
Derivation of a local diahaline Water Mass Transformation framework and application to the Baltic Sea

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Derivation of a local diahaline Water Mass Transformation framework and application to the Baltic Sea

ABSTRACT

In this dissertation, the theoretical Water Mass Transformation (WMT) framework has been extended to the formulation of a local WMT framework, that considers the water mass transformation in local water columns. In the classical WMT theory, a volume of water mass is defined by a bounding isoscalar surface of physical significance, e.g., an isopycnal or isohaline, and the mass or volume per unit time of seawater crossing this surface is then quantified. The classical framework does not contain any spatial information on the water mass transformation processes. This knowledge gap is filled by the extension to a local WMT framework, where the diasurface circulation is spatially decomposed for every water column. The presented theory includes the analytical derivation of relations between the classical WMT quantities and tracer variance decay.

The theoretical framework has been applied to the diahaline (across surfaces of constant salinity) fluxes of the Baltic Sea, such that maps of the diahaline fluxes and diahaline mixing could be produced from a two year simulation of the Baltic Sea. In this way hot spots of mixing and circulation could be visualized. These terms are connected through relations that were analytically derived as part of the extended theory. The analytically derived relations were verified and shown to hold in the two-year Baltic Sea simulation. One major result of this application was that around 50% of the diahaline circulation patterns were generated by spurious mixing from the truncation error of the advection scheme in the numerical model. Such a significant percentage was created despite the fact that an anti-diffusive advection scheme and vertically adaptive coordinates had been used, which are measures that reduce the spurious mixing.

Furthermore, a single-model ensemble simulation was developed for the Baltic Sea as part of this dissertation, and was combined with the local diahaline WMT framework, in order to enable a study of local and short-term dynamics up to daily temporal scales in salinity space. The diahaline dynamics in deep Baltic basins during the Major Baltic Inflow event of 2014/2015 could be investigated with this combined method. The analysis in salinity space clearly displayed two distinct inflow periods in the deep Gotland Basin.

Herleitung eines lokalen diahalinen Wassermassentransformationsansatzes und Anwendung auf der Ostsee

ZUSAMMENFASSUNG

In dieser Dissertation wurde der theoretische Ansatz der Wassermassentransformation (WMT) um die Formulierung eines lokalen WMT-Ansatzes erweitert, der die Wassermassentransformation in lokalen Wassersäulen berücksichtigt. In der klassischen WMT-Theorie wird ein Volumen der Wassermasse durch eine begrenzende isoskalige Fläche von physikalischer Bedeutung definiert, z. B. eine Isopykne oder Isohaline. Die Masse oder das Volumen des Meerwassers pro Zeiteinheit, das diese Fläche durchquert, wird dann quantifiziert. Der klassische Ansatz enthält keine räumlichen Informationen über die Wassermassentransformationsprozesse. Diese Wissenslücke wird durch die Erweiterung zu einem lokalen WMT-Ansatzes geschlossen, in dem die Diasurface-Zirkulation für jede Wassersäule räumlich zerlegt wird. Die vorgestellte Theorie beinhaltet die analytische Herleitung von Gleichungen zwischen den klassischen WMT-Größen und dem Zerfall der Tracer-Varianz.

Der theoretische Ansatz wurde auf die diahalinen Flüsse (über Oberflächen mit konstantem Salzgehalt) in der Ostsee angewandt, sodass Karten der diahalinen Flüsse und Durchmischung aus einer zweijährigen Simulation der Ostsee erstellt werden konnten. Auf diese Weise konnten Hot Spots der Durchmischung und Zirkulation sichtbar gemacht werden. Diese Terme sind durch Gleichungen miteinander verbunden, die als Teil der erweiterten Theorie analytisch hergeleitet wurden. Die analytisch hergeleiteten Gleichungen wurden in der zweijährigen Ostseesimulation verifiziert und haben sich als gültig erwiesen. Ein wesentliches Ergebnis dieser Anwendung war, dass etwa 50% der diahalinen Zirkulationsmuster durch numerische Vermischung aufgrund des Trunkierungsfehlers des Advektionsschemas im numerischen Modell erzeugt wurden. Ein solch signifikanter Prozentsatz entstand trotz der Tatsache, dass ein antidiffusives Advektionsschema und vertikal adaptive Koordinaten verwendet wurden, also Maßnahmen, die die unerwünschte Vermischung reduzieren.

Darüber hinaus wurde im Rahmen dieser Dissertation eine Einzelmodell-Ensemblesimulation für die Ostsee entwickelt und mit dem lokalen diahalinen WMT-Ansatz kombiniert, um eine Untersuchung der lokalen und kurzfristigen Dynamik bis hin zu täglichen Zeitskalen im Salinitätsraum zu ermöglichen. Mit dieser kombinierten Methode konnte die diahaline Dynamik in tiefen Ostseebecken während des Major Baltic Inflow-Ereignisses von 2014/2015 untersucht werden. Die Analyse im Salinitätsraum zeigte deutlich zwei unterschiedliche Einstromphasen im tiefen Gotland-Becken.

Dérivation d'un cadre de transformations diahalins de masses d'eau et application sur la mer Baltique

RÉSUMÉ

Dans cette thèse, le cadre théorique de la Transformation de la Masse d'Eau (TME) a été étendu à la formulation d'une approche TME qui prend en compte la TME dans des colonnes d'eau à une échelle locale. Dans la théorie TME classique, un volume de masse d'eau est défini par une surface isoscalaire délimitée ayant une signification physique, par exemple une isopycnales ou une isohaline, et la masse ou le volume par unité de temps de l'eau de mer traversant cette surface est alors quantifiée. Le cadre classique ne contient aucune information spatiale sur les processus de TME. Cette lacune est comblée par l'extension à un cadre TME local, où la circulation de diasurface est décomposée spatialement pour chaque colonne d'eau. La théorie présentée comprend la dérivation analytique des relations entre les quantités TME classiques et la décroissance de la variance du traceur.

Le cadre théorique a été appliqué aux flux diahalins (à travers des surfaces de salinité constante) de la mer Baltique, de sorte que des cartes des flux diahalins et du mélange diahalin ont pu être produites à partir d'une simulation de deux ans. De cette manière, les hot spots du mélange et de la circulation peuvent être visualisés. Ces termes sont reliés par des relations qui ont été dérivées analytiquement dans le cadre de la théorie étendue. Les relations dérivées analytiquement ont été vérifiées et se sont avérées valables dans la simulation de deux ans de la mer Baltique. L'un des principaux résultats de cette application a été qu'environ 50% des schémas de circulation diahaline ont été générés par des schémas de circulation diahaline qui étaient eux-mêmes générés par des mélanges parasites dus à l'erreur de troncature du schéma d'advection dans le modèle numérique. Un pourcentage aussi important a été obtenu malgré l'utilisation d'un schéma d'advection anti-diffusif et de coordonnées verticalement adaptatives, deux mesures permettant de réduire le mélange parasite.

En outre, une simulation d'ensemble à modèle unique a été développée pour la mer Baltique dans le cadre de cette thèse, et a été combinée avec le cadre TME diahalin local, afin de permettre une étude de la dynamique locale et jusqu'à des échelles temporelles quotidiennes dans l'espace de salinité. Cette méthode combinée a permis d'étudier la dynamique de la circulation diahaline dans les bassins profonds de la mer Baltique pendant l'épisode de l'afflux majeur d'eau de la mer du Nord dans la mer Baltique en 2014/2015. L'analyse dans l'espace de salinité a clairement mis en évidence deux périodes d'afflux distinctes dans le bassin profond de Gotland.

Derivation of a local diahaline Water Mass Transformation framework and application to the Baltic Sea

PLAIN LANGUAGE SUMMARY

The circulation in the Baltic Sea is governed by the mixing of water masses. In this dissertation, a theoretical framework is applied, which replaces depth with salinity. Salinity is an appropriate choice, since it is descriptive of the circulating water masses in the Baltic Sea. The circulation is then described from a point of view, where the flow crosses areas of constant salinity. This is called the diahaline circulation. The framework breaks down the circulation into smaller chunks, and gives information on how the circulating flow depends on mixing. An application of this theory in a two-year long simulation of the Baltic Sea is demonstrated.

Moreover, the framework is combined with a, so called, single-model ensemble simulation with up to 26 ensemble members. Each member can be regarded as giving a slightly different picture of the Baltic Sea circulation. Studying all the different members therefore describes the variability of the dynamics within one and the same computer model. The combination of the theory with the ensemble makes it possible to study the local diahaline dynamics up to daily temporal scales, as opposed to the two year average, which was used before.

Herleitung eines lokalen diahalinen Wassermassentransformationsansatzes und Anwendung auf der Ostsee

ZUSAMMENFASSUNG IN EINFACHER SPRACHE

Die Zirkulation in der Ostsee wird durch die Vermischung der Wassermassen bestimmt. In dieser Dissertation wird ein theoretischer Ansatz angewandt, in dem die Tiefe durch den Salzgehalt ersetzt wird. Der Salzgehalt ist eine geeignete Wahl, da er die zirkulierenden Wassermassen in der Ostsee beschreibt. Die Zirkulation wird dann von einem Standpunkt aus beschrieben, an dem die Strömung Flächen mit konstantem Salzgehalt durchquert. Dies wird als diahaline Zirkulation bezeichnet. Die Theorie zerlegt die Zirkulation in kleinere Teile und gibt Aufschluss darüber, wie die zirkulierende Strömung von der Durchmischung abhängt. Eine Anwendung dieser Theorie in einer zweijährigen Simulation der Ostsee wird demonstriert.

Außerdem wird die Theorie mit einer so genannten Einzelmodell-Ensemblesimulation mit bis zu 26 Ensemblemitgliedern kombiniert. Jedes Mitglied kann als ein leicht verändertes Bild der Ostseezirkulation betrachtet werden. Die Untersuchung aller verschiedenen Mitglieder beschreibt daher die Variabilität der Dynamik innerhalb ein und desselben Computermodells. Die Kombination der Theorie mit dem Ensemble macht es möglich, die lokale diahaline Dynamik bis hin zu täglichen Zeitskalen zu untersuchen, im Gegensatz zum zweijährigen Durchschnitt, der zuvor verwendet wurde.

Dérivation d'un cadre de transformations diahalins de masses d'eau et application sur la mer Baltique

RÉSUMÉ EN LANGUAGE SIMPLE

La circulation dans la mer Baltique est régie par le mélange des masses d'eau. Dans cette thèse, un cadre théorique est appliqué qui remplace la profondeur par la salinité. La salinité est un choix approprié car elle décrit les masses d'eau circulant dans la mer Baltique. La circulation est ensuite décrite d'un point de vue où le flux traverse des surfaces de salinité constante. C'est ce qu'on appelle la circulation diahaline. L'approche suivie ici décompose la circulation en éléments plus petits et fournit des informations sur la manière dont le flux circulant dépend du mélange des masses d'eau. Une application de cette théorie dans une simulation de deux ans de la circulation de la mer Baltique est démontrée.

En outre, cette approche est combinée avec une simulation d'ensemble à modèle unique comprenant jusqu'à 26 membres. Chaque membre peut être considéré comme donnant une image légèrement différente de la circulation de la mer Baltique. L'étude de tous les membres différents décrit donc la variabilité de la dynamique au sein d'un seul et même modèle océanique. La combinaison de la théorie et de l'ensemble permet d'étudier la dynamique diahaline jusqu'à des échelles temporelles journalières, contrairement à la moyenne sur deux ans utilisée auparavant.

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Publications

PUBLICATIONS FOR THE CUMULATIVE DISSERTATION

Klingbeil, K., and **E. Henell** (2023).

A Rigorous Derivation of the Water Mass Transformation Framework, the Relation between Mixing and Diasurface Exchange Flow, and Links to Recent Theories in Estuarine Research.

Journal of Physical Oceanography, 53, 2953–2968, <https://doi.org/10.1175/JPO-D-23-0130.1>.

Henell, E., Burchard, H., Gräwe, U., and Klingbeil, K. (2023).

Spatial composition of the diahaline overturning circulation in a fjord-type, non-tidal estuarine system.

Journal of Geophysical Research: Oceans, 128, e2023JC019862. <https://doi.org/10.1029/2023JC019862>

Henell, E., Burchard, H., Gräwe, U., Holtermann, P., Umlauf, L., Naumann, M. and Klingbeil, K. (submitted).

Exploring the variability of a non-tidal marginal sea with a single- model ensemble

Ocean Modelling

Conferences

Warnemünde Turbulence Days (WTD),

Warnemünde (Germany), September 2023, **talk**

Application of a local diahaline Water Mass Transformation framework to the Baltic Sea

Virtual European Physical Oceanography and Shelf Sea Seminar Series (VEPOSSSS),

Menai Bridge (Wales, UK), September 2023, **talk**

Applying a local diahaline Water Mass Transformation framework to a fjord-type, non-tidal estuarine system to investigate diahaline mixing and exchange flow

International Union of Geodesy and Geophysics General Assembly (IUGG),

Berlin (Germany), July 2023, **talk**

How local diahaline mixing drives the overturning circulation in the Baltic Sea

Gordon Research Conference Coastal Ocean Dynamics (GRC),

Smithfield (Rhode Island, USA), June 2023, **poster**

Spatial Composition of the Diahaline Overturning Circulation in a Fjord-Type, Non-Tidal Estuarine System

European Geophysical Union General Assembly (EGU),

Vienna (Austria), May 2022, **talk**

Analyzing Diahaline Exchange and Mixing in the Baltic Sea

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1

Introduction

Oceans cover about 71% of the Earth's surface ([Pidwirny, 2006](#)). While most of us live along or close to its shores, and depend on the ocean, not many of us would reflect on what is happening beneath its surface. Yet, so many important dynamical processes are taking place incessantly. For instance, those of us living in northwestern Europe are directly impacted by the effects of the ocean through the Gulf Stream, or the Atlantic Meridional Overturning Circulation (AMOC), as oceanographers call the circulation cell, that it is a branch of. Water masses circulate and mix with each other. Understanding AMOC, in particular, and how it might change under the stresses of climate change is important. A part of this puzzle is to quantify the circulation and mixing. This dissertation will show you how this can be done – on the example of the Baltic Sea to start with.

For the Baltic Sea, the circulation and mixing is described in this work from a theoretical point of view, or framework, where depth is replaced by salinity. This works for the Baltic Sea, since its dynamics are governed by the salinity differences. This is not the case for the World Ocean, however. To be able to study AMOC with this framework, one needs to use density instead of salinity, but that would be beyond the scope of this work.

Here, the attention is thus directed to salinity as a first step in completing the puzzle.

1.1 STRUCTURE OF THE THESIS

The introduction presents the theoretical Water Mass Transformation framework from a general point of view, and specifies how it is adapted to the Baltic Sea as study area. Section 1.3 introduces the concept of mixing and how this quantity can be described theoretically. The important quantities of diahaline velocity $u_{\text{dia},z}$ and diahaline diffusive salt flux $j_{\text{dia},z}$ are presented in the subsequent sections

(Sections 1.4 and 1.5). The last part of the introduction is dedicated to the Baltic Sea, as well as the numerical model that has been used to carry out the different simulations for this thesis. The results chapter (Chapter 2) summarizes the key results from the three papers that constitute this cumulative thesis. In the first section (Section 2.1), a simplified version of the theory underlying the thesis is presented, which was published in Klingbeil & Henell (2023) and can be found in Appendix B. Next (Section 2.2), the theory was applied in a numerical model study of the Baltic Sea, where a temporal average over two years was taken (Henell et al., 2023). And lastly (Section 2.3), short-term and local physical processes were studied in the Baltic Sea, again applying the theory, but now combined with single-model ensemble simulations (Henell et al., 2025). Chapter 3 finishes with the main conclusions that are drawn from the work of this thesis, and gives an outlook on future work.

1.2 THE WATER MASS TRANSFORMATION (WMT) FRAMEWORK

When trying to understand the ocean circulation, oceanographers face the problem of a lack of sufficient direct in-situ measurements. To bypass this challenge, the Water Mass Transformation (WMT) framework serves as a complimentary indirect means of investigating the circulation. A short definition of WMT is given in Groeskamp et al. (2019) as "the mass transport of seawater through a surface with a constant property value". WMT also compliments the Eulerian and Lagrangian description of the flow. In the Eulerian perspective, a point in space is focused on, and the properties of the fluid element passing through the point is recorded. However, in the Lagrangian description, a fluid particle is followed as it moves through the flow. WMT describes a water mass using a tracer, such as, e.g., temperature, salinity, buoyancy, among others. The idea for a WMT framework was originally developed by Walin (1977) using salinity as a tracer, and applying the framework to the Baltic Sea. In Walin (1982) he went on to focus on the sea surface heat flow and thermal circulation. In Walin (1977), the volume is bounded by an isohaline surface, such that all water within a semi enclosed basin with salinities larger than salinity S is considered (Fig. 1.1a). Integral budget equations for this volume $\mathbb{V}_{>}(S)$ and its salt content $\mathbb{S}_{>}(S)$ (not shown in Fig. 1.1a) were presented as follows:

$$\frac{\partial \mathbb{V}_{>}(S)}{\partial t} - Q_{>}(S) - Q_{\text{dia}}(S) = 0, \quad (1.1a)$$

$$\frac{\partial \mathbb{S}_{>}(S)}{\partial t} - \mathcal{F}_{>}(S) - \mathcal{F}_{\text{dia}}(S) = 0, \quad (1.1b)$$

where $Q_{>}(S)$ and $\mathcal{F}_{>}(S)$ are, respectively, the integrated volume and salt fluxes entering across the open ocean boundary with salinities larger than S . $Q_{\text{dia}}(S)$ and $\mathcal{F}_{\text{dia}}(S)$ are, respectively, the integrated diahaline volume and salt flux entering across the isohaline. The diahaline salt flux consists of its contributions from advection (former) and diffusion (latter):

$$\mathcal{F}_{\text{dia}}(S) = SQ_{\text{dia}}(S) + \mathcal{J}_{\text{dia}}(S). \quad (1.2)$$

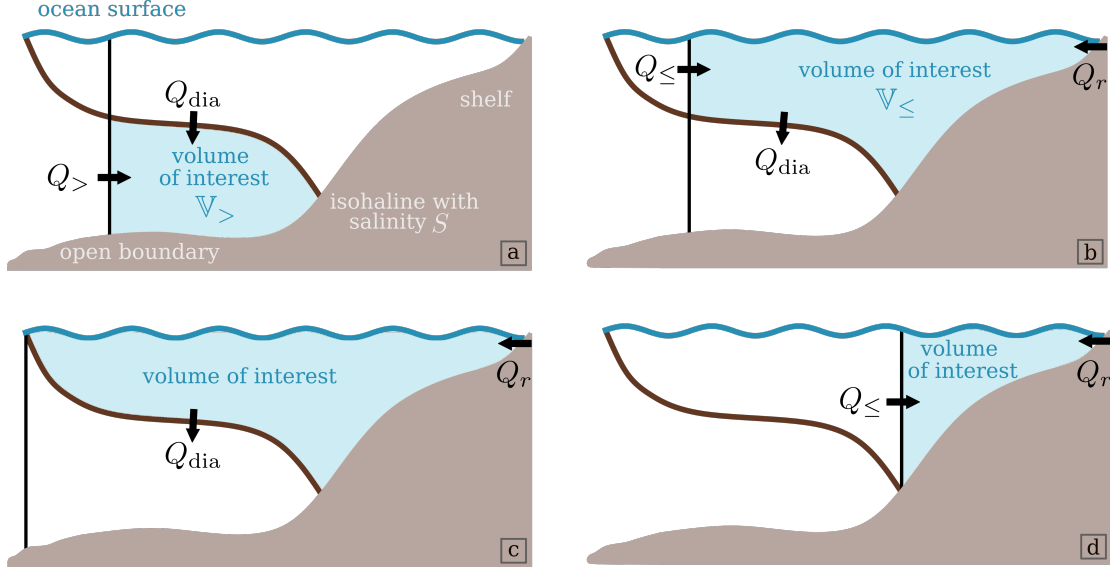


Figure 1.1: Idealized illustration of control volumes bounded by an isohaline with salinity S and a boundary transect toward the open ocean. For simplicity, I assume a stably stratified salinity distribution. (a) The volume $V_>$ contains water with salinities larger than S , and is located below the isohaline. This case was originally presented by Walin (1977). The integrated diahaline volume flux Q_{dia} is a measure for the water mass transformation. Integrated open boundary volume fluxes are depicted as $Q_>$. The arrows indicate the direction of positive fluxes. (b) The remaining volume $V_≤$ contains water with salinities less or equal to S , and is situated above the isohaline. In this case, $Q_≤$ is the open boundary flux, and, additionally, the integrated freshwater river discharge Q_r has to be included. I have chosen to focus on this case in Section 2.1. (c,d) These two cases are a special case of (b), where in (c) the volume is completely bounded by an isohaline, and in (d) the open boundary instead bounds the volume. Therefore, the open boundary flux $Q_≤$ is zero in (c), and the diahaline volume flux Q_{dia} is zero in (d).

Furthermore, Walin (1977) demonstrated that the integrated diahaline volume flux is determined by the integrated diahaline diffusive salt flux as follows:

$$Q_{\text{dia}}(S) = -\frac{\partial \mathcal{J}_{\text{dia}}(S)}{\partial S}, \quad (1.3)$$

under the assumption that there is no diffusive salt flux across the open ocean boundary. MacCready et al. (2002) built upon Walin's theory, focusing on classical estuaries. They neglected surface boundary fluxes, but included the freshwater river discharge Q_r . Moreover, they consider the water masses with salinities smaller than S (Fig. 1.1b), thus yielding the integrated volume $V_≤(S)$ and salt content

$\mathbb{S}_{\leq}(S)$ (not shown in Fig. 1.1b) budget equations:

$$\frac{\partial \mathbb{V}_{\leq}(S)}{\partial t} - Q_{\leq}(S) + Q_{\text{dia}}(S) = Q_r \quad (1.4a)$$

$$\frac{\partial \mathbb{S}_{\leq}(S)}{\partial t} - \mathcal{F}_{\leq}(S) + \mathcal{F}_{\text{dia}}(S) = 0. \quad (1.4b)$$

Note, that there is no salt discharge from the river, as the salinity is considered to be zero. [MacCready & Geyer \(2001\)](#) and [Hetland \(2005\)](#) investigated the special case, where the estuarine volume is completely bounded by an isohaline (Fig. 1.1c), that is, where there are no fluxes across the open boundary ($Q_{\leq} = \mathcal{F}_{\leq} = 0$). The opposite case, of the open boundary restricting the estuarine volume (Fig. 1.1d), was studied by [MacCready \(2011\)](#) and [Burchard et al. \(2019\)](#), among others. In this case, the diahaline fluxes would be zero.

As has been seen, water masses are considered as volumes in the general WMT framework. This is very useful, but does not contain detailed information on the location of the water masses in physical space. The framework can be extended to consider the water mass inside each single water column of the studied volume. This extension is carried out in [Klingbeil & Henell \(2023\)](#), and is presented at a later point in Section 2.1, since the theory is part of the work carried out for this cumulative thesis. This step fills a very important knowledge gap in understanding the movement and location of water masses, and thereby the ocean circulation at large. As will be seen in the following chapters, the new theory also makes it possible to visualize hot spots for mixing. Moreover, the spurious overturning circulation can be demonstrated, which is a part of the circulation produced solely by the numerical model. For the purposes of climate projection this is a key step: knowing to what extent the simulated circulation is close to the actual, real circulation, and how much the numerical model itself adds to the circulation.

1.2.1 SALINITY CLASSES

In the introduction to the WMT framework, the sights were set on the use of salinity as tracer, and working in the so called "salinity space". The principal idea is that you start from the original depth (z -) axis, and map the quantities of interest onto the salinity axis. This process is also known as sorting or binning into salinity classes. This sorting is an essential first step to work in an isohaline framework, where salinity describes the dynamics. The process can be described using, e.g., the zonal velocity variable u . This is visualized in Fig. 1.2, where an analogy for the salinity classes or salinity bins is shown in the shape of cupboard drawers. The smaller the bins are, the higher the resolution of the variable is after the binning procedure. The higher the number of entries in each bin, the smoother the result is after binning. The example here was shown for the velocity, but the same can be done for other variables, such as the volume.

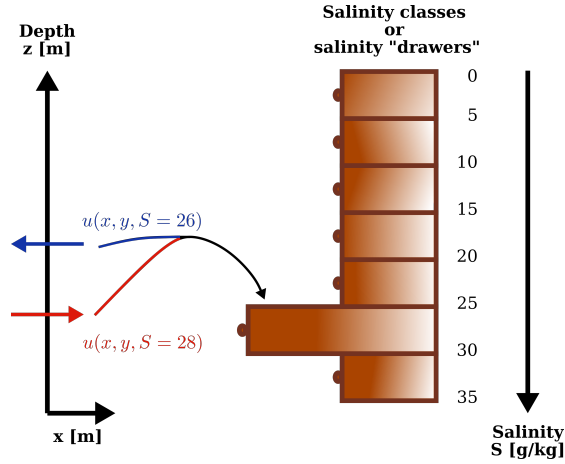


Figure 1.2: Sketch visualizing the mapping to salinity space, or sorting into salinity classes, from depth space. The cupboard of drawers is used as a visual help of how one can imagine the sorting process. In the example displayed here, velocity at two different depths and with two different salinities – 26 and 28 g/kg – are shown to be binned into the same salinity class ranging from 25 to 30 g/kg.

1.3 DEFINING MIXING

Within the context of this work, the interest lies in the mixing of water masses. The circulation of water masses and their mixing are highly connected. Which one leads or drives which has been subject to discussion for long (Burchard et al., 2024).

In order to combine different water masses, the processes of (i) stirring and (ii) mixing are involved. Stirring is the stretching of the bulk fluid, whereas mixing is the exchange of materials on the molecular level due to diffusion. Very little exchange between two neighboring fluids is enabled by molecular motions of molecules. Two different water masses can move along together without mixing properties. Eventually, though, the two fluids would mix through molecular diffusion, but this would happen on a very long time scale. However, turbulent stirring would stretch the two water masses and thereby increase the area of contact between them. This stretching, induced by the stirring, enables the mixing to occur on much shorter time scales, since the molecular diffusion randomly exchanges molecules over a larger area. It is important to note that stirring without diffusion is not the same as mixing, and can be reversed. Mixing, on the other hand, is irreversible. An intuitive view of stirring versus mixing is shown in Welander (1955) and in his Fig. 3, which is displayed here in Fig. 1.3. The small dye patch in Fig. 1.3a is stirred and starts extending. Mixing occurs along the dye boundary, which extends and elongates with time, as seen here in the evolution from Fig. 1.3a to g. At the same time, molecular processes act on the boundary to limit the extension.

MacCready et al. (2018) give an overview of different ways of studying mixing. They state that the most common way of describing mixing is in terms of eddy viscosity or diffusivity κ , both in the ocean (Polzin et al., 1997, Wunsch & Ferrari, 2004), as well as in estuaries (Fischer, 1976, Basdurak

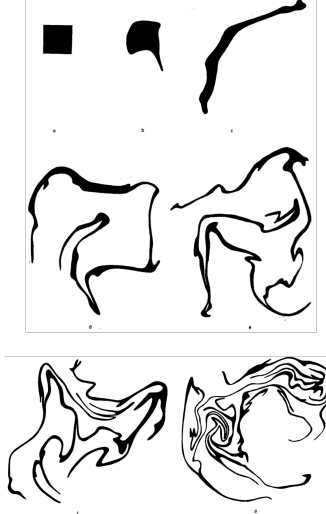


Figure 1.3: Sketch by [Welander \(1955\)](#) to indicate the difference between stirring and mixing. The dye patch shown in the sketch is stirred and starts to extend. The dye boundary also extends and elongates with time. The mixing takes place across this boundary.

[et al., 2017](#)). This measure of mixing is not suitable for all parts of estuaries, such as the Baltic Sea studied here. This is because of the well-mixed nature of many estuaries, where salinity has already been fully mixed. Therefore, salinity mixing vanishes, whereas the eddy diffusivity remains high. Furthermore, mixing can be treated in terms of the vertical component of Reynolds-averaged turbulent salt flux and the buoyancy flux in budgets of potential energy or available potential energy. However, the representation of mixing as the dissipation of salinity variance χ (also called salinity variance decay) is, according to [MacCready et al. \(2018\)](#), "recognized by the ocean turbulence community as one of the most important quantities representing mixing in the ocean" ([Nash & Moum, 2002](#), [Oakey, 1982](#)). This is also the definition that is used in this dissertation. More information on how χ is computed can be found in Chapter 1.3.1.

Mixing defined as salinity variance decay χ is visualized in Fig. 1.4a with a simple example of how the variance changes before and after mixing. The variance is found to decrease after mixing has taken place, hence encouraging the use of variance *decay* as a measure for mixing. The second view in Fig. 1.4b visualizes a peak of tracer concentration and how the tracer gradient is smoothed out, that is, flattened, when mixing is taking place. The contrary to mixing, which we denote as *demixing*, would result in a steepening of the tracer gradient. The volume-integrated and time-averaged salinity mixing within an estuarine volume is then defined as:

$$\mathbb{M} = \left\langle \int_V \chi dV \right\rangle, \quad (1.5)$$

where χ is the salinity mixing per unit volume, V the time-varying estuarine volume bounded by the

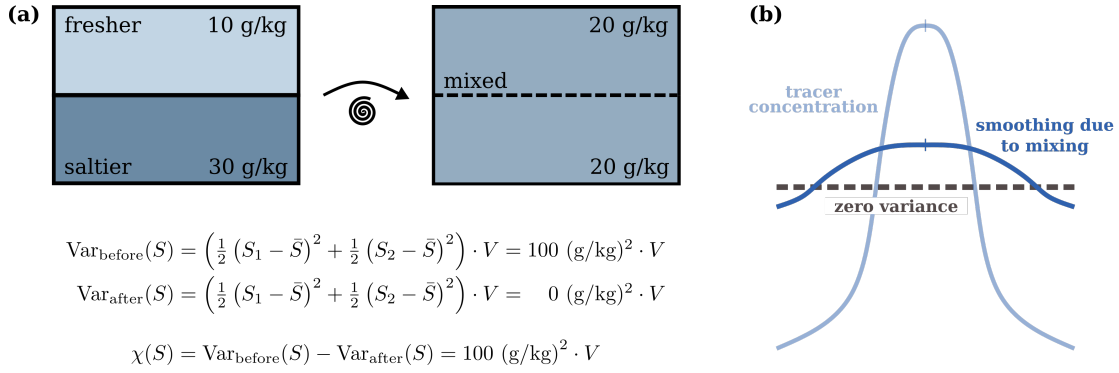


Figure 1.4: Sketches showing two ways of visualizing estuarine mixing defined as salinity variance dissipation χ . (a) Visualization of mixing defined as variance decay in terms of a simple box model. A box before mixing has two layers, where the upper layer contains fresher and the lower saltier water. After the mixing has taken place, the same salinity is present everywhere in the box, in both layers. This process of mixing can be computed using the mathematical definition of variance as $\text{Var}(X) = \frac{1}{n} \sum_{i=1}^n (x_i - \mu)^2$, where $\mu = \frac{1}{n} \sum_{i=1}^n x_i$. Applying this to the example at hand, yields a χ of 100 (g/kg)^2 times the volume of the box. (b) Mixing is shown in terms of the change in tracer concentration. A peak in tracer concentration will be smoothed out and reduced due to mixing. The tracer gradient is therefore reduced. Spurious numerical mixing can have the opposite effect, however, and sharpen the tracer gradient. This is called "demixing" here.

transect and the angular brackets denote the time-averaging.

1.3.1 ADVECTION-DIFFUSION EQUATION

The mathematical starting point for the quantification of mixing, defined as salinity variance decay χ , is the advection-diffusion equation for salinity S . Advection is the process describing the moving about of a substance by ocean currents. The advective flux can therefore be defined as the fluid velocity times the concentration of the substance. Using salinity S as tracer, the advection equation in three dimensions reads as follows:

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x} (uS) + \frac{\partial}{\partial y} (vS) + \frac{\partial}{\partial z} (wS) = 0, \quad (1.6)$$

where incompressibility of the flow has been assumed. Multiplying (1.6) with $2S$ yields:

$$\frac{\partial S^2}{\partial t} + \frac{\partial}{\partial x} (uS^2) + \frac{\partial}{\partial y} (vS^2) + \frac{\partial}{\partial z} (wS^2) = 0, \quad (1.7)$$

and shows that the advection equation does not yield any mixing, since the term on the right hand side is zero. However, when implementing Eq. (1.7) into a numerical model, mixing does in fact arise, such that a source term $-\chi_{\text{num}}$ appears on the right hand side. This term is referred to as spurious numerical mixing – that is, unphysical mixing, which does not exist in nature.

