Mixing Pathways in Simple Box Models

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ABSTRACT: Tracer variance budgets can be used to estimate bulk mixing in a control volume. For example, simple, analytical, bulk formulations of salt mixing, defined here as the destruction of salinity variance, can be found for estuaries with a riverine source of freshwater and a two-layer exchange flow at the mouth using salinity as a representative tracer. For a steady case, the bulk salt mixing $M$ can be calculated as $M = Q_R S_{out}^2 + Q_m (S_{out} - S_{in})^2$, where $S_{in}$ and $S_{out}$ are the representative salinities in the estuarine exchange flow, and $Q_R$ and $Q_m$ are the river and landward volume fluxes, respectively. The bulk salt mixing $M$ can be considered as the sum of mixing pathways, where each pathway has a mixing of $Q(RS)^2$, where $Q$ is the volume transport and $RS$ is the salinity difference across the pathway. For the estuary case, one mixing path is associated with the river inflow, and the other is associated with the inflow of salty, oceanic water. This concept of linking mixing to input–output pathways is extended, in simple box models, from estuaries to scenarios with multiple inputs/outputs, as might be found in a complex estuarine/fjord network, in a region on a continental shelf, or any other control volume with multiple exchanges. This approach allows for the estimation of the relative contributions of each input–output pathway to the total mixing within a control volume.

KEYWORDS: Salinity; Coastal flows; Mixing

1. Introduction

Mixing can be defined as the destruction of variance. For microstructure variations in momentum, this is written as $\epsilon$, the rate of turbulent kinetic energy dissipation; for tracers it is written as $\chi$, the rate of tracer microstructure variance destruction. In both cases, the destruction of variance is an irreversible process. Currently, not even very high-resolution numerical ocean models that focus on estuarine and coastal ocean domains are able to resolve microstructure gradients, and the effect of small, subgrid-scale mixing on the relatively larger, resolved scales must be parameterized. However, the effect of mixing at the resolved scales may still be defined using the concept of variance destruction. That is, regardless of the scales at which tracer variance is actually destroyed, the reduction of tracer variance within a control volume defines the mixing within that volume.

The idea that tracer variance budgets can be used to investigate mixing within an estuary (Wang et al. 2017; MacCready et al. 2018; Burchard et al. 2019) or enclosed sea (Lorenz et al. 2020) was based on the idea that complex, time-dependent solutions could be analyzed in a way consistent with a box model. For estuaries, this means writing a salt balance in a way that is consistent with Knudsen’s relation (Knudsen 1900), taking into account all possible processes that contribute to the exchange flow by averaging in space and time the inflowing and outflowing transport across a set of salinity classes; in other words, a transport-weighted histogram of salinity across a defined cross section. This technique was first introduced by MacCready (2011) and is referred to as the total exchange flow (TEF).

MacCready et al. (2018) and Burchard et al. (2019) later derive that, for a steady case, the total mixing $M$ in an estuary can be approximated as

$$M = S_{in} S_{out} Q_R,$$

where $S_{in}$ and $S_{out}$ are the representative salinities of the inflow and outflow calculated through the TEF analysis framework, and $Q_R$ is the inflowing transport of freshwater from a river. The bulk mixing $M$ represents the average rate of destruction of salinity variance over the volume of the estuary. This simple approximation provides a direct link between the mixing and the estuarine exchange flow that was found to be a good estimate of the average total mixing within an estuary, even for more complicated, unsteady cases (Burchard 2020; Lorenz et al. 2021).

A different representation of estuarine mixing defined in Eq. (1) may be derived by applying volume and salt balances to get

$$M = Q_R S_{out}^2 + Q_m (S_{out} - S_{in})^2,$$

where $Q_m$ is the inflowing water from the ocean. This new equation provides another perspective on interpreting the mixing by considering $M$ as the sum of two mixing pathways: one mixing path is associated with the river inflow ($Q_R S_{out}^2$), the other is associated with the inflow of salty, oceanic water [$Q_m (S_{out} - S_{in})^2$], as shown in Fig. 1. Each pathway is corresponding to a component of the mixing $Q_i \Delta S_i^2$, where $Q_i$ is the volume flux associated with the pathway, and $\Delta S_i$ is the

1 The mixing pathway in this study refers to the mixing that a water mass experiences along its flow pathway.
The contribution of each mixing pathway is explicitly separated in the formula; the concept of dividing pathways is similar to the efflux/reflux theory of advective reaches in fjords and estuaries (Cokelet and Stewart 1985; MacCready et al. 2021).

This paper generalizes the concept of mixing pathways and presents a box model theory that allows for a simple interpretation of multiple inflows and outflows into a control volume, expanding on our understanding of the two-inflow, one-outflow case associated with estuarine mixing. The approach is to construct a series of idealized control volumes with increasing complexity to build understanding and intuition. Idealized river plume simulations are used to illustrate the application of the box model theory on a continental shelf. In general, the box model could be also applied to complex estuarine networks, fjords, bays, straits, and other basins with multiple inputs/outputs. Salinity is used as the representative tracer, building off previous work in estuaries, and acknowledging the importance of salinity in coastal flows. However, the approach is generic and could be applied to any tracer so long as the sources and sinks, if any, are well understood and represented.

