Volume and Mass Transport across Isosurfaces of a Balanced Fluid Property

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ABSTRACT

This work provides the general theory of the volume and mass conservation in terms of its transport across surfaces (open or closed) defined by a constant value of an oceanographic property obeying a balance law. This fluid property can be any spatial density ϕ (amount of quantity per unit volume), or its specific value $\hat{\phi} \equiv \alpha\phi$ (amount of quantity per unit mass, where α is the specific volume). The main expressions obtained relate the volume transport across a ϕ-surface to the flux of the quantity ($\mathbf{h}_\phi$) across the ϕ-surface boundary, and the mass transport across a $\hat{\phi}$-surface to the flux $\mathbf{h}_{\hat{\phi}}$ across the $\hat{\phi}$-surface boundary. These expressions differ, in general, from the volume and mass conservation of the ϕ-surface, being however equivalent for closed (unlimited) ϕ-surfaces. The main expressions are generalized to the three-dimensional case, and the relation to previous results is discussed.

1. Introduction

Volume and water mass conservation, and the balances of salt and heat play a primary role in the study of oceanic processes, especially in those involving water mass transformation due to interior mixing, sea surface heating, and water mass fluxes (see, e.g., Walin 1982; Tziperman 1986; Garrett et al. 1995; Garrett and Tandon 1997; Nurser et al. 1999). The main idea in these approaches is the application of balance laws and volume or mass conservation to surfaces extending from the upper ocean to the ocean interior, relating therefore fluxes in the upper layer to interior processes like heat or buoyancy diffusion.

The objective of this work is to find the most general expressions for the volume and mass transport across surfaces (open or closed) defined by a constant value of an fluid property obeying a general balance law. This fluid property can be any spatial density ϕ (amount of quantity per unit volume), or its specific value $\hat{\phi} \equiv \alpha\phi$ (amount of quantity per unit mass, where α is the specific volume). As a consequence, this work solves some mathematical problems arising in the analytical treatment of volume and mass transport across arbitrary surfaces in the ocean, and clarifies some previous results by putting them in a general framework where the relation to the first principles becomes clear. For example, we will prove that in this approach the selection of the fluid property obeying a balance law (potential density, temperature, salinity, potential vorticity, etc.) is independent of the underlying physical assumption of mass or volume conservation and therefore any balance law can be employed. We will also show that the expressions obtained are not equivalent to the conservation of mass or area (volume in the three-dimensional case) of the ϕ-surface.

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2. Balance equations and ϕ-coordinate surface

When measurements of some oceanographic field $\phi(\mathbf{x}, t)$ (e.g., the temperature or salinity field) are available, it becomes useful to apply the general theory of rates of change of integral expressions in arbitrary volumes (see appendix A for the basic mathematical theory) to the particular case where the arbitrary surfaces are isosurfaces of the spatial density ϕ, or isosurfaces of the specific value $\hat{\phi}$. In order to do so we define the velocity field $\mathbf{w}$ (introduced in a general way in appendix A) by specifying that its component normal to a ϕ-surface equals the speed of displacement of that ϕ-surface, that is,

$$\frac{d_{\mathrm{w}}\phi}{dt} = \phi_{,t} + \mathbf{w} \cdot \nabla\phi \equiv 0. \tag{1}$$

This equation defines only the component of $\mathbf{w}$ *normal* to the ϕ-surface. The component of $\mathbf{w}$ tangent to the ϕ-surface is set to zero (thus, $\mathbf{w}$ is completely defined by the field ϕ). Let $\mathbf{n}_\phi \equiv \nabla\phi|\nabla\phi|^{-1}$ be the unit vector normal to the ϕ-surface. Thus, we define

$$\mathbf{w}_\phi \equiv -\phi_{,t}|\nabla\phi|^{-1}\mathbf{n}_\phi, \tag{2}$$

and therefore the ϕ-surfaces are material surfaces with respect to the velocity $\mathbf{w}_\phi$. The label ϕ in $\mathbf{w}_\phi$ makes explicit that there is a field $\mathbf{w}_\phi$ for every fluid property ϕ, but there is only one fluid velocity field $\mathbf{u}$. The definition of the fluid velocity for a ϕ-observer (an observer moving with the field $\mathbf{w}_\phi$, or a $\mathbf{w}_\phi$-observer) reads now $\mathbf{v}_\phi = \mathbf{u} - \mathbf{w}_\phi$. As a trivial example note that $\dot{\phi} = 0 \Rightarrow \mathbf{v}_\phi \cdot \mathbf{n}_\phi = 0$, which implies, for example, that all diapycnal fluxes of a incompressible fluid ($\dot{\rho} = 0$) are zero (isopycnals are material surfaces). With $\mathbf{w}_\phi$ so defined, the following relations hold:

$$\dot{\phi} = \phi_{,t} + (\mathbf{w}_\phi + \mathbf{v}_\phi) \cdot \nabla\phi = \mathbf{v}_\phi \cdot \nabla\phi, \quad (3a)$$

$$\phi_{,t} = -\mathbf{w}_\phi \cdot \nabla\phi. \quad (3b)$$

Relation (3a) means that the rate of change of ϕ in a fluid particle is equal to the fluid advection relative to the ϕ-observer (for a ϕ-observer the fluid velocity is $\mathbf{v}_\phi$) because ϕ is constant in the places he occupies during his own motion. Relation (3b), [equivalent to (2)], means that the temporal change of ϕ in a fixed spatial point $\mathbf{x}$ is equal to minus the advection of ϕ by the $\mathbf{w}_\phi$ field. Note that the absence of time derivatives of ϕ that follows when employing, say, $-\mathbf{w}_\phi \cdot \nabla\phi$ instead of $\phi_{,t}$, is only apparent, since the temporal change is included in the definitions of $\mathbf{w}_\phi$ and $\mathbf{v}_\phi$.

