac{\partial E_W}{\partial t} + \left(\Delta t - \Delta t_I\right)\frac{\partial E_A}{\partial t} \quad : \quad \frac{\partial E_A}{\partial t} \ge 0 \quad \text{(instability in } \delta\text{)} \tag{I.1}$$

or

$$\left(\Delta t - \Delta t_\delta\right)\frac{\partial E_W}{\partial t} \quad : \quad \frac{\partial E_A}{\partial t} < 0 \quad \text{(stable stratification in } \delta\text{)} \tag{I.2}$$

where Δt_I is the time to mix to instability and Δt_δ is the time for wind mixing to mix a stabilized near-surface layer. We obtain $\partial E_A / \partial t$ from eq. **(H.21)** or **(H.22)**, depending on Δt_I, which is computed from eq. **(H.11)**. We obtain $\partial E_W / \partial t$ from the parameterization of the wind (section K.3). The reduction of wind energy by dissipation and overcoming stable stratification in the near surface region is characterized by the reduction of time for mixing using Δt_δ, computed from eq. **(J.10)** . Thus, using the above we have the total mixing energy available at $z = \eta - \delta_r$, the top of the solar penetration region, which we will write as

$$\frac{\partial E_S}{\partial t} = \begin{cases} & : \\ \dfrac{\partial E_W}{\partial t} + \dfrac{\left(\Delta t - \Delta t_I\right)}{\Delta t}\dfrac{\partial E_A}{\partial t} & : \quad \dfrac{\partial E_A}{\partial t} \ge 0 \quad \text{(instability in } \delta\text{)} \\ \dfrac{\left(\Delta t - \Delta t_\delta\right)}{\Delta t}\dfrac{\partial E_W}{\partial t} & : \quad \dfrac{\partial E_A}{\partial t} < 0 \quad \text{(stable stratification in } \delta\text{)} \end{cases} \tag{I.3}$$

In the solar penetration region, we have a profile in the rate of increase of density, obtained from eq. **(H.2)** as

$$\frac{\partial}{\partial t}\rho(z) = -\frac{\alpha(1-\gamma)}{c_p} Q_{r0} k\, e^{-k(\eta - z)} \quad : \quad -\infty < z \leq \eta - \delta_r \tag{I.4}$$

So we will need top proceed downward by sweeping a single cell at a time.

Appendix J STABILIZING THERMODYNAMICS AND WIND MIXING

If $E_M - E_U \geq 0$, (stabilizing thermodynamics), we must look at the rate at which wind-stirring energy is applied at the surface, $\partial E_W / \partial t$, along with the dissipation rate and the background TKE. If the wind energy is sufficient to overcome the stabilizing force, then we can continue with the prior mixing height as the basis for the mixing computations. However, if the wind is insufficient to mix the near-surface region, then the mixing height is determined by the stabilizing gradient. The time required for the wind stirring to completely mix the stabilizing gradient over the layer $\eta - \delta_r \leq z \leq \eta$ can be found from

$$\Delta t_\delta \left(\frac{\partial E_W}{\partial t} - \rho \delta_r \varepsilon_\delta - \delta_r \frac{\partial e_B}{\partial t} \right) = E_M - E_U \tag{J.1}$$

where we take $\partial E_W / \partial t$ as the only source of mixing energy in the near-surface region and we use Δt_δ to indicate the time used for mixing in the $\eta - \delta_r \leq z \leq \eta$ near-surface region. We have previously shown that dissipation can be scaled as in eq. **(F.17)**, which can be modified for the near-surface region as

$$\varepsilon_\delta = \frac{C_{\varepsilon 1}}{\delta_r} \left(\frac{2 e_B}{\rho} \right)^{3/2} + \frac{C_{\varepsilon 2}}{\rho \delta_r} \frac{\partial E_W}{\partial t} \tag{J.2}$$

Similarly, the rate of change of the background TKE is modeled as a modification of eq. **(F.39)** as

$$\frac{\partial e_B}{\partial t} = \frac{e_E - e_B}{C_T \delta_r} \sqrt{\frac{2 e_B}{\rho}} \tag{J.3}$$

where similar to eq. **(F.10)**

$$e_E = \frac{1}{2} \left\{ \rho^{1/2} \frac{\left(1 - C_{\varepsilon 2}\right)}{C_{\varepsilon 1}} \frac{\partial E_W}{\partial t} \right\}^{2/3} \tag{J.4}$$

and similar to eq. **(F.9)**

$$\Delta \delta_r^n \tag{J.5}$$

It follows that eq. (H.63) can be written as

$$\Delta \delta_e \tag{J.6}$$

which expands on the LHS to

$$\Delta\delta_r \tag{J.7}$$

Using eq. (J.5) this becomes

$$\begin{aligned} C_{\varepsilon 1}\sqrt{\frac{8}{\rho}}\left\{\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right\}-\left(\frac{e_E-e_B}{C_T}\right)\sqrt{\frac{2e_B}{\rho}} \\ =-\frac{1}{2}g\delta_e\left(h-\delta_e\right)\left(\frac{\Delta\rho_{er}}{\Delta t_U}+\frac{\beta\rho V_e}{\delta_e}S_\eta-\frac{\alpha}{\delta_e c_p}Q_h\right) \end{aligned} \tag{J.8}$$

We can write eq. (J.8) as an equation for the time used in the mixing process as

$$\frac{\Delta\rho_{er}}{\Delta t_\delta}=-\frac{\beta\rho V_e}{\delta_e}S_\eta+\frac{\alpha}{\delta_e c_p}Q_h-\frac{4\sqrt{2}C_{\varepsilon 1}\left\{\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right\}}{\sqrt{\rho}g\delta_e\left(h-\delta_e\right)}+\frac{2\sqrt{2e_B}\left(e_E-e_B\right)}{C_T\sqrt{\rho}g\delta_e\left(h-\delta_e\right)} \tag{J.9}$$

or

$$\Delta t_\delta=\Delta\rho_{er}\left\{-\frac{\beta\rho V_e}{\delta_e}S_\eta+\frac{\alpha}{\delta_e c_p}Q_h-\frac{4\sqrt{2}C_{\varepsilon 1}\left\{\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right\}}{\sqrt{\rho}g\delta_e\left(h-\delta_e\right)}+\frac{2\sqrt{2e_B}\left(e_E-e_B\right)}{C_T\sqrt{\rho}g\delta_e\left(h-\delta_e\right)}\right\}^{-1} \tag{J.10}$$