Diffusion is the net movement from a region of higher concentration to a region of lower concentration. Another way of defining diffusion is as a process, where larger scale gradients in a dissolved substance are erased over time, because of random movement at the molecular scale. The diffusion equation in three dimensions reads as follows:

$$\frac{\partial S}{\partial t} - \frac{\partial}{\partial x} \left(K_h \frac{\partial S}{\partial x} \right) - \frac{\partial}{\partial y} \left(K_h \frac{\partial S}{\partial y} \right) - \frac{\partial}{\partial z} \left(K_v \frac{\partial S}{\partial z} \right) = 0, \quad (1.8)$$

where $\kappa = (K_h, K_h, K_v)$ is the diffusivity, and the subscripts "h" and "v", respectively, refer to "horizontal" and "vertical". Multiplication of (1.8) with $2S$ results in:

$$\begin{aligned} & \frac{\partial S^2}{\partial t} - \frac{\partial}{\partial x} \left(K_h \frac{\partial S^2}{\partial x} \right) - \frac{\partial}{\partial y} \left(K_h \frac{\partial S^2}{\partial y} \right) - \frac{\partial}{\partial z} \left(K_v \frac{\partial S^2}{\partial z} \right) \\ &= -2 \left(K_h \left(\frac{\partial S}{\partial x} \right)^2 + K_h \left(\frac{\partial S}{\partial y} \right)^2 + K_v \left(\frac{\partial S}{\partial z} \right)^2 \right) = -\chi \end{aligned} \quad (1.9)$$

The right hand side of Eq. (1.9) is described as physical mixing, χ_{phy} . This is the mixing arising due to diffusion, that is, the simulated "real" mixing.

Combining Eqs. (1.6) and (1.8) yields the advection-diffusion equation. When this equation is implemented into a numerical model, one can quantify the physical against the numerical mixing in the model. This procedure is detailed in [Klingbeil et al. \(2014\)](#), building on work by [Burchard & Rennau \(2008\)](#).

1.3.2 VOLUME-INTEGRATED MIXING BOUNDED BY A TRANSECT

Using the definition of mixing as salinity variance decay χ , the volume-integrated mixing bounded by a transect, $\mathbb{M}$, could be derived in [MacCready et al. \(2018\)](#) as:

$$Q_{\text{in}} (S_{\text{in}})^2 + Q_{\text{out}} (S_{\text{out}})^2 = S_{\text{in}} S_{\text{out}} Q_r \approx \mathbb{M}, \quad (1.10)$$

where S_{in} (S_{out}) is the inflowing (outflowing) salinity and Q_{in} (Q_{out}) is the inflowing (outflowing) volume flux across the open boundary transect (see [MacCready et al. \(2018\)](#) and Fig. 1.5a). Q_r is the river discharge. This expression is approximately valid in steady state, e.g., when averaging over the spring-neap cycle in tidal estuaries. Eq. (1.10) extends the Knudsen relations (Eqs. (1.19)), and quantitatively links mixing to the exchange flow.

1.3.3 VOLUME-INTEGRATED MIXING BOUNDED BY AN ISOHALINE

The mixing term $\mathbb{M}$ was extended to a slightly different view in [Burchard \(2020\)](#), where the volume-integrated mixing is bounded by an isohaline instead of a transect (Fig. 1.5b). This change in how the volume is bounded enables the derivation of a mixing equation, that – in contrast to Eq. (1.10) –

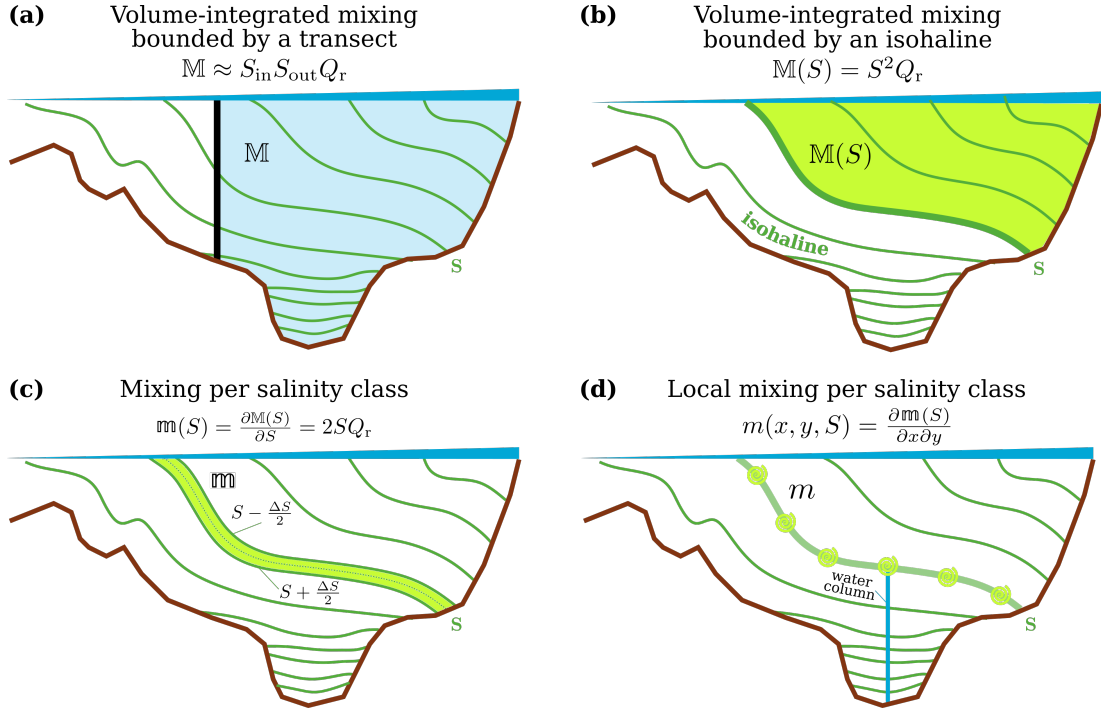


Figure 1.5: (a) Volume-integrated mixing bounded by a vertical transect. (b) Volume-integrated mixing bounded by an isohaline. (c) Mixing per salinity class. (d) Local mixing per salinity class.

is exact under certain conditions. These conditions include that the isohaline should be fully inside the considered domain, that the difference between precipitation and evaporation is zero, and that the temporal averaging is sufficiently long. By using an isohaline instead of a transect to bound the estuarine volume, the salinity of the inflow and the outflow is the same ($S_{\text{in}} = S_{\text{out}} = S$), since both flows occur along the same line of constant salinity. This implies that Eq. (1.10) can be simplified to the following new mixing relation:

$$\mathbb{M}(S) = S^2 Q_r \quad (1.11)$$

When conditions of stationarity or periodicity are fulfilled, or for long-term averaging, the river discharge Q_r and the averaged volume transport through the isohaline S are equal.

1.3.4 MIXING PER SALINITY CLASS

A special focus in this work is on the diahaline mixing, which is the mixing across isohaline surfaces. For the Baltic Sea, it is most interesting to look at this type of mixing, as the salinity gradient dominates over the temperature gradient. The Baltic Sea behaves similarly to estuaries. For estuaries, several studies have related the exchange flow to mixing by studying diahaline turbulent and advective salt fluxes (Walín, 1977, MacCready et al., 2002, Wang et al., 2017), based on the Water Mass Transformation

framework (see Section 1.2). The concept of salinity classes can be introduced (see Section 1.2.1), such that quantities *per* salinity class can be defined, for instance the mixing per salinity class $\mathfrak{m}(S)$. The mixing per salinity class is the portion of the mixing $\mathbb{M}(S)$ that occurs in between two isohalines, divided by the difference in salinity, see Fig. 1.5c. By means of Eq. (1.11), the mixing per salinity class $\mathfrak{m}$ is computed as:

$$\mathfrak{m}(S) = \frac{\partial \mathbb{M}}{\partial S} = 2SQ_r \quad (1.12)$$

The mixing per salinity class $\mathfrak{m}(S)$ is thus the infinitesimal mixing within an infinitesimal salinity interval δS centered around the isohaline. The relation (1.12) is called the "universal law of estuarine mixing" (Burchard, 2020). For any estuary, the long-term mixing per salinity class can be described as twice the salinity times the river discharge.

1.3.5 LOCAL MIXING PER SALINITY CLASS

The previously introduced ways of quantifying mixing are valuable tools to gain an understanding of the ongoing mixing. However, what is still missing, and is of importance for further research endeavors aiming to understand physical and biogeochemical processes in estuaries, is the spatial information of mixing. The introduced formulas estimate the mixing inside the entire estuary as a single value, or in different salt classes, but no information on where this mixing is taking place in physical space is given. This step further to, so called, local mixing per salinity class has been taken in the recent works by Li et al. (2022), Klingbeil & Henell (2023), Henell et al. (2023). The local mixing per salinity class m is the mixing per salinity class of a specific water column, i.e., at a specific point x and y in space, as depicted in Fig. 1.5d. It is obtained by taking the partial derivative in x - and y -direction of the mixing per salinity class $\mathfrak{m}$:

$$m(x, y, S) = \frac{\partial \mathfrak{m}(S)}{\partial x \partial y} \quad (1.13)$$

Using this equation, spatial maps can be created of the mixing, such that the location of hot spots of salinity mixing can be visualized.

Table 1.1 gives an overview of the mixing formulas presented in this dissertation. They are all linked through integration or derivation.

1.4 DIAHALINE VELOCITY

In addition to the mixing, also the circulation or dynamics are of interest. The dynamics in salinity space are described by the diahaline velocity. The diahaline velocity u_{dia} is the net volume flux through an isohaline surface per unit area ($\text{m}^3 \text{s}^{-1} \text{m}^{-2} = \text{ms}^{-1}$), and is defined as the velocity normal to an isohaline. The unit normal vector is given by $\vec{n}_S = \nabla S / |\nabla S|$, and is counted as positive in the direction of increasing salinity S . Hence, negative diahaline velocity is directed down-gradient and labeled as upward or incoming, and positive (up-gradient) as downward or outgoing (see Fig. 1.7a). In the former case, water mass volume is transformed from higher to lower salinity, whereas in the latter case

Location	water column $z(x, y, S)$ local	isohaline surface $A(S)$ per salinity class	estuarine volume $V(S)$ volume-integrated
Mixing	m $m = \frac{\partial \mathfrak{m}}{\partial x \partial y}$ $m = \frac{\partial \mathbb{M}_{\leq}}{\partial S}$	$\mathfrak{m}$ $\mathfrak{m} = 2SQ_r$ $\mathfrak{m} = \frac{\partial \mathbb{M}_{\leq}}{\partial S}$	$\mathbb{M}$ $\mathbb{M} = S^2 Q_r$
Diahaline velocity	$u_{\text{dia},z}^S$ $u_{\text{dia},z}^S = -\frac{\partial f_{\text{dia},z}^S}{\partial S}$ $u_{\text{dia},z}^S = \frac{1}{2} \frac{\partial m}{\partial S}$		Q_{dia} $Q_{\text{dia}} = -\frac{\partial \mathcal{J}_{\text{dia}}}{\partial S}$ $Q_{\text{dia}} = \frac{1}{2} \frac{\partial \mathbb{M}}{\partial S}$
Diahaline diffusive salt flux	$f_{\text{dia},z}^S$ $f_{\text{dia},z}^S = -\frac{1}{2} m$		$\mathcal{J}_{\text{dia}}$ $\mathcal{J}_{\text{dia}} = -\frac{1}{2} \mathfrak{m}$

Table 1.1: Table compiling mixing quantities over different dimensions: a water column, an isohaline surface and an estuarine volume. Integrating the relations in the water column over the longitudinal and latitudinal (x - y -)direction yields the relations per salinity class. Further integrating the relations per salinity class along salinity yields the relations for an estuarine volume. The same mathematical steps in the opposite direction through derivation, takes us from the relations for an estuarine volume to the local relations inside a water column. This table complements the visualization in Fig. 1.5b-d.

water mass volume is transformed towards higher salinity. The definition of u_{dia} as the volume flux through an isohaline surface per unit area, or, equivalently, as the difference between the fluid velocity $\vec{u}$ and the velocity of the isohaline surface $\vec{u}_S$ (Wang et al., 2017) is mathematically written as:

$$\begin{aligned}
u_{\text{dia}} &\equiv \vec{n}_S \cdot (\vec{u} - \vec{u}_S) \\
&= \frac{1}{|\nabla S|} \frac{DS}{Dt},
\end{aligned} \tag{1.14}$$

where D/Dt the material derivative. The isohaline surface can take on different shapes, as is depicted in Fig. 1.6a for three dimensions. Fig. 1.6b shows a simpler view of an isohaline surface in one dimension. For a simplified derivation for the diahaline velocity, the reader is referred to Section 2.1, and for a more rigorous derivation to Klingbeil & Henell (2023). Common to both derivations is that they consider $u_{\text{dia},z}$, instead of u_{dia} . Whereas u_{dia} is the diahaline velocity, that is, the diahaline volume flux per (complexly shaped) isohaline area element, $u_{\text{dia},z}^z$ is the diahaline volume flux per unit horizontal

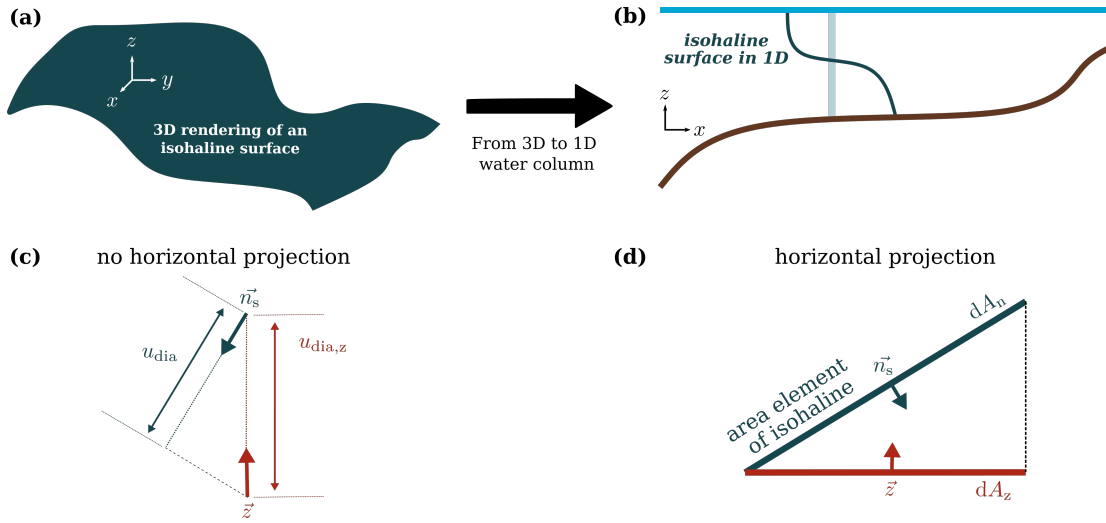


Figure 1.6: (a) A three-dimensional rendering of an isohaline surface is shown. (b) Taking the three-dimensional rendition of (a) to a one-dimensional sketch simplifies the visualization of a water column. (c) Instead of the diahaline velocity u_{dia} , the vertical diahaline velocity $u_{dia,z}$ is used in this thesis. The difference between the two is depicted here. $u_{dia,z}$ is used instead of u_{dia} . (d) $u_{dia,z}$ is *not* the horizontal projection of u_{dia} , whereas the area element dA_z is indeed the horizontal projection of dA_n . Mathematically, it is easier to handle $d\vec{A}_z$, than $d\vec{A}_n$. The reason is that $d\vec{A}_n$ can change direction often, but $d\vec{A}_z$ does not.

area. The difference is illustrated visually in Fig. 1.6c, and the relation between the two quantities can mathematically be written as:

$$u_{dia,z}^z = u_{dia} |\vec{n}_s \cdot \vec{z}|^{-1}. \quad (1.15)$$

The isohaline can change its shape in time and space, which implies that the normal vector of the isohaline area element $d\vec{A}_n$ also changes direction. If, instead, the normal vector $\vec{z}$ of the horizontal projection $d\vec{A}_z$ of $d\vec{A}_n$ (see Fig. 1.6d) is used, there is no need to deal with the changing direction of the unit vector. Hence, $u_{dia,z}$ is used instead of u_{dia} for simplicity.

1.5 DIAHALINE DIFFUSIVE SALT FLUX

Salt diffusion is the net movement of salt from a region of higher salinity to a region of lower salinity, whereas its diffusivity is the rate of diffusion. The salt diffusion is driven by the salinity gradient. In essence, the diffusion describes the ability of the salt to spread out. Fick's first law describes the (salt) diffusion flux mathematically: the diffusion flux is proportional to the negative of the concentration gradient,

$$\mathbf{j} = -\kappa \nabla S. \quad (1.16)$$

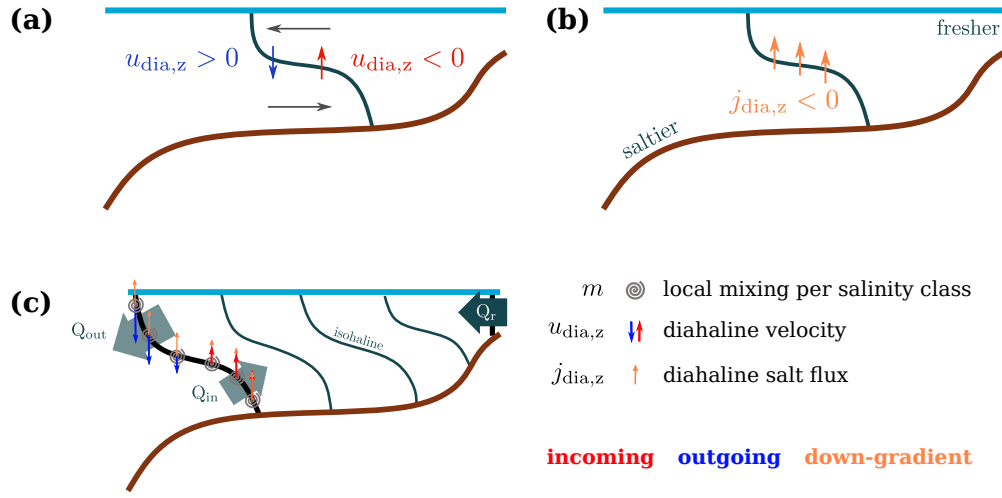


Figure 1.7: Sketch for an idealized estuary showing the sign convention used in Henell et al. (2023, 2025) and throughout this dissertation for (a) the vertical diahaline velocity $u_{\text{dia},z}$ and (b) the vertical diahaline diffusive salt flux $j_{\text{dia},z}$. Diahline fluxes are counted positive into the direction of increasing salinity. Therefore, negative diahaline velocity is counted as incoming or upward, and positive diahaline velocity as outgoing or downward. (c) Sketch visualizing the location of the diahaline quantities. Source: Henell et al. (2023)

This law postulates that the diffusive salt flux goes from regions of high, to regions of low, concentration, with a magnitude that is proportional to the concentration gradient. $\kappa = (K_h, K_h, K_v)$ is the diffusion coefficient or diffusivity, and is proportional to the squared velocity of the diffusing particles. K_h and K_v are, respectively, the horizontal and vertical diffusivity. The diahaline diffusive salt flux j_{dia} describes the diffusive salt flux crossing the isohaline in normal direction. In this work, the diahaline diffusive salt flux is counted as positive in the direction of increasing salinity. While the main focus is on the diahaline diffusive salt flux, also the advective counterpart is of interest. The advective salt flux is given by the velocity times the salinity. The total diahaline salt flux f_{dia} is obtained through the summation of its advective and diffusive partition:

$$f_{\text{dia}} = u_{\text{dia}} S + j_{\text{dia}} \quad (1.17)$$

As was the case for the diahaline velocity, again $f_{\text{dia},z}$ (and correspondingly for the advective and diffusive partition) is adopted instead of f_{dia} . For details on the mathematical derivation of the diahaline diffusive salt flux, the reader is referred to Section 2.1. The sign convention for the diahaline quantities is visualized in Fig. 1.7a,b. Lastly, a sketch of the location of $u_{\text{dia},z}$, $j_{\text{dia},z}$ and the local mixing per salinity class m in an idealized estuary is displayed in Fig. 1.7c.

Name	Unit	Description
$u_{\text{dia},z}$	m/s	Diahaline volume flux per unit horizontal area
$j_{\text{dia},z}$	m/s g/kg	Diahaline diffusive salt flux per unit horizontal area
$f_{\text{dia},z}$	m/s g/kg	Diahaline total salt flux per unit horizontal area
m	m/s g/kg	Total local mixing per salinity class
m_{phy}	m/s g/kg	Physical local mixing per salinity class
m_{num}	m/s g/kg	Numerical local mixing per salinity class
Q_{dia}	m ³ /s	Diahaline volume transport

Table 1.2: Overview of the terms from the local diahaline Water Mass Transformation theory, that are used in this thesis. The diahaline fluxes are counted as positive (negative) into the direction of increasing (decreasing) salinity. Therefore, negative diahaline fluxes, e.g., diahaline velocity, are regarded as incoming or upward, and positive are regarded as outgoing or downward.

1.6 NUMERICAL MODEL OF THE BALTIC SEA

1.6.1 THE BALTIC SEA

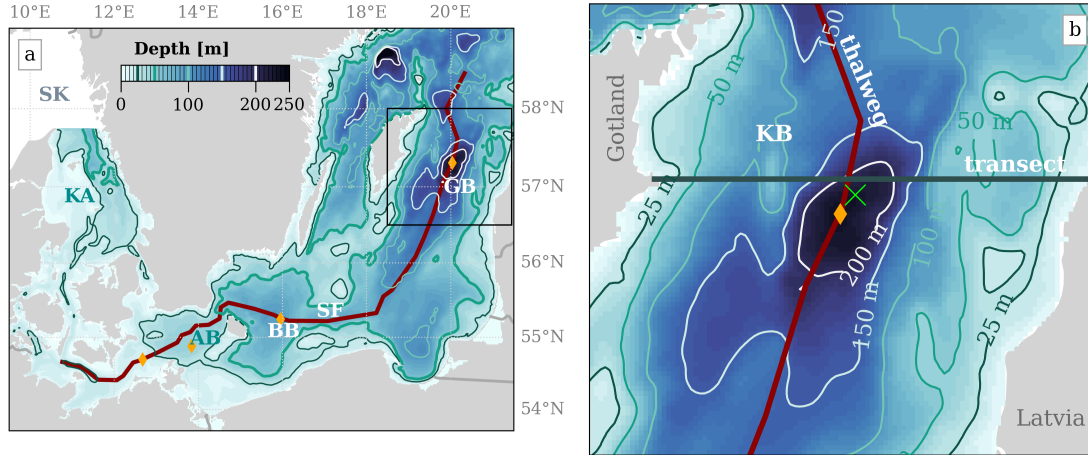


Figure 1.8: (a) Bathymetric map of the western and central Baltic Sea. (b) Zoom on the eastern Gotland Basin. Different shades of green show the isobaths of 25, 50, 100, 150 and 200 m. The main basins or features of interest are designated as SK - Skagerrak, KA - Kattegat, AB - Arkona Basin, BB - Bornholm Basin, SF - Slupsk Furrow and GB - eastern Gotland Basin in (a) and KB - Klintsbank in (b). The location of the Baltic thalweg transect is shown in bordeaux. Orange markers display the location of the stations of Darss Sill, Arkona Basin, Bornholm Basin and Gotland Basin. The green cross in (b) shows the measurement location of the GODESS station. The transect corresponds to the transect in Fig. 3.1. Source: [Henell et al. \(2025\)](#)

In this thesis work the study area of interest is the Baltic Sea (Fig. 1.8). The Baltic Sea is a brackish semi-enclosed sea located in northern Europe, and bounded by the European main continent and Scandinavia. This sea has a single connection to the North Sea, and, therefore, to the World Ocean. This connection consists of the Danish Straits – very narrow and shallow passages. Large areas of the Baltic Sea are anoxic because of eutrophication, especially at depth. As a consequence, there is a high dependence on inflow events, which originate from the North Sea, mix the Baltic waters, and ventilate the deeper basins ([Reissmann et al., 2009](#)). These inflow events carry saline and oxygen-rich water masses from the North Sea into the Baltic Sea. The inflow events can be of medium intensity and more frequent, or they can also be less frequent Major Baltic Inflow (MBI) events of either barotropic or baroclinic nature. The barotropic inflows develop as a consequence of wind and air pressure forcing due to specific weather patterns ([Franck et al., 1987](#), [Wyrski, 1954](#), [Matthäus, 2006](#)). However, the baroclinic inflows are driven by a density difference between the Kattegat and Baltic Sea ([Hela, 1944](#), [Feistel et al., 2003a,b, 2006](#), [Mohrholz et al., 2006](#), see Fig. 1.8a for the location of Kattegat). The former type of inflow is more commonly found during the winter, and the latter during the summer months. The vertical salinity stratification is very strong in the deeper basins, with a halocline at 40–

80 m depth (Liblik & Lips, 2019). This makes it difficult to mix more oxygen-rich water from diffusive fluxes at the sea surface down into the deeper basins.

Nine countries (Germany, Denmark, Sweden, Finland, Russia, Estonia, Latvia, Lithuania and Poland) border the Baltic Sea, but even more countries are included in its catchment area, which extends over an area four times the size of the Baltic Sea itself (HELCOM, 2006). The Baltic Sea also encompasses a highly unique marine ecosystem. Moreover, from an oceanographic perspective, it serves as an ideal natural laboratory, where many dynamic processes are at play, which are also found in the World Ocean. The difference between the Baltic Sea and the World Ocean, however, is the easy accessibility of the former. This gives the tremendous advantage of a long history of monitoring programs, which have produced a plethora of measurement data that are spatially and temporally well resolved.

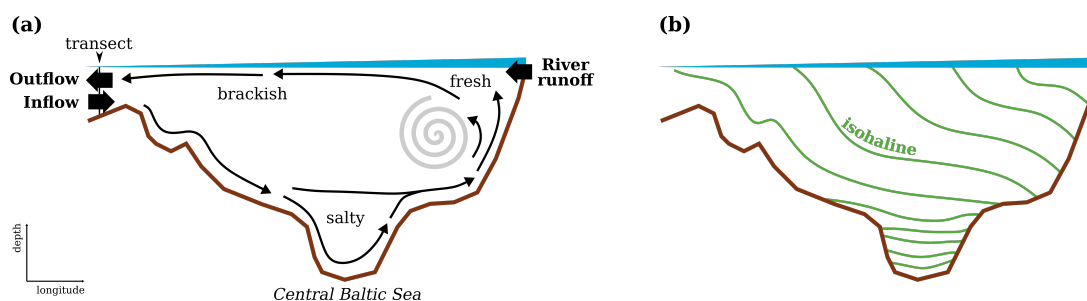


Figure 1.9: (a) Idealized sketch of the overturning circulation in the Baltic Sea. Salty and oxygen rich water flows in from the North Sea and ventilates the Baltic Sea basins. The salty water mixes with the fresh river runoff and results in brackish water masses that return to the North Sea. (b) Sketch of the location of the isohalines after sufficiently long temporal averaging. The curve in the isohalines is due to the presence of fresher water close to the surface and saltier water closer to the bottom. The denser and flat isohalines in the the deepest part of the basin is the permanent halocline and salinity stratification present at such depths in the Baltic Sea.

The dynamics of the Baltic Sea is described by a classical estuarine circulation. The fresh river runoff and precipitation in the surface waters mix with the saline and dense Atlantic waters flowing in through the straits, and result in a net outflow of mixed, brackish waters towards the North Sea: an exchange flow is formed (Fig. 1.9a). The Baltic Sea can be understood as a non-tidal estuary and acts as the brackish water zone connecting the rivers of the Baltic catchment area with the North Sea. At some point, the fresh river water enters the ocean, which can not happen without having first been transported through the estuary. During this travel, the river water is entrained through isohalines ranging continuously from low to high salinity (Fig. 1.9b). During this process turbulent mixing occurs, where the brackish, intermediate salinity water mass is formed from the mixing of fresh river and saline ocean water. From the along estuary salinity gradient, an along estuary density gradient is established. The density gradient and the tidally averaged sea surface slope generate a pressure gradient, which in turn drives the estuarine circulation. The temperature gradient does not play an important role for the dynamics of the Baltic Sea. Therefore, salinity serves as an optimal tracer to describe the dynamical processes and will be quintessential for the scope of this thesis.

In order to describe the estuarine circulation mathematically, Knudsen (1900) combined the mass (volume) and salt conservation equation,

$$Q_{\text{in}} + Q_{\text{out}} + Q_r = 0 \quad (1.18a)$$

$$Q_{\text{in}} S_{\text{in}} + Q_{\text{out}} S_{\text{out}} = 0, \quad (1.18b)$$

to derive the Knudsen relations:

$$Q_{\text{in}} = \frac{S_{\text{out}}}{S_{\text{in}} - S_{\text{out}}} Q_r, \quad Q_{\text{out}} = -\frac{S_{\text{in}}}{S_{\text{in}} - S_{\text{out}}} Q_r, \quad (1.19)$$

where S_{in} and S_{out} are the inflowing and outflowing salt, and Q_r is the river discharge. The inflowing and outflowing volume, respectively Q_{in} and Q_{out} are difficult to measure, but with the help of the Knudsen relations Eq. (1.19) bulk values could be computed already during Knudsen's time, as the other terms S_{in} , S_{out} , Q_r could be measured. The simplicity of their derivation and understanding make them useful first estimates to this day. In addition, the early work by Knudsen (1900) already contained hints about mixing and its connection to the Knudsen relations. However, more than one hundred years would elapse until the mixing would be quantified in later works.

1.6.2 THE GENERAL ESTUARINE TRANSPORT MODEL

The General Estuarine Transport Model (GETM; Burchard & Bolding, 2002, Klingbeil & Burchard, 2013) has been used for both Henell et al. (2023) and Henell et al. (2025) to carry out realistic numerical simulations of the Baltic Sea. GETM is an open source three-dimensional coastal ocean model (<https://getm.eu/>), based on state-of-the-art numerical schemes and turbulence closure. For details about the numerics of GETM, the reader is referred to Klingbeil et al. (2018). Implemented in GETM is the distinctive feature of vertically adaptive model layers (Hofmeister et al., 2010). These automatically zoom in towards areas with a strong stratification. This considerably reduces spurious numerical mixing, and is vital in order to simulate the halocline of the Baltic Sea correctly (Gräwe et al., 2015). GETM also supports the separate quantification, following Klingbeil et al. (2014), of physical and spurious numerical mixing, respectively due to turbulence parameterizations and discretization errors of the advection schemes. The variance decay caused by tracer diffusion (χ_{phy}) and tracer advection (χ_{num}) is diagnosed in each grid cell of the model. The salinity variance due to river discharge, precipitation and evaporation are also counted as "physical" contributions. Therefore, χ_{num} solely contains the spurious effects of the numerical advection scheme.

For the scope of this dissertation, GETM was extended to also diagnose the vertical diahaline velocity $u_{\text{dia},z}(S)$, the vertical diahaline diffusive salt flux $j_{\text{dia},z}$, as well as the physical and numerical mixing per salinity class m_{phy} and m_{num} , respectively. The required cumulative quantities are obtained after binning the layer heights, transports, salt contents and variance decay from the model grid cells into equidistant salinity bins of size 0.2 g/kg for every water column (following the procedure in 1.2.1). All transports are binned according to the corresponding interface salinity given by an upwind approximation. The model setup with a spatial resolution of approximately 1 nautical mile

is well validated in [Burchard et al. \(2018\)](#), [Gräwe et al. \(2019\)](#). The simulated time period covers the years of 2014 and 2015, covering the third largest Major Baltic Inflow (MBI) event starting in December 2014 ([Mohrholz et al., 2015](#)). For the first applied study of this thesis (see Section 2.2), a temporal average over these two years was taken. For the second applied study (see Section 2.3), up to daily averages were studied, focusing on the time period from July 2014 to July 2015.

2

Key results

2.1 A RIGOROUS DERIVATION OF THE WATER MASS TRANSFORMATION FRAMEWORK, THE RELATION BETWEEN MIXING AND DIA-SURFACE EXCHANGE FLOW, AND LINKS TO RECENT THEORIES IN ESTUARINE RESEARCH

2.1.1 SIMPLIFIED PRESENTATION OF THE GENERAL WATER MASS TRANSFORMATION FRAMEWORK

[Klingbeil & Henell \(2023\)](#) analytically derived the Water Mass Transformation (WMT) framework and extended the classical theory to considering individual water columns. Such an extension of the framework is of considerable research interest, as it enables a gain in spatial information of different diasurface fluxes. The theoretical framework in its most general form has been presented in [Klingbeil & Henell \(2023\)](#). Here I will not repeat the generic derivation, but will present a simplified formulation such that this chapter serves as a complementary reading to [Klingbeil & Henell \(2023\)](#). The full details of the general formulation can be found in Appendix B.