2. Theory

a. Mixing in a steady tank with two inputs and one output

Consider a tank that is attached with two sources, each with a steady volume flux and constant salinity, and one sink with a distinct salinity, also constant, and with a constant volume flux equal to the sum of the inputs. Mixing in the tank is imposed such that the salinity within the tank transitions from the salinities of sources to the sink, and both the salinity transition and mixing within the tank are steady. For the salinity field within the tank to remain steady everywhere, the turbulent diffusion of salt due to mixing must exactly balance the salt advection:

\[ \mathbf{u} \cdot \nabla s = \nabla \cdot (\kappa \nabla s), \tag{3} \]

where \( \mathbf{u} \) is the 3D velocity vector, \( s \) is the salinity, and \( \kappa \) is the turbulent diffusion coefficient treated as a scalar here for simplicity. Assuming that there are no diffusive fluxes across the open boundaries, multiplication of Eq. (3) by \( s \) and integrating over the volume of the tank yields the budget for \( s \):

\[ \int \int_{A} \mathbf{u}^2 \, dA = -2 \int \int_{V} \kappa (\nabla s)^2 \, dV, \tag{4} \]

where \( V \) is the volume, and \( A \) is the boundary of the tank. The term \( s^2 \) is referred to as salinity variance in this study for brevity. Note that the salinity variance is not referenced to a mean salinity because the mixing does not depend on a reference salinity, only the turbulent diffusion coefficient and the salinity gradients. Equation (4) implies that, in a steady state, the net salinity variance advected into and out of the volume is destroyed by the mixing within the volume. Consequently, the mixing can be estimated as the net advection of salinity variance into the volume, i.e.,

\[ M = \int \int_{A} \mathbf{u}^2 \, dA. \]

Now, let us express \( \int \int_{A} \mathbf{u}^2 \, dA \) using a box model to quantify the total mixing. A schematic of the box model is shown in Fig. 2a, with the volume fluxes (\( Q \)) and salinities (\( S \)) identified with appropriate subscripts. Volume and salt conservation may be written as

\[ Q_{11} + Q_{12} + Q_o = 0, \quad \text{and} \quad S_{11}Q_{11} + S_{12}Q_{12} + S_oQ_o = 0. \tag{6} \]

The sign convention for the volume fluxes is that \( Q \) is positive when the transport is directed into the volume, such that \( Q_o \) is negative in this case. Generally, it is clear that \( Q_o \) must be larger in magnitude than both \( Q_{11} \) and \( Q_{12} \), and that \( S_o \) is bounded by \( S_{11} \) and \( S_{12} \). Furthermore, the salinity variance balance can be found by multiplying Eq. (6) by each of \( S_{11} \), \( S_{12} \), and \( S_o \), and adding the resulting equations, to get

\[ (S_{11} + S_{12} + S_o)(Q_{11}S_{11} + Q_{12}S_{12} + Q_oS_o) = 0. \tag{7} \]

The box model variables and the TEF variables are capitalized.
Applying Eqs. (5) and (6), the equation above can be rearranged to

\[ Q_i S_i + Q_o S_o = Q_i (S_o - S_i) + Q_o (S_o - S_i)^2. \]  

(8)

The terms on the left represent the net advection of \( s^2 \) into the volume, i.e., \(-\int_{A} u s^2 \, dA\), and therefore the terms on the right must be equal to the bulk mixing. Consequently, for a steady tank with two inputs and one output, the bulk mixing in the tank is

\[ M_{\text{in, out}} = Q_i (S_o - S_i) + Q_o (S_o - S_i)^2. \]  

(9)

This mixing formulation implies that the total mixing is the sum of the mixing that is associated with the individual flows in isolation, \( Q (\Delta S)^2 \), where \( \Delta S \) is the salinity difference between an input and an output. By this formulation, the mixing can be attributed to two pathways from the inputs to the output with each individual contribution quantified.

Though labeled slightly differently, the mixing tank could represent the basic structure for an estuary following Knudsen's relation (Knudsen 1900), with \( Q_i \) representing the river input \( Q_R \) and \( Q_o \) representing the landward exchange \( Q_{in} \) and the seaward exchange \( Q_{out} \) as well. The bulk mixing in an estuary can be attributed to two mixing pathways as schematized in Fig. 1b. One specific constraint for this estuary box model is that the river input is fresh, i.e., \( S_i = 0 \). With this constraint, Eq. (9) is equivalent to Eq. (2).