If $\Delta t_\delta > \Delta t$ for $h=\delta_r$, then complete mixing of the two layers does not occur. In which case, we need to solve for h in eq. (J.8) using $\Delta t_\delta = \Delta t$

$$h=\delta_e-\frac{C_{\varepsilon 1}\sqrt{\frac{8}{\rho}}\left\{\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right\}-\left(\frac{e_E-e_B}{C_T}\right)\sqrt{\frac{2e_B}{\rho}}}{\frac{1}{2}g\delta_e\left(\frac{\Delta\rho_{er}}{\Delta t}+\frac{\beta\rho V_e}{\delta_e}S_\eta-\frac{\alpha}{\delta_e c_p}Q_h\right)} \tag{J.11}$$

or, with some algebra

$$h=\delta_e-\frac{C_{\varepsilon 1}4\sqrt{2}\left\{\left(e_E\right)^{3/2}-\left(e_B\right)^{3/2}\right\}-\frac{2}{C_T}\sqrt{2e_B}\left(e_E-e_B\right)}{\sqrt{\rho}g\left(\delta_e\frac{\Delta\rho_{er}}{\Delta t}+\beta\rho V_e S_\eta-\frac{\alpha}{c_p}Q_h\right)} \tag{J.12}$$

In this case (i.e. $\Delta t_\delta > \Delta t$), all the wind-stirring energy is used in the near-surface region so the mixed layer is set to $\phi_{e(k)}=\overline{\phi}_{(k)}$, where h is found from eq. (J.12).

If $\Delta t_{\delta} = \Delta t$, then all the wind-stirring energy is used in the near-surface region to mix down to $H^{nM} = \delta_{r}$.

If $\Delta t_{\delta} < \Delta t$, then the wind-stirring energy mixes down to δ_{r} in time $\Delta\delta_{r}$. Thus, the next part of the mixing sweep will begin with only $\Delta t_{L} = \Delta t - \Delta t_{\delta}$.

Appendix K SOME SCALING RELATIONSHIPS

K.1 Time scales for billowing

In the case of KH billows, Thorpe (1973a) defines the non-dimensional time for a KH billows as $\tau \equiv (g)(\Delta)(t) / U_0$, where the U_0 velocity scale is half the difference between the two layers, so that $U_0 = \Delta U / 2$ and the density scale is $\Delta \equiv (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$. For the present work, we note that $(g)(\Delta) = g'/2$, so

$$\tau_{\text{Thorpe}} \equiv \frac{(g)(\Delta)}{U_0} = \frac{g'}{\Delta U} t \tag{K.1}$$

Thorpe did not conduct experiments for $\tau > 20$. It is not clear how Laval et al decided to use 20 as a good number for the end of billowing. I would argue from Thorpe's results that 15 would be better. Indeed, in Thorpe (1973b , JFM) he use $\tau > 12$ as the defining "long time'. In either case, let us define

$$T_{KH} \equiv \frac{c_{tKH} g'}{\Delta U} \tag{K.2}$$

K.2 Time scale for shear mixing (without billows)

However, we need to figure out the time scale for general shear mixing that is applicable in homogeneous flows and stratified flows without KH billowing. It would seem that the most simple time scale would depend on the TKE and the mixing length scale, i.e.

$$T_m \propto \frac{h_\beta}{e_k^{1/2}} \tag{K.3}$$

However, what we are really interested in is the rate at which the mixing layer thickens, i.e.

$$\frac{dh}{dt} \propto \frac{h_\beta}{T_m} \propto e_k^{1/2} \tag{K.4}$$

We can argue that

$$\frac{dh}{dt} = w' \tag{K.5}$$

and the essentially isotropic turbulence in a shear layer provides

$$w' = \left(\frac{e_k}{3} \right)^{1/2} \tag{K.6}$$

Thus, the time scale to increase the shear layer by thickness δ_h is given by

$$T_{\delta m} = \frac{\delta_h}{dh / dt} \propto \frac{\delta_h}{e_k^{1/2}} \tag{K.7}$$

K.3 Mixing energy from wind

In Hodges et al. (2000) followed Spigel et al. (1986) in modeling the production due to wind stirring as

$$\frac{1}{2} C_N^3 u_*^3 \tag{K.8}$$

We note that this has the units m^3/s^3. If we multiply by density, we obtain (kg/m^3) (m^3/s^3), which is simply (kg /s^3), and so is then a value of $\partial E / \partial t$. Let us continue with this form and write

$$\frac{\partial E_N}{\partial t} = \frac{C_N^3}{2} \rho_0 u_*^3 \tag{K.9}$$

Appendix L ALTERNATIVE APPROACHES

In sections 3 and 4, we introduced energy scaling methods for modeling the mixing layer thickness. In developing these ideas, we also formulated some alternative approaches that are presented here, but require further exploration before implementation and testing.

