Quantification of Volume-Integrated Budgets Using Total Exchange flow

DYLAN SCHLICHTING

1. DERIVATION OF VOLUME INTEGRATED BUDGETS

Consider a three dimensional control volume with open boundaries on the four vertical faces. The continuity equation may be written as:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

where $\mathbf{u}$ is the three dimensional velocity vector $\langle u, v, w \rangle$ corresponding to the eastward, northward, and vertical velocities, respectively. We may write the volume (V) integrated continuity equation using the divergence theorem:

$$\iiint_V \nabla \cdot \mathbf{u} \, dV = \iint_A \mathbf{u} \cdot \mathbf{n} \, dA \tag{2}$$

The divergence theorem states the time rate of change of the volume is equal to net flux through the North (N), South (S), East (E), and West (W) faces of the domain:

$$-\frac{\partial}{\partial t} \iiint_V dV = A_{yz} u \Big|_E^W + A_{xz} v \Big|_N^S \tag{3}$$

with positive fluxes denoted as out of the box face, consistent with most mathematical applications.

Similarly, we can derive a volume integrated equation for salinity. First, we make some scaling arguments by assuming the horizontal mixing is much smaller than the vertical mixing. The salinity equation may be written as:

$$\frac{\partial s}{\partial t} + \mathbf{u} \cdot \nabla s - \frac{\partial}{\partial z}(K_v \frac{\partial s}{\partial z}) = 0 \tag{4}$$

where K_v is the vertical salinity diffusivity. The volume integrated budget may be written as:

$$-\frac{\partial}{\partial t} \iiint sV \, dV = A_{yz} us \Big|_E^W + A_{xz} vs \Big|_N^S \tag{5}$$

Note that vertical diffusive flux (third term) in Eqn. 4 vanishes when volume integrating because the total vertical flux is assumed to be negligible.

Next, we will derive a budget equation for salinity squared because it is of key importance to calculate mixing, which will be shown in an isohaline framework in the next section. To arrive at the salinity squared equation, we multiply Eqn. 4 by $2s$:

$$\frac{\partial s^2}{\partial t} + \mathbf{u} \cdot \nabla s^2 - \frac{\partial}{\partial z}(K_v \frac{\partial s^2}{\partial z}) = -2[K_v (\frac{\partial s^2}{\partial z})^2]. \tag{6}$$

Next, we volume integrate, applying the same scaling arguments as before:

$$-\frac{\partial}{\partial t} \iiint_V s^2 \, dV = A_{yz} us^2 \Big|_E^W + A_{xz} vs^2 \Big|_N^S - \iiint_v 2[K_v (\frac{\partial s^2}{\partial z})^2] dV. \tag{7}$$

where the third term of the RHS of Eqn 7 is referred to as mixing (see Burchard and Rennau (2008))

Last, we will derive an equation for the salinity variance budget - starting from the salinity equation but applying the decompositions $s = \overline{s} + s'$, where $\overline{s}$ denotes the mean with respect to all control surfaces of the box and the s' denotes the pertubations. Similarly we can decompose the velocity as $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$ is the relative velocity. The equation for the mean salinity may be written as:

$$\frac{\partial \overline{s}}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \overline{s} + \overline{\mathbf{u}' \cdot \nabla s'} - \frac{\partial}{\partial z}(K_v \frac{\partial \overline{s}}{\partial z}) = 0 \tag{8}$$

Taking the difference between Eqns 4 and 8 yield:

$$\frac{\partial s'}{\partial t} + \overline{\mathbf{u}} \cdot \nabla s' + \mathbf{u}' \cdot \nabla s' + \mathbf{u}' \cdot \nabla s' - \overline{\mathbf{u}' \cdot \nabla s'} - \frac{\partial}{\partial z}(K_v \frac{\partial s'}{\partial z}) = 0 \tag{9}$$

To arrive at the salinity variance equation, multiply by $2s'$:

$$\begin{aligned}\frac{\partial s'^2}{\partial t} + \bar{\mathbf{u}}\cdot\nabla s'^2 + 2\mathbf{u}'s'\cdot\nabla\bar{s} + \mathbf{u}'\cdot\nabla s'^2 - 2s'\,\overline{\mathbf{u}'\cdot\nabla s'}\\ -[2\frac{\partial}{\partial z}(K_v\frac{\partial s'^2}{\partial z}) - 2(K_v\left(\frac{\partial s'}{\partial z}\right)^2)] = 0\end{aligned} \tag{10}$$