b. Mixing in a steady volume with multiple inputs and one output

Before a general case is explored, first examine a simple case—a mixing tank, again in a steady state, with three inputs and one output (Fig. 2b). The tank can be conceptually transformed into a chain of two 2-in/1-out tanks; \( Q_m \) and \( S_m \) represent the volume flux and salinity at the intermediate stage. Volume transport and salinities are noted with \( Q \) and \( S \) with appropriate subscripts.
where $Q_m$ and $S_m$ are the volume flux and salinity at the intermediate stage. Applying the mass and salt conservation of both the child tanks, we can eliminate $Q_m$ and $S_m$ in Eq. (10) and obtain the total mixing in the parent tank as

$$M_{\text{in, out}} = M_1 + M_2 = Q_1(S_o - S_{in})^2 + Q_2(S_o - S_{in})^2 + Q_3(S_o - S_{in})^2.$$  
(11)

The total mixing is the sum of three mixing pathways between the inputs and the output. For a tank with an arbitrary number of inputs but only one output, it can be generally transformed into a form of a chain of multiple child, 2-in/1-out tanks. The procedure above can be recursively conducted to get the total mixing in the parent tank. Consequently, in the case with $N$ inputs and 1 output, the mixing is

$$M_{\text{in, out}} = \sum_{m=1}^{N} Q_m (S_o - S_{in})^2,$$  
(12)

i.e., the sum of the $N$ mixing pathways, where $S_o$ is the transport weighted mean of the input salinities,

$$S_o = -\frac{1}{Q_o} \sum_{m=1}^{N} Q_m S_{in}.$$  
(13)

Note that the total mixing is identical regardless of how the chain of 2-in/1-out tanks is configured; the mixing in each individual tank will obviously be different, but the total mixing does not depend on the order in which the inputs are mixed.

This simple example also demonstrates the limits of a box modeling approach to examine mixing. If the complexity of a system is reduced by combining inputs, the mixing associated with the reduction in input variance is lost. Thus, the assumption that the inputs and outputs are uniform may cause errors in estimated mixing if the inputs and outputs are approximated as equivalent homogeneous tracer transports using methods like TEF.

c. Mixing in a steady volume with multiple inputs and outputs

Generally, for multiple inputs and outputs, each input/output pair defines a mixing pathway, and the total mixing is the sum of the contributions associated with the mixing pathways.

As an example shown in Fig. 2c, the scenario with two inputs and two outputs yields four pathways, and the effective volume flux along each pathway is the proportion of the associated input reaching the associated output, which is governed by the flux fractions $\alpha_{in, out}$ at the inputs. The flux fractions at each input sum to unity, the concept of which follows the efflux/reflux theory by Cokelet and Stewart (1985). The salinity of a water parcel flowing through the path changes from the input salinity $S_{in}$ at the start to the output salinity $S_{out}$ at the end due to the mixing along the pathway. According to sections 2a and 2b, the associated mixing can be expressed in the form of $Q(\Delta S)^2$ as

$$M_{\text{in, out}} = \alpha_{in, out} Q_m (S_{out} - S_{in})^2,$$  
(14)

where $Q_m$ is the volume flux of the input, and $\alpha_{in, out}$ is the fraction of $Q_m$ reaching the output of the pathway ($0 \leq \alpha_{in, out} \leq 1$), thus $\alpha_{in, out} Q_m$ is the volume flux through the indexed pathway.

To get the total mixing and the relative contributions of the mixing pathways, the flux fractions need to be determined. Consider a steady tank with $N_{in}$ inputs and $N_{out}$ outputs. The system has $N_{in} \times N_{out}$ mixing pathways and thereby the same number of flux fractions which are constrained by the following principles. First, at each input, the sum of the flux fractions should be equal to unity, i.e.,

$$\sum_{m=1}^{N_{in}} \alpha_{m, n} = 1,$$  
(15)

where $\alpha_{m, n}$ is the flux fraction of $m$th input to the $n$th output; this yields $N_{in}$ constraints. Second, at each output, the sum of the fractional volume fluxes from all the inputs should match the output flux, i.e.,

$$\sum_{m=1}^{N_{in}} \alpha_{m, n} Q_m = -Q_{out},$$  
(16)

where $Q_{in}$ and $Q_{out}$ are the volume fluxes of the $m$th input and the $n$th output, respectively, and $Q_{in}$ ($Q_{out}$) is positive (negative) according the sign convention; this yields $N_{out}$ constraints. Third, at the outputs of the system, the sum of the fractional salt fluxes from all the inputs should match the total salt flux at the outputs, i.e.,

$$\sum_{m=1}^{N_{in}} Q_m S_{in} = \sum_{n=1}^{N_{out}} \sum_{m=1}^{N_{in}} \alpha_{m, n} Q_m S_{in} = -\sum_{n=1}^{N_{out}} Q_{out} S_{out},$$  
(17)

where $S_{in}$ and $S_{out}$ are the salinity of the $m$th input and the $n$th output, respectively. Last, the total mixing of all the pathways, which is defined as destruction of salinity variance, should cancel the supply of salinity variance through the open boundaries, i.e.,

$$M = \sum_{m=1}^{N_{in}} \sum_{n=1}^{N_{out}} M_{m, n} \equiv \sum_{m=1}^{N_{in}} \sum_{n=1}^{N_{out}} \alpha_{m, n} Q_m (S_{out} - S_{in})^2$$

$$= \sum_{m=1}^{N_{in}} Q_m S_{in}^2 + \sum_{n=1}^{N_{out}} Q_{out} S_{out}^2.$$  
(18)

where $M_{m, n}$ is the mixing associated with a pathway that is expressed in Eq. (14).