L.1 Alternative layer thickness approach

Eq. (5.1) can also be written as

$$\frac{dh}{dt} = \frac{\mathcal{P} - \varepsilon - \frac{de_k}{dt}}{\frac{de_b}{dh}} \tag{L.1}$$

From Appendix B.3, entraining a uniform density region of thickness δ into another uniform density region of thickness h provides

$$\frac{de_B}{dh} = \frac{1}{2} g \left(\frac{\rho_\delta - \rho_h}{\rho_h} \right) \tag{L.2}$$

So eq. (L.1) can be written as

$$\frac{dh}{dt} = \frac{2\rho_h}{g\left(\rho_\delta - \rho_h\right)} \left\{ \mathcal{P} - \varepsilon - \frac{de_k}{dt} \right\} \tag{L.3}$$

Using eq. (5.2)

$$\frac{dh}{dt} = \frac{2\rho_h}{g\left(\rho_\delta - \rho_h\right)} \left\{ \mathcal{P} - \frac{c_\varepsilon}{2L_\varepsilon} {e_k}^{3/2} - \frac{de_k}{dt} \right\} \tag{L.4}$$

Using the layer thickness as the length scale

$$\frac{dh}{dt} = \frac{2\rho_h}{g\left(\rho_\delta - \rho_h\right)} \left\{ \mathcal{P} - \frac{c_\varepsilon}{2h} {e_k}^{3/2} - \frac{de_k}{dt} \right\} \tag{L.5}$$

Thus, once we have solved for de_k / dt from eq. (5.33), we can then readily solve for dh / dt from eq. (L.5).

Let us consider what happens if we consider mixing from a gradient region. From Appendix B.4 the change in BPE is given for this case by

$$\frac{de_B}{dh} = -\frac{g}{2\rho_h}\frac{d\rho_\delta}{dz}\delta \tag{L.6}$$

Substituting into eq. (L.1) we find

$$\frac{dh}{dt} = -\frac{4\rho_h}{g\delta\frac{d\rho_\delta}{dz}}\left(P - \varepsilon - \frac{de_k}{dt}\right) \tag{L.7}$$

L.2 Alternative approach for wind-mixing

For wind mixing, the production rate is given by

$$P \sim \frac{1}{2h}\left(C_N u_*\right)^3 \tag{L.8}$$

So eq. (5.33) becomes

$$\frac{de_k}{dt} = \frac{c_\tau}{\tau}\left\{\left[\frac{\cancel{2h}}{c_\varepsilon}\left(1-R_{fc}\right)\frac{1}{\cancel{2h}}\left(C_N u_*\right)^3\right]^{2/3} - e_k\right\} \tag{L.9}$$

where τ is given by eq. (L.8) substituted into eq. (5.24) as

$$\tau = \min\left(\frac{h^{2/3}}{\frac{1}{2^{1/3}h^{1/3}}\left(C_N u_*\right)}, \frac{h}{e_k^{1/2}}\right) \quad : \quad h > 0 \tag{L.10}$$

which reduces to

$$\tau = \min\left(\frac{h\sqrt[3]{2}}{C_N u_*}, \frac{h}{e_k^{1/2}}\right) \quad : \quad h > 0 \tag{L.11}$$

The time scale is a length scale over a velocity scale, i.e.

$$\tau = \frac{h}{\tilde{u}} \tag{L.12}$$

where

$$\tilde{u} = \max\left(\frac{C_N u_*}{(2)^{1/3}}, e_k^{1/2}\right) \tag{L.13}$$

As a result, eq. (L.9) can be written as

$$\frac{de_k}{dt} = \frac{c_\tau \tilde{u}}{h}\left\{\left[\frac{1-R_{fc}}{c_\varepsilon}\right]^{2/3}\left(C_N u_*\right)^2 - e_k\right\} \tag{L.14}$$

For the rate of change of layer thickness, we have eq. (L.8) substituted into eq. (L.5), which provides

$$\frac{dh}{dt} = \frac{2\rho_h}{g\left(\rho_\delta - \rho_h\right)}\left\{\frac{1}{2h}\left(C_N u_*\right)^3 - \frac{c_\varepsilon}{2h} e_k^{\,3/2} - \frac{de_k}{dt}\right\} \tag{L.15}$$

L.3 Is it worthwhile using a linear density shear layer approximation?

The mixing by billowing is typically considered (Sherman et al?) to result in a diffuse mixing layer rather than a uniform layer as derived above. Let us consider the somewhat more complicated case where in the initial conditions are still as eq. (D.1), but the mixed conditions are

$$\rho_m(z) = \rho_2 - \frac{\Delta\rho}{h_1 + h_2} z \tag{L.16}$$

where z=0 is at the bottom of the two layers. Let us check that this satisfies continuity by integrating the total mass

$$\begin{aligned}
\int\limits_{h_1+h_2} \rho_m(z)dz &= \int\limits_{h_1+h_2} \rho_2 - \int\limits_{h_1+h_2} \frac{\Delta\rho}{h_1+h_2} zdz \\
&= \rho_2\left(h_1+h_2\right) - \frac{\Delta\rho}{h_1+h_2}\left(\frac{z^2}{2}\right)_{h_1+h_2} \\
&= \rho_2\left(h_1+h_2\right) - \frac{\Delta\rho}{\cancel{h_1+h_2}}\left(\frac{1}{2}\right)\left(h_1+h_2\right)^{\cancel{2}} \\
&= \rho_2\left(h_1+h_2\right) - \left(\rho_2-\rho_1\right)\left(\frac{1}{2}\right)\left(h_1+h_2\right) \\
&= \frac{1}{2}\rho_2\left(h_1+h_2\right) + \frac{1}{2}\rho_1\left(h_1+h_2\right)
\end{aligned} \tag{L.17}$$

if $h_1 = h_2 = \Delta z$

$$\int\limits_{\Delta z+\Delta z} \rho_m(z)dz \quad = \left(\rho_2\Delta z + \rho_1\Delta z\right) \tag{L.18}$$