Here, a strictly monotonic salinity distribution is assumed, as is often the case in the Baltic Sea (see [Burchard et al. \(2017\)](#) and [Chrysagi et al. \(2022\)](#) for exceptions). Furthermore, I focus on the water column above the isohaline (see Fig. 2.1), which is denoted by subscript $\leq$, as the water masses with salinity $\leq S$ than the isohaline are considered. Boundary fluxes across the ocean surface are not considered.

The first step in the derivation consists of performing a coordinate transformation from the geopotential z -space to the strictly monotonic S -space. A function $S^z(z)$ is introduced, which describes the vertical distribution of salinity within the water column, between the depth of the isohaline position

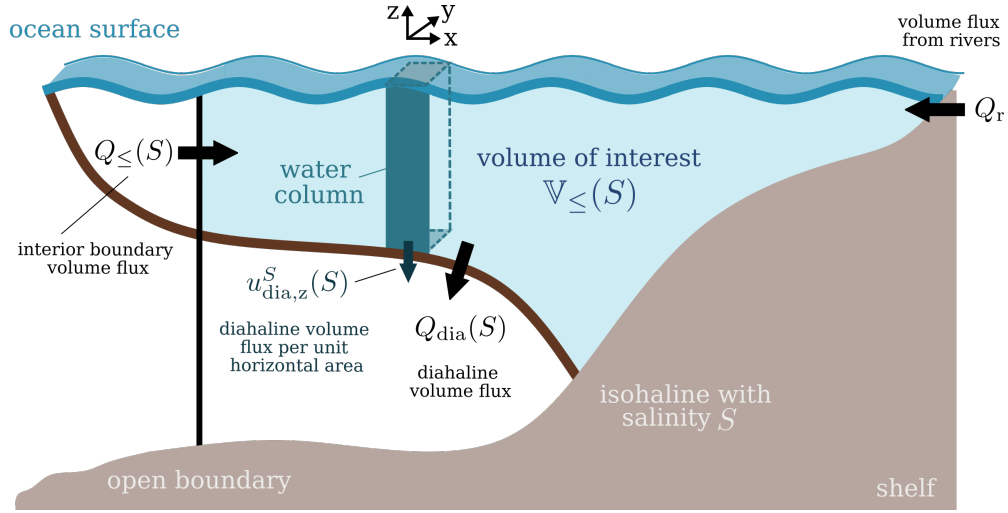


Figure 2.1: Idealized illustration of a control volume bounded by an isohaline with salinity S and a boundary transect toward the open ocean. For simplicity, a stable salinity stratification is assumed here, whereas the general theory in [Klingbeil & Henell \(2023\)](#) also covers non-monotonic tracer distributions. Moreover, only the case of the volume $\mathbb{V}_{\leq}(S)$ containing water with salinities less or equal to S , and situated above the isohaline is considered. Surface boundary fluxes $Q_{\gamma, \leq}(S)$ are assumed to be zero in this presentation. The integrated diahaline volume flux Q_{dia} is a measure for the water mass transformation. The arrows indicate the direction of positive fluxes. In the local diahaline Water Mass Transformation framework, these quantities are considered locally inside every water column, as sketched here for a single water column. Instead of the integrated diahaline volume flux, the diahaline volume flux per unit horizontal area $u_{\text{dia},z}$ is studied.

$z = z^S(S)$ and the ocean surface at $z = \eta(x, y, t)$. This means, that only the part of the water column is considered, where $S^z(z) \leq S$. In the strictly monotonic case, a unique inverse function $z^S(S)$ exists, directly providing the vertical position of the isohaline bounding the water column. Such a unique inverse function would not exist for non-monotonic functions, which would lead to a control volume containing several non-contiguous parts, as seen in Fig. 2e,f in [Klingbeil & Henell \(2023\)](#).

The continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad (2.1)$$

is given in S -space by:

$$\frac{\partial \left(\left| \frac{\partial z^S}{\partial S} \right| \right)}{\partial t} + \frac{\partial \left(\left| \frac{\partial z^S}{\partial S} \right| u \right)}{\partial x} + \frac{\partial \left(\left| \frac{\partial z^S}{\partial S} \right| v \right)}{\partial y} + \frac{\partial \left(\left| \frac{\partial z^S}{\partial S} \right| \frac{Dz^S}{Dt} \right)}{\partial S} = 0. \quad (2.2)$$

See [Klingbeil et al. \(2019\)](#) for details on the vertical coordinate transformation. In Eq. (2.2) the original

vertical velocity w is replaced by

$$u_{\text{dia},z}^S = \left| \frac{\partial z^S}{\partial S} \right| \frac{DS}{Dt}, \quad (2.3)$$

which is the diahaline volume flux per unit horizontal area and is counted positive in S -direction. Note that in the context of generalized vertical coordinates, Eq. (2.2) is often written with $|\partial z^S / \partial S|$ replaced by $\partial z^S / \partial S$ and in terms of the "new" vertical velocity $w^S = \partial z^S / \partial S DS / Dt$, which is positive in z -direction (Burchard et al., 1997). When the salinity distribution is strictly monotonic, the diahaline velocity only contains the contribution Eq. (1.15) from the one vertical position of the isohaline:

$$u_{\text{dia},z}^S = u_{\text{dia},z}^z [z^S(S)] \quad (2.4)$$

In the general non-monotonic case the isohaline may exist at multiple positions in the water column and $u_{\text{dia},z}^z$ from all of these positions contribute to the effective $u_{\text{dia},z}^S$, see Klingbeil & Henell (2023).

The diahaline salt flux per unit horizontal area ($f_{\text{dia},z}^S$) is handled analogously to the diahaline volume flux per unit horizontal area ($u_{\text{dia},z}^S$), except that the former is additionally split into its advective $u_{\text{dia},z}^S S$ and diffusive $j_{\text{dia},z}^S$ component. $j_{\text{dia},z}^S$ is the component that will henceforth be investigated.

2.1.2 THREE DIAHALINE RELATIONS

Klingbeil & Henell (2023) showed how three simple relations between the diahaline quantities can be derived, when assuming that horizontal diffusive salt fluxes can be neglected and that there are no sources and sinks. Making these assumptions simplifies the relations (46), (40) and (47) in Klingbeil & Henell (2023) to the following:

$$u_{\text{dia},z}^S(S) = - \frac{\partial f_{\text{dia},z}^S(S)}{\partial S}, \quad (2.5a)$$

$$j_{\text{dia},z}^S(S) = - \frac{1}{2} m(S), \quad (2.5b)$$

$$u_{\text{dia},z}^S(S) = \frac{1}{2} \frac{\partial m(S)}{\partial S}. \quad (2.5c)$$

where $u_{\text{dia},z}$ and $j_{\text{dia},z}$, respectively, are the diahaline velocity and diffusive salt flux per unit horizontal area and m is the mixing per (infinitesimal) salinity class.

Eq. (2.5a) can be physically understood with the help of Fig. 2.2, which is based on Fig. 1a in Ferrari et al. (2016). A water parcel, which is situated above the bottom boundary layer, experiences more diahaline mixing through the lower than the upper face, due to the enhanced mixing in the bottom boundary layer. This is the left square in Fig. 2.2. The black curly arrows represent the mixing, and their length is proportional to the strength of mixing or equivalently the diffusive salt fluxes. The increased mixing at the bottom of the left square, compared to at the top, results in the water parcel becoming saltier and possible sinking. Thus, water volume is transformed towards higher salinity. This is given by an up-gradient (positive, downward) diahaline velocity. The above describes the process

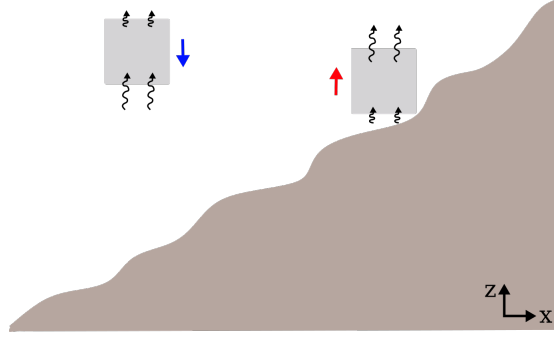


Figure 2.2: Sketch adapted from Fig. 1a in [Ferrari et al. \(2016\)](#) showing a section in longitudinal (x -) and depth (z -) direction of the ocean above a sloping topography with a rough bottom. Two water parcels are shown as gray squares. As a result of mixing, which is enhanced at the bottom, the left square experiences a higher diahaline mixing through its lower, than through its top face. The diffusive salt fluxes linked to mixing are shown as black curly arrows, and their length is proportional to the mixing strength. Therefore, water volume is transformed towards higher salinity, given by a downward diahaline velocity (blue arrow). However, the water parcel on the right experiences the opposite case. There the mixing is higher at the upper than the lower face, resulting in a water parcel which becomes fresher and lighter. This water parcel thus experiences an upward diahaline velocity (red arrow). Note that arrows indicate the transport direction of fluxes in this figure, not the direction of positive quantities.

along the z -axis. In salinity space, the described process would only result in a re-sorting of the volume between salinity classes (see Section 1.2.1, where the salt binning was described). If, instead, the water parcel is within the bottom boundary layer, the mixing is more elevated at the upper than the lower face (right square in Fig. 2.2). As a response, this water parcel would thus become fresher, lighter, and potentially rise upward. This is given by an upward diahaline velocity.

The relation between the local mixing per salinity class m and the diahaline diffusive salt flux $f_{\text{dia},z}^S$ (Eq. (2.5b)) can be understood by taking a closer look at the quantities of $\vec{j}$ and χ . The diffusive salt flux is defined as $\vec{j} = -\kappa \nabla S$, whereas χ is defined as $\chi = \vec{j} \cdot \nabla S$ with $\nabla S = (\partial_x S, \partial_y S, \partial_z S)$. From these definitions it becomes visible that the diffusive salt flux is a three dimensional vector, and therefore gives detailed information of the salt diffusion in three directions. However, χ is not a vector, and is reduced to a single dimension. With χ it is only possible to retain how big the mixing is in one spot, but not in which direction it changes. That information is given by the $\vec{j}$ -vector. In this work, the interest lies in the magnitude of the mixing, as given by χ . The diahaline diffusive salt flux $f_{\text{dia},z}^S$ is the formulation of the diffusive salt flux, that is equivalent to mixing (Eq. (2.5b)), in contrast to the three-dimensional $\vec{j}$ -vector.

Relation (2.5c) is easily derived through the combination of the previous relations, Eqs. (2.5a)–(2.5b), and combines the message from these two relations.

2.2 SPATIAL COMPOSITION OF THE DIAHALINE OVERTURNING CIRCULATION IN A FJORD-TYPE, NON-TIDAL ESTUARINE SYSTEM

2.2.1 THE ANALYTICALLY DERIVED DIAHALINE RELATIONS HOLD IN A NUMERICAL MODEL APPLICATION

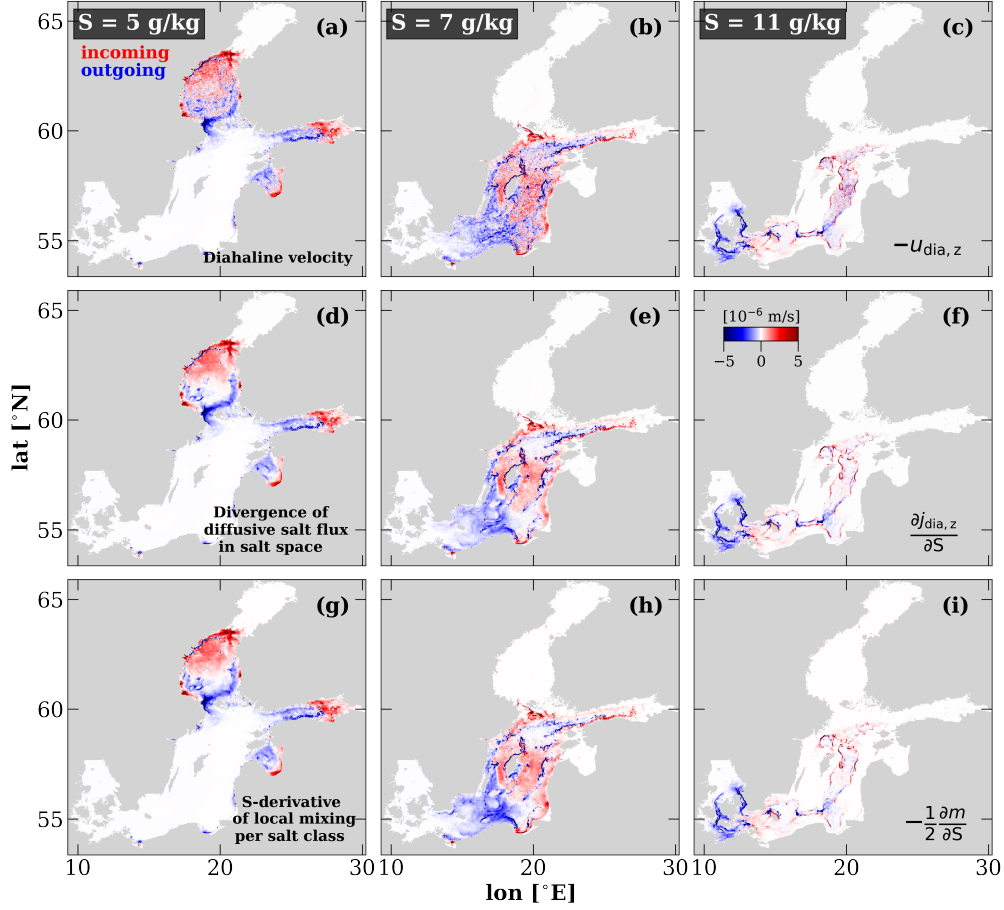


Figure 2.3: Maps of diahaline quantities temporally averaged over two years. Column 1: 5 g/kg; Column 2: 7 g/kg; Column 3: 11 g/kg. Row 1 (a–c): vertical diahaline velocity $u_{\text{dia},z}$; Row 2 (d–f): divergence of vertical diffusive salt flux in salt space $\partial j_{\text{dia},z}/\partial S$; Row 3 (g–i): derivative of mixing per salinity class with respect to salinity $\partial m/\partial S$. The similar patterns of the shown quantities for each isohaline demonstrate the approximate validity of Equations (2.5a) and (2.5c). Source: [Henell et al. \(2023\)](#)

This paper demonstrates the theory derived in [Klingbeil & Henell \(2023\)](#) in a two-year model application to the Baltic Sea. A main topic of investigation was to see whether the analytically derived relations (2.5a)–(2.5c) hold, not only in theory, but also in practice. Furthermore, an additional step

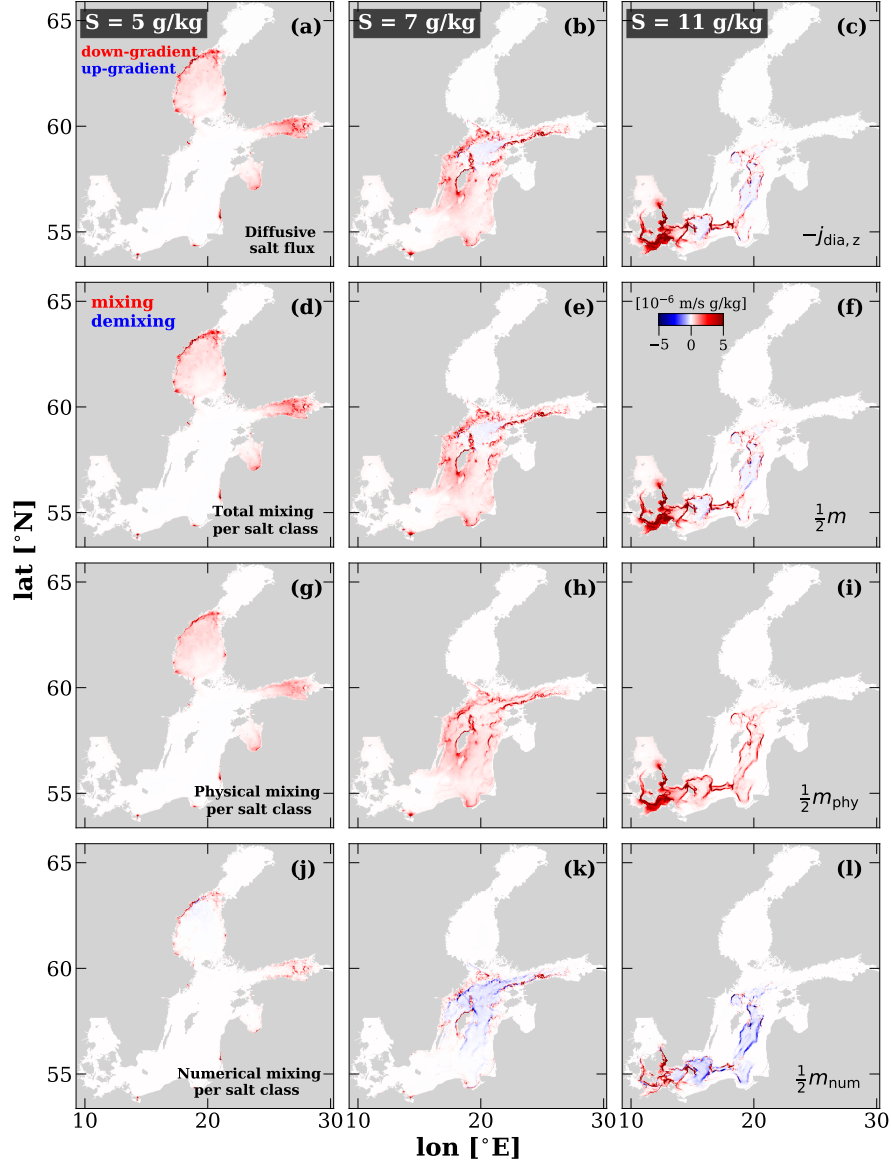


Figure 2.4: Maps of diahaline quantities temporally averaged over two years. Column 1: salt class 5 g/kg; Column 2: 7 g/kg; Column 3: 11 g/kg. Row 1 (a–c): vertical diffusive salt flux; Row 2 (d–f): mixing per salinity class; Row 3 (g–i): physical mixing per salinity class; Row 4 (j–l): numerical mixing per salinity class. The close to identical patterns in panels (a)–(c) and (d)–(f) display the validity of Equation (2.5b). Source: [Henell et al. \(2023\)](#)

has been taken in this article using relation (2.5c). This will be demonstrated in Subsection 2.2.2. But in order to enable this step, it is key that the relations hold! In addition to scatter plots and the computation of the correlation coefficient of the term on each side of the relations, horizontal maps of every term were studied. The term on each side of the relations were plotted individually, such that they could be visually compared to each other and it could be seen whether they yield the same result. The diahaline velocity on the left hand side of relation (2.5a) can, for instance, be compared with the divergence of the diffusive salt flux on the right hand side. The result for the relations (2.5a) and (2.5c) is shown in Fig. 2.3. The diahaline velocity and the mixing gradient agree well with each other (Fig. 2.3a-c,g-i). The former shows somewhat noisier patterns. Also the diahaline velocity and the divergence of the diffusive salt flux show corresponding pictures (Fig. 2.3a-c,d-f). Fig. 2.4a-c,d-f furthermore demonstrates that the patterns of the diffusive salt flux and the mixing per salinity class concur. These results were confirmed in the scatter plots and correlation coefficients of the respective terms (see Fig. 10 in [Henell et al. \(2023\)](#)). Therefore, the conclusion is that the relations (2.5a)-(2.5c) hold well.

Fig. 2.4g-i and j-l shows the mixing per salinity class separated, respectively, into its physical and numerical contributions, following $m = m_{\text{phy}} + m_{\text{num}}$. This indicates that the simulation results are dominated by the physical mixing from the well-calibrated turbulence parametrization. However, some numerical mixing is present for the three chosen isohaline surfaces, especially in Fig. 2.4l. Both contributions show similar patterns as the two depend on the salinity gradient. Fig. 2.4i,l further demonstrates the mixing contributions to be highest in shallower regions of the Western Baltic Sea, as well as in the Danish Straits which are influenced by the tides. For all salinity classes the hot spots for physical and numerical mixing are located at the rims of the basins, where the isohalines touch the bottom topography.

2.2.2 SPURIOUS OVERTURNING CIRCULATION

After having confirmed the validity of the relation in Equation (2.5c) between the effective vertical diahaline velocity and the mixing per salinity class, this relation can be used to calculate separate estimates for the physically and numerically induced portions of the diahaline exchange flow in terms of the physical and numerical mixing contributions. The physically and numerically induced effective vertical diahaline velocities are compared in Fig. 2.5a-c, d-f, respectively. Physics mostly dominates the diahaline exchange flow across the presented isohaline surfaces, yet it is also clear that numerics play a role that is far from being negligible. The physical as well as the numerical contribution is enhanced along the topographic boundaries. When each contribution is spatially integrated over the incoming and outgoing part, also the physically and numerically induced integrated incoming and outgoing diahaline transports can be obtained (Fig. 11g,h in [Henell et al. \(2023\)](#)). The resulting residual transports interestingly show opposing directions for the physical and numerical contributions across some isohalines, e.g., 7 and 11 g/kg. Indeed, the integrated transports confirm that the exchange flow across isohalines with salinities below 10 g/kg is usually dominated by the physically induced contribution. Nevertheless, the numerically induced transports contribute with up to 50% and more to the diahaline exchange flow for most isohalines (Fig. 11i in [Henell et al. \(2023\)](#)). This result is astonishing,

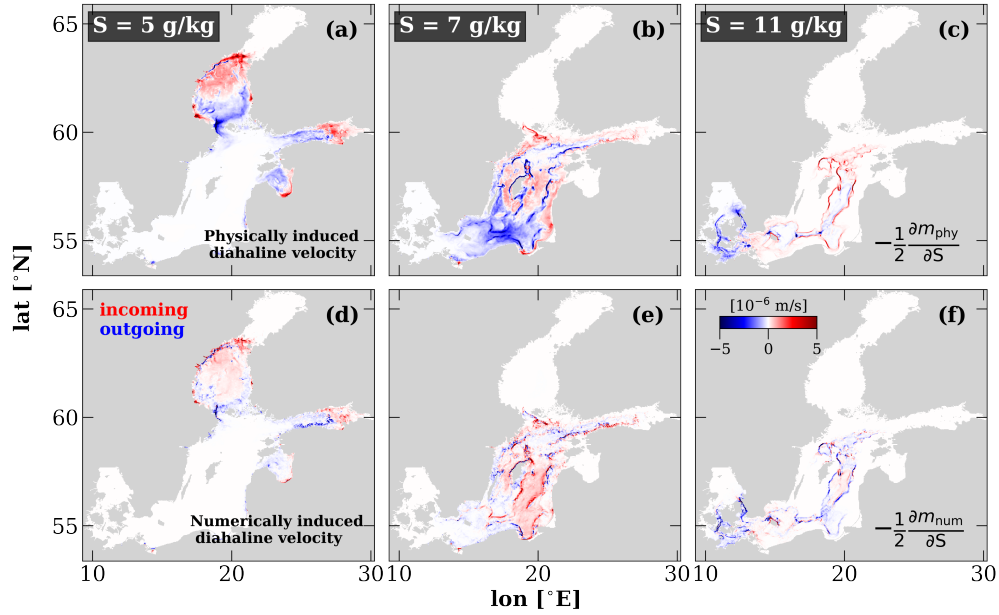


Figure 2.5: Maps of the physically (a–c) and numerically (d–f) induced vertical diahaline velocity, diagnosed by means of Equation (2.5c) in terms of the two-year temporally averaged physical and numerical mixing per salinity class, m_{phy} and m_{num} , respectively. Left column: salinity class 5 g/kg; Middle column: salinity class 7 g/kg; Right column: salinity class 11 g/kg. Source: [Henell et al. \(2023\)](#)

considering that the model uses vertically adaptive coordinates, as well as an anti-diffusive advection scheme.

2.2.3 DIAHALINE BOUNDARY MIXING

[Ferrari et al. \(2016\)](#) argue that the current consensus on the global abyssal overturning circulation neglects a key point. Before their study, the latest observations demonstrated increased mixing in the abyssal waters. The consequence of this would be sinking waters – not rising, as the consensus stated at that point. It would therefore result in an incomplete picture of the overturning circulation, if the bottom-intensified mixing would not be considered. To accommodate for this missing point, they propose that the abyssal waters should ascend to the surface along thin, turbulent bottom boundary layers. In zoomed-in versions of the two regions shown in Fig. 2.3b,c (not shown here, see Fig. 12 in [Henell et al., 2023](#)), regions of intensified diahaline velocity and mixing along bathymetric boundaries were observed. This constituted the motivation for a detailed look into these areas. Increased values are, e.g., discernible in the immediate proximity of the Gotland island, where the isohalines encounter the boundary, i.e., the bottom topography. Fig. 2.6 brought to light that the same boundary mixing structure, observed in the global ocean, is at play in the Baltic Sea as well. The mixing gradient (Fig. 2.6c,d) and the diahaline velocity (Fig. 2.6e,f) show these same patterns in different locations. Due to

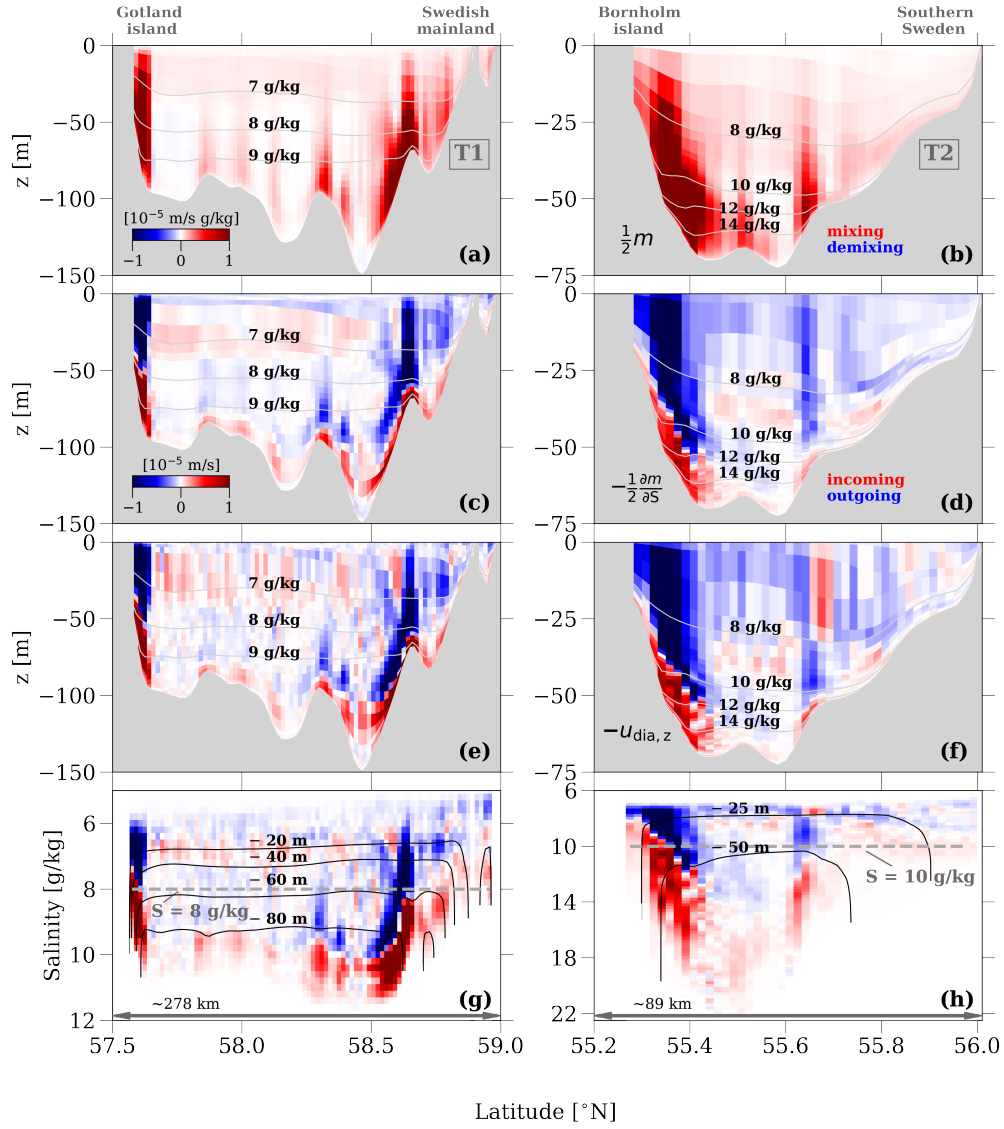


Figure 2.6: (a), (b) Local mixing per salinity class, (c), (d) derivative of the mixing per salinity class with respect to salinity, vertical diahaline velocity in (e), (f) geopotential and (g), (h) salinity space along the transects T1 and T2 shown in Fig. 12 in [Henell et al. \(2023\)](#). A temporal average is taken over two years. Isohaline contour lines are added in (a)–(f), and isobathic contour lines in (g), (h). Quantities in geopotential (z -) coordinates result from a consecutive arrangement of salt classes with their thicknesses, starting with lowest salinity at the ocean surface. The dashed gray lines in (g) and (h) correspond to the isohalines of 8 and 10 g/kg showcased in Fig. 12 in [Henell et al. \(2023\)](#). Source: [Henell et al. \(2023\)](#)

the applied local diahaline WMT framework, these quantities can also be shown in salinity space (Fig. 2.6g,h), which again confirms the pattern. As a further emphasis, also the mixing per salinity class is shown in Fig. 2.6a,b. The intention behind is to display that the mixing is indeed increased in the very same regions where the pattern is present. The sketch in Fig. 14 of [Henell et al. \(2023\)](#) explains the observed pattern in Fig. 2.6c-h. When moving away from the bathymetry within the bottom boundary layer, the mixing starts increasing as the salinity decreases, if a stable salinity stratification is assumed. Hence, the salinity gradient is negative. The mixing gradient in the numerator is positive, however, such that the overall mixing gradient $\partial m / \partial S$ is negative. Eq. (2.5c) imparts that when the mixing gradient is negative, so is the diahaline velocity, because they have the same sign. A negative diahaline velocity is counted as incoming diahaline velocity in the employed sign convention. After a maximum in mixing is reached, the mixing starts decreasing, which gives a negative gradient – but the salinity is still decreasing. Therefore, the outcome is a positive mixing gradient, a positive diahaline velocity and thus an outgoing diahaline velocity.

2.3 EXPLORING THE VARIABILITY OF A NON-TIDAL MARGINAL SEA WITH A SINGLE-MODEL ENSEMBLE

2.3.1 SINGLE-MODEL ENSEMBLE SIMULATIONS ENABLE INVESTIGATION OF SHORT-TERM AND LOCAL PROCESSES IN SALINITY SPACE

The local diahaline Water Mass Transformation framework, mathematically derived in [Klingbeil & Henell \(2023\)](#), was applied in [Henell et al. \(2023\)](#). This first application study served as a demonstration of the method. For this means, it was sufficient to study the entire Baltic Sea domain for temporally averaged quantities over the years 2014 and 2015. In this last manuscript of the PhD, I seek to apply the same method to local and short-term processes, again using the Baltic Sea as a testbed. However, in order to manage this, an additional method is necessary that can reduce the noise that was already observed in a two-year temporal average in [Henell et al. \(2023\)](#). Such noise would obscure the results of any attempts at smaller temporal and spatial resolution with the local WMT framework.

A method for reducing the noise is the use of single-model ensemble simulations, which can be used as a method to tackle deterministic chaos. One can define a chaotic system in different ways, but here it is defined with regard to how sensitive the numerical model is to the initial conditions ([Devaney, 2018](#)). [Büchmann & Söderkvist \(2016\)](#) explain that "the physical system may be seen as a stochastic process, which is executed only once". Numerical models also have such an inherent, stochastic nature, which arises chiefly from the non-linear coupled primitive equations they are built upon. As a consequence, the outcome of a numerical model ought to be regarded as a single realization of a stochastic process. If the model's initial conditions are perturbed, this can lead to highly different results. Yet, in the case that the perturbation is small enough, the additional simulation can be seen as a second realization of the same stochastic process, because the model's overarching stochastic characteristics are not changed ([Büchmann & Söderkvist, 2016](#)). In this way, one can use the variability of a single-model ensemble to estimate the uncertainty of model results, and furthermore to investigate the natural variability in a physical system. More concretely for the method applied in this work, the

ensemble members produce a wider spread of values, which are then sorted into salinity bins following the diahaline WMT theory (see Section 1.2.1). A wider spread of values goes hand in hand with a wider spread across the salinity bins. After the binning, an average over all members (all outcomes) in every salinity bin is calculated, yielding a smoother end result because of the increased amount of data. The results presented here are based on a single-model ensemble consisting of 18 ensemble members. The Bornholm and the Gotland Basin are focused on in the results presented here. Their location is shown in Fig. 1.8.