Given the tank with $N_{in}$ inputs and $N_{out}$ outputs, Eqs. (15)–(18) yield $N_{in} + N_{out} + 2$ constraints, but only $N_{in} + N_{out}$ constraints are independent. The reason is, first, one of the equations of volume flux conservation [Eq. (16)] is redundant due to the global volume flux conservation; second, the equation of salt flux conservation [Eq. (17)] is automatically satisfied by the requirement that the specified salinities obey global
salt conservation. The global conservation of volume flux and salt flux are required because of the steady state assumption, which could be relaxed if extra storage terms are considered. Consequently, there are \( N_{in} + N_{out} \) linear equations and \( N_{in} \times N_{out} \) flux fractions to be determined. If \( N_{in} > 2 \) and \( N_{out} > 2 \), the numbers of variables will exceed the number of equations, leading to an underdetermined system.

In the cases where the system is underdetermined, instead of seeking a unique solution, the space of the physically possible solutions can be explored, and some optimal solutions can be sought by minimizing certain cost functions. We will show an example following this approach with three inputs and three outputs later in section 4. For now, here we discuss the scenario with \( N_{in} = 2 \) and \( N_{out} = 2 \) where the flux fractions can be analytically and uniquely determined. The corresponding schematic is shown in Fig. 2c. The system of linear equations to be solved is

\[
\begin{align*}
\alpha_{1,1} + \alpha_{1,2} &= 1 \\
\alpha_{2,1} + \alpha_{2,2} &= 1 \\
\alpha_{1,1}Q_{11} + \alpha_{1,2}Q_{12} &= -Q_{o1} \\
\alpha_{2,1}Q_{11} + \alpha_{2,2}Q_{12} &= -Q_{o2} \\
\alpha_{1,1}Q_{11}S_{11} + \alpha_{1,2}Q_{12}S_{12} + \alpha_{1,1}Q_{11}S_{21} + \alpha_{1,2}Q_{12}S_{22} &= -Q_{o1}S_{11} - Q_{o2}S_{22} \\
\alpha_{1,1}Q_{11}(S_{11} - S_{12})^2 + \alpha_{1,2}Q_{11}(S_{12} - S_{11})^2 + \alpha_{2,1}Q_{12}(S_{21} - S_{12})^2 + \alpha_{2,2}Q_{12}(S_{21} - S_{22})^2 &= Q_{11}^2S_{11} + Q_{12}^2S_{12} + Q_{o1}^2S_{o1} + Q_{o2}^2S_{o2}. \\
\end{align*}
\]

Again, one equation of volume flux conservation and the equation of global salt flux conservation are redundant and can be excluded. The fractions can be analytically determined:

\[
\begin{align*}
\alpha_{1,1} &= \frac{Q_{o1}S_{12} - S_{11}}{Q_{11}S_{11} - S_{12}} \\
\alpha_{1,2} &= \frac{Q_{o2}S_{12} - S_{12}}{Q_{12}S_{12} - S_{11}} \\
\alpha_{2,1} &= \frac{Q_{o1}S_{11} - S_{11}}{Q_{11}S_{12} - S_{11}} \\
\alpha_{2,2} &= \frac{Q_{o2}S_{11} - S_{12}}{Q_{12}S_{12} - S_{12}}. \\
\end{align*}
\]

Given the fractions, four mixing pathways are then determined based on Eq. (14):

\[
\begin{align*}
M_{1,1} &= \alpha_{1,1}Q_{11}(S_{11} - S_{12})^2 \\
M_{1,2} &= \alpha_{1,2}Q_{11}(S_{12} - S_{11})^2 \\
M_{2,1} &= \alpha_{2,1}Q_{12}(S_{11} - S_{12})^2 \\
M_{2,2} &= \alpha_{2,2}Q_{12}(S_{12} - S_{12})^2. \\
\end{align*}
\]

The total mixing in the tank is the sum of the four mixing pathways. For a physically meaningful solution, the values of \( S_{11} \) and \( S_{12} \) are bounded by \( S_1 \) and \( S_2 \) such that all the fractions are nonnegative and thereby all the mixing pathways are nonnegative. The following section will examine the box model using an idealized 3D river plume simulation that can be considered as a 2-in/2-out case, where we map the inputs and outputs of a control volume to a mixing tank with two inputs and two outputs.