Thus, the above is consistent for uniform thickness layers only. We will require a conservation of momentum that can be written as

$$U_m \int \rho_m(z)dz = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.19}$$

where we make the modeling approximation that the momentum ends up completely mixed and we have invoked the uniform thickness layer approximation required for eq. (L.16). It follows that

$$U_m \int_{2h} \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} dz = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.20}$$

or

$$U_m \left\{ 2h\rho_2 - \frac{\Delta\rho}{2h} \left(\frac{z^2}{2} \right)_{2h} \right\} = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.21}$$

or

$$U_m \left\{ 2h\rho_2 - \frac{\Delta\rho}{2h} \left(\frac{4h^2}{2} \right) \right\} = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.22}$$

or

$$U_m h\left(2\rho_2 - \Delta\rho\right) = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.23}$$

or

$$U_m h\left(2\rho_2 - \left[\rho_2 - \rho_1\right]\right) = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.24}$$

or

$$U_m h\left(\rho_2 + \rho_1\right) = \rho_1 hU_1 + \rho_2 hU_2 \tag{L.25}$$

so that

$$U_m = \frac{\rho_1 hU_1 + \rho_2 hU_2}{h\left(\rho_2 + \rho_1\right)} \tag{L.26}$$

Noting that

$$\begin{aligned} E_{km} &= \frac{1}{2}\left(U_m{}^2\right) \int_{2h} \rho_m(z)dz \\ &= \frac{1}{2}\left(U_m{}^2\right) h\left(\rho_1 + \rho_2\right) \end{aligned} \tag{L.27}$$

we note that

$$\left(U_m{}^2\right)h\left(\rho_1+\rho_2\right)=\left(\frac{\rho_1 hU_1+\rho_2 hU_2}{h\left(\rho_2+\rho_1\right)}\right)^2 h\left(\rho_1+\rho_2\right)=\frac{\left(\rho_1 hU_1+\rho_2 hU_2\right)^2}{h\left(\rho_2+\rho_1\right)} \tag{L.28}$$

Now we write the change in the kinetic energy, i.e. eq. (D.7)

$$\left(E_{km}-E_{ku}\right)=\frac{\left(\rho_1 hU_1+\rho_2 hU_2\right)^2}{2h\left(\rho_2+\rho_1\right)}-\frac{\left(\rho_1 h+\rho_2 h\right)\left\{\rho_1 h\left(U_1{}^2\right)+\rho_2 h\left(U_2{}^2\right)\right\}}{2\left(\rho_1 h+\rho_2 h\right)} \tag{L.29}$$

where again we have taken advantage of the uniform layer approximation. Simplifying provides

$$\left(E_{km}-E_{ku}\right)=\frac{h\left(\rho_1 U_1+\rho_2 U_2\right)^2-h\left(\rho_1+\rho_2\right)\left\{\rho_1\left(U_1{}^2\right)+\rho_2\left(U_2{}^2\right)\right\}}{2\left(\rho_1+\rho_2\right)} \tag{L.30}$$

expanding the numerator

$$\cancel{\left(\rho_1 U_1\right)^2}+2\rho_1 U_1\rho_2 U_2+\cancel{\left(\rho_2 U_2\right)^2}-\cancel{\rho_1{}^2\left(U_1{}^2\right)}-\rho_1\rho_2\left(U_1{}^2\right)-\rho_1\rho_2\left(U_2{}^2\right)-\cancel{\rho_2{}^2\left(U_2{}^2\right)} \tag{L.31}$$

or

$$-\rho_1\rho_2\left(U_1-U_2\right)^2 \tag{L.32}$$

so we obtain the linear gradient result as

$$\left(E_{km}-E_{ku}\right)=\frac{-\rho_1\rho_2 h\left(U_1-U_2\right)^2}{2\left(\rho_1+\rho_2\right)} \tag{L.33}$$

Note that we previously derived for uniform density result

$$\left(E_{km}-E_{ku}\right)=\frac{-\left(\rho_1\rho_2 h_1 h_2\right)\left(U_1-U_2\right)^2}{2\left(\rho_1 h_1+\rho_2 h_2\right)} \tag{L.34}$$

Using $h=h_1=h_2$, the uniform gradient result is

$$\left(E_{km}-E_{ku}\right)=\frac{-\left(\rho_1\rho_2 h^{\cancel{2}}\right)\left(U_1-U_2\right)^2}{4\cancel{h}\left(\rho_1+\rho_2\right)} \tag{L.35}$$

comparing eq. (L.33) and (L.35) indicates that mixing only to a linear gradient releases more kinetic energy; i.e. eq. (L.33) is larger. However, this is somewhat inconsistent as it requires the momentum to be fully mixed by the density to be only linearly mixed. Thus, we prefer to use the original result, eq. (L.35), developed for complete mixing.

L.4 Is it worthwhile using linear gradient approximations for both density and velocity in shear model?

Now, if both momentum and density are only linearly mixed, and we use

$$U_m(z) = U_2 - \frac{\Delta U}{2h} z \tag{L.36}$$

where

$$\Delta U = U_2 - U_1 \tag{L.37}$$

Then the integrated kinetic energy after mixing is

$$E_{km} = \frac{1}{2} \int_{2h} \left({U_m}^2 \right) \rho_m(z) dz \tag{L.38}$$

or

$$E_{km} = \int_{2h} \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} \left\{ U_2 - \frac{\Delta U}{2h} z \right\}^2 dz \tag{L.39}$$

So

$$\begin{aligned} E_{km} &= \int_{2h} \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} \left\{ {U_2}^2 - 2U_2 \frac{\Delta U}{2h} z + \frac{\Delta U^2}{4h^2} z^2 \right\} dz \\ &= \int_{2h} \left[\left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} {U_2}^2 - \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} 2U_2 \frac{\Delta U}{2h} z + \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} \frac{\Delta U^2}{4h^2} z^2 \right] dz \end{aligned} \tag{L.40}$$

Thus, we have the change in energy as

$$\begin{aligned} E_{km} - E_{ku} = &\int_{2h} \left[\left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} {U_2}^2 - 2 \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} U_2 \frac{\Delta U}{2h} z + \left\{ \rho_2 - \frac{\Delta\rho}{2h} z \right\} \frac{\Delta U^2}{4h^2} z^2 \right] dz \\ &- \rho_1 h {U_1}^2 - \rho_2 h {U_2}^2 \end{aligned} \tag{L.41}$$