Appendix A shows that the general balance equation for $\phi(\mathbf{x}, t)$ can be written as (A8). Combining both the general balance (A8) and (3a) we obtain, in the absence of supply z_ϕ,

$$\mathbf{v}_\phi \cdot \nabla\phi + \phi\nabla \cdot \mathbf{u} = -\nabla \cdot \mathbf{h}_\phi, \quad (4a)$$

$$\rho\mathbf{v}_{\hat{\phi}} \cdot \nabla\hat{\phi} = -\nabla \cdot \mathbf{h}_\phi. \quad (4b)$$

For incompressible fluids, relation (4a) states that, at a point $\mathbf{x}$, the advection of ϕ apparent to a $\mathbf{w}_\phi$-observer equals the (minus) divergence of $\mathbf{h}_\phi$. Since $\nabla \cdot \mathbf{h}_\phi(\mathbf{x}, t)$ can be interpreted as the flux of $\mathbf{h}_\phi$ across the *boundary* of the point $\mathbf{x}$, integral expressions of (4) on arbitrary curves and surfaces (next section) are related to fluxes of $\mathbf{h}_\phi$ across the *boundary* of these arbitrary curves and surfaces. This concept is an expression of the one- and two-dimensional (2D) versions of the divergence theorem. Furthermore, the incompressibility condition does not need to be imposed if instead of (4a) we consider specific quantities and use (4b). This latter option is more general (it only assumes mass conservation) and leads to expressions involving the transport of mass across $\hat{\phi}$-surfaces.

In order to integrate (4) over a ϕ-surface it is useful to establish an orthogonal curvilinear coordinate system $(\nu^1, \nu^2, \nu^3) = [\xi(x, z), y, \phi(x, z)]$, in such a way that $\nabla\xi \cdot \nabla\phi = 0$ (see Fig. 1). This orthogonal coordinate system differs from the nonorthogonal coordinate system that considers ϕ as the vertical coordinate and (x, y) remain unchanged (e.g., the density coordinate system used by Tziperman 1986). The problems we shall consider in the next section are, for simplicity, 2D [in the (x, z) plane], and therefore functions do not depend on

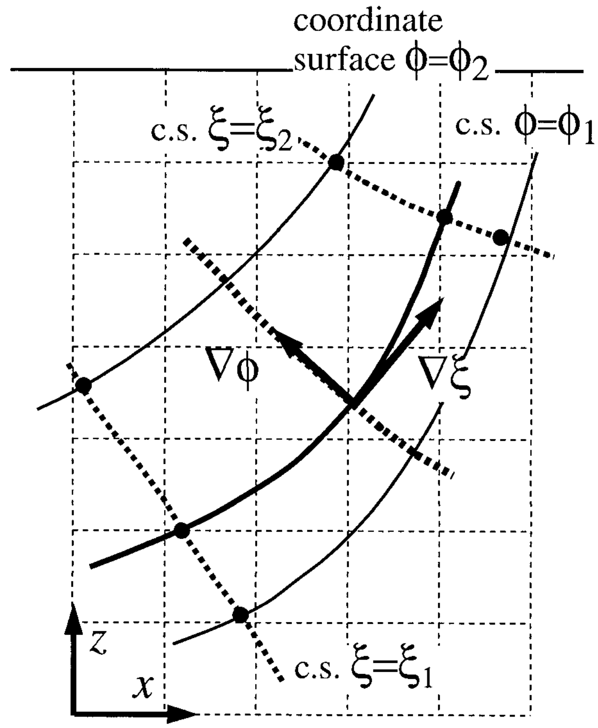

FIG. 1. Schematic showing the 2D orthogonal curvilinear coordinate system (ξ, η).

y. However, we continue working in the three-dimensional (3D) space (considering the y coordinate) in order to use the general tools of the vector and tensor algebra. The Jacobian of the transformation is $J = |\nabla\phi|^{-1}|\nabla\xi|^{-1}$. Because of the orthogonality of the transformation the reciprocal basis and tangent basis vectors are parallel:

$$\mathbf{e}^1 = \nabla\xi \qquad \mathbf{e}^2 = \nabla y = \mathbf{j} \qquad \mathbf{e}^3 = \nabla\phi$$
$$\mathbf{e}_1 = |\nabla\xi|^{-2}\mathbf{e}^1 \qquad \mathbf{e}_2 = \mathbf{e}^2 \qquad \mathbf{e}_3 = |\nabla\phi|^{-2}\mathbf{e}^3, \quad (5)$$

and therefore the unit reciprocal-basis vectors and unit tangent vectors coincide, $\mathbf{n}_\xi \equiv \hat{\mathbf{e}}^1 = \hat{\mathbf{e}}_1 = |\nabla\xi|^{-1}\nabla\xi, \hat{\mathbf{e}}^2 = \hat{\mathbf{e}}_2 = \mathbf{j}$, $\mathbf{n}_\phi \equiv \hat{\mathbf{e}}^3 = \hat{\mathbf{e}}_3 = |\nabla\phi|^{-1}\nabla\phi$. The differential arc length along the ξ-coordinate curve is $dl(1) = g_{11}^{-1/2}\, d\xi = |\nabla\xi|^{-1}\, d\xi$, and the differential area vector in the coordinate surface ϕ = constant is

$$\mathbf{dS}(3) = J\nabla\phi\, d\xi\, dy = \mathbf{n}_\phi|\nabla\xi|^{-1}\, d\xi\, dy = \mathbf{n}_\phi\, dy\, dl(1). \quad (6)$$

Having set in this section 1) the general balance equation for ϕ in terms of the fluid velocity $\mathbf{v}_\phi$ relative to a ϕ-observer (4), and 2) the orthogonal curvilinear coordinate system with ϕ providing one of the family of surfaces, we are now in a position to integrate (4) over a ϕ-surface and relate the volume and mass transport (next section) across a ϕ-surface to the vector flux $\mathbf{h}_\phi$.

3. Volume and mass transport

First, we assume the fluid is incompressible and obtain the volume transport across a ϕ-surface. In order to do so we multiply (4a) by $|\nabla\phi|^{-1}\, dl(1)\, dy = J\, d\xi\, dy$ and integrate on a ϕ-surface. Using the expression of the divergence of a vector field $\mathbf{A}$ in terms of its contravariant components A^i,

$$\nabla \cdot \mathbf{A} = J^{-1}\frac{\partial}{\partial \nu^i}(JA^i), \tag{7}$$

we obtain

$$\int_{\xi_1}^{\xi_2}\int_y \mathbf{v}_\phi \cdot \mathbf{dS}(3) = -\int_{\xi_1}^{\xi_2}\int_y \left[\frac{\partial}{\partial\xi}(Jh^1) + \frac{\partial}{\partial\phi}(Jh^3)\right] d\xi\, dy. \tag{8}$$