Note that the box-model theory does not restrict salt fluxes to be partitioned as the volume fluxes (i.e., for each output, generally \( \sum_{m=1}^{N_{in}} \alpha_{m,ex}Q_{o,m}S_{o,m} \neq -Q_{o,m}S_{o,m} \)). This is because there may be some salt exchange among the pathways due to mixing. In particular, the relaxation of the salt-flux partition differentiates this theory from the efflux/reflux theory by Cokelet and Stewart (1985). The addition of the mixing constraint [Eq. (18)] is now relative to Cokelet and Stewart (1985). However, in the 2-in/2-out case, the flux fractions of the box-model theory [Eq. (20)] are identical to the ones of the efflux/reflux theory by Cokelet and Stewart (1985), and the salt fluxes are partitioned as the volume fluxes, i.e.,

\[
\begin{align*}
\alpha_{1,1}Q_{11}S_{11} + \alpha_{2,1}Q_{12}S_{12} &= -Q_{o1}^2S_{11} \\
\alpha_{1,2}Q_{11}S_{12} + \alpha_{2,2}Q_{12}S_{22} &= -Q_{o2}^2S_{o2}. \\
\end{align*}
\]
3. Results

A numerical simulation of an idealized river plume is used to examine the performance of the box model discussed in section 2. The resolved mixing in the simulation will be compared to the mixing predicted by the box model, and the mixing pathways will be quantified. The configuration of the simulation follows Qu and Hetland (2019) and is an implementation of the Regional Ocean Modeling System (ROMS; Shchepetkin and McWilliams 2005). The model domain consists of two components: a straight estuary and a uniformly sloping shelf. The estuary is 1 km wide and 22 km long with a constant depth of 10 m. The shelf is 103 km (across shelf) × 360 km (along shelf) with a constant slope of 10−2 and the depth at the coast being 10 m. The model is forced by oscillating winds and river flows (Fig. 3a). The river input (with the salinity of zero) sinusoidally varies between 0 and 1000 m3 s−1 at M2 frequency, mimicking a tidal estuary. The wind stress oscillates at the quarter of M2 frequency with no across-shelf component. The winds are downwelling with periodic intermission. There is no source/sink of salinity at the surface and bottom. The lateral open boundaries are set with zero elevation and constant salinity (32 g kg−1). MPDATA (multidimensional positive definite advection transport algorithm) is used for the tracer advection (Smolarkiewicz 2006). The k–ε turbulence closure scheme is used for the vertical mixing parameterization (Umlauf and Burchard 2003) and no explicit horizontal viscosity/diffusion is applied. The model is initialized at rest with constant salinity of 32 g kg−1 and integrated for 30 days. The model output is at hourly frequency and a combination of average and diagnostic files is used for subsequent analysis.

This idealized simulation also serves as a toy model illustrating the use of the box model. A 3D control volume is selected to construct a box model, which covers the near field, bulge, and part of the far field of the river plume (Fig. 3b). The control volume extends from the sea floor to the sea surface, such that the incoming and outgoing flows across the boundaries of the control volume are all lateral. The across-boundary velocities averaged over the simulation period are shown in Fig. 3c. At the western boundary, the input and output are the exchange flow at the estuary mouth. Qin represents the seaward exchange flow, and Qo1 represents the landward exchange flow. At the southern boundary, the river plume exits the control volume with an outgoing volume flux of Qo2, and the incoming flux is zero. At the eastern boundary, the net transport is onshore due to the Ekman transport by the downwelling winds, although the compensating flow near the bottom is offshore. The plume never reaches the eastern boundary, and therefore the salinity remains at 32 g kg−1. MacCready (2011) notes that inflow and outflow at the same salinity class is not considered to be exchange flow, and hence one sole input is considered at the eastern boundary.
boundary. At the northern boundary, the background salty water is blown into the control volume due to the southward winds, yielding an input, and the river plume never reaches the northern boundary so that the salinity remains at 32 g kg\(^{-1}\). Noting that the inputs at the eastern and northern boundaries are from the same water mass, i.e., the shelf water with the salinity of 32 g kg\(^{-1}\), they are combined to be one sole incoming flux, \(Q_{in}\). Overall, this control volume creates a box model with two inputs and two outputs, and the box model with the mixing pathways will inform the mixing occurring between the riverine water and the shelf water.

The TEF analysis is applied at each boundary of the control volume to get the volume transport and the transport-weighted salinities. The TEF procedure is conducted in three steps, which follows MacCready et al. (2018). The first step is to get the incoming and outgoing transport. At each boundary, the volume transport in each grid cell is binned into 250 salinity bins (that range from 0 to 35) according to the hourly salinity, and the volume transport in each salinity class (an hourly time series) is temporally averaged with a rolling window of four tidal periods of M\(_2\) (50 h). The fluctuations induced by the tides and winds are removed. The averaged transport of all the salinity classes is then grouped by the transport direction at each time and integrated to get the incoming and outgoing transport. The dividing salinity method is used to get the incoming and outgoing transport (Lorenz et al. 2019). The volume transport at each boundary is shown in Fig. 4a. The \(Q_{in}\) terms balance the \(Q_{out}\) terms when the system reaches a steady, periodic state. The second step is to get the incoming and outgoing salt fluxes at each boundary. The incoming (outgoing) fluxes are calculated by integrating the incoming (outgoing) volume transport times the corresponding salinity class. At the steady, periodic state, the incoming salt flux balances the outgoing salt flux (Fig. 4c). The last step is to get the transport-weighted salinities by dividing the salt fluxes by the corresponding volume transport. The transport-weighted salinities, \(S_{in}\) and \(S_{out}\), at the quasi-steady state are shown in Fig. 4b. This TEF procedure was tested with different numbers of salinity bins (250, 500, and 1000), and the TEF quantities are not sensitive to the number of salinity bins.