Then integrated momentum conservation requires is

$$\int U_m \rho_m(z) dz = \rho_1 h U_1 + \rho_2 h U_2 \tag{L.42}$$

or

$$\int_{2h} \left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\}\left\{U_2 - \frac{\Delta U}{2h} z\right\} dz = \rho_1 h U_1 + \rho_2 h U_2 \tag{L.43}$$

The LHS can be written as

$$\int_{2h} \left[\left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\} U_2 - \left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\}\frac{\Delta U}{2h} z\right] dz = \rho_1 h U_1 + \rho_2 h U_2 \tag{L.44}$$

Multiplying through by U$_2$

$$\int_{2h} \left[\left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\} U_2{}^2 - \left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\} U_2 \frac{\Delta U}{2h} z\right] dz = \rho_1 h U_1 U_2 + \rho_2 h U_2{}^2 \tag{L.45}$$

This can be substituted into eq. (L.41) to obtain

$$\begin{aligned} E_{km} - E_{ku} = {} & \rho_1 h U_1 U_2 + \cancel{\rho_2 h U_2{}^2} + \int_{2h} \left[-\left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\} U_2 \frac{\Delta U}{2h} z + \left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\}\frac{\Delta U^2}{4h^2} z^2\right] dz \\ & - \rho_1 h U_1{}^2 - \cancel{\rho_2 h U_2{}^2} \end{aligned} \tag{L.46}$$

Next, we apply eq. (L.37) to say

$$\rho_1 h U_1 U_2 = \rho_1 h U_1 \left(U_1 + \Delta U\right) \tag{L.47}$$

so that

$$\begin{aligned} E_{km} - E_{ku} = {} & \cancel{\rho_1 h U_1{}^2} + \rho_1 h U_1 \Delta U + \int_{2h} \left[-\left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\} U_2 \frac{\Delta U}{2h} z + \left\{\rho_2 - \frac{\Delta\rho}{2h} z\right\}\frac{\Delta U^2}{4h^2} z^2\right] dz \\ & - \cancel{\rho_1 h U_1{}^2} \end{aligned} \tag{L.48}$$

The integral term

$$\int_{2h} \left[-\rho_2 U_2 \frac{\Delta U}{2h} z + \frac{\Delta U}{4h^2}\left\{\Delta\rho U_2 + \rho_2 \Delta U\right\} z^2 - \frac{\Delta\rho \Delta U^2}{8h^3} z^3\right] dz \tag{L.49}$$

which evaluates as

$$-\rho_2 U_2 \frac{\Delta U}{2h}\left(\frac{4h^2}{2}\right) + \frac{\Delta U}{4h^2}\left\{\Delta\rho U_2 + \rho_2 \Delta U\right\}\left(\frac{8h^3}{3}\right) - \frac{\Delta\rho \Delta U^2}{8h^3}\left(\frac{16h^4}{4}\right) \tag{L.50}$$

or

$$-h\rho_2 U_2 \Delta U + \frac{2}{3} h \Delta U \left\{\Delta\rho U_2 + \rho_2 \Delta U\right\} - \frac{1}{2} h \Delta\rho \Delta U^2 \tag{L.51}$$

or

$$-h\rho_2 U_2 \Delta U + \frac{2}{3} h \Delta\rho U_2 \Delta U + \frac{2}{3} h\rho_2 \Delta U^2 - \frac{1}{2} h \Delta\rho \Delta U^2 \tag{L.52}$$

or

$$-h\rho_2 U_2 \Delta U + \frac{2}{3} h \Delta\rho U_2 \Delta U + \frac{2}{3} h\rho_2 \Delta U^2 - \frac{1}{2} h \Delta\rho \Delta U^2 \tag{L.53}$$

so that eq. (L.48) is

$$E_{km} - E_{ku} = h\rho_1 U_1 \Delta U - h\rho_2 U_2 \Delta U + \frac{2}{3} h \Delta\rho U_2 \Delta U + + \frac{2}{3} h\rho_2 \Delta U^2 - \frac{1}{2} h \Delta\rho \Delta U^2 \tag{L.54}$$

This can be expanded as

$$E_{km} - E_{ku} = h\left(\rho_2 - \Delta\rho\right)\left(U_2 - \Delta U\right)\Delta U - h\rho_2 U_2 \Delta U + \frac{2}{3} h \Delta\rho U_2 \Delta U + + \frac{2}{3} h\rho_2 \Delta U^2 - \frac{1}{2} h \Delta\rho \Delta U^2 \tag{L.55}$$

or

$$\begin{aligned} \frac{E_{km} - E_{ku}}{h} &= \rho_2 U_2 \Delta U - \rho_2 \Delta U^2 - \Delta\rho U_2 \Delta U + \Delta\rho \Delta U^2 - \rho_2 U_2 \Delta U \\ &\quad + \frac{2}{3} \Delta\rho U_2 \Delta U + \frac{2}{3} \rho_2 \Delta U^2 - \frac{1}{2} \Delta\rho \Delta U^2 \end{aligned} \tag{L.56}$$

Grouping

$$\frac{E_{km} - E_{ku}}{h} = \cancel{\rho_2 U_2 \Delta U} - \frac{1}{3} \rho_2 \Delta U^2 - \frac{1}{3} \Delta\rho U_2 \Delta U + \frac{1}{2} \Delta\rho \Delta U^2 - \cancel{\rho_2 U_2 \Delta U} \tag{L.57}$$

or

$$E_{km} - E_{ku} = \frac{1}{2} h \Delta\rho \Delta U^2 - \frac{1}{3} h\rho_2 \Delta U^2 - \frac{1}{3} h \Delta\rho U_2 \Delta U \tag{L.58}$$

or

$$E_{km} - E_{ku} = -\frac{1}{3} h\rho_2 \Delta U^2 + \Delta\rho \left\{ \frac{1}{2} h \Delta U^2 - \frac{1}{3} h U_2 \Delta U \right\} \tag{L.59}$$

or

$$E_{km} - E_{ku} = -\frac{1}{3} h\rho_2 \Delta U^2 + h \Delta\rho \Delta U \left\{ -\frac{1}{3} U_2 + \frac{1}{2} \Delta U \right\} \tag{L.60}$$