(For clarity we drop momentarily the symbol ϕ from $\mathbf{h}_\phi$). Since $Jh^1 = |\nabla\phi|^{-1}|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{e}^1 = |\nabla\phi|^{-1}\mathbf{h}\cdot\mathbf{n}_\xi$, and $Jh^3 = |\nabla\phi|^{-1}|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{e}^3 = |\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi$, relation (8) can be partly integrated,

$$\Delta y\int_{\mathcal{L}_\phi(\xi_1,\xi_2)} \mathbf{v}_\phi\cdot\mathbf{n}_\phi\, dl(1) = -\Delta y[|\nabla\phi|^{-1}\mathbf{h}\cdot\mathbf{n}_\xi]_{\xi_1}^{\xi_2} - \Delta y\int_{\xi_1}^{\xi_2}\frac{\partial}{\partial\phi}(|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi)\, d\xi. \tag{9}$$

Note that $\mathbf{v}_\phi \cdot \mathbf{n}_\phi\, dl(1)$ is the volume transport (by unit distance in the y direction) across the differential surface element $\mathbf{dS}(3)$. Here $dl(1)$ is the distance measured on the ϕ-surface along the ξ-coordinate curve. Symbol $\mathcal{L}_\phi(\xi_1, \xi_2)$ stands for the path on the ϕ-surface from $\xi = \xi_1$ to $\xi = \xi_2$. In the most general case the limits $\xi_1 = \tilde{\xi}_1(\phi)$ and $\xi_2 = \tilde{\xi}_2(\phi)$ are arbitrary and therefore depend on ϕ (see Fig. 2a). Since these limiting functions, $\tilde{\xi}_1$ and $\tilde{\xi}_2$, must be specified for every case, we can employ Leibniz's rule to relate the integral of the derivative to the derivative of the integral, and write the second term on the right-hand side of (9) as

$$\int_{\tilde{\xi}_1(\phi)}^{\tilde{\xi}_2(\phi)}\frac{\partial}{\partial\phi}(|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi)\, d\xi = -\left[\frac{\partial\tilde{\xi}_2}{\partial\phi}|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi\right]_{\xi=\xi_2} + \left[\frac{\partial\tilde{\xi}_1}{\partial\phi}|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi\right]_{\xi=\xi_1} + \frac{\partial}{\partial\phi}\int_{\tilde{\xi}_1(\phi)}^{\tilde{\xi}_2(\phi)}|\nabla\xi|^{-1}\mathbf{h}\cdot\mathbf{n}_\phi\, d\xi. \tag{10}$$

Note that $|\nabla\xi|^{-1}\partial\tilde{\xi}_{1,2}/\partial\phi = |\nabla\xi|^{-1}\nabla\xi\cdot\partial\mathbf{R}_{1,2}(\phi)/\partial\phi = \mathbf{n}_\xi\cdot\partial\mathbf{R}_{1,2}(\phi)/\partial\phi$, where $\mathbf{R}_{1,2}(\phi)$ is the position vector of the points in the limiting curves.

For limits ξ_1 and ξ_2 not depending on ϕ (as in Fig. 2b) the first two terms on the right-hand side of (10) can be removed and relation (9) is finally written (dividing by Δy) as

$$\int_{\mathcal{L}_\phi(\xi_1,\xi_2)} \mathbf{v}_\phi\cdot\mathbf{n}_\phi\, dl(1) = -[|\nabla\phi|^{-1}\mathbf{h}\cdot\mathbf{n}_\xi]_{(\xi_1,\phi)}^{(\xi_2,\phi)} - \frac{\partial}{\partial\phi}\int_{\mathcal{L}_\phi(\xi_1,\xi_2)}\mathbf{h}\cdot\mathbf{n}_\phi\, dl(1). \tag{11}$$

This equation is one of the main results of this work. Note that it is independent of the parameterisation chosen for the ξ-coordinate curves (this must be the case because only ϕ is a physically measurable field). Physically, relation (11) means that the volume transport across a limited ϕ-surface equals the flux of $\mathbf{h}$ across the ϕ-surface *boundary* in the (ξ, y, ϕ) space. The boundary of the ϕ-surface in this space is formed by the two points $[(\xi_1, \phi)$ and $(\xi_2, \phi)]$ plus the two limited surfaces $\phi \pm \delta\phi =$ constant. This latter concept (the flux of $\mathbf{h}$ across these two boundary surfaces) can be understood by considering that

$$\frac{\partial}{\partial\phi}\int_{\xi_1(\phi)}^{\xi_2(\phi)} f(\phi, \xi)\, d\xi = \lim_{\delta\phi\to 0}(2\delta\phi)^{-1}\left[\int_{\xi_1(\phi^+)}^{\xi_2(\phi^+)} f(\phi^+, \xi)\, d\xi - \int_{\xi_1(\phi^-)}^{\xi_2(\phi^-)} f(\phi^-, \xi)\, d\xi\right], \tag{12}$$

where $\phi^\pm \equiv \phi \pm \delta\phi$. In order to compute the second term on the right-hand side of (11), choose two points $[(\xi_1, \phi)$ and $(\xi_2, \phi)]$ over any ϕ-surface (see Fig. 3); move normal from the ϕ-surface to get the four points, $(\xi_1, \phi^\pm)$ and $(\xi_2, \phi^\pm)$; integrate $\mathbf{h}\cdot\mathbf{n}_\phi$ along the surfaces $\phi^\pm$ (curves in 2D space) from ξ_1 to ξ_2; compute the difference; and divide by $2\delta\phi$. These arguments show that (11) is in fact an expression of the divergence theorem ($\int_{\mathcal{V}}\nabla\cdot\mathbf{h}\, dv = \oint_{\partial\mathcal{V}}\mathbf{h}\cdot\mathbf{ds}$) applied to a curve. Previous formulations related to this development are derived and discussed in appendix B.

The physical dimensions of (11) are those of volume transport (volume/time), and therefore (11) is independent of the physical dimensions of the balanced quantity ϕ. In this sense (11) may be interpreted as an expression for the volume conservation in terms of the volume transport across a ϕ-surface. If the divergence term in (4) were kept in the previous development, we would have obtained a relation similar to (11) (with some additional terms) which, while not expressing volume conservation, would be a mathematical identity since no constitutive equation for the flux $\mathbf{h}$ has been adopted. Thus, the balance equation for ϕ is used, in this development, with the purpose of taking into account the relative motion and geometry of the ϕ-surfaces.