Given the TEF \(Q\) and \(S\) terms, the mixing pathways can be determined based on Eq. (21), and the total mixing in the control volume is equal to the sum of the mixing pathways. At the same time, the mixing resolved by the model can be quantified using the budget of \(s^2\):

\[
\frac{\partial s^2}{\partial t} = -\int_{A_h} u s^2 \, dA - 2 \int_V \kappa \frac{\partial s^2}{\partial z} \, dV
\]

where \(\kappa\) is the turbulent diffusion in the vertical direction, \(V\) is the control volume marked in Fig. 3b, and \(A_h\) and \(A_v\) are the lateral and vertical boundaries of the control volume, respectively. Each term in the budget is temporally averaged to remove the fluctuations induced by the tides and winds. The budget is shown in Fig. 5a. The storage term gradually vanishes, indicating that the system reaches a steady, periodic state.

Fig. 4. TEF analysis results from the simulation with one river. (a) TEF volume transport terms. (b) Transport-weighted TEF salinities. (c) TEF salinity fluxes. Gold arrows represent inflow terms, and blue arrows represent outflow terms. All the terms are calculated when the system reaches a steady, periodic state.
state. The numerical mixing is small due to the smooth nature of the simulation. The box-model mixing is in great agreement with the resolved mixing. The individual contribution of each pathway (schematized in Fig. 5) to the total mixing is quantified in the box model (Fig. 5c). The main mixing pathway \( (P_{1,2}) \) is from the estuary mouth to the southern boundary, contributing 91.5% of the total mixing. The physical interpretation is that the estuarine water introduced to the river plume mixes with the shelf water through wind-, tide-, shear-driven mixing processes, leading to the largest fraction of salinity variance destruction. The second largest mixing pathway is from the eastern/northern boundaries to the southern boundary \( (P_{2,2}) \), contributing 8.2% of the total mixing.

4. Discussion

For a tank with more than two inputs and two outputs, the system of linear equations to be solved for the flux fractions [i.e., Eqs. (15), (16), and (18)] is underdetermined. To get a solution, the space of physically possible solutions is first explored, and an optimization approach is applied by minimizing and maximizing the variance of mixing pathways. Here, we use a case with three inputs and three outputs to illustrate this approach. The river plume simulation is revisited with one more river added. The added river and estuary are located at \( y = -10 \) km (Fig. 6). The new river has the same input flux as the original river with the same amplitude and phasing. The only difference is the input salinity, 10 g kg\(^{-1}\) for the new river and 0 g kg\(^{-1}\) for the original. The simulation is run for 30 days with the same wind forcing to reach a steady, periodic state. The same control volume is used to create a

![Diagram showing mixing pathways and flux fractions](image-url)
box model with three inputs and three outputs. The exchange flows at the southern estuary mouth are the added pair of input and output, denoted as $Q_{i3}$ and $Q_{o3}$. The same procedure of TEF analysis is applied with the results shown in Fig. 6.

As illustrated in the schematic (Fig. 7), the box model consists of nine pathways and thereby nine flux fractions. First, we list the constraints for the flux fractions. As demonstrated in section 2c, there are eight equality constraints and nine inequality constraints of this system:

$$
\begin{align*}
\alpha_{1,1} + \alpha_{1,2} + \alpha_{1,3} &= 1 \\
\alpha_{2,1} + \alpha_{2,2} + \alpha_{2,3} &= 1 \\
\alpha_{3,1} + \alpha_{3,2} + \alpha_{3,3} &= 1 \\
\alpha_{3,1}Q_{11} + \alpha_{1,2}Q_{21} + \alpha_{3,1}Q_{31} &= -Q_{o1} \\
\alpha_{3,2}Q_{12} + \alpha_{1,2}Q_{22} + \alpha_{3,2}Q_{32} &= -Q_{o2} \\
\alpha_{3,3}Q_{13} + \alpha_{3,3}Q_{23} + \alpha_{3,3}Q_{33} &= -Q_{o3} \\
\sum_{m=1}^{3} \sum_{n=1}^{3} a_{m,n}Q_{i,m}S_{i,n} &= -\sum_{n=1}^{3} Q_{o,n}S_{o,n} \\
\sum_{m=1}^{3} \sum_{n=1}^{3} M_{m,n} &= \sum_{m=1}^{3} Q_{i,m}S_{i,m} + \sum_{n=1}^{3} Q_{o,n}S_{o,n} \\
0 \leq \alpha_{m,n} \leq 1, & m, n = 1, 2, 3
\end{align*}
$$