If $U_2 \sim \Delta U$ then

$$\mathrm{E}_{\mathrm{km}} - \mathrm{E}_{\mathrm{ku}} = -\frac{1}{3}\mathrm{h}\rho_2\Delta\mathrm{U}^2 + O(\Delta\rho) \tag{L.61}$$

Without approximation, we might write

$$\mathrm{E}_{\mathrm{km}} - \mathrm{E}_{\mathrm{ku}} = -\frac{1}{3}\mathrm{h}\rho_2\Delta\mathrm{U}^2 + \Delta\rho\mathrm{h}\Delta\mathrm{U}\left\{\frac{1}{2}\Delta\mathrm{U} - \frac{1}{3}\mathrm{U}_2\right\} \tag{L.62}$$

Note that for the uniform slab mixing, we had

$$\left(\mathrm{E}_{\mathrm{km}} - \mathrm{E}_{\mathrm{ku}}\right) = \frac{-(\rho_1\rho_2\mathrm{h})(\Delta\mathrm{U})^2}{4(\rho_1 + \rho_2)} \tag{L.63}$$

which is approximately

$$\left(\mathrm{E}_{\mathrm{km}} - \mathrm{E}_{\mathrm{ku}}\right) = -\frac{1}{4}\rho_2\mathrm{h}\Delta\mathrm{U}^2 \tag{L.64}$$

Thus, since eq. (L.61) is larger (negatively) than eq. (L.64), this implies that there will be slightly more kinetic energy released when computed from mixing to linear gradients. However, this might not be correct since if $\mathrm{U}_2 < \Delta\mathrm{U}$, i.e. for a low velocity layer, then the leading additional term is $\mathrm{h}\Delta\rho\Delta\mathrm{U}^2 / 2$, which reduces the energy released.

This approach does not seem to be significantly better given the nature of the approximations involved.

Appendix M PSEUDO-CODE OF SHEAR MIXING

```
%% required data at start of mixing
$\Delta t_M$
$U^n_{R(i,j,k)}$ , $V^n_{R(i,j,k)}$ , $\rho^n_{R(i,j,k)}$ , $h^n_{T(i,j,k)}$ , $h^n_{B(i,j,k)}$


%% compute shear mixing ====================


%% initialize mixing time remaining
  $\Delta t^{(1)}_{L(k+1/2)} = \Delta t_M$
%% initialize representative gradients
  $\Delta U^{(1)}_{R(i,j,k+1/2)} = U^n_{R(i,j,k+1)} - U^n_{R(i,j,k)}$
  $\Delta V^{(1)}_{R(i,j,k+1/2)} = V^n_{R(i,j,k+1)} - V^n_{R(i,j,k)}$
  $\Delta \rho^{(1)}_{R(i,j,k+1/2)} = \rho^n_{R(i,j,k+1)} - \rho^n_{R(i,j,k)}$
%% time for KH billows, eq.
  $T^{(1)}_{KH(k+1/2)} = -\frac{20\rho_0}{g\,\Delta\rho^{(1)}_{R(k+1/2)}}\sqrt{\left(\Delta U^{(1)}_{R(k+1/2)}\right)^2 + \left(\Delta V^{(1)}_{R(k+1/2)}\right)^2}$
%% time left for KH billow computation
  $T^{(1)}_{LKH(k+1/2)} = T^{(1)}_{KH(k+1/2)}$
%% KH billow thickness
  $\delta^{(1)}_{KH(k+1/2)} = -\frac{0.3\rho_0}{g\,\Delta\rho^{(1)}_{R(k+1/2)}}\left\{\left(\Delta U^{(1)}_{R(k+1/2)}\right)^2 + \left(\Delta V^{(1)}_{R(k+1/2)}\right)^2\right\}$
%% define initial mixing time step
  $\Delta t^{(1)}_{U(k+1/2)} = \min\left\{\Delta t^{(1)}_{L(k+1)}, T^{(1)}_{KH(k+1/2)}\right\}$   %% over all cells
%% define the mixing thickness during the time step
```

$$\delta^{(1)}_{m(k+1/2)} = \frac{\Delta t^{(1)}_{U(k+1/2)}}{T^{(1)}_{KH(k+1/2)}} \delta^{(1)}_{KH(k+1/2)}$$

%% define the mixing anomaly (the amount greater than local dz)

$$a\delta^{(1)}_{m(k+1/2)} = \delta^{(1)}_{m(k+1/2)} - \Delta z_{(k+1/2)}$$

%% define the set of cell faces for single-step mixing and multistep mixing

aa = where ($a\delta^{(1)}_{m(k+1/2)} \le 0$) %% single step

ff = where not (aa) faces %% multi-step

%% set the time used to zero for multi-step (ff) cell faces so that they are not altered by the

%% single-step mixing

$\Delta t^{(1)}_{U(k+1/2)} = 0$ %% over ff cell faces

%% the additional mixing completed

$\Delta h^{(1)}_{(k+1/2)} = \frac{1}{2}\left\{\delta^{(1)}_{m(k+1/2)} - \left[h^{n}_{T(k)} + h^{n}_{B(k+1)}\right]\right\}$ %% over (aa) faces

%% define the cells where the existing gradient was larger than the KH billow gradient

bb = k or k+1 where $\Delta h^{(1)}_{(k+1/2)} > 0$

%% apportion the mixing change equally on both sides

$h^{(2)}_{T(k)} = h^{(1)}_{T(k)} + \Delta h^{(1)}_{(k+1/2)}$ %% over (bb) cells

$h^{(2)}_{B(k+1)} = h^{(1)}_{B(k+1)} + \Delta h^{(1)}_{(k-1/2)}$ %% over (bb) cells