Next, we can make some simplifications by noting that $\bar{s}$ is constant in space, yielding $\nabla\bar{s} = 0$. After some rearranging, the variance equation may be written as:

$$\frac{\partial s'^2}{\partial t} + \nabla\cdot(\mathbf{u}s'^2) - 2s'\,\overline{\mathbf{u}'\cdot\nabla s'} = 2\frac{\partial}{\partial z}(K_v\frac{\partial s'^2}{\partial z}) - 2(K_v\left(\frac{\partial s'}{\partial z}\right)^2) \tag{11}$$

where the first term on the RHS represents the vertical diffusive flux and the second term will represents the destruction of salinity variance, or termed mixing. Note that this is identical to equation 5 of Li et al. (2018) without the horizontal diffusive fluxes and mixing terms. To obtain the volume integrated salinity variance budget, we note that the vertical integral of the divergence of vertical diffusive flux vanishes because the vertical turbulent flux is zero at both the top and bottom of the water column. We also note that the volume integral of $\overline{s'}$ is zero, allowing the third term in equation X to cancel out. So the volume budget may be written as:

$$-\frac{\partial}{\partial t}\iiint_V s'^2\,dV = A_{yz}u(s-\bar{s})^2\Big|_E^W + A_{xz}v(s-\bar{s})^2\Big|_N^S - 2\iiint_v K_v\left(\frac{\partial s}{\partial z}\right)^2 dV. \tag{12}$$

The salinity variance budget in Eqn 12 indicates that the rate of change of salinity variance is controlled by the boundary fluxes and the dissipation due to difference. The major difference between the salinity variance budget of an estuary compared to a system with no closed boundaries is that the salinity variance flux is averaged with respect to a particular control surface, not the entire domain.

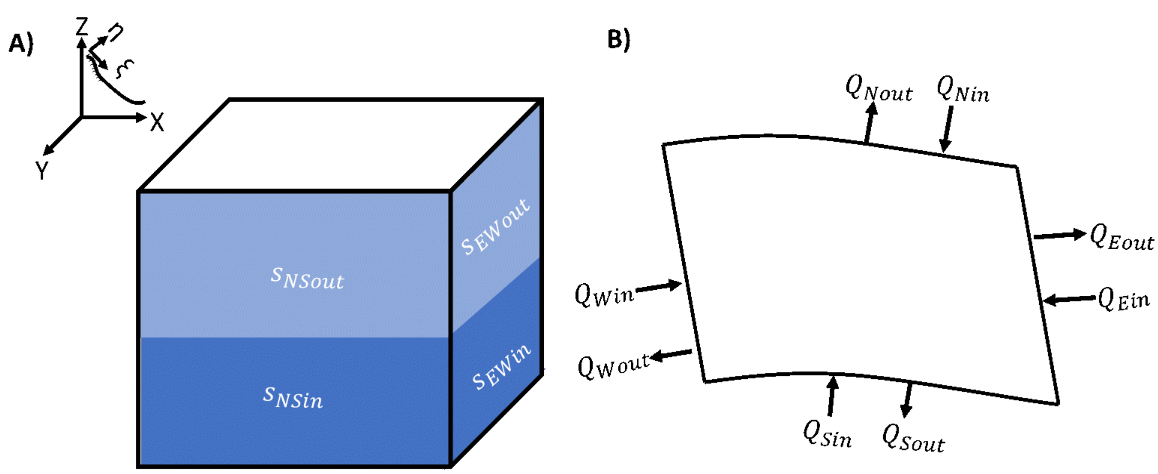

Figure 1: A) Conceptual schematic of exchange flow for a control volume with open boundaries with two layer flow. Subscripts N, S, E, and W refer to the north, south, east, and west box faces. Vertical fluxes are neglected. Box is shaded qualitatively for salinity concentration, with darker values indicating higher salinity concentrations. B) 2D representation (plan view) of control volume in curvilinear coordinates. Arrows shown are indicate the direction of inflows and outflows with each face of the control volume