Relation (11) is however different from the expression of volume conservation of the ϕ-surface (area conservation in the 2D case). This latter concept is instead presented in the appendix A and is given by (A4). Ap-

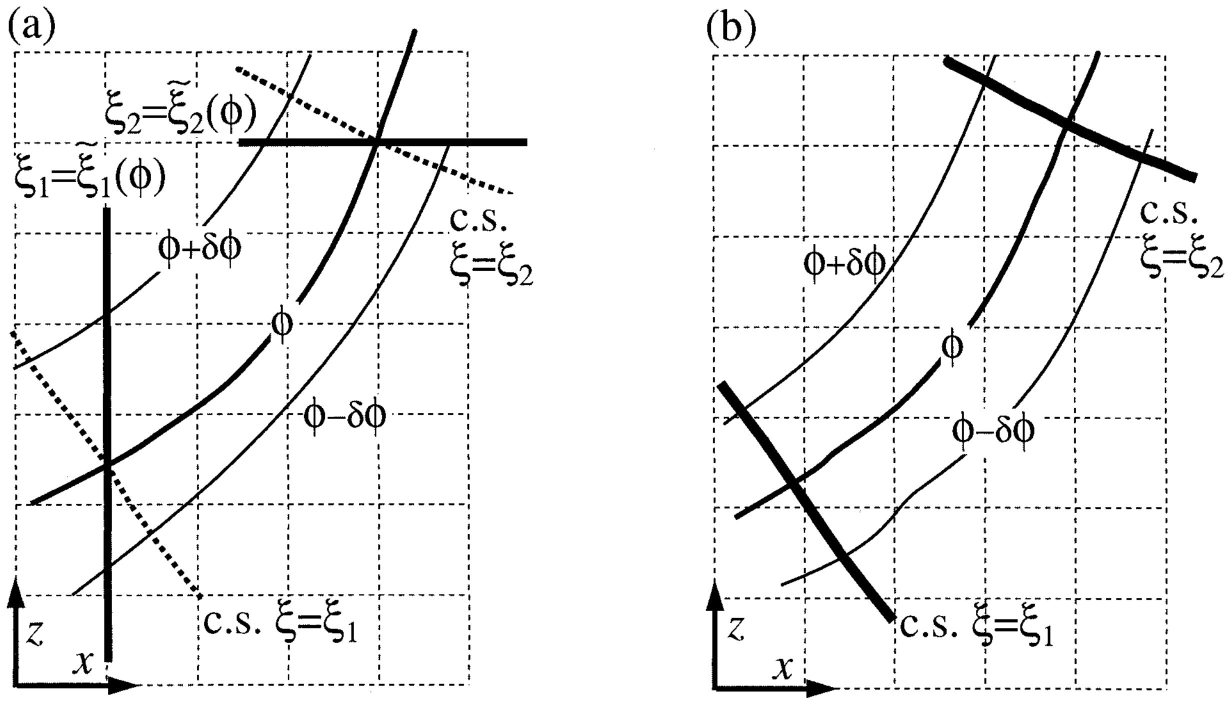

FIG. 2. Schematic showing (a) the ϕ-surfaces limited by functions $\xi_1 = \tilde{\xi}_1(\phi)$ and $\xi_2 = \tilde{\xi}_2(\phi)$, and (b) the ϕ-surfaces limited by ξ-coordinate surfaces (C.S.).

plied to $\mathbf{w}_\phi$, this means that the rate of change of the ϕ-surface volume (area) equals the volume transport, across the ϕ-surface boundary, of the incompressible fluid. Both concepts are however related when the arbitrary volume is defined by a closed (unlimited) ϕ-surface (or a number of closed ϕ_i-surfaces). In this case we have

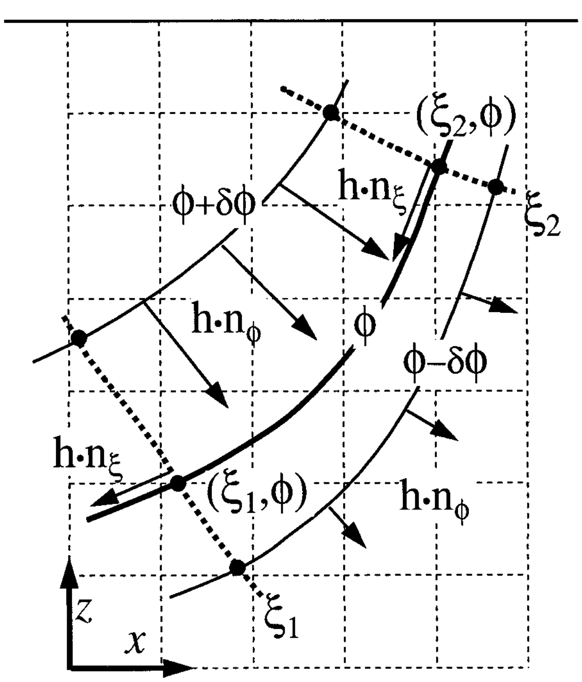

FIG. 3. Schematic showing the volume transport across a limited ϕ-surface and the flux of $\mathbf{h}_\phi$ across the ϕ-surface boundary.

$$\frac{d_{\mathbf{w}_\phi}}{dt}\int_{\mathcal{V}(\phi)} dv \overset{(A4)}{=} -\oint_{\partial\mathcal{V}(\phi)} \mathbf{v}_\phi \cdot \mathbf{dS}(3)$$

$$\overset{(11)}{=} \frac{\partial}{\partial\phi}\oint_{\partial\mathcal{V}(\phi)} \mathbf{h}_\phi \cdot \mathbf{dS}(3), \qquad (13)$$

meaning that the rate of change of the volume enclosed by a ϕ-surface equals the flux of $\mathbf{h}_\phi$ across the ϕ-surface boundary.