2.3.2 THE 2014/2015 MAJOR BALTIC INFLOW EVENT IS SENSITIVE TO DETERMINISTIC CHAOS

The inter-ensemble spread of salinity and temperature at the deepest point in the Gotland Basin is shown in Fig. 2.7 in order to assess the uncertainty and variability in the individual ensemble simulations. Thereby, the general predictability of the evolution of Major Baltic Inflows (MBIs) can be evaluated. The ensemble-wide spread of the arrival date of the saltier MBI water masses is shown to span over four days, from 19 to 23 February 2015 (see inset axis in Fig. 2.7). This is an increase from the Bornholm Basin, where all ensemble members agreed on the same date for the arrival of the MBI (see Fig. 60 in [Henell et al. \(2025\)](#)). Even though the inflow can successfully be captured by the ensemble, there is a general overestimation in bottom salinity and temperature. A reason for this could be the insufficient plume mixing, when the inflowing water masses travel from the Bornholm Basin into the Gotland Basin. However, when the large error margins in model intercomparison projects for the Baltic Sea ([Placke et al., 2018](#)) are considered, the deviations of approximately 0.5 g/kg and 1 K in, respectively, salinity and temperature can be deemed relatively small. With the focus turned on the arrival of the inflow event, distinct modes can be identified. By some ensemble members, the inflow is described as a massive, abrupt front, whereas other members depict the inflow to arrive more gradually over time (respectively, the upper or lower ensemble members). It is interesting to see that some ensemble members show a small perturbation in salinity starting in mid-April (Fig. 2.7o). This perturbation forms two distinct branches of equilibrium states from May and spans over a range of approximately 0.25 g/kg.

The time series of bottom temperatures in the Gotland Basin discloses periods of large ensemble variability before the arrival of the MBI (Fig. 2.7p). Two mechanisms can be held responsible for this variability in temperature. The first can be characterized as a "shortcut", where a pre-inflow is initiated. The inflowing waters pushed water from the deep Arkona Basin (see Fig. 1.8 for the location) into the Bornholm Basin. The water masses were not particularly dense, such that they could slide on top of the dense, stagnant bottom water in the Bornholm Basin. By sliding on top, they could directly go on into the Gotland Basin. For the second mechanism, old and stagnant Bornholm Basin bottom water is lifted by the denser inflowing water masses. In this way, the old water masses are displaced by the newly arrived, denser water, which are subsequently pushed into the Gotland Basin. This generated a second peak in the pre-inflow. In both the first and the second mechanism the water masses' density is similar, because they have similar salinity. Therefore, temperature can give an insight into different pathways. The measurements indicate that the temperature spread of the pre-inflow can

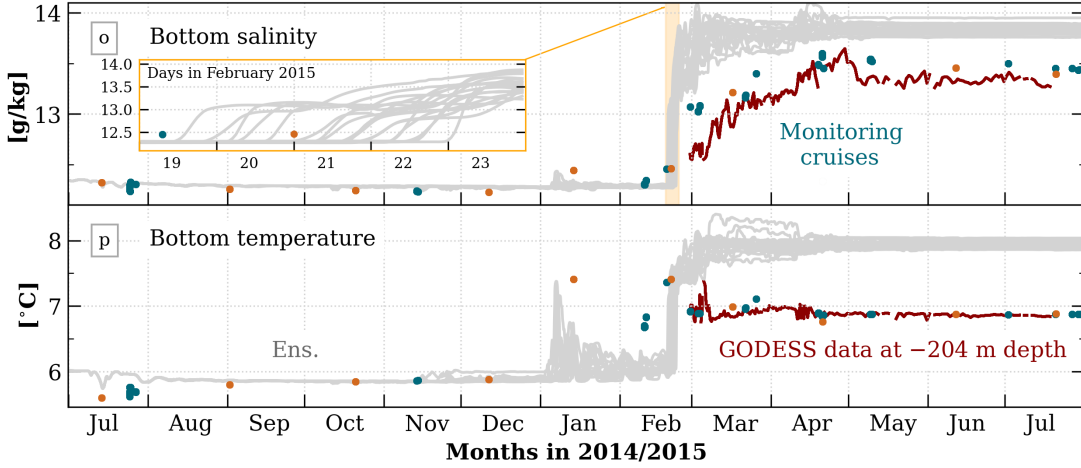


Figure 2.7: Time series of bottom salinity and temperature at station Gotland Basin (see Fig. 1.8 for position): The gray lines show the individual realizations in the model ensemble, whereas the dots are the measurement data. This figure is extracted from Fig. 7 in [Henell et al. \(2025\)](#).

attain up to 1.5 K (Fig. 2.7p). This suggests that the individual member are still too conservative in capturing this variability.

2.3.3 INTEGRAL WATER MASS TRANSFORMATION IN DEEP BALTIC BASINS

In the following, results are presented for the integral water mass transformation quantities in the Bornholm and Gotland Basin, which are both closed off with a virtual lid at a fitting depth level, such that the deep basins can be studied during the MBI.

BORNHOLM BASIN

Here, the Bornholm Basin, with a maximum depth of 92 m, is closed off with a virtual lid at $z = -61$ m. Waters can spill over this lid, and continue to flow on towards the Gotland Basin. Fig. 2.8a gives an understanding of the water mass composition in the deep basin. Starting in December 2014, the Bornholm Basin was filled with water masses of salinities between 16 and 22 g/kg. This increased volume below high salinity isohalines lifts the low salinity waters, and their isohalines, above the virtual lid, and out of the deep basin (Fig. 2.8a). The previously mentioned volume changes occur because of fluxes across the lateral and vertical boundary of the Bornholm Basin, i.e., for non-diahaline reasons. Additionally, the volume in salinity classes can be altered by converging, or diverging, diahaline volume fluxes, as seen in the quantity $\partial Q_{\text{dia}} / \partial S$ in Fig. 2.8c. There, a significant decrease of the inflowing high salinity volumes, because of divergence of the diahaline volume flux, is observed. This explains why, in particular, the 21 and 22 g/kg isohalines do not show up in Fig. 2.8a. The underlying diahaline volume flux Q_{dia} in Fig. 2.8d assesses the water mass transformation between salinity classes, which are

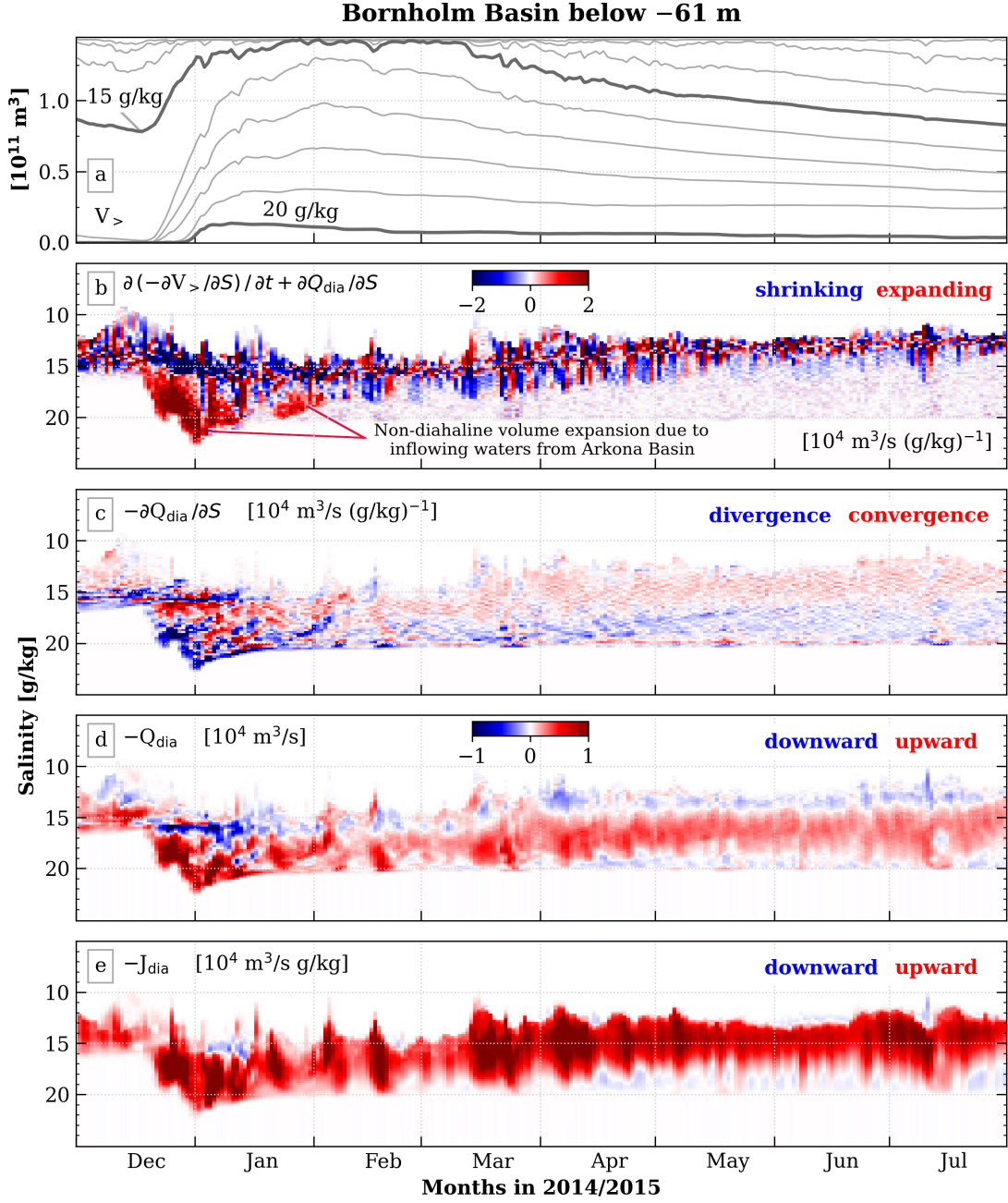


Figure 2.8: Time series ensemble-averaged quantities in salinity space for the Bornholm Basin below a virtual lid placed at $z = -61$ m: (a) stacked volume in salinity classes with the height of an isohaline representing the cumulative volume $V_{>}$ below it, (b) non-diahaline volume change per salinity class $\partial(-\partial V_{>}/\partial S)/\partial t + \partial Q_{\text{dia}}/\partial S$ due to lateral fluxes and fluxes across the virtual lid, (c) volume change per salinity class due to the convergence of diahaline volume fluxes $-\partial Q_{\text{dia}}/\partial S$, (d) diahaline volume flux Q_{dia} , and (e) diahaline diffusive salt flux J_{dia} . Fluxes towards lower salt classes are called "upward". The same colorbars are respectively shared by panels (a) and (b), as well as (c) and (d). Source: [Henell et al. \(2025\)](#)

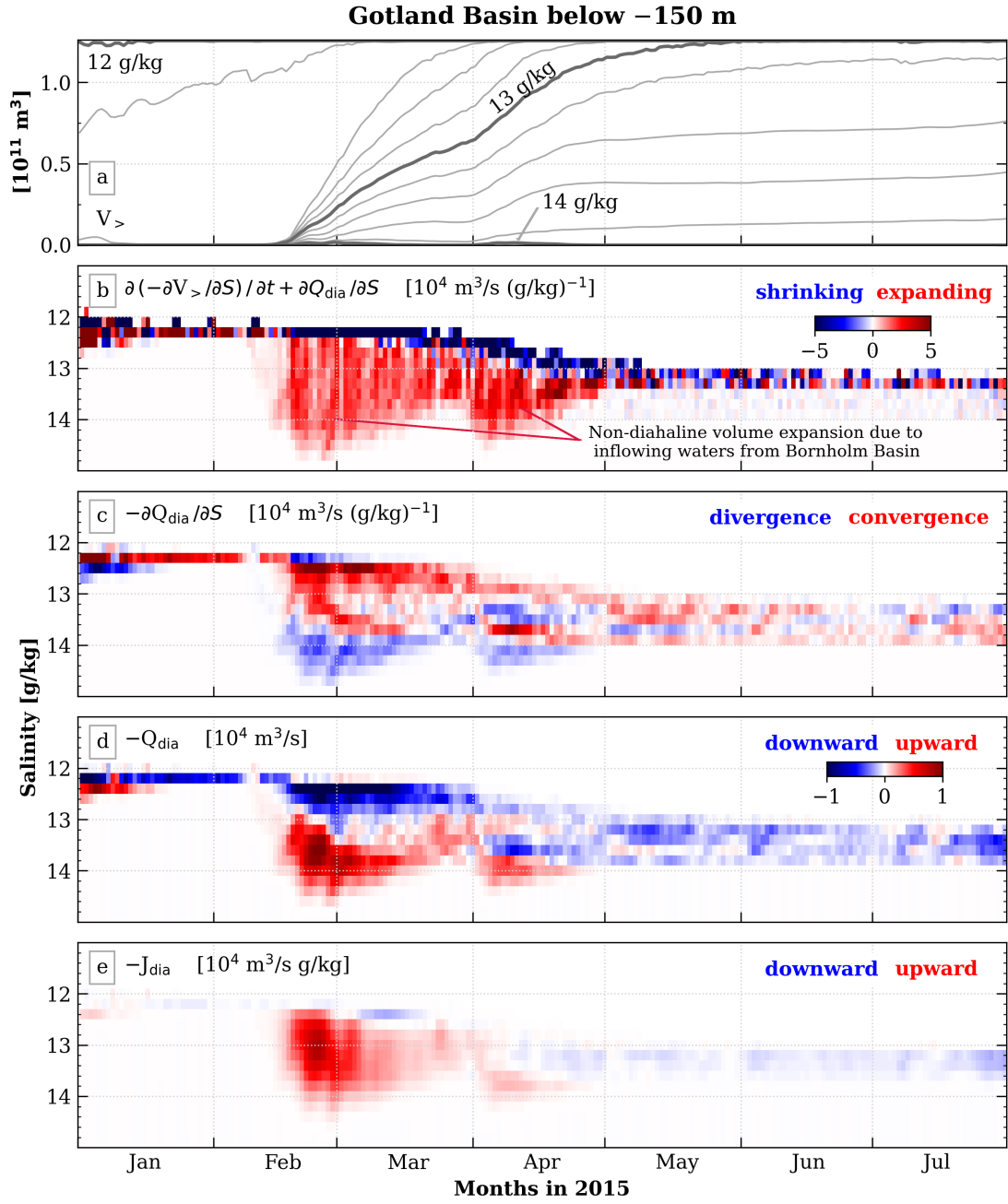


Figure 2.9: Same as for the Bornholm Basin in Fig. 2.8, but for the Gotland Basin and below a virtual lid at $z=-150$ m. Fig. 2.10 shows the spatial distribution of the diahaline volume fluxes Q_{dia} within the basin for selected isohalines. Source: [Henell et al. \(2025\)](#)

associated with diahaline diffusive fluxes J_{dia} (Fig. 2.8e). The diahaline diffusive fluxes are induced by turbulent mixing (Burchard, 2020). Their relation to the diahaline volume fluxes is described by Eq. (1.3): $Q_{\text{dia}} = -\partial J_{\text{dia}} / \partial S$ (Walín, 1977). The direction of J_{dia} is from higher to lower salinity classes, here called the "upward" direction. Because of discretization errors in advection schemes, slight anti-diffusive fluxes can result from the numerical model (Klingbeil et al., 2014, Mohammadi-Aragh et al., 2015). This is showcased by the presence of "downward" J_{dia} in Fig. 2.8e. As a result of the strong diahaline diffusive flux between the inflowing waters of high salinity, and the initial low salinity waters, water is moved from both towards intermediate salinity classes. The former causes an upward flux, whereas the latter causes a downward flux (Fig. 2.8d). Therefore, the outcome is an area of convergence, as seen in Fig. 2.8c. A second, smaller inflow of waters with high salinity is visible at the end of January 2015 (Fig. 2.8b). However, this secondary inflow could not be detected previously, when the bottom salinity of the Bornholm Basin was shown in Fig. 60 in Henell et al. (2025). The reason is that the inflowing volumes of the second inflow did not have a higher salinity than the water mass already present at the bottom of the basin. For the remaining time period, from February to July 2015, the volumes below the 15 g/kg isohaline shrank, resulting in low salinity isohalines sinking back down across the virtual lid into the deep basin (Fig. 2.8a). This change in volume is explainable by the persistent mixing visible in Fig. 2.8e, and the resulting divergence of diahaline volume flux in Fig. 2.8c.

With the help of the evolution of the water mass composition in Fig. 2.8a, the total volume of inflowing high salinity waters into the deep part of the Bornholm Basin can be estimated. At the beginning of the inflow, in December 2014, the isohaline of 16 g/kg was already present, but with almost no volume below it. Subsequently, this isohaline was raised until February 2015 by an inflow volume of approximately 125 km³ below it. The volume of waters with lower salinity than 16 g/kg is not considered in our estimate. These water masses interleaved above the virtual lid, sliding directly towards Slupsk Skill and on into the Gotland Basin. These lower salinity waters are, however, included in the estimate in Gräwe et al. (2015) of a total inflow volume of 298 km³ into the Arkona Basin. Naturally, the present method of estimating the total volume of inflowing high salinity waters into the deep Bornholm Basin with the water mass composition – calculated from the integrated volume below the virtual lid – cannot represent the complex shape, and changing vertical position, of the isohalines in three-dimensional space. The consequence of this is shown in Fig. 2.8b, where a wide band of strong non-dihaline volume changes in lower salinity classes can be discerned. This band arises due to isohalines, that in Fig. 2.8a seem to be sufficiently below the virtual lid, actually cross the lid in some areas of the basin. Therefore, also water masses with salinities higher than 15 g/kg were pushed out above the lid, toward the Gotland Basin, during the inflow from end of December 2014 to January 2015. This will be further studied in the Gotland Basin in the next section, where indeed two distinct inflow periods are present. The first results from the pushed out, old waters from the Bornholm Basin, and the second is caused by the late inflow waters from the Arkona Basin, which can slide on top of the the early inflow waters, that had filled the deep Bornholm Basin.

GOTLAND BASIN

The same analyses of water masses below a virtual lid in the Bornholm Basin is also carried out in the Gotland Basin. The virtual lid in this case is placed at a depth of $z = -150$ m for the Gotland Basin with a maximum depth of 248 m. Fig. 2.9a provides the water mass composition in the deep Gotland Basin. Starting in January 2015, the basin was filled with water masses of salinities between 12.0 and 12.4 g/kg. Over the longer timer period from February to April 2015, the basin was filled substantially by two inflow periods bringing along high salinity waters (Fig. 2.9b). The first inflow period, which lasted from mid-February to the end of March 2015, represents the inflowing old Bornholm Basin waters, which were pushed out there by the early MBI waters. The second inflow period in April 2015 consists of the later inflowing MBI waters, which slid over the deep Bornholm Basin, that had already been filled with saltier MBI waters, and directly on into the Gotland Basin. This was already described in the previous section about the Bornholm Basin. As observed in Fig. 2.9b, the volume between 12.4 and 14.8 g/kg increases during the first inflow. Simultaneously, the volume in salinity classes higher than 13.8 g/kg rapidly transforms into waters of lower salinity (Fig. 2.9c,d). During the second inflow, the volumes between 12.8 and 14.6 g/kg increase (Fig. 2.9b), but with volumes with salinities higher than 14.0 g/kg being transformed into lower salinities, as was also seen for the first inflow (Fig. 2.9c,d). After the two periods of inflowing water masses, the deep Gotland Basin is filled with water masses spanning from 13.0 to 14.0 g/kg. Throughout the stagnation period after the inflow, the volume of the highest salinity waters between 13.4 and 14.0 g/kg expands (Fig. 2.9a,c). The underlying "downward" volume fluxes and up-gradient diffusive fluxes (Fig. 2.9d,e) are unphysical fluxes, caused by the anti-diffusive advection schemes of the numerical model.

The previous analyses carried out in salinity space revealed the two distinct inflow periods into the Gotland Basin, which was not possible to distinguish from the evolution of bottom salinity in Fig. 2.7o. Furthermore, the analyses could also show that the second period of inflow waters pushed out the just arrived, first phase of inflow waters. The first inflow phase can be estimated from Fig. 2.9a to have completely filled the deep basin with approximately 125 km^3 , as the 12.4 g/kg isohaline was lifted above the virtual lid by end of March 2015. The second period fills the basin with approximately another 50 km^3 of highly saline waters. This could be estimated by the lift of the 12.8 g/kg isohaline. This secondary filling confirms the superposition of the old Bornholm Basin (also estimated to around 125 km^3), and later MBI waters. Any further less saline inflowing waters masses into the Gotland Basin can be assumed to stay above the virtual lid.

2.3.4 LOCAL WATER MASS TRANSFORMATION IN THE GOTLAND BASIN

In the previous section and Fig. 2.9, I discussed the integral diahaline volume fluxes Q_{dia} as a metric for the water mass transformation in the Gotland Basin. Here, this analysis is deepened through the study of the spatial distribution of Q_{dia} within the basin. This is given by $u_{\text{dia},z}$. Three isohalines are focused on for this purpose: 12.4 g/kg, 13.2 g/kg and 13.8 g/kg. The 12.4 g/kg and 13.8 g/kg isohalines were chosen, since they were shown in Fig. 2.9a to define the band of salinity classes substantially filled during the inflow. The intermediate isohaline of 13.2 g/kg was selected as it shows interesting features

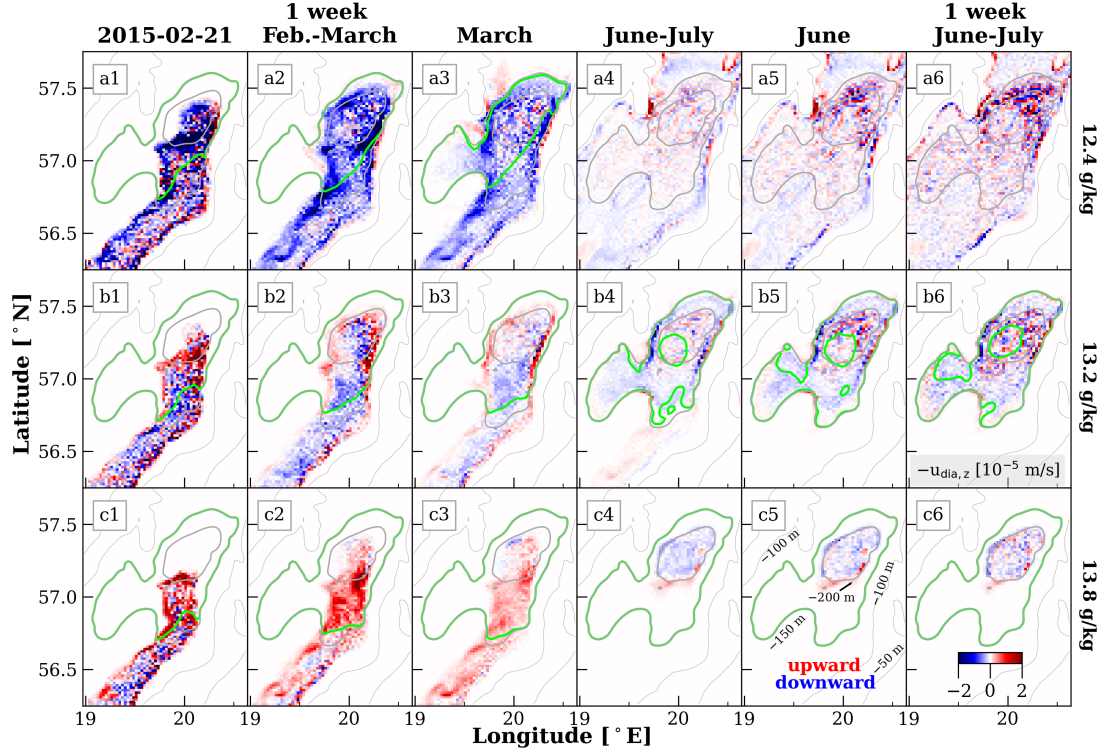


Figure 2.10: Maps of ensemble-averaged local water mass transformation rates (dialine volume flux per unit horizontal area $u_{\text{dia},z}$) across the isohaline surfaces of salinities 12.4 g/kg (row a), 13.2 g/kg (row b) and 13.8 g/kg (row c) in the Gotland Basin, averaged over different periods (columns 1 to 6). The first three columns cover the first inflow period, while the last three columns cover the stagnation period after the inflow. Fluxes towards lower salt classes are labeled "upward". Gray contour lines depict isobaths, while the green contour lines enclose the parts in the basin where the isohalines are below the virtual lid at $z = -150$ m. Areas that are above the virtual lid are not considered in the integrated dialine volume fluxes Q_{dia} below the lid shown in Fig. 2.9d. Source: [Henell et al. \(2025\)](#).

due to being within the vicinity of the virtual lid after the inflow. The local dialine volume fluxes per unit horizontal area $u_{\text{dia},z}$ across the chosen isohalines is shown in Fig. 2.10 over different averaging periods.

I present fluxes averaged over a single day in column 1 of Fig. 2.10, because the dynamics during the arrival of the inflow in February 2015 take place on short time scales. On 21 February 2015, the inflowing plume is seen to have reached the center of the Gotland Basin. Even though I have used averaged data from a large single-model ensemble simulation, the daily data of $u_{\text{dia},z}$ are still noisy. Coherent structures can, however, already be diagnosed despite the presence of noise. Various layers of different salinities make up the inflowing plume. The deviation between the $z = -150$ m isobath and the green contour line shows that the three chosen layers are not the ones that are closest to the bottom. The latter contour line encloses the area in the basin, where the isohalines are below the

virtual lid placed at $z = -150$ m. Any deviation between this contour line and the $z = -150$ m isobath therefore shows that the layer is further from the bottom. But, because of the Coriolis force the plume adheres to the eastern slope of the basin, such that the three layers are exposed to the bottom boundary layer on eastern side (Umlauf & Arneborg, 2010a,b). This is the reason, in addition to entrainment with surrounding waters at the plume front and on the other side, that the highest $u_{\text{dia},z}$ for all salinities is discernible along the margins of the plume (Fig. 2.10a1–c1). The bottom waters with highly saline water masses show an upward velocity towards lower salinities (Fig. 2.10b1–c1), whereas the less saline top layers of the plume show downward velocities towards higher salinities (Fig. 2.10a1,b1). This structure leads to a transformation of water masses toward intermediate salinities. While averaging over longer time scales creates a slightly clearer vision of certain features (Fig. 2.10a2–c2 and a3–c3), this also removes the relevant short-term hotspots of the dynamics, which is induced by the passing inflow plume.

During the stagnation period, the isohaline of 12.4 g/kg (Fig. 2.10a4) is above the virtual lid at $z = -150$ m, i.e., outside the deep basin. This indicates that water mass transformation is taking place at some boundaries, as well as in the basin's interior (Fig. 2.10a4–c6). Fig. 2.10b4–b6 shows that the 13.2 g/kg isohaline is partly above, partly below the virtual lid. The part of the isohaline that domes above the lid, in the center of the basin, is caused by rim currents. This was already described and shown in the Fig. 9a by Holtermann et al. (2014). Moreover, the rim currents are expected to induce water mass transformations in the center of the basin. The isohaline of 13.8 g/kg displays low levels of increased water mass transformations at the boundaries (Fig. 2.10c4–c6). Additionally, slight downward velocities are present in the remaining parts. These are unphysical and due to the anti-diffusive advection schemes in the numerical model.

With the exception of a few locations, the typical upward/downward pattern of the secondary circulation in sloping bottom boundary layers (Garrett, 1990, Ferrari et al., 2016, Henell et al., 2023) and Section 2.2 could not be observed. A tentative explanation for this are the steep topographic slopes and the coarse resolution in the numerical model.

3

Summary and conclusions

This dissertation contributed to the extension of the theoretical Water Mass Transformation (WMT) framework to the formulation of a local WMT framework with [Klingbeil & Henell \(2023\)](#), that considers the water mass transformation in local water columns. When it comes to the understanding of ocean dynamics, the lack of sufficient direct in-situ measurement data poses a major challenge. The theoretical WMT framework complements the measurements by providing an indirect means of investigating the dynamics. The classical framework does not contain any spatial information on the water mass transformation processes. This knowledge gap is filled by the extension to a local WMT framework, where the diasurface circulation is spatially decomposed for every water column. The presented theory includes the analytical derivation of relations between the classical WMT quantities and tracer variance decay.

The theoretical framework has been applied in [Henell et al. \(2023\)](#) to the diahaline fluxes of the Baltic Sea, such that maps of the diahaline fluxes and diahaline mixing could be produced from a two year simulation of the Baltic Sea. In this way hot spots of mixing and circulation could be visualized. These terms are connected through relations that were analytically derived as part of the extended theory. The analytically derived relations were verified and shown to hold in the two-year Baltic Sea simulation. One major result of this application was that around 50% of the diahaline circulation patterns were generated by spurious mixing from the truncation error of the advection scheme in the numerical model. Such a significant percentage was created despite the fact that an anti-diffusive advection scheme and vertically adaptive coordinates had been used, which are measures that reduce the spurious mixing.

Furthermore, a single-model ensemble simulation was developed for the Baltic Sea in [Henell et al. \(2025\)](#), and was combined with the local diahaline WMT framework ([Klingbeil & Henell, 2023](#)),

in order to enable a study of local and short-term dynamics up to daily temporal scales in salinity space. The diahaline dynamics in deep Baltic basins during the Major Baltic Inflow (MBI) event of 2014/2015 could be investigated with this combined method. The analysis in salinity space clearly displayed two distinct inflow periods in the deep Gotland Basin.

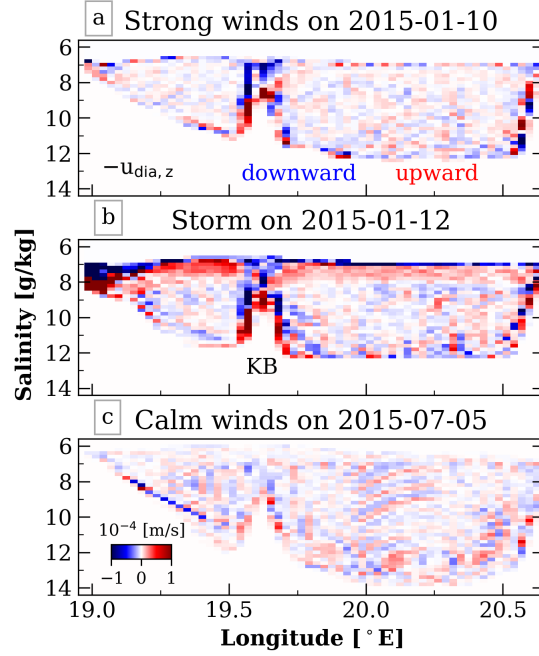


Figure 3.1: Ensemble-averaged local water mass transformation rates (diahline volume flux per unit horizontal area $u_{dia,z}$) along a transect through the Gotland Basin across the Klintsbank under the influence of (a) strong and (b) calm wind conditions. See Fig. 1.8b for location of the transect and of Klintsbank. Source: [Henell et al. \(2025\)](#)

In Fig. 3.1 an outline is presented for the analysis of daily water mass transformation ensemble data from a local, short wind event. The diahaline volume fluxes do indeed show hot spots of water mass transformation rates at the surface (Fig. 3.1b) and the topographic slopes (Fig. 3.1a,b). The enhancement by the surface is only visible during storm events, whereas the increased water mass transformation rates along the topographic slopes remain for a longer time because of generated currents. Moreover, the latter is ubiquitous during the winter season due to the regularity of strong winds. Fig. 3.1 has thus shown the feasibility of studying very local and short term water mass transformations in high-resolution simulations, when combined with single-model ensemble realizations. This result opens up doors for many future research endeavors. The combined method used in [Henell et al. \(2025\)](#) could be carried out for different types of estuaries to study very local, short term diahaline water mass transformations. Only within the geographical bounds of the Baltic Sea, many opportunities already present themselves. More analyses of the 2014/2015 MBI with this method are certainly still possible. For instance, the pursuit of the daily water mass transformations following in the tracks

of the MBI event. Investigations could also be carried out on smaller inflow events. More generally, the diahaline circulation in the Baltic Sea could be studied up to daily scales at essentially any location of interest.