2. Derivation using TEF

In this section we will derive the budgets using the isohaline framework described by MacCready (2011) and Burchard et al. (2019). For any tracer c, its time averaged flux through a cross section may be expressed in salinity coordinates:

$$\langle \int_{A(S)} F^c \, dA \rangle = \int_0^{s_{max}} q^c(s) ds, \tag{13}$$

where

$$q^c(s) = \frac{\partial Q^c(S)}{\partial S} \text{ and } Q^c(s) = \langle \int_{A(S)} uc \, dA \rangle. \tag{14}$$

where $Q^c(S)$ is the transport of the tracer through cross-sectional area $A(S)$ with salinities s higher than S, and $q^c(S)$ is the boundary flux of the tracer per salinity class. In practice, $q^c(S)$ is calculated as a transported weighted histogram with salinity bins as the sorting property. The bulk inflows and outflows of the tracer may be expressed as:

$$\begin{aligned} Q^c_{in} &= \int_0^{s_{max}} (q^c)^- dS \leq 0, \\ Q^c_{out} &= \int_0^{s_{max}} (q^c)^+ dS \geq 0, \end{aligned} \tag{15}$$

where the $-$ refers to all areas where the transport per salinity class is negative, and the $+$ refers to all areas where the transport is positive, resulting in negative inflows and positive outflows, consistent with most mathematical applications. The corresponding inflowing and outflowing tracer concentrations are defined as:

$$c_{in} = \frac{Q^c_{in}}{Q_{in}}; \; c_{out} = \frac{Q^c_{out}}{Q_{out}}. \tag{16}$$

Note that the dropping of the c superscipt indicates volume flux. There only difference between the current derivation and MacCready (2011) is that the signs for outflows and inflows are reversed.

Consider a fully three dimensional control volume as in Section 1. First, we write the bulk transport of a tracer for the control volume as:

$$Q^c_{net}(s) = \langle \iint_{A(S)} uc \cdot \, dA \rangle = \langle A(S)_{yz} uc \rangle \Big|_E^W + \langle A(S)_{xz} vc \rangle \Big|_N^S \tag{17}$$

Which is similar in form to one dimensional transport, except here the tracer transport is averaged temporally and is in salinity coordinates. Note that the definition of q^c and F^c are subsequently redefined as well. In practice, individual control surfaces are isolated and binned (resulting in four separate histograms), averaged temporally, and then the divergence theorem is applied to obtain the bulk transport. The advantage of binning at each individual face is that it establishes context for the bulk values. A simple example would be that eastward transport contributed say 75% of the volume budget of the box.

For a more complex system like the inner shelf or open ocean, the water column may consist of a series of asymmetrical inflows and outflows. Lorenz et al. (2019) developed an extension of the TEF concept to multilayered flow by determining the salinities S_{div} that divide each layer. The idea is to find the extrema of the discrete Q^c profiles, which shares the same salinity as the zero crossing points. The fluxes in the individual layers Q^c_n are calculated as:

$$\int_{S_{div,n}}^{S_{div,n+1}} q^c \, dS = Q^c(S_{div,n+1} - S_{div,n}). \tag{18}$$

The net transport may be written discretely as:

$$Q^C_{net} = \sum_{i=1}^{N} \sum_{j=1}^{M} Q^c_{in,i} + Q^c_{out,j} \tag{19}$$

where N and M represent the total number of inflows and outflows, respectively. Similarly, the net tracer concentration may be calculated as

$$c_{net} = \frac{\sum_{i=1}^{N}\sum_{j=1}^{M} Q^c_{in,i} + Q^c_{out,j}}{\sum_{i=1}^{N}\sum_{i=1}^{M} Q_{in,i} + Q_{out,j}}. \tag{20}$$

Note that one may easily split apart the net tracer concentration to consider the net inflows and outflows. To examine this in a budget context, we must derive a an expression for the time rate of change of the volume integrated tracers in salinity coordinates.

$$\frac{\partial}{\partial t}\iiint_V cdV \rightarrow \Phi^c = \frac{\partial}{\partial t}\langle \int_{V_s} \frac{\partial \phi^c}{\partial s}\, ds\rangle \tag{21}$$

where $V(S)$ is a volume with salinities S higher than s and $\frac{\partial \phi^c}{\partial S}$ represents the volume integrated tracer per salinity class. We switch notation here so that there is no confusion between the north velocity and volume integrated terms. Similar to the tracer flux per salinity class, this is essentially a histogram of volume with salinity as the sorting class. Both the time rate of change of volume integrated tracer per layer and net quantities may be written as:

$$\Phi^c_n = \Phi^c(S_{div(n)+1}) + \Phi^c(S_{div(n)}),\ \ \Phi^c_{net} = \sum_{i=1}^{N}\sum_{j=1}^{M} \Phi^c_i + \Phi^c_j. \tag{22}$$