A more general way of dealing with similar problems is based on the conservation of mass instead of the conservation of volume. This alternative approach starts from the balance equation (4b), using therefore the specific field $\hat{\phi} \equiv \alpha\phi$ instead of the spatial density ϕ. Now $\mathbf{v}_{\hat{\phi}}$ is the velocity of a fluid particle relative to the observer moving with velocity $\mathbf{w}_{\hat{\phi}}$ on the surface $\hat{\phi}$ = constant. The relation equivalent to (11), and the second main equation of this article, is

$$\int_{\mathcal{L}_{\hat{\phi}}(\xi_1,\xi_2)} \rho\mathbf{v}_{\hat{\phi}} \cdot \mathbf{n}_{\hat{\phi}}\, dl(1) = -[|\nabla\hat{\phi}|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\xi]_{(\xi_1,\hat{\phi})}^{(\xi_2,\hat{\phi})} - \frac{\partial}{\partial\hat{\phi}}\int_{\mathcal{L}_{\hat{\phi}}(\xi_1,\xi_2)} \mathbf{h}_\phi \cdot \mathbf{n}_{\hat{\phi}}\, dl(1). \qquad (14)$$

The first term on the left-hand side is the transport of *mass* through the limited surface $\hat{\phi}$ = const. The terms on the right-hand side are the flux of $\mathbf{h}_\phi$ across the boundary of the limited $\hat{\phi}$-surface. In an analogous way to (11), relation (14) means that the mass transport across a limited $\hat{\phi}$-surface equals the flux of $\mathbf{h}_\phi$ across the $\hat{\phi}$-surface boundary. Note that, as long as the mass of a fluid body is conserved and there is no supply z_ϕ, relation (14) is exact. However, it is apparent that most applications of (14) require the density field be known. The difference between (11) and (14) is important for non-isochoric motions (div$\mathbf{u} \neq 0$), like compressible phenomena in the ocean or in atmospheric applications when spatial coordinates are used.

Relation (14) is different from the expression of mass conservation of the fluid particles on the ϕ-surface. This latter concept is instead given by (A6), applied to $\mathbf{w}_{\hat{\phi}}$, and means that the rate of change of the mass of the fluid in the $\hat{\phi}$-surface (which, in general, is not a material surface, and therefore is not formed by the same fluid particles at different times) equals the mass transport, across the ϕ-surface boundary, of the (mass-conserved) fluid. Both concepts are again related when the arbitrary volume is defined by a closed $\hat{\phi}$-surface (or a number of closed $\hat{\phi}_i$-surfaces) by

$$\frac{d_{\mathbf{w}_{\hat{\phi}}}}{dt}\int_{\mathcal{V}(\hat{\phi})} \rho\, dv \overset{\text{(A6)}}{=} -\oint_{\partial\mathcal{V}(\hat{\phi})} \rho \mathbf{v}_{\hat{\phi}} \cdot \mathbf{dS}(3) \overset{\text{(14)}}{=} \frac{\partial}{\partial\hat{\phi}} \oint_{\partial\mathcal{V}(\hat{\phi})} \mathbf{h}_\phi \cdot \mathbf{dS}(3), \qquad (15)$$

meaning that the rate of change of the mass in the volume enclosed by the $\hat{\phi}$-surface equals the flux of $\mathbf{h}_\phi$ across the $\hat{\phi}$-surface boundary.

When the flux field $\mathbf{h}_\phi$ and the ϕ-surface are of a full 3D nature the procedure given above must be generalized by the establishment of an orthogonal curvilinear coordinate system $(\nu^1, \nu^2, \nu^3) = [\xi(x, y, z), \eta(x, y, z), \phi(x, y, z)]$. Thus $J = |\nabla\xi|^{-1}|\nabla\eta|^{-1}|\nabla\phi|^{-1}$, $dl(1) = |\nabla\xi|^{-1}\, d\xi$, $dl(2) = |\nabla\eta|^{-1}\, d\eta$, $\mathbf{dS}(3) = J\nabla\phi\, d\xi\, d\eta = \mathbf{n}_\phi|\nabla\xi|^{-1}|\nabla\eta|^{-1}\, d\xi\, d\eta$; $Jh^1_\phi = |\nabla\phi|^{-1}|\nabla\eta|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\xi$, $Jh^2_\phi = |\nabla\phi|^{-1}|\nabla\xi|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\eta$, and $Jh^3_\phi = |\nabla\xi|^{-1}|\nabla\eta|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\phi$. For control surfaces limited by ξ- and η-coordinate lines, the generalization of (11) is

$$\int \mathbf{v} \cdot \mathbf{dS}(3) = -\left[\int |\nabla\phi|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\xi\, dl(2)\right]_{\xi_1}^{\xi_2} - \left[\int |\nabla\phi|^{-1}\mathbf{h}_\phi \cdot \mathbf{n}_\eta\, dl(1)\right]_{\eta_1}^{\eta_2} - \frac{\partial}{\partial\phi}\int \mathbf{h}_\phi \cdot \mathbf{n}_\phi\, dl(1)\, dl(2), \qquad (16)$$

meaning that the volume transport across a ϕ-surface limited by orthogonal coordinate surfaces $\xi = \xi_1$, $\xi = \xi_2$, $\eta = \eta_1$, and $\eta = \eta_2$, equals the flux of $\mathbf{h}_\phi$ across the ϕ-surface boundary (see Fig. 4). The interpretation of these terms is analogous to the 2D case. A relation equivalent to (16) but for the mass transport [analogous to (14)] may be also derived in a similar way.

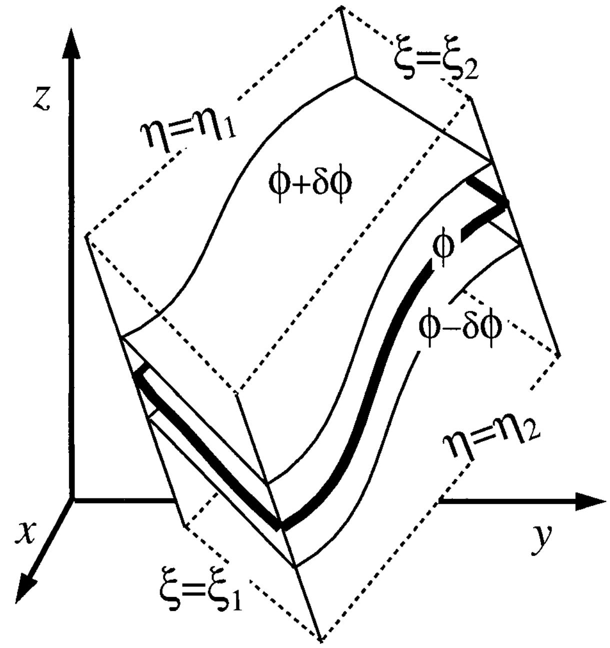

FIG. 4. Schematic showing a ϕ-surface limited by two ξ- and η-coordinate curves in the 3D space.