Future work lies in the further extension of the local WMT framework to fully consider diapycnal fluxes. This extension is a vital step in improving the accuracy of current climate models by reducing diapycnal spurious mixing. The extension would be possible by either combining the diahaline and diathermal theory, or by directly deriving it for diapycnal fluxes. While the current framework ([Klingbeil & Henell, 2023](#)) can also be applied to density or temperature, many complications in terms of effects such as thermobaricity and cabbeling arise, whichever path is chosen. Both thermobaricity and cabbeling are effects that result from the combination of eddy mixing and nonlinearities in the nonlinear equation of state ([Groeskamp et al., 2016](#)). These effects can not yet be fully handled.

4

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Declaration of my contributions to the publications

A.1 A RIGOROUS DERIVATION OF THE WATER MASS TRANSFORMATION FRAMEWORK, THE RELATION BETWEEN MIXING AND DIA-SURFACE EXCHANGE FLOW, AND LINKS TO RECENT THEORIES IN ESTUARINE RESEARCH

This first manuscript provided the mathematical background and details for the second and third manuscript and is published in Journal of Physical Oceanography in 2023. I am the second author of this manuscript. The first author is Knut Klingbeil (KK). KK wrote the text. My contribution was given in the form of many hours of discussions with KK on the mathematical theory during the course of the first two years of my PhD. I independently cross-checked the derivations. I also contributed with reading and commenting on the manuscript, and making it more available for a broader public by simplifying the structure and mathematical details. Also, the explanatory sketches of the manuscript were created by me.

A.2 SPATIAL COMPOSITION OF THE DIAHALINE OVERTURNING CIRCULATION IN A FJORD-TYPE, NON-TIDAL ESTUARINE SYSTEM

The second manuscript is the first implementation of new theory from the first manuscript to the estuary of the Baltic Sea. It is published in the Journal of Geophysical Research: Oceans in 2023. I am the first author. Co-authors are my supervisors Hans Burchard (HB) and KK, as well as my

colleague Ulf Gräwe (UG). HB and KK have contributed with the idea for this study, since they had already developed parts of the theory before I started my PhD. They have also contributed with many discussions and by supervising me. UG ran all simulations for this study. All figures and sketches of the manuscript were produced by me. The text is written by me. KK reformulated parts of the text to make it as concise and short as possible. HB contributed with specific lines of text in the subsection on boundary mixing and the abstract. I carried out all the revision steps and received valuable comments by KK.

A.3 EXPLORING THE VARIABILITY OF A NON-TIDAL MARGINAL SEA WITH A SINGLE-MODEL ENSEMBLE

The third manuscript combines the theory from the first one, and serves as an additional short-term and local application study the western and central Baltic Sea, but additionally implementing the method of a single-model ensemble. It is submitted to *Ocean Modelling* in 2025. I am the first author. Co-authors are my supervisors KK and HB, as well as my colleagues UG, Peter Holtermann (PH), Lars Umlauf (LU) and Michael Naumann (MN). HB came up with the idea to use a single-model ensemble to enable a study of short-term and local processes. I carried out the analyses and produced the figures of the study. Together with KK and UG, I wrote the text of the manuscript. KK supervised me. UG ran all the ensemble simulations. All co-authors have contributed with comments.

B

Publications

A Rigorous Derivation of the Water Mass Transformation Framework, the Relation between Mixing and Diasurface Exchange Flow, and Links to Recent Theories in Estuarine Research

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ABSTRACT: In this paper we present the analytical derivation of a local water mass transformation (WMT) framework for an individual water column. We exactly formulate the mapping of the governing equations from geopotential coordinates to an arbitrary tracer space. Unique definitions for the local effective vertical diasurface fluxes are given. In tracer space we derive new relations between the local diatracer fluxes and the mixing per tracer class. The key relation between the effective vertical diatracer velocity and the mixing per tracer class directly formulates how the overturning circulation is linked to local tracer variance dissipation. Horizontal integration of the governing equations in tracer space and the relations between the diatracer quantities finally recovers the well-known integral WMT formulations.

KEYWORDS: Diapycnal mixing; Thermohaline circulation; Water masses/storage

1. Introduction

In his seminal work, Walin (1977) presented integral budget equations for the volume $\mathbb{V}_>(S)$ and salt content $\mathbb{S}_>(S)$ of all water within a semiclosed basin with salinities larger than a prescribed salinity S ,

$$\frac{\partial \mathbb{V}_>(S)}{\partial t} - Q_>(S) - Q_{\text{dia}}(S) = 0, \quad (1a)$$

$$\frac{\partial \mathbb{S}_>(S)}{\partial t} - \mathcal{F}_>(S) - \mathcal{F}_{\text{dia}}(S) = 0. \quad (1b)$$

The volume $\mathbb{V}_>(S)$ and its salt content $\mathbb{S}_>(S)$ are illustrated in Fig. 1. The reference to the original equations in Walin (1977), and a comparison to the original notation, is given in Table 1. The integrated volume and salt fluxes entering across the open ocean boundary with salinities larger than S are given by $Q_>(S)$ and $\mathcal{F}_>(S)$. Across the isohaline the integrated diahaline fluxes $Q_{\text{dia}}(S)$ and $\mathcal{F}_{\text{dia}}(S)$ are entering, with the diahaline salt flux consisting of advective (SQ_{dia}) and diffusive contributions ($\mathcal{J}_{\text{dia}}$):

$$\mathcal{F}_{\text{dia}}(S) = SQ_{\text{dia}}(S) + \mathcal{J}_{\text{dia}}(S). \quad (2)$$

Walin (1977) showed that for no diffusive fluxes across the open boundary, i.e., $\mathcal{F}_>(S) = \int_S^\infty S'q(S')dS'$ with $q(S) = -\partial Q_>/\partial S$ being the volume flux per salinity class, the integrated diahaline volume flux is determined by the integrated diahaline diffusive salt flux

$$Q_{\text{dia}}(S) = -\frac{\partial \mathcal{J}_{\text{dia}}(S)}{\partial S}. \quad (3)$$

In analogy, Walin (1982) presented budgets for volumes $\mathbb{V}_\leq(T)$ of all water with temperatures smaller or equal to T , and

additionally considered integrated volume and temperature fluxes across the ocean surface, $Q_{\eta,\leq}(T)$ and $\mathcal{F}_{\eta,\leq}(T)$, respectively. For $\mathcal{F}_{\eta,\leq}(T) = \int_{-\infty}^T T'q_\eta(T')dT' + \mathcal{J}_{\eta,\leq}(T)$, with $q_\eta(T) = \partial Q_{\eta,\leq}/\partial T$ being the volume flux per temperature class, and $\mathcal{J}_{\eta,\leq}(T)$ being the integrated nonadvective temperature flux across the ocean surface, relation (3) was extended to

$$Q_{\text{dia}}(T) = -\frac{\partial \mathcal{J}_{\text{dia}}(T)}{\partial T} + \frac{\partial \mathcal{J}_{\eta,\leq}(T)}{\partial T}. \quad (4)$$

Walin's concept of analyzing budgets of water masses defined by a distinct property, e.g., salinity or temperature, is the foundation of the water mass transformation (WMT) framework. The transformation of water masses due to interior and boundary processes leads to mass fluxes (volume fluxes under the Boussinesq approximation) between water masses, i.e., across the isosurface of the defining property, and is measured by Q_{dia} , see (3) and (4). A review of the integral WMT framework, its derivation from differential volumes in tracer space and references for the numerous applications can be found in Groeskamp et al. (2019).

With the focus on integrated diahaline fluxes in classical estuaries, MacCready et al. (2002) presented the budgets for $\mathbb{V}_\leq(S)$ and $\mathbb{S}_\leq(S)$, neglecting surface boundary fluxes but including explicit freshwater river discharge Q_r ,

$$\frac{\partial \mathbb{V}_\leq(S)}{\partial t} - Q_\leq(S) + Q_{\text{dia}}(S) = Q_r, \quad (5a)$$

$$\frac{\partial \mathbb{S}_\leq(S)}{\partial t} - \mathcal{F}_\leq(S) + \mathcal{F}_{\text{dia}}(S) = 0. \quad (5b)$$

The budgets (5a) and (5b) offer to study the water masses *inside* a classical estuary. The special case of an estuarine volume completely bounded by an isohaline, i.e., without open boundary fluxes ($Q_\leq, \mathcal{F}_\leq$), was considered by MacCready and Geyer (2001) and Hetland (2005). Contrary, if the estuarine volume is completely bounded by the open boundary, see, e.g., MacCready (2011) or Burchard et al. (2019), the diahaline fluxes ($Q_{\text{dia}}, \mathcal{F}_{\text{dia}}$)

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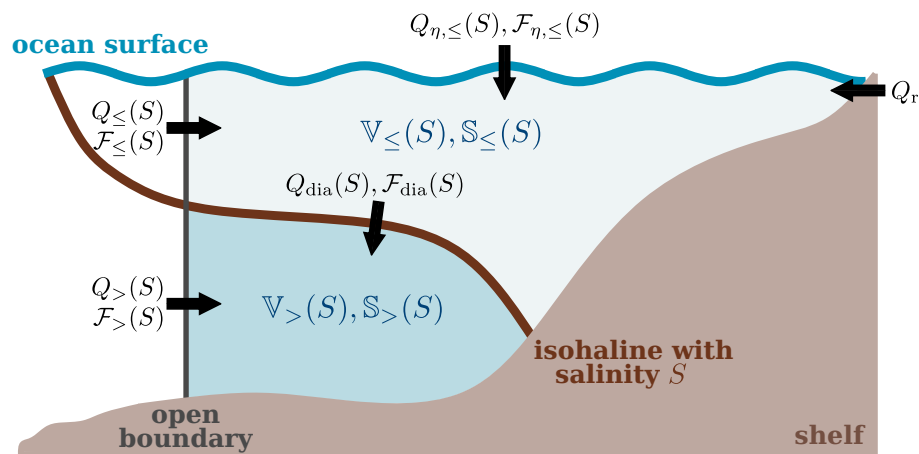


FIG. 1. Idealized illustration of control volumes bounded by an isohaline with salinity S and a boundary transect toward the open ocean. For simplicity a stable salinity stratification is assumed, such that the volume $V_{>}(S)$ containing water with salinities larger than S is located below the isohaline, and the remaining volume $V_{\leq}(S)$ containing water with salinities less or equal to S above the isohaline. The integrated diahaline volume flux Q_{dia} is a measure for the water mass transformation. Integrated surface boundary and open boundary volume fluxes are depicted as $Q_{\eta,\leq}$, $Q_{\leq}$, and $Q_{>}$, defined based on how the salinity of the transported water relates to S . Integrated salt fluxes are denoted by $\mathcal{F}$ and alter the salt contents $S_{\leq}(S)$ and $S_{>}(S)$ inside the corresponding volumes. Surface boundary fluxes $Q_{\eta,>}$ and $\mathcal{F}_{\eta,>}$, transporting or exchanging water with salinities larger than S , are not sketched for simplicity. Additional freshwater river discharge is depicted as Q_r . The arrows indicate the direction of positive fluxes. Walin (1977) presented the budget equations for $V_{>}(S)$ and $S_{>}(S)$; see (1a) and (1b). In many studies on estuaries the budgets for $V_{\leq}(S)$ and $S_{\leq}(S)$, (5a) and (5b) are used.

drop out. For this case, MacCready (2011) developed the concept of total exchange flow (TEF): based on the volume flux per salinity class $q(S) = \partial Q_{\leq} / \partial S = -\partial Q_{>} / \partial S$, the time-averaged open boundary fluxes can be decomposed into net

in- and outflow contributions, and associated salinities for the in- and outflowing water masses can be calculated, finally recovering the Knudsen relations (Knudsen 1900; Burchard et al. 2018).

TABLE 1. Overview of main quantities in an isohaline framework with salinities larger than the specific isohaline, and comparison to earlier publications. Wang et al. (2017) and Walin (1977) presented the equivalent equations horizontally integrated over a single water column and an ocean basin with vertical transects, respectively. In the integrated equations relation (23) holds and there is no need to distinguish between diahaline and effective vertical diahaline fluxes.

	Individual water column		Volume integrated		
	This work	Li et al. (2022, $\partial S / \partial z < 0$)	Wang et al. (2017)	Walin (1977)	This work
Volume budget	(C15)	Their (12)	Their (2.4)	His (4)	(1a)
Cumulative thickness/volume	$D_{>}$	$l^> = z(S) + H$	V	V	$V_{>}$
Cumulative volume transports	$U_{>}, V_{>}$	$p^{x>}, p^{y>}$	Q	M	$Q_{>}$
Local diahaline velocity/transport	u_{dia}^z	u_{dia}^z	$-Q_e$	$-G$	Q_{dia}
Effective vertical diahaline velocity/transport	$u_{\text{dia},z}^S$	$-w_e$			
Salt content budget	(C16)	Their (16)	Their (2.7)	His (5)	(1b)
Cumulative salt content	$S_{>}$	—	V_s	S	$S_{>}$
Cumulative salt transports	$F_{x,>}, F_{y,>}$	—	—	—	$\mathcal{F}_{>}$
Cumulative diffusive salt transports	$J_{x,>}, J_{y,>}$	$=0$	$=0$	$=0$	$\mathcal{J}_{>}$
Local diahaline salt flux	f_{dia}^z	—	$-F_s$	$-H$	$\mathcal{F}_{\text{dia}}$
Effective vertical diahaline salt flux	$f_{\text{dia},z}^S$	—			
Diahaline diffusive salt flux	$\tilde{f}_{\text{dia}}^z$	f_{diff}^S	$-F_m$	$-F$	$\mathcal{J}_{\text{dia}}$
Effective vertical diahaline diffusive salt flux	$\tilde{f}_{\text{dia},z}^S$	$-f_{\text{diff}}^S / \mathbf{n} \cdot \mathbf{z}$			
Salt mixing per salinity class	m	m_{lo}	—	—	m
Relation diahaline volume and salt flux	(46)	Their (18)	Their (2.13)	His (6a)	(3)/(54)
Relation diahaline diffusion and mixing	(40)	Their (9)	[Their (4.5)]	—	(8)/(51)
Relation diahaline volume flux and mixing	(47)	—	—	—	(9)/(55)

TABLE 2. Overview of main integrated quantities in an isohaline framework with salinities smaller or equal to the specific isohaline, and comparison to earlier publications.

	Volume integrated		
	This work	Li et al. (2022)	Bladwell et al. (2021)
Volume budget	(5a)/(48a)	Their (1)	Their (2)
Cumulative volume	$\mathbb{V}_{\leq}$	V	$\mathbb{V}$
Integrated cumulative volume flux	$\mathcal{Q}_{\leq}$	—	$-\Psi$
Integrated diahaline volume flux	$\mathcal{Q}_{\text{dia}}$	Q	$\mathcal{G}$
Salt content budget	(5b)/(48b)	Their (2)	Their (3)
Integrated cumulative salt content	$\mathbb{S}_{\leq}$	—	$\mathbb{S}$
Integrated cumulative salt flux	$\mathcal{F}_{\leq}$	—	$\mathcal{A}$
Integrated cumulative diffusive salt flux	$\mathcal{J}_{\leq}$	$= 0$	$\mathcal{A}_{\text{diff}}$
Integrated diahaline salt flux	$\mathcal{F}_{\text{dia}}$	—	—
Integrated diahaline diffusive salt flux	$\mathcal{J}_{\text{dia}}$	F^s	$\mathcal{D}$
Internal salt content budget	(52)/(53)	[Their (7)]	Their (10)
Integrated internal salt content	$\mathbb{S}_{I,\leq}$	—	$\mathbb{S}_I$
Integrated internal salt flux	$\mathcal{F}_{I,\leq}$	—	$\mathcal{A}_I$
Integrated salt mixing	$\mathbb{M}_{\leq}$	M	—
Integrated salt mixing per salinity class	$\mathfrak{m}$	m	—
Relation diahaline volume and salt flux	(3)/(54)	—	—
Relation diahaline diffusion and mixing	(8)/(51)	Their (6)	—
Relation diahaline volume flux and mixing	(9)/(55)	—	—

Burchard (2020) supplemented (5a) and (5b) by a budget equation for the content of squared salinity. Its sink term $\mathbb{M}_{\leq}(S) = \int_{\mathbb{V}_{\leq}(S)} \chi \, dV$, being the volume-integrated dissipation of salinity variance χ (Burchard and Rennau 2008), is a measure for mixing inside $\mathbb{V}_{\leq}(S)$. With

$$\mathfrak{m}(S) = \frac{\partial \mathbb{M}_{\leq}}{\partial S} \quad (\text{integrated mixing per salinity class}), \quad (6)$$

Burchard (2020) derived the linear relation

$$\langle \mathfrak{m}(S) \rangle = 2S \langle \mathcal{Q}_r \rangle \quad (7)$$

as the *universal law of estuarine mixing* for estuarine volumes completely bounded by the isohaline with salinity S , and assuming sufficiently long time averaging (denoted by angle brackets). Burchard et al. [2021, their (19)] showed the general relation between the integrated diahaline diffusive salt flux and the integrated mixing per salinity class

$$\mathcal{J}_{\text{dia}}(S) = -\frac{1}{2} \mathfrak{m}(S). \quad (8)$$

Although the integrated diahaline fluxes and mixing ($\mathcal{Q}_{\text{dia}}$, $\mathcal{J}_{\text{dia}}$, and $\mathfrak{m}$) provide valuable information about interior processes, they do not provide information on how these quantities are distributed on the isohaline within the basin. Separating the domain into individual water columns facilitates a detailed view of the horizontal distribution. Volume integrated WMT budget equations for individual water columns have been presented in, e.g., Wang et al. (2017) and Holmes et al. (2021). However, in those works no analytical derivation and definition of the local diahaline quantities was done. Under the assumption of a stable salinity stratification, Li et al. (2022) derived budget equations for the thickness $D_{>}(S)$ of all water with salinities larger than S as the distance of the isohaline from the bottom, and the

corresponding salt content $S_{>}(S)$. They also introduced the local diahaline volume flux per unit horizontal area $u_{\text{dia},z}$ and the local mixing per salinity class $m(S)$. Differences in notations are again compared in Tables 1 and 2. However, because of the conceptual limitation due to the assumed stable salinity stratification, their formulated relations are not generally valid.

In this manuscript we present the analytical derivation of a local WMT framework and generally valid mathematical definitions for the corresponding local quantities. In contrast to Groeskamp et al. (2019), we start our derivations in classical geopotential coordinates and exactly formulate the mapping to tracer space. Our new unified presentation easily links the various existing integrated formulations. One major new result of our derivations is an analytical equation that shows how the overturning circulation is linked to local small-scale tracer variance dissipation. Until now, this can only be anticipated from the integrated formulation

$$\mathcal{Q}_{\text{dia}}(S) = \frac{1}{2} \frac{\partial \mathfrak{m}(S)}{\partial S}, \quad (9)$$

that we obtain by combining (3) and (8).

The paper starts with the governing equations in Cartesian coordinates (section 2a) and the mathematical formulation for the mapping from vertical coordinates to a general coordinate space of an arbitrary property s in section 2b. The mapping of the local budgets for volume, tracer content and squared tracer content, as well as the definitions for the local diasurface quantities, are presented in the following sections 2c–2e. The relations between these diasurface quantities in tracer coordinates are derived in section 2f. In section 2g we show how the local budgets and relations recover the well-known integral formulations presented in the introduction. The new local relations are demonstrated in section 3. A summary and conclusions are given in section 4. In the appendixes, details can be found about the unified notation (appendix A), the relation between the general mapping and

coordinate transformations (appendix B), the mapping of the budget equations (appendix C), integral relations in tracer space (appendix D), and the used Leibniz rule (appendix E).

2. Derivation of a local WMT formulation

a. Governing equations in Cartesian coordinates

Under the Boussinesq approximation, mass conservation is turned into volume conservation which is locally described by the incompressibility constraint

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (10)$$

In (10) the flux divergence is written in Cartesian coordinates x, y, z , and the velocity components in the corresponding directions are given by u, v , and w , respectively. Kinematic boundary conditions at the ocean surface and the bottom are given by

$$\frac{\partial \eta}{\partial t} + u(\eta) \frac{\partial \eta}{\partial x} + v(\eta) \frac{\partial \eta}{\partial y} - w(\eta) = u_{\eta,z}, \quad (11a)$$

$$u(-H) \frac{\partial H}{\partial x} + v(-H) \frac{\partial H}{\partial y} + w(-H) = 0, \quad (11b)$$

with $u_{\eta,z}$ being the volume flux across the ocean surface per unit horizontal area (positive into the water column), e.g., due to precipitation, evaporation, ice melting, or freezing.

The local budget equation for an arbitrary tracer with concentration $c^z(x, y, z, t)$ reads

$$\begin{aligned} \frac{\partial c^z}{\partial t} + \underbrace{\frac{\partial}{\partial x} \left(u c^z - K_h \frac{\partial c^z}{\partial x} \right)}_{=f_x} + \underbrace{\frac{\partial}{\partial y} \left(v c^z - K_h \frac{\partial c^z}{\partial y} \right)}_{=f_y} \\ + \underbrace{\frac{\partial}{\partial z} \left(w c^z - K_v \frac{\partial c^z}{\partial z} \right)}_{=f_z} = \pi. \end{aligned} \quad (12)$$

The notation c^z is used to indicate the functional dependence on z coordinates. The tracer flux in the x direction is given by f_x and consists of advective ($u c^z$) and diffusive (j_x) contributions. The fluxes into the other directions are defined accordingly. Diffusive fluxes are given in terms of horizontal and vertical diffusivities K_h and K_v , respectively, but can also be extended to consider more advanced diffusivity tensors. The source term π on the right-hand side of (12) accounts for local tracer production, e.g., due to shortwave radiation for temperature. Flux boundary conditions at the ocean surface and bottom are given by

$$c^z(\eta) \frac{\partial \eta}{\partial t} + f_x(\eta) \frac{\partial \eta}{\partial x} + f_y(\eta) \frac{\partial \eta}{\partial y} - f_z(\eta) = f_{\eta,z}, \quad (13a)$$

$$f_x(-H) \frac{\partial H}{\partial x} + f_y(-H) \frac{\partial H}{\partial y} + f_z(-H) = 0, \quad (13b)$$

with $f_{\eta,z}$ being the surface tracer flux per unit horizontal area (positive into the water column). Bottom tracer fluxes, e.g., geothermal heating, are neglected but can easily be added to the equations.

b. Mapping to an arbitrary s space

In this work we follow Walin's construction of control volumes bounded by a distinct water mass property. But, in contrast to Walin, we will apply the construction to a water column. Let the function $s^z(z)$ describe the vertical distribution of an arbitrary property (e.g., temperature, salinity or density) within the water column between the bottom at $z = -H(x, y)$ and the ocean surface at $z = \eta(x, y, t)$. For any prescribed property value s we need to identify the parts of the water column, i.e., the vertical positions z , where water masses with $s^z(z) \leq s$ or $s^z(z) > s$ are located. This is straight forward for strictly monotonic functions $s^z(z)$, e.g., for stably stratified temperature or salinity distributions as sketched in Figs. 2a and 2c. Only in this monotonic case there exists a unique inverse function $z^s(s)$, which directly provides the vertical position of the prescribed s isosurface that separates the two control "volumes" in the water column. This inverse function does not exist for nonmonotonic functions $s^z(z)$, e.g., for tracer distributions with inversions as sketched in Fig. 2e. In this nonmonotonic case the isosurface exists at multiple positions within the water column and the control volumes consist of noncontiguous parts. Following Wolfe (2014) and Klingbeil et al. (2019), a general mathematical formulation that correctly considers also these noncontiguous parts, is possible by means of the Heaviside step function $\mathcal{H}\{x\}$ and the filter functions

$$\mathcal{H}_{\leq}\{x\} = 1 - \mathcal{H}\{x\} = \begin{cases} 1, & \text{for } x \leq 0, \\ 0, & \text{for } x > 0, \end{cases} \quad (14a)$$

$$\mathcal{H}_{>}\{x\} = \mathcal{H}\{x\} = \begin{cases} 0, & \text{for } x \leq 0, \\ 1, & \text{for } x > 0. \end{cases} \quad (14b)$$

With these filter functions the cumulative thickness of the control volumes, i.e., all parts of the water column where $s^z(z) \leq s$ or $s^z(z) > s$, respectively, can be calculated as

$$D_{\leq}(s) = \int_{-H}^{\eta} \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (15a)$$

$$D_{>}(s) = \int_{-H}^{\eta} \mathcal{H}_{>}\{s^z(z) - s\} dz. \quad (15b)$$

Due to the filter functions in the integrands of (15a) and (15b), the integrals only count those parts of the water column where $s^z(z) \leq s$ or $s^z(z) > s$, respectively. Figure 2 illustrates the functioning of the filter functions, as well as the resulting cumulative thicknesses $D_{\leq}$ and $D_{>}$ for strictly monotonic and nonmonotonic functions $s^z(z)$. For strictly monotonic functions $s^z(z)$, and depending on the sign of $\partial s^z / \partial z$, the cumulative thickness represents the distance of the isosurface to the ocean surface or bottom. For nonmonotonic functions the cumulative thickness consists of the thicknesses from the individual noncontiguous parts.

In the following we will present the derivations only for the " $\leq$ " case for simplicity. The unified derivation for both cases

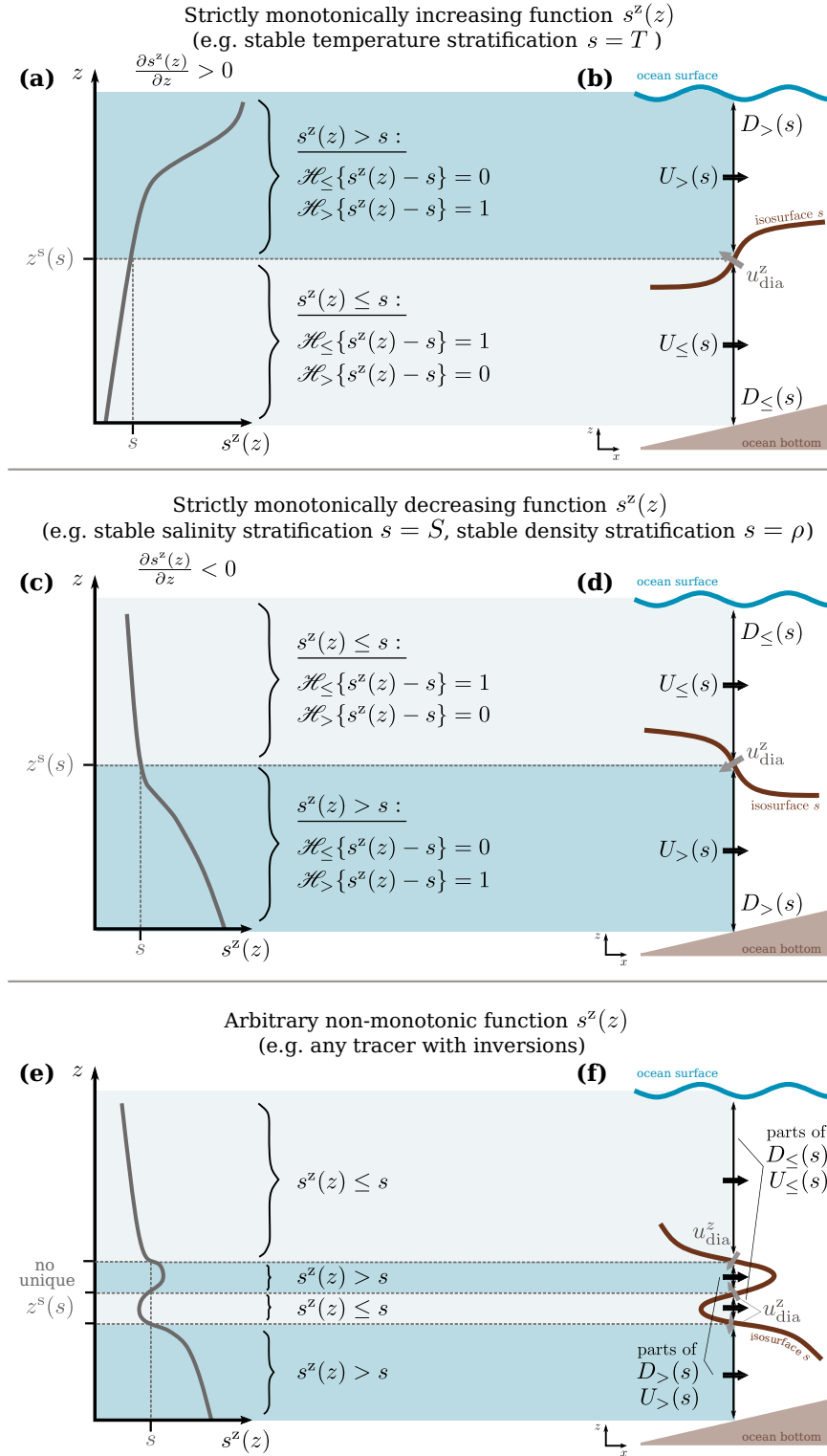


FIG. 2. Control volumes within a water column separated by an isosurface of property s . The vertical distribution of the property is given by the function $s^z(z)$. (a),(c),(e) Examples for strictly monotonic and nonmonotonic distributions are illustrated. For a prescribed value s the filter functions $\mathcal{H}_{\leq}$ and $\mathcal{H}_{>}$, defined in (14a) and (14b), identify the parts of the water column with $s^z(z) \leq s$ or $s^z(z) > s$, respectively. (b),(d),(f) Examples for the location of the isosurface in xz space in the vicinity of the water column are sketched. The local volume budget (18) describes the relation between the cumulative thickness $D_{\leq}$ and horizontal transport $U_{\leq}$, as well as the diasurface velocities u_{dia}^z for the two control volumes.

can be found in the appendixes. The differential thickness, i.e., the thickness per s class, is given by

$$\frac{\partial D_{\leq}(s)}{\partial s} \stackrel{(15a)}{=} \int_{-H}^{\eta} \delta\{s^z(z) - s\} dz, \quad (16)$$

and $\partial D_{\leq}/\partial s ds$ represents the thickness of the infinitesimal ds band around the s isosurface. The Dirac delta distribution $\delta\{x\} = \partial \mathcal{H}\{x\}/\partial x$ is the derivative of the Heaviside step function. It only lets vertical positions contribute to the integral, where the specific isosurface s is present. In analogy to $D_{\leq}$ and $\partial D_{\leq}/\partial s$, the cumulative and differential formulations for any quantity ψ^z can be obtained by

$$\Psi_{\leq}(s) = \int_{-H}^{\eta} \psi^z(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (17a)$$

$$\frac{\partial \Psi_{\leq}(s)}{\partial s} = \int_{-H}^{\eta} \psi^z(z) \delta\{s^z(z) - s\} dz. \quad (17b)$$

The cumulative and differential quantities in (17a) and (17b) are defined for any value of s . Therefore, these relations can be used to map data from z coordinates to an arbitrary s space, similar to a classical coordinate transformation, but applicable also for nonmonotonic functions $s^z(z)$. See [appendix B](#) for more details.

c. Local volume budget

Following the derivation of (C15) in [appendix C](#), vertical integration of (10) over the parts of the water column where $s^z(z) \leq s$ yields the cumulative volume budget in s space

$$\frac{\partial D_{\leq}(s)}{\partial t} + \frac{\partial U_{\leq}(s)}{\partial x} + \frac{\partial V_{\leq}(s)}{\partial y} + u_{\text{dia},z}^s(s) = u_{\eta,z} \mathcal{H}_{\leq}\{s_{\eta} - s\}, \quad (18)$$

with the cumulative thickness $D_{\leq}$ from (15a), the cumulative transports

$$U_{\leq}(s) = \int_{-H}^{\eta} u(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (19a)$$

$$V_{\leq}(s) = \int_{-H}^{\eta} v(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (19b)$$

and the effective vertical diasurface velocity (positive into the direction of increasing s)

$$u_{\text{dia},z}^s(s) = \int_{-H}^{\eta} u_{\text{dia},z}^z(z) \left| \frac{\partial s^z}{\partial z} \right| \delta\{s^z(z) - s\} dz \quad (\text{effective vertical diasurface velocity}). \quad (20)$$

The cumulative transports in (19a) and (19b) are the basis for generalized streamfunctions in s space (Döös and Webb 1994; Nurser and Lee 2004; MacCready 2011; Wolfe 2014). The effective vertical diasurface velocity $u_{\text{dia},z}^s$ in s space, defined in (20), represents the

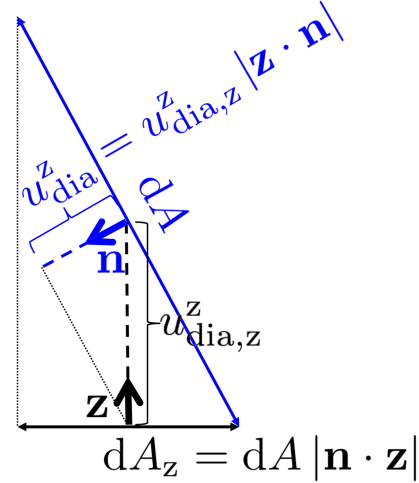


FIG. 3. Sketch for relation between area elements and diasurface velocities (u_{dia}^z , $u_{\text{dia},z}^z$). The infinitesimal area element dA is located on the isosurface with the local unit normal vector $\mathbf{n}$. Its horizontal projection is given by dA_z , with $\mathbf{z}$ being the vertical unit vector. By construction $u_{\text{dia}}^z dA = u_{\text{dia},z}^z dA_z$ holds; see (23). The same relations are valid for the total and diffusive tracer fluxes (f_{dia}^z , $f_{\text{dia},z}^z$) and (j_{dia}^z , $j_{\text{dia},z}^z$), respectively.

volume flux across the given s isosurface per unit horizontal area.¹ It is a key quantity in this paper. The term *effective* stresses that the integrand can contribute with compensating values from multiple positions in the water column where the specific isosurface s is present (see Fig. 2f). At each vertical position in the water column, the local diasurface volume flux per unit horizontal area, $u_{\text{dia},z}^z$ in z space in the integrand of (20), is given by

$$u_{\text{dia},z}^z(z) = u_{\text{dia}}^z(z) |\mathbf{n}(z) \cdot \mathbf{z}|^{-1} = u_{\text{dia}}^z(z) \left| \frac{\partial s^z}{\partial z} \right|^{-1} |\nabla s^z|, \quad (21)$$

in terms of the diasurface velocity u_{dia}^z . The relation between u_{dia}^z and $u_{\text{dia},z}^z$ in (21) is illustrated in Fig. 3. The diasurface velocity u_{dia}^z is the component of the relative velocity normal to the isosurface that is currently located at the specific position z and moving with velocity $\mathbf{u}_s$,

$$u_{\text{dia}}^z(z) = [\mathbf{u}(z) - \mathbf{u}_s(z)] \cdot \mathbf{n}(z) = \frac{1}{|\nabla s^z|} \frac{Ds^z}{Dt} \quad (\text{diasurface velocity}), \quad (22)$$

with $\mathbf{n}(z) = \nabla s^z / |\nabla s^z|$ and $\mathbf{z}$ denoting the unit normal vectors at the isosurface and in the vertical, respectively. The term D/Dt is the material derivative. As sketched by the geometric relations in Fig. 3, the diasurface transport across an infinitesimal isosurface area element dA can be reformulated in terms of the local diasurface volume flux per unit horizontal area $u_{\text{dia},z}^z$ and the horizontal projection of the isosurface area dA_z ,

¹ In this paper all diasurface fluxes measured as “per unit horizontal area” are denoted by subscript “dia,z”.

$$u_{\text{dia}}^z dA \stackrel{(21)}{=} \underbrace{u_{\text{dia},z}^z [\mathbf{z} \cdot \mathbf{n}]}_{=dA_z} dA = u_{\text{dia},z}^z dA_z. \quad (23)$$

Relation (23) is well known from the treatment of boundary fluxes at the ocean surface and bottom, e.g., (C4a) and (C5a), because the mathematical formulation is identical for any surface (Griffies 2004, section 6.7).