Note that the volume between two layers is added together because they correspond to the tracer flux per salinity class, which have opposite signs. The layer equation is written above to accommodate asymmetrical inflows/outflows. Now, we may write the volume and salt budget for the control volume using the TEF framework:

$$\Phi_{net} = Q_{net} \tag{23}$$

$$\Phi^s_{net} = Q^s_{net} \tag{24}$$

Now, we may combine the above two equations (with some manipulation) to derive separate equations for $Q_{in,net}$ and $Q_{out,net}$, which can be thought of as the time dependent Knudsen relations without a river discharge term:

$$Q_{out,net} = \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{s_{in,i}}{s_{in,i} - s_{out,j}}(\Phi_i + \Phi_j) - \frac{1}{s_{in,i} - s_{out,j}}(\Phi^s_i + \Phi^s_j) \tag{25}$$

$$Q_{in,net} = \sum_{i=1}^{N}\sum_{j=1}^{M} -\frac{s_{out,i}}{s_{in,i} - s_{out,j}}(\Phi_i + \Phi_j) + \frac{1}{s_{in,i} - s_{out,j}}(\Phi^s_i + \Phi^s_j) \tag{26}$$

Now, we may write the salinity squared and salinity variance budgets as:

$$\Phi^{s^2}_{net} = Q_{in,net}(s)^2_{in,net} + Q_{out,net}(s)^2_{out,net} - \langle M\rangle \tag{27}$$

$$\Phi^{s'^2}_{net} = Q_{in,net}(s'^2)_{in,net} + Q_{out,net}(s'^2)_{out,net} - \langle M\rangle. \tag{28}$$

Note that the dissipation of salinity variance has been abbreviated as M. Now, we can use our 'modified' Knudsen relations and rearrange the salinity variance equation to solve for an equation for M. In Burchard et al. (2019)'s framework, $\langle M\rangle$ has been rewritten using using the time dependent Knudsen relations, yielding:

$$\langle M_{s^2,net}\rangle = \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{s_{out,j}(s^2)_{in,i} - s_{in,j}(s^2)_{out,j}}{s_{in,i} - s_{out,j}}(-(\Phi_i+\Phi_j)) + \frac{(s^2)_{in,i} - (s'^2)_{out,j}}{s_{in,i} - s_{out,j}}(\Phi^s_i+\Phi^s_j) - (\Phi^{s^2}_i+\Phi^{s^2}_j). \tag{29}$$

,

$$\langle M_{svar,net}\rangle = \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{s_{out,j}(s'^2)_{in,i} - s_{in,j}(s'^2)_{out,j}}{s_{in,i} - s_{out,j}}(-(\Phi_i+\Phi_j)) + \frac{(s^2)_{in,i} - (s'^2)_{out,j}}{s_{in,i} - s_{out,j}}(\Phi_i^s+\Phi_j^s) - (\Phi_i^{s'^2}+\Phi_j^{s'^2}). \tag{30}$$

3. DISCUSSION

The key distinction between the derived definition of mixing is that they differ for the salinity square and variance budgets. If you go back and read Burchard et al. (2019), how is it possible for M to be the same for the variance and the s^2 budget? The derivation is based on the Knudsen relations, then applied to a specific budget. All they are essentially doing is rearranging the s^2 equation and solving for M, which I dislike because M depends on the advection terms. For the figures in the other PDF, I didn't actually apply the dividing salinity method - I used the sign method. The budgets here still close.

I did some simple numerical experiments to try to 'break' the budget by using some of my incorrect approximations of the advection terms. For example, I defined $\overline{s}$ to be the volume averaged salinity, not the salinity of a particular control surface. Budget still closes. I also accidentally ran a trial where I multiplied the variance flux by salinity - so totally overestimating the advection, but since mixing scales with the advection, the budget still closed. The result is that the variance was an order of magnitude smaller than both advection/mixing, but it didn't matter.

There are two different conceptual models to define mixing: scalar dissipation of tracer variance per unit volume, and in a budget sense through the extended Knudsen relations. Either I'm really over-complicating this, or the derivation of mixing needs a shift at the conceptual level. Or does it make sense that in this framework you need two definitions of mixing? Maybe I'm just misunderstanding the paper, but the intuition I got from building the toy model has lead me to an obstacle.

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