where $M_{m,n} = \alpha_{m,n}Q_{i,m}(S_{i,m} - S_{o,n})^2$ is the mixing along the pathway from the $m$th input to the $n$th output. One equation of volume flux conservation and the equation of salt flux conservation in Eq. (24) are redundant due to the global conservation of volume flux and salt flux and can be excluded. Second, the upper and lower limits of each flux fraction are explored by individually maximizing and minimizing the flux fraction under the constraints Eq. (24). The limits of all the fractions are shown in Table 1. The space of physically possible fractions is small with less than 3% of variations in each fraction. Third, the optimal fractions are sought by minimizing the variance of the mixing pathways, i.e.,

$$
\min \sum_{m=1}^{3} \sum_{n=1}^{3} M_{m,n}^2, \quad (25)
$$

which will tend to spread the mixing as evenly as possible across all pathways; and by maximizing the variance of the mixing pathways, i.e.,

$$
\max \sum_{m=1}^{3} \sum_{n=1}^{3} M_{m,n}^2, \quad (26)
$$

which will tend to put as much mixing as possible in one or a few major mixing pathways. The optimization employs the sequential least squares programming (Kraft 1988). To get around the local minima/maxima, we use Monte Carlo simulations to initialize the optimization with 10,000 sets of random $\alpha (0 < \alpha < 1)$ and get an approximate global minimum/maximum from the randomized simulations. The solutions of the minimization and maximization are shown in Fig. 7a.
As the two solutions are quite similar and describe the same qualitative mixing pathways (see Tables 1 and 2), we will only discuss the solution of the minimization. Here, 98.2% of the estuarine water of the northern river \((a_{1,2})\), 92.0% of the shelf water \((a_{2,2})\), and 100.0% of the estuarine water of the southern river \((a_{3,2})\) exit the domain through the southern boundary \((O_2)\). Of the shelf water, 8.0% \((a_{2,1} + a_{2,3})\) enters the estuaries \((O_1\) and \(O_3)\). With these optimal fractions, the individual contribution of each pathway to the total mixing can be quantified, which is shown in Fig. 7b (values in Table 2). The two leading pathways are the ones from the estuary mouths to the southern boundary \((P_{1,2} \text{ and } P_{3,2})\). The estuarine water mixes with the shelf water through various mixing processes, contributing most of the total mixing. The northern river contributes more than the southern river (51.0% versus 34.1%) due to its fresher input \((S_{i1} < S_{i3})\) and larger volume flux \((Q_{i1} > Q_{i3}; \text{ Fig. } 6)\). The third largest mixing pathway is from the eastern/northern boundaries to the southern boundary \((P_{2,3})\), contributing 13.7% of the total mixing. Other mixing pathways are negligibly small due to either small salinity contrast or small flux fractions.

5. Conclusions

The primary result of this study is a box model that links the total mixing in a control volume to the mixing pathways for multiple inputs and outputs. The amount of mixing a particular water mass experiences relative to the total mixing can be easily calculated. The total mixing is broken down into the pathway from every input to each output; each individual mixing pathway can be compared to the total. This new perspective on mixing allows us to better understand dominant sources of mixing. For example, in an estuary, Eq. (2) allows us to separate the contribution of mixing from the river input and oceanic input.

### Table 1. Flux fractions in the 3-in/3-out case under the constraints of Eq. (24).

<table>
<thead>
<tr>
<th></th>
<th>(a_{1,1})</th>
<th>(a_{1,2})</th>
<th>(a_{1,3})</th>
<th>(a_{2,1})</th>
<th>(a_{2,2})</th>
<th>(a_{2,3})</th>
<th>(a_{3,1})</th>
<th>(a_{3,2})</th>
<th>(a_{3,3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Individual (\alpha) minima</td>
<td>0.000%</td>
<td>98.187%</td>
<td>0.000%</td>
<td>4.649%</td>
<td>91.963%</td>
<td>3.173%</td>
<td>0.000%</td>
<td>97.409%</td>
<td>0.000%</td>
</tr>
<tr>
<td>Individual (\alpha) maxima</td>
<td>1.416%</td>
<td>100.000%</td>
<td>1.813%</td>
<td>4.649%</td>
<td>91.987%</td>
<td>3.364%</td>
<td>2.023%</td>
<td>100.000%</td>
<td>2.590%</td>
</tr>
<tr>
<td>Minimize (\sum_m \sum_n M_{mn}^2)</td>
<td>0.000%</td>
<td>98.187%</td>
<td>1.813%</td>
<td>4.649%</td>
<td>91.987%</td>
<td>3.364%</td>
<td>2.023%</td>
<td>97.977%</td>
<td>0.000%</td>
</tr>
<tr>
<td>Maximize (\sum_m \sum_n M_{mn}^2)</td>
<td>0.000%</td>
<td>100.000%</td>
<td>0.000%</td>
<td>4.649%</td>
<td>91.987%</td>
<td>3.364%</td>
<td>2.023%</td>
<td>97.977%</td>
<td>0.000%</td>
</tr>
</tbody>
</table>
Table 2. Mixing pathway fractions $P_{m,n} \equiv M_{m,n}/M$ in the 3-in/3-out case. The first row shows the mixing pathway fractions calculated using the optimal fractions in the second row of Table 1 that are obtained by minimizing the variance of mixing pathways. The second row shows the mixing pathway fractions calculated using the optimal fractions in the third row of Table 1 that are obtained by maximizing the variance of mixing pathways.