4. Summary

This work has introduced the general theory of the volume and mass conservation in terms of its transport across isosurfaces (open or closed) of an oceanographic quantity obeying a general balance law. In the volume conservation case the moving surface (neither material nor steady) is defined by a constant value of the spatial density ϕ and the general expressions obtained relate the volume transport across the ϕ-surface to the flux of $\mathbf{h}_\phi$ across the ϕ-surface *boundary*. In the more general case only mass conservation is assumed, the surface is defined by a constant value of the specific quantity $\hat{\phi} \equiv \alpha\phi$, and the expressions relate the mass transport across the $\hat{\phi}$-surface to the flux $\mathbf{h}_\phi$ across the $\hat{\phi}$-surface boundary. These relations [(11) and (14)], together with the 3D generalisation (16), are the main results of this work. These expressions differ in general from the expressions for the volume (or area) and mass conservation of the ϕ-surface, being however equivalent for closed (unlimited) ϕ-surfaces.

Some previous results have been derived as particular cases of the general theory, and have been clarified at the light of the present generalization and interpretation (appendix B). These previous results are not as complete as the main relations (11) or (14). For example, the flux of **h** across the two points (ξ_i, ϕ), $i = 1, 2$, in (11), seem never been simultaneously included in previous developments. The general expression (10), valid even when limits ξ_1 and ξ_2 *depend* on ϕ, the mass transport equation (14), and the 3D generalization (16), are, to the best of my knowledge, also new.

The development introduced here makes also clear that the selection of the fluid property obeying a balance law is independent of the underlying physical assumption of mass or volume conservation, and therefore any balance law can be employed. Thus, the role of the flux $\mathbf{h}_\phi$ in this theory is to modify the geometry (shape, gradients, and location) of the ϕ-surfaces, the final expressions being independent of the physical dimensions of the balanced quantity used. The final equations are independent of the constitutive equation chosen for the flux field $\mathbf{h}_\phi$, and the boundary conditions, being therefore a general development where many physical processes (as interior diffusion and mixing, balance of potential vorticity, balance of energy, etc.) can be considered.

APPENDIX A

Mathematical Preliminaries

This appendix introduces the mathematical tools for dealing with rates of change of integral expressions in arbitrary volumes, the general balance equations, and the relevant curvilinear coordinate transformation. Let the rate of change of a field A measured by an observer at point $(\mathbf{x}, t)$ having a velocity $\mathbf{c}(\mathbf{x}, t)$ be denoted by

$$d_\mathbf{c}A/dt \equiv A_{,t} + \mathbf{c}\cdot\nabla A, \tag{A1}$$

where ∇ is the 3D gradient operator, and $A_{,t}$ denotes the partial derivative of $A(\mathbf{x}, t)$ with respect to time. Let $\mathbf{u}$ be the fluid velocity field. For $\mathbf{c} = \mathbf{u}$ we simplify $d_\mathbf{u}A/dt = dA/dt = \dot{A}$. For managing balance equations in integral form in arbitrary control volumes (i.e., neither material nor steady) it is useful to employ the kinematic identity

$$\frac{d_\mathrm{w}}{dt}\int_\mathcal{V} f\,dv = \int_\mathcal{V}\left(\frac{d_\mathrm{w}f}{dt} + f\nabla\cdot\mathbf{w}\right)dv$$

$$= \int_\mathcal{V}[f_{,t} + \nabla\cdot(f\mathbf{w})]\,dv, \tag{A2}$$

[see Truesdell and Toupin (1960, section 81)]. The symbol d_w/dt indicates that the volume of integration $\mathcal{V}$ is material with respect to the velocity $\mathbf{w}$. The field $\mathbf{w}$ is the velocity of the points that form the arbitrary volume $\mathcal{V}$. The balance equation for $\mathcal{V}$ is obtained from (A2) for f = constant, $(d_\mathrm{w}/dt)(\int_\mathcal{V} dv) = \int_\mathcal{V}\nabla\cdot\mathbf{w}\,dv = \oint_{\partial\mathcal{V}}\mathbf{w}\cdot\mathbf{ds}$, and states that the volume change equals the compression or expansion of the volume boundary. A steady volume ($\mathbf{w} = \mathbf{0}$) is trivially conserved. The field $\mathbf{v} \equiv \mathbf{u} - \mathbf{w}$ is the velocity of a fluid particle relative to an observer having velocity $\mathbf{w}$, that is, the fluid velocity for a $\mathbf{w}$-observer. From (A1) follows that $d_\mathrm{w}f/dt = \dot{f} - \mathbf{v}\cdot\nabla f$, and therefore

$$\frac{d_\mathrm{w}}{dt}\int_\mathcal{V} f\,dv = \frac{d}{dt}\int_\mathcal{V} f\,dv - \oint_{\partial\mathcal{V}} f\mathbf{v}\cdot\mathbf{ds}, \tag{A3}$$

meaning that the rate of change of the extensive quantity with spatial density f in an arbitrary volume equals the rate of change of the extensive quantity in the *fluid* particles in the arbitrary volume minus the flux of $f\mathbf{v}$ (or transport of f) relative to the moving boundary $\partial\mathcal{V}$. The rate of change of volume in terms of $\mathbf{v}$ is obtained from (A3) for f = constant.

For an incompressible fluid, $\nabla\cdot\mathbf{u} = 0$, $\nabla\cdot\mathbf{w} = -\nabla\cdot\mathbf{v}$, thus $(d/dt)(\int_\mathcal{V} f\,dv) = \int_\mathcal{V}\dot{f}\,dv$, and therefore (A3) reads $(d_\mathrm{w}/dt)(\int_\mathcal{V} f\,dv) = \int_\mathcal{V}\dot{f}\,dv - \oint_{\partial\mathcal{V}} f\mathbf{v}\cdot\mathbf{ds}$; that is, the rate of change of f in an arbitrary volume is related to the change of f in the fluid particles inside the volume ($\dot{f}$) minus the the f-transport relative to the moving boundaries ($f\mathbf{v}$). For f = constant we have

$$\frac{d_\mathrm{w}}{dt}\int_\mathcal{V} dv = -\int_\mathcal{V}\nabla\cdot\mathbf{v}\,dv = -\oint_{\partial\mathcal{V}}\mathbf{v}\cdot\mathbf{ds}, \tag{A4}$$

which states that the rate of change of an arbitrary volume equals the (minus) volume transport (of an incompressible fluid) relative to the moving volume. For a material volume $\mathbf{w} = \mathbf{u}$, $\mathbf{v} = \mathbf{0}$, and therefore, for a incompressible fluid, (A4) states that the volume of a material element is conserved ($d\mathcal{V}/dt = \dot{\mathcal{V}} = 0$).