%% adjust for mixing regions greater than grid cell size – height anomaly

$ah_{(k)} = h^{(2)}_{T(k)} + h^{(2)}_{B(k)} - \Delta z_{k}$ %% over (bb) cells

%% identify the areas where the net top and bottom mixing is larger than the grid cell

cc = where ($ah_{(k)} > 0$) %% over (bb) cells

%% reset mixing thickness for cells that mixing is greater than grid cell size

%% this neglects an interaction between upper and lower boundaries of a cell, but this should be
%% a small term

%% To make this conservative, we must change the mixing layer equally on both sides.

```
  $h^{(2)}_{T(k)} = h^{(2)}_{T(k)} - \frac{1}{2}\max\left\{ah_{(k)}, ah_{(k+1)}\right\}$ %% over (cc) cells
  $h^{(2)}_{B(k)} = h^{(2)}_{B(k)} - \frac{1}{2}\max\left\{ah_{(k)}, ah_{(k-1)}\right\}$ %% over (cc) cells
%% error checking
  if $h^{(2)}_{B(k)} < 0$ or $h^{(2)}_{T(k)} < 0$ and error has occurred (investigate)
%% update grid-cell average values
  $\overline{\phi}^{(2)}_{(k)} = \overline{\phi}^{(2)}_{(k)} + \frac{1}{2\Delta z_{(k)}}\left(\Delta\phi^{n}_{R(k+1/2)}\left\{\frac{\left[h^{(2)}_{T(k)}\right]^2}{h^{(2)}_{T(k)} + h^{(2)}_{B(k+1)}} - \frac{\left[h^{n}_{T(k)}\right]^2}{h^{n}_{T(k)} + h^{n}_{B(k+1)}}\right\} - \Delta\phi^{n}_{R(k-1/2)}\left\{\frac{\left[h^{(2)}_{T(k-1)}\right]^2}{h^{(2)}_{T(k-1)} + h^{(2)}_{B(k)}} - \frac{\left[h^{n}_{T(k-1)}\right]^2}{h^{n}_{T(k-1)} + h^{n}_{B(k)}}\right\}\right)$ %% over (bb) cells
%% define the time left for mixing
  $\Delta t^{(2)}_{L(k+1/2)} = \Delta t^{(1)}_{L(k+1/2)} - \Delta t^{(1)}_{U(k+1/2)}$ over all cells (requires $\Delta t_{U} = 0$ for ff faces)
  $T^{(2)}_{LKH(k+1/2)} = T^{(1)}_{LKH(k+1/20} - \Delta t^{(1)}_{U(k+1/2)}$
%% finished with single-step mixing.


%% Begin multi-step mixing over cell boundaries (ff) =========================
%% set the loop counter
  m=3
%% count the number of cells with multi-step mixing
  $n_{cells}$ = number of cell faces in (ff)
%% main loop for multi-step mixing
  while $n_{cells} > 0$ %% outer iteration
      %% compute mean gradients over cell faces (ff)
      $\Delta\overline{U}^{(m-1)}_{(i,j,k+1/2)} = \overline{U}^{(m-1)}_{(i,j,k+1)} - \overline{U}^{(m-1)}_{(i,j,k)}$
      $\Delta\overline{V}^{(m-1)}_{(i,j,k+1/2)} = \overline{V}^{(m-1)}_{(i,j,k+1)} - \overline{V}^{(m-1)}_{(i,j,k)}$
```

```
    $\Delta\overline{\rho}^{(m-1)}_{(i,j,k+1/2)} = \overline{\rho}^{(m-1)}_{(i,j,k+1)} - \overline{\rho}^{(m-1)}_{(i,j,k)}$

    %% time for KH billows using mean gradients over cell faces (ff)

    $T^{(m)}_{KH(k+1/2)} = -\frac{20\rho_0}{g\,\Delta\overline{\rho}^{(m-1)}_{(k+1/2)}}\sqrt{\left(\Delta\overline{U}^{(m-1)}_{(k+1/2)}\right)^2 + \left(\Delta\overline{V}^{(m-1)}_{(k+1/2)}\right)^2}$

    %% time left for KH billow computation over cell faces (ff)

    $T^{(m)}_{LKH(k+1/2)} = T^{(m)}_{KH(k+1/2)}$

    %% KH billow thickness using mean gradients over cell faces (ff)

    $\delta^{(m)}_{KH(k+1/2)} = -\frac{0.3\rho_0}{g\,\Delta\overline{\rho}^{(m-1)}_{(k+1/2)}}\left\{\left(\Delta\overline{U}^{(m-1)}_{(k+1/2)}\right)^2 + \left(\Delta\overline{V}^{(m-1)}_{(k+1/2)}\right)^2\right\}$

    %% Reset the cumulative thickness counter and billow time over cell faces (ff)

    $\Delta t^{(m-1)}_{c(k+1/2)} = 0$
    $\delta^{(m-1)}_{c(k+1/2)} = 0$

    %%  Define new faces (ff) for the multi-step

    ff = where $T^{(m)}_{LKH(k+1/2)} > 0$ and $\Delta t^{(m)}_{L(k+1/2)} > 0$

    %% set the $n_{cells}$

    $n_{cells}$ = number of cell faces in (ff)


    %% begin inner iteration

    while $n_{cells} > 0$  %% inner iteration

        %% find the dz anomaly; the amount of a grid cell that has not been mixed by the
        %% billow.  If this is negative, then mixing must go to an outer iteration.

        $a\Delta z^{(m)}_{U(k+1/2)} = \Delta z_{(k+1)} - \frac{1}{2}\delta_{c(k+1/2)}$
        $a\Delta z^{(m)}_{L(k+1/2)} = \Delta z_{(k)} - \frac{1}{2}\delta_{c(k+1/2)}$

        %% compute the allowed mixing height in the sub-time step