<table>
<thead>
<tr>
<th>$P_{1,1}$</th>
<th>$P_{1,2}$</th>
<th>$P_{1,3}$</th>
<th>$P_{2,1}$</th>
<th>$P_{2,2}$</th>
<th>$P_{2,3}$</th>
<th>$P_{3,1}$</th>
<th>$P_{3,2}$</th>
<th>$P_{3,3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000%</td>
<td>51.005%</td>
<td>1.177%</td>
<td>0.002%</td>
<td>13.703%</td>
<td>0.032%</td>
<td>0.000%</td>
<td>34.082%</td>
<td>0.000%</td>
</tr>
<tr>
<td>0.000%</td>
<td>51.923%</td>
<td>0.000%</td>
<td>0.002%</td>
<td>13.695%</td>
<td>0.033%</td>
<td>0.969%</td>
<td>33.377%</td>
<td>0.002%</td>
</tr>
</tbody>
</table>

This is split as $M = M_{\text{river}} + M_{\text{ocean}} = Q_R S_{\text{out}}^2 + Q_m (S_{\text{in}}^2 - S_{\text{out}}^2)$, then

$$
\frac{M_{\text{ocean}}}{M_{\text{river}}} = \left( \frac{S_{\text{in}}^2}{S_{\text{out}}^2} - 1 \right) = \left( - \frac{Q_{\text{out}}}{Q_{\text{in}}} - 1 \right) = \frac{Q_R}{Q_m}.
$$

(27)

So, the relative magnitude of bulk mixing can be estimated from either volume fluxes or salinity. As an example, consider a case with $S_{\text{in}} = 32$ g kg$^{-1}$ and $S_{\text{out}} = 28$ g kg$^{-1}$. The mixing associated with the freshwater input is 7 times greater. If $S_{\text{out}}$ is increased to 30, this ratio increases to 15 times greater. In general, the box model could be applied to complex networks of estuaries and fjords, in a region on a continental shelf, bays, straits, and other basins with multiple inputs/outputs.

The box model developed in this paper assumes that the mixing and input/output flow are all in a steady state. An appropriate averaging time scale where the integrated inputs and outputs can be considered as steady can be estimated by calculating the adjustment time. For simple estuary cases, the adjustment time scale has been shown to be proportional to the flushing time scale for estuaries ($T = V/Q_R$) divided by some $O(10)$ factor (Kranenburg 1986; Hetland and Geyer 2004; Rayson et al. 2015). Averaging over a spring–neap cycle has also been shown to be appropriate (Burchard et al. 2019). For the single source plume case described here, the adjustment time shown in Fig. 5 is about a week, allowing the solution to equilibrate over a number of adjustment periods and averaging over a periodic wind cycle was sufficient for approximating steady conditions.

For the 2-in/2-out case presented above there are two primary mixing pathways ($P_{1,2}$ and $P_{2,2}$ in Fig. 5c) where the estuary outflow and ambient water combine to form a single dominant outflow associated with the river plume leaving the control volume. In this case, the mixing in the plume mirrors mixing in an estuary, as the dominant mixing pathways mirror a 2-in/1-out configuration. Indeed, an accurate estimate of the mixing pathways—with calculated mixing pathway fractions within 1% of the complete calculation—can be derived just knowing the salinity and inflow/outflow at the boundaries. For the 3-in/3-out case presented above, the two river inputs are the dominant mixing pathways ($P_{1,2}$ and $P_{3,2}$ in Fig. 7b), with ambient water entrained into the outflowing plume being the third largest pathway ($P_{2,2}$ in Fig. 7b); other mixing pathways appear negligible. Thus, the dominant mixing pathways mirror a 3-in/1-out case, and this assumption results in mixing pathway fractions within 5% of the complete calculation. We expect many complicated mixing pathway networks, based on realistic ocean model applications, to simplify into a few dominant pathways that can be more easily interpreted, as is the case with the idealized examples shown here.

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Data availability statement. The data for both numerical simulations are available online at https://doi.org/10.5281/zenodo.6773581. All data needed to evaluate the conclusions in the paper are present in the paper. Additional data or code related to this paper may be requested from the authors.

REFERENCES