The *density of mass* ρ is defined by $\mathcal{M} = \int_\mathcal{B} dm = \int_\mathcal{V}\rho\,dv$, and mass conservation is

$$\frac{d\mathcal{M}}{dt} = \frac{d}{dt}\int_\mathcal{V}\rho\,dv = \int_\mathcal{V}(\dot{\rho} + \rho\nabla\cdot\mathbf{u})\,dv = 0,$$

$$\dot{\rho} + \rho\nabla\cdot\mathbf{u} = 0, \tag{A5}$$

in integral and local form, respectively. Using (A3) with $f = \rho$ the mass conservation in an arbitrary volume may be written as

$$\frac{d_\mathrm{w}}{dt}\int_\mathcal{V}\rho\,dv = -\oint_{\partial\mathcal{V}}\rho\mathbf{v}\cdot\mathbf{ds}, \tag{A6}$$

which states that the rate of change of mass in an arbitrary (changing) volume equals the (minus) mass transport across the volume boundary.

Next, we consider some extensive fluid property $\Phi = \int\phi\,dv$ having a *spatial volume density* $\phi = \phi(\mathbf{x}, t)$ obeying the general balance equation

$$\frac{d}{dt}\int_\mathcal{V}\phi\,dv + \int_{\partial\mathcal{V}}\mathbf{h}_\phi\cdot\mathbf{n}\,ds = \int_\mathcal{V} z_\phi\,dv. \tag{A7}$$

The field $\phi(\mathbf{x}, t)$ is the spatial volume density of the balanced quantity, $\mathbf{h}_\phi(\mathbf{x}, t)$ is the true flux vector, $z_\phi(\mathbf{x}, t)$ is the spatial volume density of the rate of supply of the balanced quantity, and $\mathbf{n}$ is a unit vector normal to the surface boundary. A balance equation expresses the time derivative of an extensive quantity contained in a volume in terms of its flux through the boundary and the external source of the quantity. With the concept of mass available ($\alpha \equiv \rho^{-1}$ is the specific volume) we introduce also the specific value $\hat{\phi} \equiv \alpha\phi$, that is, the amount of the quantity per unit mass. The local form of (A7) may therefore be written in the following equivalent ways:

$$\phi_{,t} + \nabla \cdot (\phi \mathbf{u} + \mathbf{h}_\phi) = z_\phi, \tag{A8a}$$

$$\dot{\phi} + \phi \nabla \cdot \mathbf{u} = -\nabla \cdot \mathbf{h}_\phi + z_\phi, \tag{A8b}$$

$$\rho \dot{\hat{\phi}} = -\nabla \cdot \mathbf{h}_\phi + z_\phi. \tag{A8c}$$

Given the mass conservation (A5), Eqs. (A8b) and (A8c), express the balance of the same quantity though using different fields (the spatial density and the specific value).

The previous results have been expressed in direct vector notation in order to show their coordinate-free nature. Now we assume that $|\nabla\phi| \neq 0$ (the ϕ-surfaces provide therefore a family of surfaces) and will consider this set of ϕ-surfaces as a new coordinate surface family. In order to do this we establish a one-to-one curvilinear transformation $\mathbf{R}(\nu^1, \nu^2, \nu^3)$: $(x, y, z) = [x(\nu^1, \nu^2, \nu^3), y(\nu^1, \nu^2, \nu^3), z(\nu^1, \nu^2, \nu^3)]$, which can be inverted $(\nu^1, \nu^2, \nu^3) = [\nu^1(x, y, z), \nu^2(x, y, z), \nu^3(x, y, z)]$. [This notation mimics that in D'haeseleer et al. (1991) but note that $\nu^3 = \phi$.] There are three families of coordinate surfaces (ν^i = constant, the other two ν^j, ν^k variable), and three families of coordinates curves produced when one coordinate ν^i is allowed to vary while the other two, ν^j and ν^k, are held fixed. Summation convection is implicit in repeated indices (i, j, k), except for caret (^) indices. Tangent-basis vectors (tangent to the ν^j coordinate surfaces) are $\mathbf{e}_i \equiv \partial\mathbf{R}/\partial\nu^i$, and unit tangent vectors $\hat{\mathbf{e}} \equiv |\mathbf{e}_{\hat{\imath}}|^{-1}\mathbf{e}_{\hat{\imath}}$, where $|\mathbf{e}_i|^{-1}$ is the scale factor. Reciprocal-basis vectors (perpendicular to the coordinate surfaces $\nu^i = c^i$) are $\mathbf{e}^i \equiv \nabla\nu^i$. The covariant and contravariant components of a vector $\mathbf{d}$ are defined by $d_i \equiv \mathbf{d} \cdot \mathbf{e}_i$ and $d^i \equiv \mathbf{d} \cdot \mathbf{e}^i$, respectively. The metric coefficients $g_{ij} \equiv \mathbf{e}_i \cdot \mathbf{e}_j$, and $g^{ij} \equiv \mathbf{e}^i \cdot \mathbf{e}^j$; $g \equiv \det[g_{ij}] = \det[g^{ij}]^{-1}$. The Jacobian of the coordinate transformation $J = J(\nu^1, \nu^2, \nu^3) \equiv \partial(x, y, z)/\partial(\nu^1, \nu^2, \nu^3) = \mathbf{e}_1 \cdot \mathbf{e}_2 \times \mathbf{e}_3 = (\mathbf{e}^1 \cdot \mathbf{e}^2 \times \mathbf{e}^3)^{-1} = g^{-1/2}$. The differential arc length along a coordinate curve ν^i is $dl(i) \equiv (g_{\hat{\imath}\hat{\imath}})^{1/2}\, d\nu^{\hat{\imath}} = J|\nabla\nu^j \times \nabla\nu^k|\, d\nu^i$ (i, j, k cyc 1, 2, 3). The differential element of area in the coordinate surface ν^i = constant is $dS(i) \equiv |\mathbf{e}_{\hat{\jmath}} \times \mathbf{e}_{\hat{k}}|\, d\nu^{\hat{\jmath}}\, d\nu^{\hat{k}} = J|\nabla\nu^i|\, d\nu^j\, d\nu^k$; and the differential area vector $\mathbf{dS}(i) = |\nabla\nu^{\hat{\imath}}|^{-1}\nabla\nu^{\hat{\imath}}\, dS(\hat{\imath}) = J\, d\nu^j\, d\nu^k \nabla\nu^i$.