The local diasurface volume flux per unit horizontal area, $u_{\text{dia},z}^z$ in (21), is formally not defined for vertical isosurface elements, i.e., for $\partial s^z/\partial z = 0$. In our framework for a vertical water column this does not pose a problem, because the formally infinite $u_{\text{dia},z}^z$ is multiplied with $|\partial s^z/\partial z| = 0$ in (20) and an associated horizontal area $dA_z = 0$ in (23). Instead, the diasurface transport through a vertical isosurface is already accounted for as part of the cumulative horizontal transports (19a) and (19b). Moreover, due to the associated modified horizontal transport divergence in (18), this “missing” contribution to $u_{\text{dia},z}^s$ in (20) will simply appear in an adjacent water column. Therefore, the globally integrated diasurface volume flux

$$Q_{\text{dia}}(s) = \int u_{\text{dia},z}^s(s) dA_z \quad (\text{integrated diasurface volume flux}) \quad (24)$$

again correctly accounts for all contributions. In case of a nonmonotonic coordinate distribution, with an isosurface occurring at multiple positions within the water column, the area dA_z is still only counted once for the specific s (and not for every position z) in (24), because the effect of multiple isosurfaces is already accounted for in the multiple contributions of $u_{\text{dia},z}^s$ to $u_{\text{dia},z}^s$ in (20).

For strictly monotonic coordinate distributions $s^z(z)$, and depending on the sign of $\partial s^z/\partial z$, the cumulative transports (19a) and (19b) represent the transports below or above the isosurface, respectively (see Figs. 2b,d). In this monotonic case a unique inverse function $z^s(s)$ exists, and the effective vertical diasurface velocity in (20) only contains the contribution from the one vertical position of the isosurface,

$$u_{\text{dia},z}^s(s) \stackrel{(20), (B3)}{=} \int_{-H}^{\eta} u_{\text{dia},z}^z [z^s(s')] \delta\{s' - s\} ds' \stackrel{(B3)}{=} u_{\text{dia},z}^z [z^s(s)] \quad \text{for strictly monotonic } s^z(z). \quad (25)$$

Finally, the term on the right hand side of (18) with $u_{\eta,z}$ considers the volume fluxes across the ocean surface into water column volumes that contain the isosurface s_{η} . In case of geometric coordinates s_{η} refers to the coordinate value at the ocean surface $s^z(\eta)$. In case of s being a water mass property s_{η} refers to the property value that is transported with the volume flux.

d. Local tracer budget

Following the derivation of (C16) in appendix C, vertical integration of (12) over the parts of the water column where $s^z(z) \leq s$ yields the cumulative tracer budget in s space

$$\frac{\partial C_{\leq}(s)}{\partial t} + \frac{\partial F_{x,\leq}(s)}{\partial x} + \frac{\partial F_{y,\leq}(s)}{\partial y} + f_{\text{dia},z}^s(s) = \Pi_{\leq}(s) + f_{\eta,z} \mathcal{H}_{\leq}\{s_{\eta} - s\}, \quad (26)$$

with the cumulative tracer content

$$C_{\leq}(s) = \int_{-H}^{\eta} c^z(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (27)$$

the cumulative tracer fluxes

$$F_{x,\leq}(s) = \int_{-H}^{\eta} f_x(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (28a)$$

$$F_{y,\leq}(s) = \int_{-H}^{\eta} f_y(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (28b)$$

the cumulative tracer production

$$\Pi_{\leq}(s) = \int_{-H}^{\eta} \pi(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz, \quad (29)$$

and the effective vertical diasurface tracer flux (positive into the direction of increasing s)

$$f_{\text{dia},z}^s(s) = \int_{-H}^{\eta} f_{\text{dia},z}^z(z) \left| \frac{\partial s^z}{\partial z} \right| \delta\{s^z(z) - s\} dz \quad (\text{effective vertical diasurface tracer flux}). \quad (30)$$

For the interpretation of the effective vertical diasurface tracer flux, and the quantities in the following relations, we refer to the analogous explanations for the effective diasurface velocity $u_{\text{dia},z}^s$ in (20). The local diasurface tracer flux per unit horizontal area in the integrand of (30) is defined as

$$f_{\text{dia},z}^z(z) = f_{\text{dia}}^z(z) |\mathbf{n}(z) \cdot \mathbf{z}|^{-1} = f_{\text{dia}}^z(z) \left| \frac{\partial s^z}{\partial z} \right|^{-1} |\nabla s^z|, \quad (31)$$

with the diasurface tracer flux f_{dia}^z being the component of the tracer flux normal to the moving isosurface that is currently located at the specific position z ,

$$\begin{aligned} f_{\text{dia}}^z(z) &= c^z(z) u_{\text{dia}}^z(z) + \underbrace{\mathbf{j}(z) \cdot \mathbf{n}(z)}_{=f_{\text{dia}}^z(z)} \\ &\stackrel{(22)}{=} \frac{1}{|\nabla s^z|} \left(c^z \frac{Ds^z}{Dt} + j_x \frac{\partial s^z}{\partial x} + j_y \frac{\partial s^z}{\partial y} + j_z \frac{\partial s^z}{\partial z} \right) \\ &= \frac{1}{|\nabla s^z|} \left(c^z \frac{\partial s^z}{\partial t} + f_x \frac{\partial s^z}{\partial x} + f_y \frac{\partial s^z}{\partial y} + f_z \frac{\partial s^z}{\partial z} \right) \\ &\quad (\text{diasurface tracer flux}). \end{aligned} \quad (32)$$

For strictly monotonic coordinate distributions $s^z(z)$ the effective vertical diasurface tracer flux in (30) only contains the contribution from the one vertical position of the isosurface, analogously to the relation for the diasurface velocity (25), such that

$$f_{\text{dia},z}^s(s) = c^s(s) u_{\text{dia},z}^s(s) + f_{\text{dia},z}^s(s) \quad \text{for strictly monotonic } s^z(z) \quad (33)$$

holds, with the diffusive contribution $j_{\text{dia},z}^s$ defined equivalently to $f_{\text{dia},z}^s$ in (30),

$$j_{\text{dia},z}^s(s) = \int_{-H}^{\eta} j_{\text{dia},z}^s(z) \left| \frac{\partial s^z}{\partial z} \right| \delta\{s^z(z) - s\} dz \quad (34a)$$

$$= \int_{-H}^{\eta} \left(-K_h \frac{\partial c^z}{\partial x} \frac{\partial s^z}{\partial x} - K_h \frac{\partial c^z}{\partial y} \frac{\partial s^z}{\partial y} - K_v \frac{\partial c^z}{\partial z} \frac{\partial s^z}{\partial z} \right) \times \delta\{s^z(z) - s\} dz. \quad (34b)$$

Finally, the last term on the right hand side of (26) with $f_{\eta,z}$ considers the tracer flux across the ocean surface into water column volumes that contain the isosurface s_{η} . In case of salinity, that is for $c = S$, there is no salt flux across the atmosphere–ocean interface, but potentially across ice–ocean interfaces.

e. Local squared tracer budget

Following Burchard and Rennau (2008), and according to (C3), an equation for the squared tracer can be derived from the tracer equation (12),

$$\frac{\partial (c^z)^2}{\partial t} + \frac{\partial f_x^{(2)}}{\partial x} + \frac{\partial f_y^{(2)}}{\partial y} + \frac{\partial f_z^{(2)}}{\partial z} = 2c^z \pi - \chi, \quad (35)$$

with the fluxes of squared tracer defined in (C1) and the tracer variance dissipation

$$\chi = 2 \left[K_h \left(\frac{\partial c^z}{\partial x} \right)^2 + K_h \left(\frac{\partial c^z}{\partial y} \right)^2 + K_v \left(\frac{\partial c^z}{\partial z} \right)^2 \right]. \quad (36)$$

Flux boundary conditions at the ocean surface and the bottom are given by (C4d) and (C5d). Note, that the boundary fluxes of squared tracer are already determined by the volume and tracer fluxes according to (C4e) and (C5e).

Following the derivation of (C14) in appendix C, vertical integration of (35) over the parts of the water column where $s^z(z) \leq s$ yields a budget equation for the cumulative squared tracer content in s space. Its sink term is given by the cumulative content of variance dissipation and quantifies the mixing inside $D_{\leq}$:

$$M_{\leq}(s) = \int_{-H}^{\eta} \chi(z) \mathcal{H}_{\leq}\{s^z(z) - s\} dz \quad (\text{cumulative tracer mixing}). \quad (37)$$

From (37) the mixing per s class can be defined as

$$m(s) = \frac{\partial M_{\leq}}{\partial s} = \int_{-H}^{\eta} \chi(z) \delta\{s^z(z) - s\} dz \quad (\text{mixing per } s \text{ class}). \quad (38)$$

f. Mapping to tracer coordinates

In the previous sections we derived the governing equations in a general coordinate space by mapping to an arbitrary property s . In the following we will demonstrate, that for the special choice of tracer coordinates, i.e., $s = c$ with c being the tracer in the tracer equation (12), useful relations between the diasurface

(now diatracer) quantities can be derived. These relations in tracer space are the local equivalents of the integrated formulations presented in the introduction.

1) RELATION BETWEEN DIATRACER DIFFUSIVE TRACER FLUXES AND MIXING

If the tracer is mapped to its own coordinate system, the effective vertical diatracer tracer flux (30) can be written as

$$j_{\text{dia},z}^c(c) = cu_{\text{dia},z}^c(c) + j_{\text{dia},z}^c(c), \quad (39)$$

which, in contrast to (33), does not require any monotonicity constraints on the tracer distribution. The effective vertical diatracer diffusive tracer flux $j_{\text{dia},z}^c$ obeys

$$j_{\text{dia},z}^c(c) \stackrel{(34b)}{=} - \int_{-H}^{\eta} \underbrace{\left[K_h \left(\frac{\partial c^z}{\partial x} \right)^2 + K_h \left(\frac{\partial c^z}{\partial y} \right)^2 + K_v \left(\frac{\partial c^z}{\partial z} \right)^2 \right]}_{\stackrel{(36)}{=} \chi/2} \delta\{c^z(z) - c\} dz \quad (40)$$

$$\stackrel{(37)}{=} - \frac{1}{2} \underbrace{\left(\frac{\partial M_{\leq}}{\partial c} \right)}_{\stackrel{(38)}{=} m(c)},$$

with the cumulative mixing $M_{\leq}$ defined in (37) and $m(c)$ being the mixing per tracer class. Relation (40) is the local equivalent of the integrated formulation (8) and the correct generalization of (9) in Li et al. (2022).

2) OCEAN SURFACE BOUNDARY FLUXES

The volume and tracer fluxes across the ocean surface in (18) and (26) are formally considered in water column volumes that contain the isosurface s_{η} . In tracer space the individual fluxes enter different tracer classes and thus are considered in different water column volumes:

$$u_{\eta,z} \mathcal{H}_{\leq}\{s_{\eta} - s\} \rightarrow u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\}, \quad (41a)$$

$$f_{\eta,z} \mathcal{H}_{\leq}\{s_{\eta} - s\} \rightarrow c_{\eta} u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\} + j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\}. \quad (41b)$$

Each advective contribution enters the tracer class that corresponds to the tracer concentration c_{η} transported by $u_{\eta,z}$. The nonadvective tracer flux $j_{\eta,z}$ is assumed to enter the tracer class that is currently located at the ocean surface, given by $c^z(\eta)$. The consideration of advective contributions in tracer classes with concentrations different from the actual sea surface tracer concentration is mathematically valid, because tracer coordinates are not required to be monotonic and layers of c_{η} can be constructed anywhere in the water column. For example, incoming freshwater volume fluxes always enter the zero salinity class, independent of the actual sea surface salinity.

3) BUDGET FOR INTERNAL TRACER CONTENT

With (39), (41a), and (41b) a budget equation for the internal tracer content $C_{I,\leq}$ can be derived by combining (18) and (26),

$$\begin{aligned}
& \frac{\partial}{\partial t} \overbrace{(C_{\leq} - cD_{\leq})}^{=C_{I,\leq}(c)} + \frac{\partial}{\partial x} \overbrace{(F_{x,\leq} - cU_{\leq})}^{F_{Ix,\leq}(c)} + \frac{\partial}{\partial y} \overbrace{(F_{y,\leq} - cV_{\leq})}^{F_{Iy,\leq}(c)} + j_{\text{dia},z}^c(c) \\
& = \Pi_{\leq}(c) + (c_{\eta} - c)u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\} + j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\},
\end{aligned} \quad (42)$$

with internal tracer fluxes $F_{Ix,\leq}$ and $F_{Iy,\leq}$. As motivated by Holmes et al. (2019) and Bladwell et al. (2021) for the integrated internal heat and salt content, respectively, $C_{I,\leq}$ quantifies the tracer content relative to the bounding tracer concentration c and the so-called external tracer content $cD_{\leq}$. As shown below, in this work the budget for the internal tracer content will be used to derive a relation between the diatracer velocity and the diatracer diffusive tracer fluxes. Alternative expressions for the internal tracer content and the associated internal tracer fluxes can be derived by means of (D1a) and partial integration:

$$C_{I,\leq}(c) = - \int_{-\infty}^c D_{\leq}(c') dc', \quad (43a)$$

$$F_{Ix,\leq}(c) = - \int_{-\infty}^c U_{\leq}(c') dc' + J_{x,\leq}(c), \quad (43b)$$

$$F_{Iy,\leq}(c) = - \int_{-\infty}^c V_{\leq}(c') dc' + J_{y,\leq}(c). \quad (43c)$$

4) RELATION BETWEEN DIATRACER VELOCITY AND DIFFUSIVE TRACER FLUXES

With (43a)–(43c) and (18), the budget for the internal tracer content (42) can be reformulated² to

$$\begin{aligned}
& \int_{-\infty}^c u_{\text{dia},z}^c(c') dc' + j_{\text{dia},z}^c(c) + \frac{\partial J_{x,\leq}(c)}{\partial x} + \frac{\partial J_{y,\leq}(c)}{\partial y} \\
& = \Pi_{\leq}(c) + j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\}.
\end{aligned} \quad (44)$$

Taking the derivative with respect to c yields the differential formulation

$$\begin{aligned}
& u_{\text{dia},z}^c(c) + \frac{\partial j_{\text{dia},z}^c}{\partial c} + \frac{\partial}{\partial x} \left(\frac{\partial J_{x,\leq}}{\partial c} \right) + \frac{\partial}{\partial y} \left(\frac{\partial J_{y,\leq}}{\partial c} \right) \\
& = \frac{\partial \Pi_{\leq}}{\partial c} + j_{\eta,z} \delta\{c^z(\eta) - c\}.
\end{aligned} \quad (45)$$

Neglecting horizontal diffusive tracer fluxes and tracer production simplifies the general relation to

$$u_{\text{dia},z}^c(c) = - \frac{\partial j_{\text{dia},z}^c}{\partial c} + j_{\eta,z} \delta\{c^z(\eta) - c\}. \quad (46)$$

Following (46), the local diatracer velocity (positive into the direction of increasing tracer concentration) across

² Due to $-\int_{-\infty}^c u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c'\} dc' = (c_{\eta} - c)u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\}$ the advective flux across the ocean surface in (42) cancels with the one from (18).

isosurfaces in the interior of the water column is always into the direction of larger $-j_{\text{dia},z}^c$, i.e., into the direction of stronger diasurface diffusive tracer fluxes. Of course, the net diffusive tracer transport is always into the direction of decreasing tracer concentration, but it can be either diverging ($\partial j_{\text{dia},z}^c / \partial c > 0$, i.e., dominated by the transport from the present tracer concentration toward lower one), or converging ($\partial j_{\text{dia},z}^c / \partial c < 0$, i.e., dominated by the transport from higher tracer concentration toward the present one). Divergence is associated with a decreasing volume of high tracer concentrations and an increasing volume of lower ones, i.e., a volume transport from high to low tracer concentrations ($u_{\text{dia},z}^c < 0$). Vice versa, convergence is associated with water mass being transformed from low to high tracer concentrations ($u_{\text{dia},z}^c > 0$). Relation (46) is the local equivalent³ of the integrated formulation (4) and the correct generalization of (18) in Li et al. (2022).

5) RELATION BETWEEN DIATRACER VELOCITY AND MIXING

The combination of (40) and (46) directly formulates how the diatracer exchange flow is linked to local tracer variance dissipation:

$$u_{\text{dia},z}^c(c) = \frac{1}{2} \frac{\partial m}{\partial c} + j_{\eta,z} \delta\{c^z(\eta) - c\}. \quad (47)$$

Following (47), the local diatracer velocity across isosurfaces in the interior of the water column is always into the direction of increased mixing. Relation (47) is the local equivalent of the integrated formulation (9), deduced in the introduction for salinity without salt fluxes across the ocean surface.

g. Integrated budgets and relations

Finally, we will show that integration of the local budgets and relations, derived in the previous sections, recovers the integral formulations presented in the introduction.

1) INTEGRATED VOLUME AND TRACER CONTENT BUDGETS

Integration of the local volume and tracer content budgets (18) and (26) in tracer space over a horizontal area A_z , and combination with (41a) and (41b) yields prognostic equations for volumes $\mathbb{V}_{\leq}(c)$ of all water with tracer concentrations $\leq c$ and their tracer content $\mathbb{C}_{\leq}(c)$:

$$\begin{aligned}
& \frac{\partial}{\partial t} \overbrace{\int D_{\leq}(c) dA_z}^{=\mathbb{V}_{\leq}(c)} + \overbrace{\int \left[\frac{\partial U_{\leq}(c)}{\partial x} + \frac{\partial V_{\leq}(c)}{\partial y} \right] dA_z}^{=-Q_{\leq}(c) - Q_{r,\leq}(c)} + \overbrace{\int u_{\text{dia},z}^c(c) dA_z}^{=Q_{\text{dia}}(c)} \\
& = \underbrace{\int u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\} dA_z}_{=Q_{\eta,\leq}(c)},
\end{aligned} \quad (48a)$$

³ Here, $j_{\eta,z} \delta\{c^z(\eta) - c\} = \partial(j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\}) / \partial c$ holds.

$$\begin{aligned}
& \frac{\partial}{\partial t} \int \overbrace{C_{\leq}(c) dA_z}^{=C_{\leq}(c)} + \int \left[\overbrace{\frac{\partial F_{x,\leq}(c)}{\partial x} + \frac{\partial F_{y,\leq}(c)}{\partial y}}^{=-\mathcal{F}_{\leq}(c)-\mathcal{F}_{r,\leq}(c)} \right] dA_z + \int \overbrace{f_{\text{dia},z}^c(c) dA_z}^{=\mathcal{F}_{\text{dia}}(c)} \\
&= \int \overbrace{\Pi_{\leq}(c) dA_z}^{=\mathbb{P}_{\leq}(c)} \\
&+ \underbrace{\int [c_{\eta} u_{\eta,z} \mathcal{H}_{\leq}\{c_{\eta} - c\} + j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\}] dA_z}_{=\mathcal{F}_{\eta,\leq}(c)}. \quad (48b)
\end{aligned}$$

The volumes are bounded by an open boundary and the isosurface with tracer concentration c . Figure 1 illustrates volumes for the special case of a stable salinity stratification. The equations derived here are also valid for nonmonotonic tracer distributions with inversions and noncontiguous volumes. The evolution of the volumes and their tracer content depends on the integrated fluxes entering across the open boundary ($Q_{\leq}$, $\mathcal{F}_{\leq}$), integrated diatracer fluxes (Q_{dia} , $\mathcal{F}_{\text{dia}}$) and integrated fluxes entering across the ocean surface (Q_{η} , $\mathcal{F}_{\eta}$). Incoming integrated fluxes due to rivers ($Q_{r,\leq}$, $\mathcal{F}_{r,\leq}$) are treated separately from the integrated open boundary fluxes. The integrated tracer production is denoted by $\mathbb{P}_{\leq}$. The integrated diatracer tracer flux is given by

$$\mathcal{F}_{\text{dia}}(c) \stackrel{(39)}{=} cQ_{\text{dia}}(c) + \underbrace{\int f_{\text{dia},z}^c(c) dA_z}_{=\mathcal{J}_{\text{dia}}(c)}, \quad (49)$$

and recovers (2).

The general formulation of integrated fluxes across the ocean surface and due to rivers in (48a) and (48b) supports loads with different tracer concentrations. For the special case of freshwater fluxes in salinity space the formulation simplifies, because the associated volume fluxes per salinity class are given by $q_{\eta}(S) = \partial Q_{\eta,\leq}/\partial S = Q_{\eta}\delta\{S_{\eta} - S\}$ and $q_r(S) = \partial Q_{r,\leq}/\partial S = Q_r\delta\{S_r - S\}$ with $S_{\eta} = S_r = 0$, respectively. Then the integrated fluxes become

$$\begin{aligned}
Q_{\eta,\leq}(S) &= Q_{\eta}, \quad \mathcal{J}_{\eta,\leq} = \mathcal{F}_{\eta,\leq} = 0 \\
&\text{(integrated freshwater surface fluxes),} \quad (50a)
\end{aligned}$$

$$\begin{aligned}
Q_{r,\leq}(S) &= Q_r, \quad \mathcal{J}_{r,\leq} = \mathcal{F}_{r,\leq} = 0 \\
&\text{(integrated freshwater river discharge).} \quad (50b)
\end{aligned}$$

With these integrated freshwater fluxes the integral budgets (48a) and (48b) recover (5a) and (5b) used by, e.g., MacCready et al. (2002). Analogously, horizontal integration of (C15) and (C16) also recover Walin's (1a) and (1b).

2) RELATION BETWEEN INTEGRATED DIATRACER DIFFUSIVE TRACER FLUX AND MIXING

The integrated diatracer diffusive tracer flux $\mathcal{J}_{\text{dia}}$ obeys

$$\mathcal{J}_{\text{dia}}(c) \stackrel{(40)}{=} -\frac{1}{2} \underbrace{\int m(c) dA_z}_{=\mathbb{M}(c)} = -\frac{1}{2} \frac{\partial}{\partial c} \underbrace{\int M_{\leq}(c) dA_z}_{=\mathbb{M}_{\leq}(c)}, \quad (51)$$

which recovers (8). The integrated mixing per tracer class m can be either obtained by horizontal integration of the local mixing per tracer class m , or following (6) as the derivative of the integrated tracer mixing $\mathbb{M}_{\leq}$.

3) INTEGRATED INTERNAL TRACER CONTENT BUDGET

By combination of the integral budgets (48a) and (48b), or directly by horizontal integration of the local formulation (42), the budget for the integrated internal tracer content can be obtained as

$$\begin{aligned}
& \frac{\partial}{\partial t} \left(\overbrace{C_{\leq} - cV_{\leq}}^{=C_{I,\leq}(c)} - \overbrace{(\mathcal{F}_{\leq} - cQ_{\leq})}^{=\mathcal{F}_{I,\leq}(c)} - \overbrace{(\mathcal{F}_{r,\leq} - cQ_{r,\leq})}^{=\mathcal{F}_{Ir,\leq}(c)} \right) + \mathcal{J}_{\text{dia}}(c) \\
&= \mathbb{P}_{\leq}(c) + \underbrace{(\mathcal{F}_{\eta,\leq} - cQ_{\eta,\leq})}_{=\mathcal{F}_{I\eta,\leq}(c)}, \quad (52)
\end{aligned}$$

which recovers the internal heat content budget (12) in Holmes et al. (2019) and the internal salt content budget (10) in Bladwell et al. (2021). A comparison to the notation of Bladwell et al. (2021) is given in Table 2.

With the budget for the internal salt content, the mixing per salinity class inside a classical estuarine volume can be diagnosed,

$$\begin{aligned}
m(S) &= 2 \left\{ \frac{\partial}{\partial t} [\mathbb{S}_{\leq}(S) - S\mathbb{V}_{\leq}(S)] - [\mathcal{F}_{\leq}(S) - SQ_{\leq}(S)] \right. \\
&\quad \left. + S(Q_r + Q_{\eta}) \right\}, \quad (53)
\end{aligned}$$

where (50a), (50b), and (51) has been used. This formulation generalizes (7) in Li et al. (2022) by including integrated fluxes across the ocean surface and the open boundary. For an estuarine volume completely bounded by the isohaline the integrated open boundary fluxes $Q_{\leq}(S)$ and $\mathcal{F}_{\leq}(S)$ do not exist (MacCready and Geyer 2001; Burchard 2020). In this case, and after sufficiently long time averaging, (53) recovers the universal law of estuarine mixing (7).

4) RELATION BETWEEN INTEGRATED DIATRACER VOLUME AND DIFFUSIVE TRACER FLUXES

The integrated formulation of relation (46) reads

$$Q_{\text{dia}}(c) = -\frac{\partial \mathcal{J}_{\text{dia}}}{\partial c} + \frac{\partial}{\partial c} \underbrace{\int j_{\eta,z} \mathcal{H}_{\leq}\{c^z(\eta) - c\} dA_z}_{=\mathcal{J}_{\eta,\leq}}, \quad (54)$$

and recovers (4). In contrast to the local relation (46), by means of the divergence theorem the integral relation (54) does not require to neglect horizontal diffusive tracer fluxes in general, but only across the open boundary. For a global volume such an open boundary does not even exist, and relation (54) holds for any horizontal diffusive tracer fluxes.

5) RELATION BETWEEN INTEGRATED DIATRACER VOLUME FLUX AND MIXING

Combination of (51) and (54), or direct integration of the local relation (47), yields

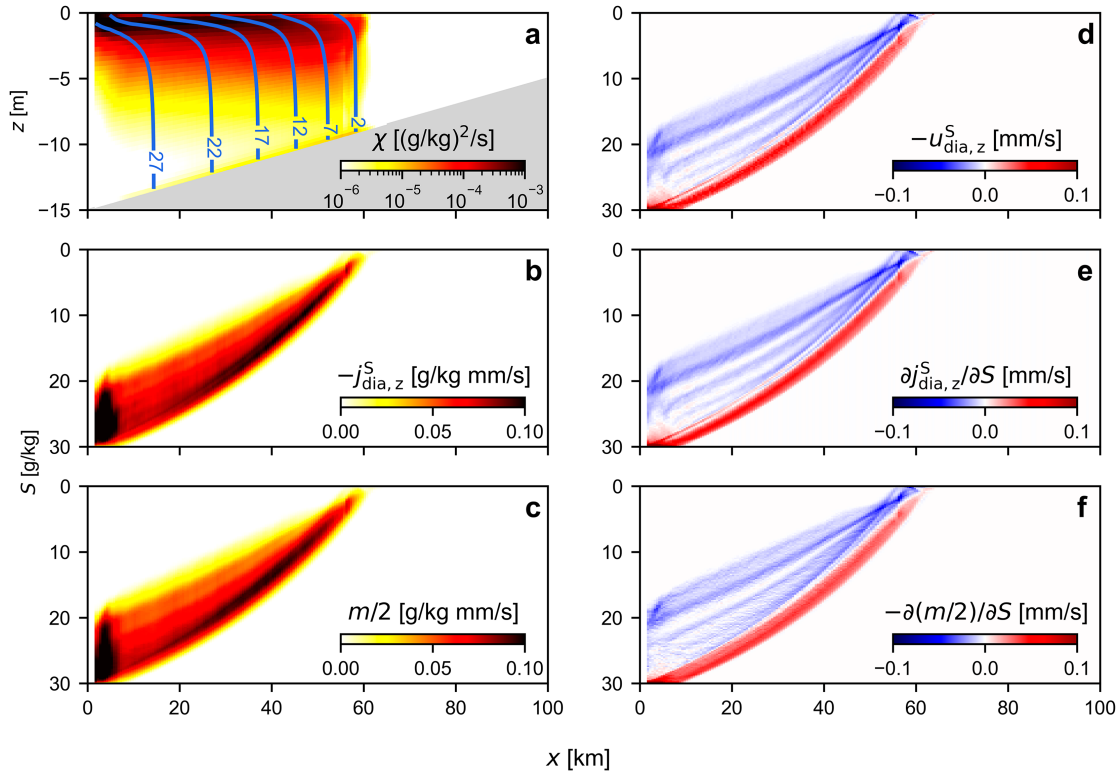


FIG. 4. Model results for an idealized tidal estuary in a periodic state. (a) Tidally averaged salinity distribution (blue contours) and salinity variance dissipation χ (colored) are shown. (b)–(d) The tidal mean diahaline diffusive salt flux $j^S_{\text{dia},z}$, mixing per salinity class m , and diahaline velocity $u^S_{\text{dia},z}$ have been diagnosed during model runtime, independently from (26), (38), and (18), respectively. In (b) and (d), the diahaline fluxes from higher to lower salinity are negative. (e),(f) The quantities are calculated from (b) and (c), respectively. The almost perfect agreement between the diahaline quantities in (b) and (c), as well as in (d)–(f) demonstrates the analytically derived relations (40), (46), and (47).

$$Q_{\text{dia}} = \frac{1}{2} \frac{\partial \mathfrak{m}}{\partial c} + \frac{\partial \mathcal{J}_{\eta, \leq}}{\partial c}, \quad (55)$$

and generalizes (9) deduced in the introduction.