        $\delta^{(m)}_{f} = \min\left\{\frac{\Delta z_{(k)}}{2}, \frac{\Delta z_{(k+1)}}{2}, a\Delta z^{(m)}_{U(k+1/2)}, a\Delta z^{(m)}_{L(k+1/2)}\right\}$
```

```
%% find where a negative might have occurred (indicating that no further mixing
%% in the cell is possible in this step)
  where $(\delta^{(m)}_{f(k+1/2)} < 0)$  set $(\delta^{(m)}_{f(k+1/2)} = 0)$
%% compute the time required for a fraction of the cell volume to flux across a
%% boundary
  $\Delta t^{(m)}_{R(k)} = \frac{-g\left[\delta^{(m)}_{f(k+1/2)}\right]^2 \Delta\bar{\rho}^{(m-1)}_{(k+1/2)}}{C_C\rho_0}\left\{\left(\Delta\bar{U}^{(m-1)}_{(k+1/2)}\right)^2 + \left(\Delta\bar{V}^{(m-1)}_{(k+1/2)}\right)^2\right\}^{-3/2}$
%% ... above is over (ff) cell faces
%% compute the allowable mixing time used in this mixing sub-time step
  $\Delta t^{(m)}_{U(k+1/2)} = \min\left[\Delta t^{(m-1)}_{L(k+1/2)}\ T^{(m-1)}_{LKH(k+1/2)},\ \Delta t^{(m)}_{R(k+1)},\right]$ %% over (ff) cell faces
%% compute the actual height mixed based on the time used over (ff) cell faces
  $\delta^{(m)}_{f(k+1/2)} = \sqrt{\frac{-C_C\rho_0\Delta t^{(m)}_{U(k+1/2)}}{g\Delta\bar{\rho}^{(m-1)}_{(k+1/2)}}\left\{\left(\Delta\bar{U}^{(m-1)}_{(k+1/2)}\right)^2 + \left(\Delta\bar{V}^{(m-1)}_{(k+1/2)}\right)^2\right\}^{3/2}}$
%% compute the cumulative mixing time for this billow
  $\Delta t^{(m)}_{c(k+1/2)} = \Delta t^{(m-1)}_{c(k+1/2)} + \Delta t^{(m-1)}_{U(k+1/2)}$ %%  over (ff) cell faces
%% compute the cumulative mixing height for this inner iteration
  $\delta^{(m)}_{c(k+1/2)} = \delta^{(m-1)}_{c(k+1/2)} + \delta^{(m)}_{f(k+1/2)}$
%% define cell centers where a face is in (ff)
  gg = where (k+1/2 in ff or k-1/2 in ff)
%% update the cell mean values.  Note that this will also compute over cells with
%% faces
%% where  $(\delta^{(m)}_{f(k+1/2)} = 0)$.  This extra computation shouldn't be an issue since
%% $\Delta t_U = 0$ will be required for these cells
```

```
        $\overline{\phi}^{m}_{(k)} = \overline{\phi}^{m-1}_{(k)} + \frac{1}{2\Delta z_{(k)}}\left(\frac{C_C\rho_0}{g}\right)^{1/2}\left(\Delta\overline{\phi}^{m-1}_{(k+1/2)}\left\{\frac{\Delta t^{m}_{U(k+1/2)}}{-\Delta\overline{\rho}^{m-1}_{(k+1/2)}}\right\}^{1/2}\left\{\left[\Delta\overline{U}^{m-1}_{(k+1/2)}\right]^2+\left[\Delta\overline{V}^{m-1}_{(k+1/2)}\right]^2\right\}^{3/4} - \Delta\overline{\phi}^{n}_{k-1/2}\left\{\frac{\Delta t^{m}_{U(k-1/2)}}{-\Delta\overline{\rho}^{m-1}_{(k-1/2)}}\right\}^{1/2}\left\{\left[\Delta\overline{U}^{m-1}_{(k-1/2)}\right]^2+\left[\Delta\overline{V}^{m-1}_{(k-1/2)}\right]^2\right\}^{3/4}\right)$
        %% ...the above is over (gg) cells
        %% update the time left for the KH billow and the mixing over (ff) cell faces
          $T^{(m)}_{LKH(k+1/2)} = T^{(m-1)}_{LKH(k+1/2)} - \Delta t^{(m-1)}_{U(k+1/2)}$
          $\Delta t^{(m)}_{L(k+1/2)} = \Delta t^{(m-1)}_{L(k+1/2)} - \Delta t^{(m-1)}_{U(k+1/2)}$
        %% find cells to continue with another iteration.  These cells must have time left
        %% in the time step, in the billow evolution, and must not have "run out" of grid
        %% cells space.
          ff = where $T^{(m)}_{LKH(k+1/2)} > 0$ and $\Delta t^{(m)}_{L(k+1/2)} > 0$ and $(\delta^{(m)}_{f(k+1/2)} > 0)$
        %% loop counter
          m=m+1
        %% loop control
          $n_{cells}$ = number of cell faces in (ff)
        %% compute mean gradients for next loop over faces (ff)
          $\Delta\overline{U}^{(m-1)}_{(i,j,k+1/2)} = \overline{U}^{(m-1)}_{(i,j,k+1)} - \overline{U}^{(m-1)}_{(i,j,k)}$
          $\Delta\overline{V}^{(m-1)}_{(i,j,k+1/2)} = \overline{V}^{(m-1)}_{(i,j,k+1)} - \overline{V}^{(m-1)}_{(i,j,k)}$
          $\Delta\overline{\rho}^{(m-1)}_{(i,j,k+1/2)} = \overline{\rho}^{(m-1)}_{(i,j,k+1)} - \overline{\rho}^{(m-1)}_{(i,j,k)}$
    end while %% inner ncells > 0
end while %% outer ncells > 0
```

Appendix N REFERENCES

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