APPENDIX B

Relation to Previous Developments

Walin (1982) derived his basic equation for the heat balance for a particular configuration of isotherms and heat fluxes. In order to present in general terms his procedure and relate it to the framework introduced here we start from the balance (4a), $\nabla \cdot \mathbf{u} = 0$, and assume that every ϕ-surface at a fixed time *t defines a volume* in such a way there is a one-to-one correspondence between ϕ and the volume $\tilde{\mathcal{V}}(\phi, t)$. Since $dv = J\, d\phi\, d\xi\, dy$, volume integration of (4a) and use of $\mathbf{dS}(3) = J\nabla\phi\, d\xi\, dy$ leads to $\iint \mathbf{v}_\phi \cdot \mathbf{dS}(3)\, d\phi = -\int \nabla \cdot \mathbf{h}_\phi\, dv$. Using the divergence theorem,

$$\iint \mathbf{v}_\phi \cdot \mathbf{dS}(3)\, d\phi = -\oint \mathbf{h}_\phi \cdot \mathbf{ds}. \tag{B1}$$

Differentiating with respect to ϕ (for a fixed time t), in the 2D space (x, z), we obtain

$$\int_{[\partial\mathcal{V}](\phi)} \mathbf{v}_\phi \cdot \mathbf{dS}(3) = -\frac{\partial}{\partial\phi}\oint_{[\partial\mathcal{V}](\phi)} \mathbf{h}_\phi \cdot \mathbf{ds}. \tag{B2}$$

The symbol $[\partial\mathcal{V}](\phi)$ denotes the boundary of $\mathcal{V}$ which, though assumed a function of ϕ, need not be a closed ϕ-surface. However, when the ϕ-surface is only a small part of the boundary of $\mathcal{V}$ this expression has redundant information in the term on the right-hand side, caused by the application of two (in part) inverse operations—namely, 3D volume integration and partial differentiation. Two-dimensional integration on the ϕ-surface leading to relation (11) is instead a more clear and direct approach, expressing in an explicit way the flux of $\mathbf{h}_\phi$ across the ϕ-surface boundary. Walin's (1982) main result is a particular case of relation (B2). He used the thermodynamic equation with $\dot{T} = -\nabla \cdot \mathbf{h}_T$ to obtain a relation between sea surface heat flow and volume transport across isotherms. The 2D control volume used in Walin's derivation consists in four surfaces ($\mathcal{S}_1, \ldots, \mathcal{S}_4$), two of them are isotherms (T_1 and T_3), one vertical deep surface $\mathcal{S}_4$, and one horizontal upper surface $\mathcal{S}_2$. It is assumed that the heat flux $\mathbf{h}_T(\mathcal{S}_4) = \mathbf{h}_T(\mathcal{S}_3) = \mathbf{0}$. Thus (B1) applied to the present case is

$$\iint_{T_3}^{T_1} \mathbf{v} \cdot \mathbf{dS}(3)\, dT' = -\oint \mathbf{h}_T \cdot \mathbf{ds}$$
$$= -(H_1 + H_2), \tag{B3}$$

where $H_n \equiv \int_{\mathcal{S}_n} \mathbf{h}_T \cdot \mathbf{ds}$ is the heat flux through surface $\mathcal{S}_n$. Denoting $G \equiv \int_{T=T_1} \mathbf{v}_T \cdot \mathbf{dS}(3)$, Walin's (1982) main eq. (2.7), $G = -[\partial H_1/\partial T]_{T_1} - [\partial H_2/\partial T]_{T_2}$, is derived in a simple way.

Garrett et al. (1995) and Garrett and Tandon (1997) deal with water mass formation and surface fluxes of volume and heat in terms of *mean* flow and averaged buoyancy. Buoyancy $b \equiv -g(\rho - \rho_o)/\rho_o$, where g is the acceleration due to gravity, and ρ_o is a constant reference density. It is assumed that the fluxes correspond to the averaged flow $\overline{\mathbf{u}}$. The decomposition used is $b = \overline{b} + b'$, $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$, with $\overline{b'} = 0$ and $\overline{\mathbf{u}'} = \mathbf{0}$. The averaged buoyancy balance is

$$\overline{b}_{,t} + \overline{\mathbf{u}} \cdot \nabla\overline{b} + \overline{b}\nabla \cdot \overline{\mathbf{u}} = -\nabla \cdot (\overline{b'\mathbf{u}'}).$$

A constitutive equation for $\nabla \cdot (\overline{b'\mathbf{u}'})$ of the form $\kappa_E\nabla \cdot (\nabla\overline{b}) = -\nabla \cdot (\overline{b'\mathbf{u}'})$, where κ_E is the buoyancy eddy diffusivity, is also introduced. We proceed for the averaged buoyancy $\overline{b}$ in a similar way to that used for ϕ and define the velocity of $\overline{b}$-surfaces $\mathbf{w}_{\overline{b}} = -\overline{b}_{,t}|\nabla\overline{b}|^{-1}\mathbf{n}_{\overline{b}}$, so $d_{\mathbf{w}_{\overline{b}}}\overline{b}/dt = 0$, and $\mathbf{v}_{\overline{b}} \equiv \overline{\mathbf{u}} - \mathbf{w}_{\overline{b}}$. Since the average operator and partial spatial derivatives are assumed to commute, incompressibility implies $\nabla \cdot \overline{\mathbf{u}} = 0$. Assuming that 1) the flux at the ocean surface ($h_s \equiv \mathbf{h}_{\overline{b}} \cdot \mathbf{n}_{\overline{b}}$) is given by sea surface heating and fresh water transport (evaporation minus precipitation), and 2) the flux in the ocean interior is given by the constitutive equation for $\nabla \cdot (\overline{b'\mathbf{u}'})$ above, so that $-\mathbf{n}_{\overline{b}} \cdot \overline{b'\mathbf{u}'} = \kappa_E\mathbf{n}_{\overline{b}} \cdot \nabla\overline{b} = \kappa_E\delta\overline{b}/\delta n_{\overline{b}}$, where $\delta(\ )/\delta n \equiv \mathbf{n} \cdot \nabla(\ )$ is the *directional* derivative in the direction of $\mathbf{n}$, and defining $A \equiv \int \mathbf{v}_{\overline{b}} \cdot \mathbf{n}_{\overline{b}}\ dl(1)$, and $D \equiv -\int \kappa_E\delta\overline{b}/\delta n_{\overline{b}}\ dl(1)$, we obtain, from (11), Garrett et al. (1995)'s main Eq. (1.3), $A = -|\nabla\overline{b}|_s^{-1}h_s - \partial D/\partial\overline{b}$, as a particular case of (11) and with no approximations regarding the control volume.

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