3. Demonstration

a. Idealized steady state and a word of caution

In a steady-state balance between vertical advection and vertical diffusion the tracer equation (12) reduces to $w \partial c^z / \partial z = \partial (K_v \partial c^z / \partial z) / \partial z$. Assuming the resulting horizontally homogeneous tracer distribution is strictly monotonic with $\partial c^z / \partial z > 0$, the mixing inside an arbitrary dz interval is given by $dM = \chi dz = 2K_v (\partial c^z / \partial z)^2 dz = 2K_v \partial c^z / \partial z dc \equiv mdc$. Combination of both equations yields $w \partial c^z / \partial z = \partial (m/2) / \partial z = \partial (m/2) / \partial c \partial c^z / \partial z$ and thus $w = \partial (m/2) / \partial c$, which resembles the newly derived relation between the diatracer velocity and mixing (47). Indeed, for this special setting $u^c_{\text{dia},z} \stackrel{(25)}{=} u^z_{\text{dia},z} \stackrel{(21), (22)}{=} w$ holds, and the simplified notation (omitting the superscripts for the actual coordinate space) is appropriate as long as the quantities are evaluated in the correct space. However, in more general settings we strongly encourage the use of the precise notation developed during the course of the manuscript, clearly indicating the coordinate

space and preventing misunderstandings about derivatives. In this context, it is also important to remember that derivatives of the local quantities with respect to a tracer are evaluated at constant horizontal position (x, y) , i.e., should not be misinterpreted as three-dimensional gradients in tracer direction.

b. Model results for an idealized tidal estuary

To demonstrate the derived relations in salinity space, the diagnostic calculation of diahaline mixing, volume and salt fluxes has been implemented into the coastal ocean model GETM (Burchard and Bolding 2002; Klingbeil et al. 2018). A simulation has been carried out for an idealized tidal estuary, which already represents realistic features of water mass transformation and overturning circulation, while still being a simple benchmark test case. Detailed results from realistic ocean modeling applications are presented in Henell et al. (2023) and Reese et al. (2023).

The estuary has a length of 100 km and a width of 500 m. The water depth decreases linearly from 15 m at the open ocean boundary to 5 m at the river end (see Fig. 4a). The estuary is forced by a harmonic semidiurnal tide with an elevation amplitude of 0.6 m and a constant salinity of 30 g kg^{-1} at the ocean boundary. At the river end a freshwater discharge of $50 \text{ m}^3 \text{ s}^{-1}$ is prescribed. Horizontal diffusive fluxes

are switched off. The estuarine circulation is discussed in detail in Burchard et al. (2019) and Klingbeil et al. (2019), such that we focus on the new diahaline analyses here. Figures 4b and 4c show the diagnosed diahaline diffusive fluxes and mixing between incoming high-saline ocean water and estuarine water of lower salinities. The resulting diahaline exchange flow in Figs. 4d–f indicates the transformation of the incoming high-saline water masses into lower-salinity water all the way up to the reversal point 60 km up-estuary, and the transformation of the outflowing brackish water masses into higher-salinity water again while flowing back toward the open ocean. This overturning circulation in salinity space complements the classical picture of estuarine circulation (e.g., Hansen and Rattray 1965).

4. Summary and conclusions

In this paper we analytically derived the local water mass transformation (WMT) framework for an individual water column. The derivation is based on the mapping of the governing equations from geopotential coordinates to an arbitrary tracer space. Exact local definitions for the effective vertical diasurface velocity, tracer flux and its diffusive contribution are given in (20), (30), and (34a), respectively. Mixing is defined in terms of the dissipation of tracer variance according to (37) and (38). In tracer space new relations between the local diatracer quantities and the mixing per tracer class have been derived as (46), (40), and (47). The key relation (47) between the effective vertical diatracer velocity and the mixing per tracer class directly formulates how the overturning circulation is linked to local tracer variance dissipation. It was demonstrated for different settings. The relations could also be used to study the diapycnal mixing and circulation in bottom boundary layers in the abyssal ocean described by Ferrari et al. (2016), and consistently link it to the large-scale overturning circulation. The local quantities and relations in tracer space represent an intermediate formulation between the direct ones in geopotential coordinates, for example presented by Garrett et al. (1995) and Ferrari et al. (2016), and the ones from the integral WMT framework presented in the introduction. The effective vertical diasurface quantities offer a convenient calculation of integrated diasurface fluxes by simple integration over the horizontal area instead of the complexly shaped area of the isosurface. By horizontally integrating the budget equations in tracer space and the relations between the diatracer quantities we finally recovered the well-known integral WMT formulations. Similar to the extension of the integral formulation by Hieronymus et al. (2014), an extension of our local formulation to multidimensional tracer space is possible. A summary of local and integral quantities and equations presented in this paper, as well as a comparison with published formulations, is given in Tables 1 and 2. The local diatracer fluxes and the local diatracer mixing provide new and valuable information on the spatial distribution of these quantities, and will enable new insights for coastal and large-scale oceanography.

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Data availability statement. Model data shown in Fig. 4 have been obtained from a simulation with the coastal ocean model GETM (www.getm.eu). The model setup, simulation data, and scripts are archived at <https://doi.org/10.5281/zenodo.8136528> (Klingbeil 2023a). The used model source code is archived at <https://doi.org/10.5281/zenodo.8137091> (Klingbeil 2023b).

APPENDIX A

Unified Notation

For brevity we will use

$$D_{\leq, >}(s) = \int_{-H}^{\eta} \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz \quad (\text{A1})$$

as a combined notation for (15a) and (15b) throughout the appendixes. In both cases the differential thickness is given by

$$\pm \frac{\partial D_{\leq, >}(s)}{\partial s} \stackrel{(\text{A1})}{=} \int_{-H}^{\eta} \delta\{s^z(z) - s\} dz. \quad (\text{A2})$$

In (A2) and in the following the upper sign (here “+”) always refers to the “ $\leq$ ” case and the lower sign (here “−”) to the “ $>$ ” case. In analogy to $D_{\leq, >}$ and $\pm \partial D_{\leq, >}/\partial s$, for any quantity ψ^z the cumulative and differential formulations in s space can be obtained by

$$\Psi_{\leq, >}(s) = \int_{-H}^{\eta} \psi^z(z) \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz, \quad (\text{A3})$$

$$\pm \frac{\partial \Psi_{\leq, >}(s)}{\partial s} = \int_{-H}^{\eta} \psi^z(z) \delta\{s^z(z) - s\} dz. \quad (\text{A4})$$

APPENDIX B

Mapping as a Generalized Coordinate Transformation

In this paper the vertical coordinate z is replaced by an arbitrary coordinate s . For geometric coordinates, e.g., geopotential ($s = z$) or sigma coordinates with $s = \sigma = (z - \eta)/(\eta + H)$, the coordinate distribution $s^z(z)$ is strictly monotonic between the bottom at $z = -H(x, y)$ and the ocean surface at $z = \eta(x, y, t)$. The same holds for stably stratified temperature or salinity distributions (see Figs. 2a,c). Under this monotonicity constraint there exists a well-defined coordinate transformation to a unique inverse function $z^s(s)$ such that an arbitrary quantity ψ can be uniquely defined in s coordinates by

$$\psi^s(s) = \psi^z[z^s(s)] \quad \text{for strictly monotonic } s^z(z), \quad (\text{B1})$$

with superscripts indicating the coordinate space the different functions are defined for. In contrast, for nonmonotonic distributions $s^z(z)$, e.g., for tracer coordinates where single tracer values may occur at multiple positions in the water column (e.g., Fig. 2e), there exists no function $z^s(s)$ and the usual transformation procedure (B1) cannot be applied. In this case a general mapping to s space can formally be defined by thickness-weighted quantities in infinitesimally small bins according to (B2a),

$$\psi^s(s) = \frac{\int_{-H}^{\eta} \psi^z(z) \delta\{s^z(z) - s\} dz}{\int_{-H}^{\eta} \delta\{s^z(z) - s\} dz}, \quad (\text{B2a})$$

$$= \frac{\pm \frac{\partial \Psi_{\leq, >}(s)}{\partial s}}{\pm \frac{\partial D_{\leq, >}(s)}{\partial s}}. \quad (\text{B2b})$$

The equivalent formulation (B2b) is of more practical use and is based on the cumulative thickness $D_{\leq, >}$ and the cumulative quantity $\Psi_{\leq, >}$ defined in (A1) and (A3). By construction (B2a) and (B2b) map data from z coordinates to s levels, and do not require any monotonicity constraints on the coordinate distribution $s^z(z)$. For strictly monotonic functions the integrals in (B2a) can be transformed by means of

$$\begin{aligned} \int_{-H}^{\eta} \psi^z(z) \delta\{s^z(z) - s\} dz &= \int_{-\infty}^{+\infty} \psi^z[z^s(s')] \left| \frac{\partial z^s}{\partial s} \right| \delta\{s' - s\} ds' \\ &= \psi^z[z^s(s)] \left| \frac{\partial z^s}{\partial s} \right| \end{aligned} \quad (\text{B3})$$

for strictly monotonic $s^z(z)$,

where in the last step the sampling property of the δ distribution was used. Analogously, the differential thickness $\pm \partial D_{\leq, >}/\partial s$ simplifies to the magnitude of the Jacobian of the coordinate transformation,

$$\pm \frac{\partial D_{\leq, >}}{\partial s} = \left| \frac{\partial z^s}{\partial s} \right| = \left| \frac{\partial s^z}{\partial z} \right|^{-1} \quad \text{for strictly monotonic } s^z(z), \quad (\text{B4})$$

and (B2a) recovers (B1). The formulations (B2a) and (B2b) are motivated by (13) and (14) in Klingbeil et al. (2019) from the context of generalized thickness-weighted averaging.

APPENDIX C

Derivation of the p-Generalized Tracer Budget in s Space

Because the integrations for volume, tracer and tracer-square content are similar, the following derivations consider the tracer concentration c to the power of an arbitrary integer $p \geq 0$. The flux of c^p in the x direction (the fluxes into the other directions are defined accordingly) is given by

$$\begin{aligned} f_x^{(p)} &= u(c^z)^p - \overbrace{K_h \frac{\partial (c^z)^p}{\partial x}}^{=f_x^{(p)}}, \\ &= p(c^z)^{p-1} f_x - (p-1)(c^z)^p u, \end{aligned} \quad (\text{C1})$$

with $f_x^{(0)} = u$ and $f_x^{(1)} = f_x$ being the velocity and tracer flux, respectively. According to (C1), for $p \geq 2$, $f_x^{(p)}$ is determined by u and f_x . With the incompressibility constraint (10) it can be shown that

$$\begin{aligned} \frac{\partial f_x^{(p)}}{\partial x} + \frac{\partial f_y^{(p)}}{\partial y} + \frac{\partial f_z^{(p)}}{\partial z} &= p(c^z)^{p-1} \left(\frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z} \right) \\ &\quad - \frac{p(p-1)}{2} (c^z)^{p-2} \times \underbrace{2 \left[K_h \left(\frac{\partial c^z}{\partial x} \right)^2 + K_h \left(\frac{\partial c^z}{\partial y} \right)^2 + K_v \left(\frac{\partial c^z}{\partial z} \right)^2 \right]}_{=\chi}. \end{aligned} \quad (\text{C2})$$

Multiplication of the tracer equation (12) by $p(c^z)^{p-1}$ and reformulating the fluxes with (C2) yields the prognostic equation for $(c^z)^p$:

$$\frac{\partial (c^z)^p}{\partial t} + \frac{\partial f_x^{(p)}}{\partial x} + \frac{\partial f_y^{(p)}}{\partial y} + \frac{\partial f_z^{(p)}}{\partial z} = p(c^z)^{p-1} \pi - \frac{p(p-1)}{2} (c^z)^{p-2} \chi. \quad (\text{C3})$$

Boundary fluxes across the ocean surface and the bottom per unit horizontal area (positive into the water column) are defined by

$$f_{\eta, z}^{(p)} = f_{\eta}^{(p)} |\mathbf{n}_{\eta} \cdot \mathbf{z}|^{-1} \quad (\text{C4a})$$

$$= f_{\eta}^{(p)} |\nabla(\eta - z)| \quad (\text{C4b})$$

$$= \{[c^z(\eta)]^p [\mathbf{u}(\eta) - \mathbf{u}_{\eta}] + \mathbf{j}^{(p)}(\eta)\} \cdot \nabla(\eta - z) \quad (\text{C4c})$$

$$= [c^z(\eta)]^p \frac{\partial \eta}{\partial t} + f_x^{(p)}(\eta) \frac{\partial \eta}{\partial x} + f_y^{(p)}(\eta) \frac{\partial \eta}{\partial y} - f_z^{(p)}(\eta) \quad (\text{C4d})$$

$$\stackrel{(\text{C1})}{=} p[c^z(\eta)]^{p-1} f_{\eta, z} - (p-1)[c^z(\eta)]^p u_{\eta, z}, \quad \text{and} \quad (\text{C4e})$$

$$f_{-H, z}^{(p)} = f_{-H}^{(p)} |\mathbf{n}_{-H} \cdot \mathbf{z}|^{-1} \quad (\text{C5a})$$

$$= f_{-H}^{(p)} |\nabla(z + H)| \quad (\text{C5b})$$

$$= \{[c^z(-H)]^p [\mathbf{u}(-H) + \mathbf{j}^{(p)}(-H)]\} \cdot \nabla(z + H) \quad (\text{C5c})$$

$$= f_x^{(p)}(-H) \frac{\partial H}{\partial x} + f_y^{(p)}(-H) \frac{\partial H}{\partial y} - f_z^{(p)}(-H) \quad (\text{C5d})$$

$$\stackrel{(\text{C1})}{=} p[c^z(-H)]^{p-1} f_{-H, z} - (p-1)[c^z(-H)]^p u_{-H, z}, \quad (\text{C5e})$$

with the unit normal vectors $\mathbf{n}_{\eta} = \nabla(\eta - z)/|\nabla(\eta - z)|$ and $\mathbf{n}_{-H} = \nabla(z + H)/|\nabla(z + H)|$, and the vertical unit vector $\mathbf{z}$. For $p = 0$ the relations (C4d) and (C5d) recover the well-known kinematic boundary conditions (11a) and (11b), and for $p = 1$ the tracer flux boundary conditions (13a) and

(13b). According to (C4e) and (C5e), for $p \geq 2$ the boundary fluxes are determined by the ones for volume and tracer.

Following (A3) the p -generalized cumulative tracer content is defined as

$$C_{\leq, >}^{(p)}(s) = \int_{-H}^{\eta} [c^z(z)]^p \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz, \quad (\text{C6})$$

with $C_{\leq, >}^{(0)} = D_{\leq, >}$ and $C_{\leq, >}^{(1)} = C_{\leq, >}$. In analogy the p -generalized cumulative tracer fluxes are defined as

$$F_{x, \leq, >}^{(p)}(s) = \int_{-H}^{\eta} f_x^{(p)}(z) \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz, \quad (\text{C7a})$$

$$F_{y, \leq, >}^{(p)}(s) = \int_{-H}^{\eta} f_y^{(p)}(z) \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz, \quad (\text{C7b})$$

with $F_{x, \leq, >}^{(0)} = U_{\leq, >}$, $F_{y, \leq, >}^{(0)} = V_{\leq, >}$, $F_{x, \leq, >}^{(1)} = F_{x, \leq, >}$ and $F_{y, \leq, >}^{(1)} = F_{y, \leq, >}$. For (C6)–(C7b) Leibniz rule (E1) yields

$$\begin{aligned} \frac{\partial C_{\leq, >}^{(p)}(s)}{\partial t} = & \mp \int_{-H}^{\eta} (c^z)^p \frac{\partial s^z}{\partial t} \delta \{s^z(z) - s\} dz \\ & + \int_{-H}^{\eta} \frac{\partial (c^z)^p}{\partial t} \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz \\ & + [c^z(\eta)]^p \frac{\partial \eta}{\partial t} \mathcal{H}_{\leq, >} \{s_{\eta} - s\}, \end{aligned} \quad (\text{C8a})$$

$$\begin{aligned} \frac{\partial F_{x, \leq, >}^{(p)}(s)}{\partial x} = & \mp \int_{-H}^{\eta} f_x^{(p)} \frac{\partial s^z}{\partial x} \delta \{s^z(z) - s\} dz \\ & + \int_{-H}^{\eta} \frac{\partial f_x^{(p)}}{\partial x} \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz \\ & + f_x^{(p)}(\eta) \frac{\partial \eta}{\partial x} \mathcal{H}_{\leq, >} \{s_{\eta} - s\} \\ & + f_x^{(p)}(-H) \frac{\partial H}{\partial x} \mathcal{H}_{\leq, >} \{s_{-H} - s\}, \end{aligned} \quad (\text{C8b})$$

$$\begin{aligned} \frac{\partial F_{y, \leq, >}^{(p)}(s)}{\partial y} = & \mp \int_{-H}^{\eta} f_y^{(p)} \frac{\partial s^z}{\partial y} \delta \{s^z(z) - s\} dz \\ & + \int_{-H}^{\eta} \frac{\partial f_y^{(p)}}{\partial y} \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz \\ & + f_y^{(p)}(\eta) \frac{\partial \eta}{\partial y} \mathcal{H}_{\leq, >} \{s_{\eta} - s\} \\ & + f_y^{(p)}(-H) \frac{\partial H}{\partial y} \mathcal{H}_{\leq, >} \{s_{-H} - s\}. \end{aligned} \quad (\text{C8c})$$

Application of (E2) for the vertical flux gives

$$\begin{aligned} & \int_{-H}^{\eta} \frac{\partial}{\partial z} [\mathcal{H}_{\leq, >} \{s^z(z) - s\} f_z^{(p)}] dz \\ & = \mp \int_{-H}^{\eta} \delta \{s^z(z) - s\} f_z^{(p)} \frac{\partial s^z}{\partial z} dz + \int_{-H}^{\eta} \mathcal{H}_{\leq, >} \{s^z(z) - s\} \frac{\partial f_z^{(p)}}{\partial z} dz \\ & \equiv f_z^{(p)}(\eta) \mathcal{H}_{\leq, >} \{s_{\eta} - s\} - f_z^{(p)}(-H) \mathcal{H}_{\leq, >} \{s_{-H} - s\}. \end{aligned} \quad (\text{C9})$$

With (C4d), (C5d), and (C9), summation of (C8a)–(C8c) yields

$$\begin{aligned} & \frac{\partial C_{\leq, >}^{(p)}(s)}{\partial t} + \frac{\partial F_{x, \leq, >}^{(p)}(s)}{\partial x} + \frac{\partial F_{y, \leq, >}^{(p)}(s)}{\partial y} \\ & = \mp \int_{-H}^{\eta} \left[(c^z)^p \frac{\partial s^z}{\partial t} + f_x^{(p)} \frac{\partial s^z}{\partial x} + f_y^{(p)} \frac{\partial s^z}{\partial y} + f_z^{(p)} \frac{\partial s^z}{\partial z} \right] \delta \{s^z(z) - s\} dz \\ & \quad + \int_{-H}^{\eta} \left[\frac{\partial (c^z)^p}{\partial t} + \frac{\partial f_x^{(p)}}{\partial x} + \frac{\partial f_y^{(p)}}{\partial y} + \frac{\partial f_z^{(p)}}{\partial z} \right] \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz \\ & \quad + f_{\eta, z}^{(p)} \mathcal{H}_{\leq, >} \{s_{\eta} - s\} + f_{-H, z}^{(p)} \mathcal{H}_{\leq, >} \{s_{-H} - s\}. \end{aligned} \quad (\text{C10})$$

The integrand of the first integral on the right hand side of (C10) can be further reformulated in terms of the local diasurface flux $f_{\text{dia}}^{(p), z}$, defined as the component of the relative flux normal to the isosurface that is currently located at the specific position z and moving with velocity $\mathbf{u}_s$:

$$\begin{aligned} f_{\text{dia}}^{(p), z} &= (c^z)^p (\mathbf{u} - \mathbf{u}_s) \cdot \mathbf{n} + \mathbf{j}^{(p)} \cdot \mathbf{n} \\ &= \frac{1}{|\nabla s^z|} \left[(c^z)^p \frac{Ds^z}{Dt} + f_x^{(p)} \frac{\partial s^z}{\partial x} + f_y^{(p)} \frac{\partial s^z}{\partial y} + f_z^{(p)} \frac{\partial s^z}{\partial z} \right] \end{aligned} \quad (\text{C11a})$$

$$= \frac{1}{|\nabla s^z|} \left[(c^z)^p \frac{\partial s^z}{\partial t} + f_x^{(p)} \frac{\partial s^z}{\partial x} + f_y^{(p)} \frac{\partial s^z}{\partial y} + f_z^{(p)} \frac{\partial s^z}{\partial z} \right] \quad (\text{C11b})$$

$$\stackrel{(\text{C1})}{=} p(c^z)^{p-1} f_{\text{dia}}^z - (p-1)(c^z)^p u_{\text{dia}}^z. \quad (\text{C11c})$$

The local diasurface velocity and the local diasurface tracer flux are given by $f_{\text{dia}}^{(0), z} = u_{\text{dia}}^z$ in (22) and $f_{\text{dia}}^{(1), z} = f_{\text{dia}}^z$ in (32), respectively. With the unit normal vector $\mathbf{n} = \nabla s^z / |\nabla s^z|$, the diasurface fluxes are positive into the direction of increasing s . In analogy to the formulations of the fluxes across the ocean surface and bottom (C4a) and (C5a), the associated local diasurface tracer flux per unit horizontal area formally can be defined as

$$f_{\text{dia}, z}^{(p), z} = f_{\text{dia}}^{(p), z} |\mathbf{n} \cdot \mathbf{z}|^{-1} = f_{\text{dia}}^{(p), z} \left| \frac{\partial s^z}{\partial z} \right|^{-1} |\nabla s^z|. \quad (\text{C12})$$

Using (C11b) and (C12), the first integral on the right hand side of (C10) can be defined as the effective vertical diasurface flux

$$f_{\text{dia}, z}^{(p), s}(s) = \int_{-H}^{\eta} f_{\text{dia}, z}^{(p), z}(z) \left| \frac{\partial s^z}{\partial z} \right| \delta \{s^z(z) - s\} dz, \quad (\text{C13})$$

The integrand of the second integral on the right hand side of (C10) can be replaced by inserting the prognostic equation for $(c^z)^p$, (C3), such that the following budget equation for the p -generalized cumulative tracer content can be derived:

$$\begin{aligned} & \frac{\partial C_{\leq, >}^{(p)}(s)}{\partial t} + \frac{\partial F_{x, \leq, >}^{(p)}(s)}{\partial x} + \frac{\partial F_{y, \leq, >}^{(p)}(s)}{\partial y} \pm f_{\text{dia}, z}^{(p), s}(s) \\ & = \int_{-H}^{\eta} \left[p(c^z)^{p-1} \pi - \frac{p(p-1)}{2} (c^z)^{p-2} \chi \right] \mathcal{H}_{\leq, >} \{s^z(z) - s\} dz \\ & \quad + f_{\eta, z}^{(p)} \mathcal{H}_{\leq, >} \{s_{\eta} - s\} + f_{-H, z}^{(p)} \mathcal{H}_{\leq, >} \{s_{-H} - s\}. \end{aligned} \quad (\text{C14})$$

Neglecting bottom fluxes, for $p = 0$ the volume budget

$$\frac{\partial D_{\leq, >}(s)}{\partial t} + \frac{\partial U_{\leq, >}(s)}{\partial x} + \frac{\partial V_{\leq, >}(s)}{\partial y} \pm u_{\text{dia}, z}^s(s) = u_{\eta, z}^s \mathcal{H}_{\leq, >} \{s_{\eta} - s\}, \quad (\text{C15})$$

and for $p = 1$ the tracer budget

$$\begin{aligned} & \frac{\partial C_{\leq, >}(s)}{\partial t} + \frac{\partial F_{x, \leq, >}(s)}{\partial x} + \frac{\partial F_{y, \leq, >}(s)}{\partial y} \pm f_{\text{dia}, z}^s(s) \\ &= \Pi_{\leq, >}(s) + f_{\eta, z} \mathcal{H}_{\leq, >}\{s_{\eta} - s\}, \end{aligned} \quad (\text{C16})$$

with the cumulative tracer production

$$\Pi_{\leq, >}(s) = \int_{-H}^{\eta} \pi(z) \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz \quad (\text{C17})$$

are obtained, respectively. Taking the derivative of (C14) with respect to s and using (B2b) yields the differential formulation

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\pm \frac{\partial D_{\leq, >}}{\partial s} c^{(p), s} \right) + \frac{\partial}{\partial x} \left(\pm \frac{\partial D_{\leq, >}}{\partial s} f_x^{(p), s} \right) + \frac{\partial}{\partial y} \left(\pm \frac{\partial D_{\leq, >}}{\partial s} f_y^{(p), s} \right) \\ &+ \frac{\partial f_{\text{dia}, z}^{(p), s}}{\partial s} = \int_{-H}^{\eta} \left[p(c^z)^{p-1} \pi - \frac{p(p-1)}{2} (c^z)^{p-2} \chi \right] \delta\{s^z(z) - s\} dz \\ &+ f_{\eta, z}^{(p)} \delta\{s_{\eta} - s\} + f_{-H, z}^{(p)} \delta\{s_{-H} - s\}, \end{aligned} \quad (\text{C18})$$

with the thickness-weighted quantities in s space, $c^{(p), s} = (\partial C_{\leq, >}^{(p)} / \partial s) / (\partial D_{\leq, >} / \partial s)$, $f_x^{(p), s} = (\partial F_{x, \leq, >}^{(p)} / \partial s) / (\partial D_{\leq, >} / \partial s)$ and $f_y^{(p), s}$ accordingly, from (B2b). For strictly monotonic coordinates, i.e., with (B4), the budget (C18) with $p = 0$ and $p = 1$ recovers the budget equations in generalized vertical coordinates which are the basis for the layer-integrated equations in ocean models, see, e.g., Griffies (2004) and Klingbeil et al. (2018).

APPENDIX D

Further Relations in Tracer Space

For tracer coordinates, i.e., for $s = c$, and by means of the Newton–Leibniz theorem the following useful transformation relation holds for an arbitrary quantity ψ :

$$\begin{aligned} & \int_{-H}^{\eta} (c^z)^p \psi^z \mathcal{H}_{\leq, >}\{c^z(z) - c\} dz \\ &= \int_{-H}^{\eta} (c^z)^p \psi^z \mathcal{H}_{\leq, >}\{c^z(z) - (\mp \infty)\} dz \\ &+ \int_{\mp \infty}^c \left[\frac{\partial}{\partial c'} \int_{-H}^{\eta} (c^z)^p \psi^z \mathcal{H}_{\leq, >}\{c^z(z) - c'\} dz \right] dc' \\ &= \pm \int_{\mp \infty}^c \left[\int_{-H}^{\eta} (c^z)^p \psi^z \delta\{c^z(z) - c'\} dz \right] dc' \\ &= \pm \int_{\mp \infty}^c (c')^p \left[\int_{-H}^{\eta} \psi^z \delta\{c^z(z) - c'\} dz \right] dc' \\ &= \pm \int_{\mp \infty}^c (c')^p \left[\pm \frac{\partial}{\partial c'} \int_{-H}^{\eta} \psi^z \mathcal{H}_{\leq, >}\{c^z(z) - c'\} dz \right] dc' \\ &\stackrel{(\text{A3})}{=} \pm \int_{\mp \infty}^c (c')^p \left(\pm \frac{\partial \Psi_{\leq, >}}{\partial c'} \right) dc' \quad (\text{D1a}) \\ &= \int_{-\infty}^{+\infty} (c')^p \left(\pm \frac{\partial \Psi_{\leq, >}}{\partial c'} \right) \mathcal{H}_{\leq, >}\{c^z(z) - c'\} dc' \\ &\stackrel{(\text{B2b})}{=} \int_{-\infty}^{+\infty} (c')^p \left[\pm \frac{\partial D_{\leq, >}}{\partial c'} \psi^z(c') \right] \mathcal{H}_{\leq, >}\{c^z(z) - c'\} dc'. \end{aligned}$$

By means of (D1a), the integration on the right hand side of (C14) can be carried out in tracer space,

$$\begin{aligned} & \frac{\partial C_{\leq, >}^{(p)}(c)}{\partial t} + \frac{\partial F_{x, \leq, >}^{(p)}(c)}{\partial x} + \frac{\partial F_{y, \leq, >}^{(p)}(c)}{\partial y} \pm f_{\text{dia}, z}^{(p), c}(c) \\ &= \pm \int_{\mp \infty}^c \left[p(c')^{p-1} \left(\pm \frac{\partial \Pi_{\leq, >}}{\partial c'} \right) - \frac{p(p-1)}{2} (c')^{p-2} \left(\pm \frac{\partial M_{\leq, >}}{\partial c'} \right) \right] dc' \\ &+ f_{\eta, z}^{(p)} \mathcal{H}_{\leq, >}\{c_{\eta} - c\} + f_{-H, z}^{(p)} \mathcal{H}_{\leq, >}\{c_{-H} - c\}, \end{aligned} \quad (\text{D2})$$

with the cumulative tracer production $\Pi_{\leq, >}$ defined in (C17), and the cumulative tracer mixing $M_{\leq, >}(s) = \int_{-H}^{\eta} \chi(z) \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz$. Subsequent derivation with respect to c yields

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\pm \frac{\partial D_{\leq, >}}{\partial c} c^p \right) + \frac{\partial}{\partial x} \left[\pm \frac{\partial D_{\leq, >}}{\partial c} f_x^{(p), c} \right] + \frac{\partial}{\partial y} \left[\pm \frac{\partial D_{\leq, >}}{\partial c} f_y^{(p), c} \right] \\ &+ \frac{\partial f_{\text{dia}, z}^{(p), c}}{\partial c} = p c^{p-1} \left(\pm \frac{\partial \Pi_{\leq, >}}{\partial c} \right) - \frac{p(p-1)}{2} c^{p-2} \left(\pm \frac{\partial M_{\leq, >}}{\partial c} \right) \\ &+ f_{\eta, z}^{(p)} \delta\{c_{\eta} - c\} + f_{-H, z}^{(p)} \delta\{c_{-H} - c\}, \end{aligned} \quad (\text{D3})$$

which simplifies the first term and the right hand side from the general formulation (C18).

APPENDIX E

Leibniz Rule

For $\xi \in \{x, y, t\}$ the Leibniz rule reads

$$\begin{aligned} & \frac{\partial}{\partial \xi} \int_{-H(\xi)}^{\eta(\xi)} \psi^z(\xi, z) \mathcal{H}_{\leq, >}\{s^z(\xi, z) - s\} dz \\ &= \mp \int_{-H}^{\eta} \psi^z \frac{\partial s^z}{\partial \xi} \delta\{s^z(\xi, z) - s\} dz + \int_{-H}^{\eta} \frac{\partial \psi^z}{\partial \xi} \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz \\ &+ \psi^z(\eta) \frac{\partial \eta}{\partial \xi} \mathcal{H}_{\leq, >}\{s^z(\eta) - s\} + \psi^z(-H) \frac{\partial H}{\partial \xi} \mathcal{H}_{\leq, >}\{s^z(-H) - s\}. \end{aligned} \quad (\text{E1})$$

But note that the bottom topography H will be considered as constant in time t in this manuscript.

For the vertical direction it can be shown that

$$\begin{aligned} & \int_{-H}^{\eta} \frac{\partial}{\partial z} [\psi^z \mathcal{H}_{\leq, >}\{s^z(z) - s\}] dz \\ &= \mp \int_{-H}^{\eta} \psi^z \frac{\partial s^z}{\partial z} \delta\{s^z(z) - s\} dz + \int_{-H}^{\eta} \frac{\partial \psi^z}{\partial z} \mathcal{H}_{\leq, >}\{s^z(z) - s\} dz, \\ &\equiv \psi^z(\eta) \mathcal{H}_{\leq, >}\{s^z(\eta) - s\} - \psi^z(-H) \mathcal{H}_{\leq, >}\{s^z(-H) - s\}, \end{aligned} \quad (\text{E2})$$

where the third line follows directly from the first one, using the Newton–Leibniz theorem.

In the rest of the manuscript we replace $s^z(\eta)$ and $s^z(-H)$ in the arguments of the Heaviside functions in (E1) and (E2) by s_{η} and s_{-H} .

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**Key Points:**

- The local diahaline mixing per salinity class is associated with the overturning circulation
- The spurious numerical contribution to the total diahaline exchange flow is around 50% over a large range of salinity classes
- Hot spots for diahaline exchange flow are located at sloping topography and where isohalines encounter surface (outflow) or bottom (inflow)

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Spatial Composition of the Diahline Overturning Circulation in a Fjord-Type, Non-Tidal Estuarine System

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Abstract In this study we present new insights into the overturning circulation in non-tidal, fjord-type estuarine systems associated with diahaline mixing. As a realistic example we analyze 2 years of numerical model results for the Baltic Sea, a brackish semi-enclosed marginal sea, characterized by strong freshwater surplus. An isohaline water mass transformation framework is applied to quantify and decompose the diahaline exchange flow. Time-averaged effective vertical diahaline velocity is directly calculated from the divergence of the transports below the respective isohaline surface. It is furthermore indirectly estimated from the gradient of local mixing per salinity class with respect to salinity. Under the assumption of negligible horizontal diffusive salt transports both estimates should be identical. Our analysis shows a high correlation between the spatial patterns of the two estimates for the diahaline exchange flow. Two dominant types of diahaline exchange flow are analyzed. First of all there is a large scale overturning circulation with inflow at places where the isohaline surface is close to the bottom and with outflow at places where the isohaline is surfacing. Secondly, there is the well-known small-scale overturning circulation localized inside the bottom boundary layer over sloping bathymetry, associated with boundary mixing. Both types of circulation are visualized across selected vertical transects in physical and in salinity space. One major result is that about 50% of the diahaline exchange flow patterns are generated by numerical mixing caused by the truncation error of the advection scheme, despite the fact that an anti-diffusive advection scheme and vertically adaptive coordinates are used.

Plain Language Summary We study the major circulation in estuaries controlled by mixing of water masses. A theoretical framework is applied that replaces depth with salinity, since the latter is descriptive of the circulating water masses. The circulation is described from a point of view where the flow crosses areas of constant salinity. This is the diahaline circulation. The framework breaks down the circulation into smaller chunks, and allows us to deduce how the circulating flow depends on mixing. An application of this theory in a 2-year long computer simulation of the large and non-tidal estuary of the Baltic Sea is demonstrated. Two dominant types of diahaline circulation are analyzed. The first is a large-scale circulation where water masses flow into the estuary where the areas of constant salinity touch the bottom, and out where they encounter the surface. The second is a small-scale circulation close to the bottom where the ocean bathymetry is sloping, and is controlled by boundary mixing. Both types of diahaline circulation are visualized in this study. One major result is that around 50% of the circulation is generated by unwanted spurious mixing, which is created by the computer simulation and does not exist in reality.

1. Introduction

Estuaries can be termed as “mixing machines,” as Wang et al. (2017) put it, where saline ocean water is mixed with freshwater from rivers and precipitation, to form brackish water with intermediate salinity. Due to salinity being an ideal tracer for the different water masses in estuaries, an isohaline framework (a space where the vertical coordinate is replaced by salinity) is well suited for the analysis of the estuarine mixing and the resulting exchange flow.

The isohaline framework builds on the early Knudsen theorem (Knudsen, 1900), which quantifies the exchange flow in terms of bulk values for the inflowing and outflowing volume fluxes, as well as representative salinities. This initial theory was extended several decades later by Walin (1977), and even later by MacCready (2011). In these works, the stratification and flow are permitted to be continuous and to vary with space and time. The following step is essential in these theories: the time-averaged volume transport per salinity class $q(S)$ is calculated by binning and averaging the transport in salinity classes. A balance must hold inside the estuary between (a) the net inflow of volume and salt with salinities above the salinity of a reference isohaline

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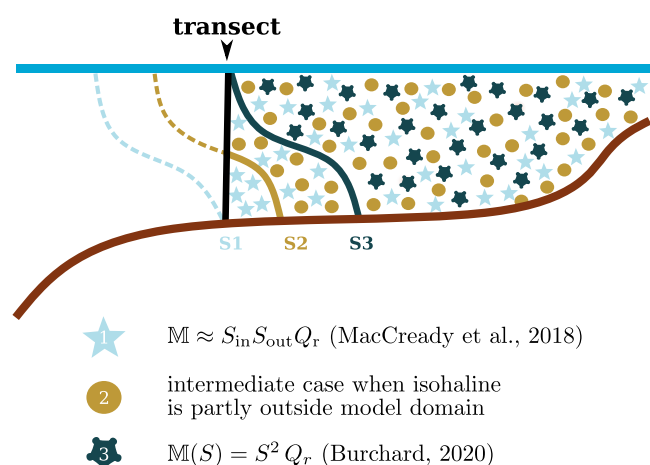


Figure 1. Sketch showing the differences in which areas the mixing formulas encompass. In mixing formula 1 (MacCready et al., 2018) the estuarine volume is bounded by the transect. In mixing formula 3 (Burchard, 2020) the volume of interest is bounded entirely by an isohaline (S3). In regional models, the intermediate scenario is often encountered, where the bounding isohaline (S2) is partially inside, partially outside of the model domain. Then the volume of interest is partly bounded by the isohaline and the transect.

at an estuarine control section, and (b) respectively the volume transports or advective and diffusive salt transports across the isohaline surface with the reference salinity (Walin, 1977). Furthermore, the inflow (outflow) volume transport, Q_{in} (Q_{out}), is obtained through integration of $q(S)$ in salinity space for inflows (outflows) according to MacCready (2011). This theoretical framework was termed the Total Exchange Flow (TEF) analysis framework (MacCready, 2011). Various studies have adopted the TEF analysis framework to investigate diverse types of estuarine systems (Burchard et al., 2018; Chen et al., 2012; Gräwe et al., 2016; Purkiani et al., 2016; Sutherland et al., 2011, among others). Analyses of dynamics in estuaries and river plumes using isohaline surfaces as reference have been carried out by MacCready and Geyer (2001), MacCready et al. (2002), and Hetland (2005). The TEF analysis, however, is limited to the study of transports at a single transect in space. The spatial information remains unknown in this analysis, so does the knowledge about diahaline fluxes.

Subsequent research has taken the TEF theory further by linking it to different quantities, notably estuarine mixing. In these various research endeavors, the following suggestion by Burchard and Rennau (2008) has proven to be key: quantify mixing as the (local) destruction of salinity variance per unit volume χ^S . The integrated mixing within a given volume can then be quantified as $\mathbb{M} = \int \chi^S dV$. Moreover, this method for the analysis of mixing, renders it possible in numerical models to accurately separate the mixing into physical and numerical contributions (Burchard & Rennau, 2008; Klingbeil

et al., 2014). The physical contribution is associated with the explicit diffusion from turbulence parameterizations. The numerical contribution is associated with the implicit diffusion due to the truncation errors of advection schemes in a numerical model.

The TEF was linked to the entrainment and diffusive salt flux, which in turn disclosed a relationship between mixing and TEF (Wang et al., 2017). The latter relationship was further developed in MacCready et al. (2018), where it was shown that the long-term time-averaged mixing in an estuary behind a fixed transect is approximately given by the relation $\mathbb{M} \approx S_{in} S_{out} Q_r$, where S_{in} (S_{out}) is the inflow (outflow) salinity at the boundary transect, and Q_r describes the volume flux discharged by the river. Exact mixing formulas allowing for continuous and time-dependent exchange flow was derived in Burchard et al. (2019). Furthermore, a universal law of estuarine mixing was derived in Burchard (2020). These approaches resulted in the relation $\mathbb{M}(S) = S^2 Q_r$ for the long-term averaged mixing inside an estuarine volume bounded by the isohaline of salinity S . A visual distinction between the different mixing relations described here is compiled in Figure 1. The universal law can also be formulated as $m(S) = \partial \mathbb{M}(S) / \partial S = 2S Q_r$, with $m(S)$ being the salinity variance dissipation per unit salinity. In the following m will be referred to as mixing per salinity class (per infinitesimal salinity bin).

The isohaline framework also offers to diagnose diahaline fluxes that give new insights, as was done in Wang et al. (2017). They showed the overturning circulation in salinity space along the Hudson River (respectively their Figures 5b and 5c). The exchange flow was observed to drive the saline water landward, and the brackish water oceanward. Mixing was seen to show maxima around the interface between the inflowing and outflowing water. The diahaline transport (referred to as entrainment there) was in upward direction (toward lower salinity classes) below the interface and in downward direction (toward higher salinity classes) above. Similarly, the diahaline exchange flow was studied for the Pearl River Estuary (Li et al., 2022). They find that the diahaline exchange flow shows a classical exchange flow consisting of inflow in the deeper and outflow in the shallower water layers. The magnitude of the inflowing and outflowing diahaline transport is found to increase with salinity, while the net diahaline transport stays constant, amounting to Q_r after long enough temporal averaging. The progress made by Li et al. (2022) is that horizontal maps were shown of the diahaline velocity and the *local* mixing per salinity class (their Figure 6). They found that high diahaline velocity correlated with strong mixing. Along the same line of research are the horizontal maps of the diapycnal velocity to study the spatial composition of the Atlantic Meridional Overturning Circulation in Sidorenko et al. (2020, their Figures 5 and B4). In studies of numerical diapycnal mixing, diapycnal velocity maps of the Southern Ocean and the World Ocean were presented in, respectively, Lee et al. (2002, their Figure 7) and Megann (2018, his Figure 9).

Next to the large-scale overturning circulation, also local processes are present. One such process is boundary mixing, which occurs in the near-bottom region. Boundary mixing is a major contributor to the vertical transport of salt, heat, and matter across the whole basin, whether it be a basin the size of the Baltic Sea, a small lake or the World Ocean (Holtermann et al., 2014, and references therein). Despite its importance, the quantification of boundary mixing has been a challenging task. Recent advances on the subject, such as the modeling study by Holtermann et al. (2014), have been made possible by (a) the implementation of a vertically adaptive numerical grid that resolves the bottom boundary layer (Hofmeister et al., 2010), and (b) by state-of-the-art turbulence models (Umlauf & Burchard, 2005). The modeling study by Holtermann et al. (2014) is motivated by their previous results from observation data of the Baltic Sea Tracer Release Experiment (Holtermann & Umlauf, 2012; Holtermann et al., 2012). In the early work by Garrett (1990), the role of bidirectional flow in boundary mixing was investigated. An idealized one-dimensional model was used by Umlauf and Burchard (2011) to investigate how shear, stratification and turbulence interact in the boundary layer on sloping topography. Their velocity profile showed an exchange flow with up-slope velocity near the bottom, and down-slope velocity above (Umlauf & Burchard, 2011, their Figure 5). The consensus in 2016 on the global abyssal overturning circulation misses a key point according to Ferrari et al. (2016). They argue that recent observations prior to their study had shown bottom-intensified mixing in abyssal waters, and that this is not considered in the theory. The enigma that arises when considering these measurements in the light of the theory, is that a reversed picture emerges. These measurements indicate that waters should sink due to the increased mixing, but the theory considers rising water masses. Therefore, they strongly argue for the inclusion of bottom-intensified mixing in the theory. Their proposal to accommodate for this missing point, is that the abyssal waters ascend to the surface along thin, turbulent bottom boundary layers. In this paper, we carry out a three-dimensional numerical model study and investigate the boundary mixing in an isohaline framework, comprising both features (a) and (b) mentioned above.

The theory of the isohaline framework is based on the water mass transformation (WMT) framework. WMT was introduced by Walin (1977, 1982), originally, in the former work, for the description of estuaries. In a recent review by Groeskamp et al. (2019), a more general WMT is discussed. WMT is defined in Groeskamp et al. (2019) as the “mass transport of seawater through a surface with a constant property value.” The benefit of WMT is that it provides an indirect means of studying the ocean circulation based on tracers. This way of indirectly analyzing the ocean circulation complements direct measurements. Air-sea fluxes and mixing are the main processes causing WMT (Groeskamp et al., 2019). The study by Walin (1977) introduced a WMT framework using salinity as an essential scalar property for a WMT analysis of the Baltic Sea. Further studies used WMT in thermohaline coordinates to study the thermohaline ocean circulation (Döös et al., 2012; Groeskamp et al., 2014; Zika et al., 2012). The meridional circulation cells in the Southern Ocean were studied using WMT in the form of overturning stream functions in latitude-density space (Döös & Webb, 1994). In the later study by Döös et al. (2004), the overturning circulation of the Baltic Sea is viewed by using meridional stream functions as functions of the four vertical coordinates depth, salinity, temperature and density. While the TEF analysis framework studies the exchange flow at individual transects in space, the stream function as shown in Döös et al. (2004) makes it possible to illustrate the circulation by concatenating the TEF profiles from different transects.

All the methods presented up to this point are important diagnostic tools to study estuarine dynamics. In particular, maps of diahaline velocity and diffusive salt fluxes, as seen in Wang et al. (2017) and Li et al. (2022), allow for studying the link between mixing and diahaline exchange flow. Recently, Klingbeil and Henell (2023) derived a *local* WMT framework and provided exact definitions for local diasurface quantities. Moreover, they derived relations between these quantities, thereby generalizing the formulations by Li et al. (2022). In particular, they provided an equation that directly formulates how small-scale mixing, that is, local dissipation of tracer variance, is associated with the local dia-surface exchange flow. In this paper we verify these local relations for the first time in an isohaline framework using a realistic model for the non-tidal, fjord-type Baltic Sea. The use of an isohaline framework to study the circulation in salinity space is particularly appropriate since the density-driven estuarine circulation is mainly controlled by the salinity gradient. We quantify local and integrated contributions to the diahaline volume transport, diahaline diffusive salt transport and diahaline mixing. Moreover, we separate the mixing into physical and numerical contributions and quantify the associated physical and numerical diahaline exchange flow. With our local diagnostics we investigate diahaline boundary mixing in detail and contribute to existing theories on boundary mixing.

This paper has the following structure. First, it introduces the applied methods in Section 2. Therein, the theory of the isohaline framework is described, focusing on the diahaline quantities presented in this work. This section

further includes a description of the study area that the theory is applied to, and of the numerical model used to produce the results. The results are presented in seven subchapters on the hydrographic state (Section 3.1), diahaline volume transport (Section 3.2), diahaline diffusive salt transport (Section 3.3), diahaline mixing (Section 3.4), relations between the diahaline quantities (Section 3.5), physically and numerically induced diahaline exchange flow (Section 3.6), and a more detailed view on boundary mixing (Section 3.7). Concluding remarks are made concerning new insights into the isohaline framework, and further applications of this method are discussed in Section 4.

2. Methods

2.1. Budgets and Relations in Salinity Space

Adapting the general Equations 18 and 26 from Klingbeil and Henell (2023) to salinity yields:

$$\frac{\partial D_{\leq}(S)}{\partial t} + \frac{\partial U_{\leq}(S)}{\partial x} + \frac{\partial V_{\leq}(S)}{\partial y} + u_{\text{dia},z}(S) = P - E, \quad (1)$$

$$\frac{\partial S_{\leq}(S)}{\partial t} + \frac{\partial F_{x,\leq}(S)}{\partial x} + \frac{\partial F_{y,\leq}(S)}{\partial y} + f_{\text{dia},z}(S) = 0. \quad (2)$$

These budgets describe how the thickness $D_{\leq}(S)$ and salt content $S_{\leq}(S)$ of all water with salinities smaller or equal to S in an individual water column evolve in terms of the divergence of horizontal transports with salinities $\leq S$, diahaline fluxes (per unit horizontal area) across the isohaline with salinity S , and surface freshwater fluxes due to precipitation (P) and evaporation (E). The diahaline salt flux in Equation 2 consists of advective and diffusive contributions:

$$f_{\text{dia},z}(S) = Su_{\text{dia},z}(S) + j_{\text{dia},z}(S). \quad (3)$$

Exact mathematical expressions for $u_{\text{dia},z}(S)$ and $f_{\text{dia},z}(S)$ have been derived in Klingbeil and Henell (2023, their (20) and (34a)), but are not required in this study, because they will be diagnosed from Equations 1 and 2. Mathematically, the cumulative quantities in Equations 1 and 2 are defined by vertical integration over the parts of the water column where the salinity is $\leq S$,

$$D_{\leq}(S) = \int_{S(z) \leq S} dz \quad U_{\leq}(S) = \int_{S(z) \leq S} u(z) dz, \quad (4)$$

$$S_{\leq}(S) = \int_{S(z) \leq S} S(z) dz \quad F_{x,\leq}(S) = \int_{S(z) \leq S} f_x(z) dz, \quad (5)$$

with u and f_x being the zonal velocity and salt flux (accordingly for the transports in y -direction). Analogously, a cumulative salinity mixing can be defined as

$$M_{\leq}(S) = \int_{S(z) \leq S} \chi(z) dz, \quad (6)$$

with the salinity variance dissipation rate

$$\chi = 2 \left(K_h \left(\frac{\partial S}{\partial x} \right)^2 + K_h \left(\frac{\partial S}{\partial y} \right)^2 + K_v \left(\frac{\partial S}{\partial z} \right)^2 \right) \quad (7)$$

associated with salinity diffusion by horizontal and vertical diffusivities K_h and K_v , respectively. From Equation 6 the mixing per (infinitesimal) salinity class is obtained as

$$m(S) = \frac{\partial M_{\leq}(S)}{\partial S}. \quad (8)$$

An intuitive view of the local diahaline fluxes and mixing is given in a sketch of an idealized estuary in Figure 2c. The sign convention applied in this work is described in Figures 2a and 2b. Klingbeil and

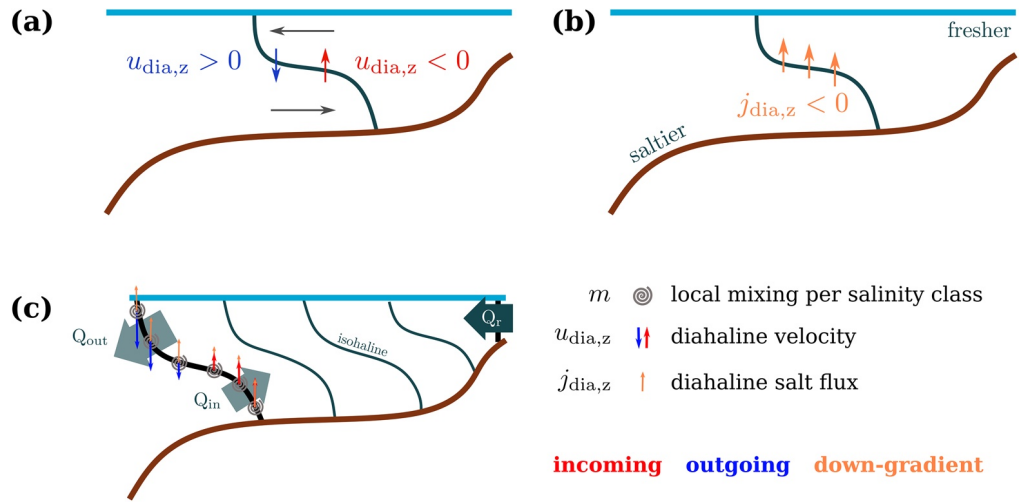


Figure 2. Sketch for an idealized estuary displaying the sign convention for (a) the effective vertical diahaline velocity $u_{dia,z}$ and (b) the effective vertical diahaline diffusive salt flux $j_{dia,z}$. Dihaline fluxes are counted positive into the direction of increasing salinity. Therefore, negative diahaline velocity is counted as incoming, and positive diahaline velocity as outgoing. (c) Sketch visualizing the location of the terms in Equations 9a–9c.

Henell (2023) showed how, under the assumption of negligible horizontal diffusive salt fluxes and no sources and sinks, the following simple relations between the diahaline quantities can be derived (their (46), (40) and (47)):

$$u_{dia,z}(S) = -\frac{\partial j_{dia,z}(S)}{\partial S}, \quad (9a)$$

$$j_{dia,z}(S) = -\frac{1}{2}m(S), \quad (9b)$$

$$u_{dia,z}(S) = \frac{1}{2}\frac{\partial m(S)}{\partial S}. \quad (9c)$$

To which extent Equations 9a–9c hold in realistic applications has to be investigated. Integrated diahaline quantities can be obtained by horizontal integration over all water columns,

$$Q_{dia}(S) = \int u_{dia,z}(x, y, S) dx dy, \quad (10a)$$

$$J_{dia}(S) = \int j_{dia,z}(x, y, S) dx dy, \quad (10b)$$

$$m(S) = \int m(x, y, S) dx dy, \quad (10c)$$

and the integral formulations of Equations 9a–9c read

$$Q_{dia}(S) = -\frac{\partial J_{dia}(S)}{\partial S}, \quad (11a)$$

$$J_{dia}(S) = -\frac{1}{2}m(S), \quad (11b)$$

$$Q_{dia}(S) = \frac{1}{2}\frac{\partial m(S)}{\partial S}. \quad (11c)$$

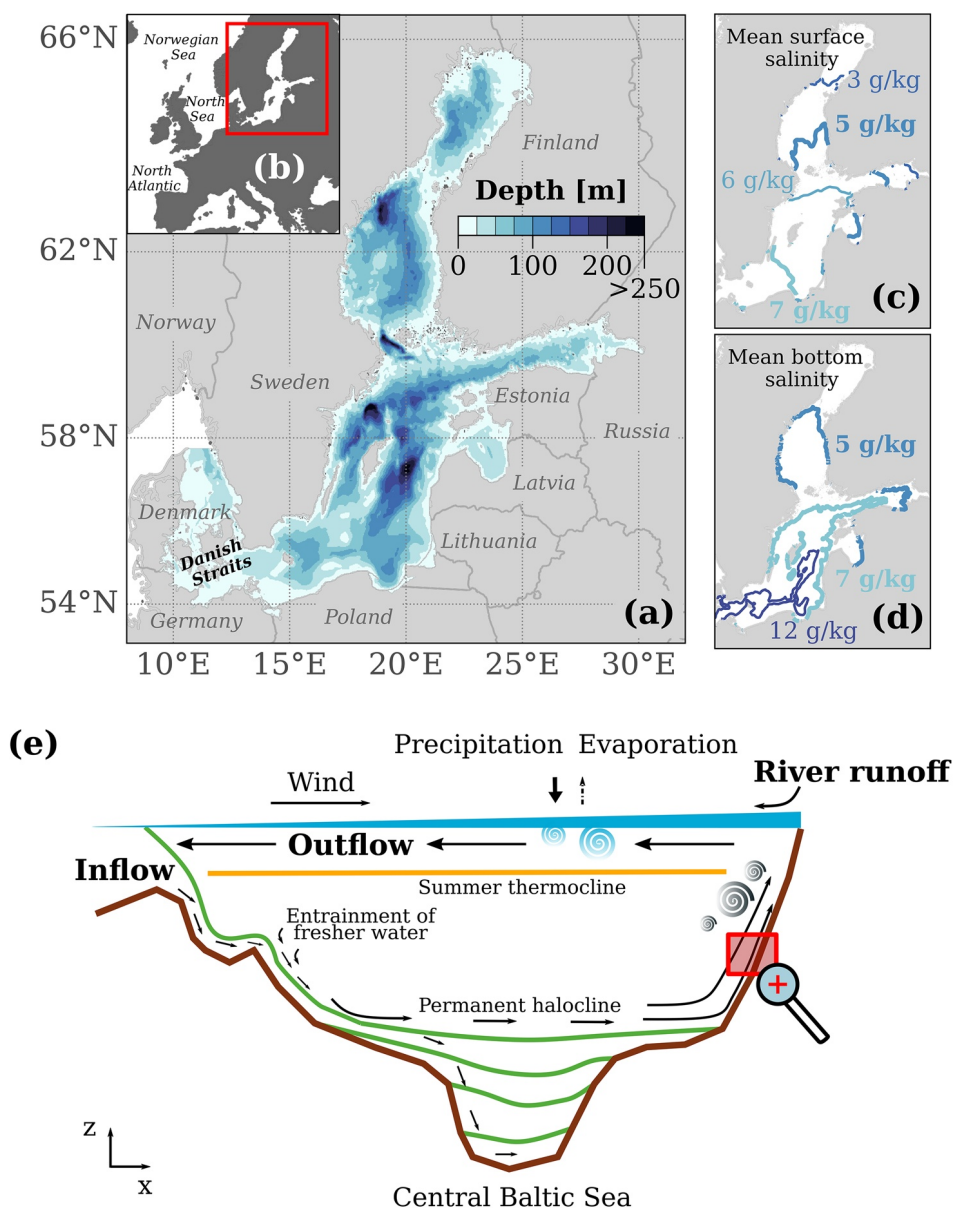


Figure 3. (a) Bathymetric map of the Baltic Sea. (b) Location of the Baltic Sea in Europe. (c) Mean surface salinity contour lines for 3, 5, 6, and 7 g/kg. (d) Mean bottom salinity contour lines for 5, 7, and 12 g/kg. (e) Schematic of the water balance and overturning circulation in the Baltic Sea in longitude–depth space based on Matthäus (2006, his Figure 1.2). The magnifying glass refers to Section 3.7 and Figure 14 where diahaline boundary mixing is studied.

2.2. Study Area

In the present study, we demonstrate the analytical power of Equations 9a–9c for the estuary of the Baltic Sea, because a detailed understanding of diahaline processes is highly relevant for its ecosystem.

The Baltic Sea is an almost non-tidal marginal sea located in northern Europe, and bounded by the European main continent and Scandinavia. The only connection to the North Sea (and the World Ocean) is established through the narrow and shallow Danish Straits (see Figure 3a). The catchment area of the Baltic Sea includes many rivers with the largest river runoff originating from the Neva river near St. Petersburg in Russia (Bergström & Carlsson, 1994). This fresh river runoff, and precipitation, in the surface waters mix with the saline and dense Atlantic waters flowing in through the straits, and result in a net outflow of the mixed, brackish waters toward the North Sea. An exchange flow is formed. For this circulation—consisting of the inflow of salty, dense

bottom waters, upwelling and mixing with fresh surface waters, and outflow of brackish waters in the upper water layers—Döös et al. (2004) coined the term “Baltic Haline Conveyor Belt.”

A prominent feature of the Baltic Sea is the halocline at 40–80 m depth in the deeper basins (Liblik & Lips, 2019), from which ensues a permanent salinity stratification. This halocline serves as an efficient delimiter between surface and bottom water masses. A general idea of how the isohalines are located in the Baltic Sea is given by displaying the mean surface and bottom salinity of, respectively, isohalines 3, 5, 6, and 7 g/kg in the former, and 5, 7, and 12 g/kg in the latter case (Figures 3c and 3d). In addition to the permanent halocline, a seasonal thermocline between depths of 10–30 m develops during the summer months (Reissmann et al., 2009), see Figure 3e. The bathymetry of the Baltic Sea contains several basins such as the Arkona Basin, the Bornholm Basin and the Gotland Basin. Of these, the Gotland Basin is the deepest with a depth of 459 m in its western and 248 m in its eastern branch. The mean depth of the Baltic Sea, however, is only at about 52 m.

The inflowing saline water is dense, therefore heavy, and also oxygen-rich, and thus ventilates the deeper basins of the Baltic Sea. These inflows are the main source of deepwater salt and oxygen in the Baltic Sea and are therefore important for the Baltic Sea ecosystem and its maintenance. The only other source of oxygen is from diffusive flux at the sea surface, which can not enter the deeper basins efficiently due to the strong vertical stratification (Döös et al., 2004; Mohrholz et al., 2015). The inflows can be either more frequent medium-intensity salinity inflow events from the Kattegat, or less frequent major barotropic and baroclinic inflow events (MBIs). The occurrence of the inflow events is linked to the weather patterns over this region. The *barotropic* inflow events are forced by the differences in sea level between the Arkona Basin and the Kattegat due to wind and air pressure forcing (Franck et al., 1987; Matthäus, 2006; Wyrki, 1954). This type of inflow is more frequent during the winter season, but may also occur during the other seasons. *Baroclinic* inflows, on the other hand, are driven by the density gradient between the Kattegat and the Baltic, and are common during long and calm summer periods (Feistel, Günther, et al., 2003; Feistel, Nausch, et al., 2003; Feistel et al., 2006; Hela, 1944; Knudsen, 1900; Mohrholz et al., 2006).

A detailed review of current knowledge gaps concerning the Baltic Sea, with special emphasis on its salinity dynamics, has been provided by Lehmann et al. (2022). Among other things, they emphasize the lack of knowledge about regional coastal processes and small-scale variability. They also point out that we do not yet understand all branches of the general circulation of the Baltic Sea. The methods applied in our work serve to better understand the Baltic Sea circulation and mixing hotspots, which in turn may be useful for understanding different branches of the circulation. In addition, it provides insight into possible future research opportunities, for example, by applying the isohaline framework to improve knowledge of MBIs.

2.3. Numerical Model

Realistic numerical simulations of the Baltic Sea have been carried out with the General Estuarine Transport Model (GETM; Burchard and Bolding (2002); Klingbeil and Burchard (2013)). GETM is an open source three-dimensional coastal ocean model. General details about the numerics can be found in Klingbeil et al. (2018). A special feature of GETM are vertically adaptive model layers (Hofmeister et al., 2010). Their automatic zooming toward areas of strong stratification significantly reduces spurious numerical mixing and is fundamental for the proper simulation of the halocline in the Baltic Sea (Gräwe et al., 2015). GETM supports the separate quantification of physical mixing due to turbulence parameterizations and spurious numerical mixing due to discretization errors of the advection schemes according to Klingbeil et al. (2014). In each grid cell the variance decay caused by tracer diffusion (χ_{phy}) and tracer advection (χ_{num}) is diagnosed. The changes of salinity variance due to river discharge, precipitation and evaporation are also counted as “physical” contributions, such that χ_{num} solely contains the spurious effects of the numerical advection scheme. For the present study, GETM was extended to also diagnose the effective vertical diahaline velocity $u_{\text{dia},z}(S)$ from Equation 1, the effective vertical diahaline diffusive salt flux $j_{\text{dia},z}(S)$ by means of Equation 3 from Equation 2, as well as the physical and numerical mixing per salinity class $m_{\text{phy}}(S)$ and $m_{\text{num}}(S)$ from Equation 8, respectively. For every water column the required cumulative quantities in Equations 4–6 are obtained after binning the layer heights, transports, salt contents and variance decay from the model grid cells into equidistant salinity bins of size 0.2 g/kg. All transports are binned based on the corresponding interface salinity given by an upwind approximation.

The model setup with a spatial resolution of approximately 1 nautical mile is described and validated in Burchard et al. (2018) and Gräwe et al. (2019). The simulated time period covers the years of 2014 and 2015, with a

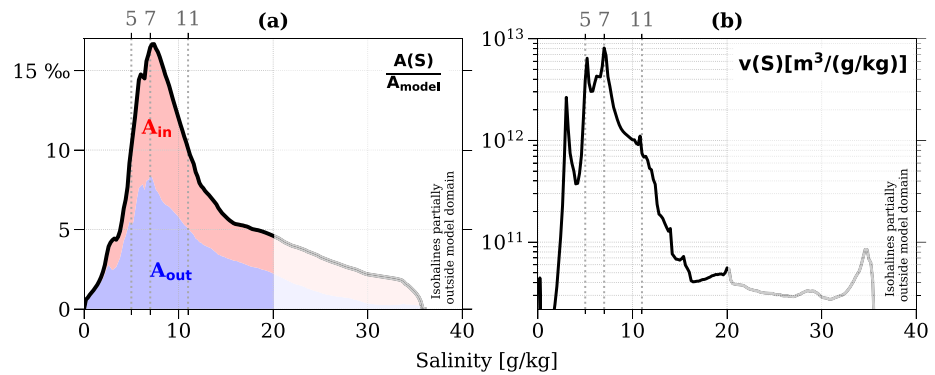


Figure 4. Isohaline area $A(S)$ and volume per salinity class $v(S)$ are shown in (a) and (b), respectively. The isohaline area is the respective surface covered by every present isohaline. The isohaline volume is the total volume encompassed by the respective salt class. A_{in} is the isohaline surface of the incoming, and A_{out} of the outgoing flow, calculated by means of Equation 14. The paler patch shows the isohalines already extending outside the model domain, and thus do not account for all near surface areas across which outflow occurs. This is the intermediate case 2 in Figure 1.

measured MBI event occurring at the end of 2014 (Mohrholz et al., 2015). A temporal average was taken over these 2 years.

3. Results

3.1. Hydrographic State

The isohaline surface $A(S)$ and the isohaline volume per salinity class $v(S)$ serve as means of describing the hydrographic state of the Baltic Sea (Walin, 1977). Due to the small slope of the isohalines, the isohaline surface can be approximated by the horizontal footprint area of all water columns, where the particular isohaline is present. The isohaline volume per salinity class is defined as follows:

$$v(S) = \frac{\partial V(S)}{\partial S}, \quad (12)$$

where $V(S)$ is the volume of all water with salinity smaller than or equal to a specific salinity S . The mean isohaline surface, scaled with the area of the entire Baltic Sea, is shown in Figure 4a, and the isohaline volume per salinity class in Figure 4b. Both quantities have a maximum at a salinity of 7 g/kg, with a sharp increase prior and a slower decrease after the peak. This result can be expected since the 7 g/kg isohaline accounts for the surface water in large parts of the central Baltic Sea. For salinities larger than 20 g/kg the isohalines (partially) and the isohaline volumes extend outside the model domain. This corresponds to the intermediate case in Figure 1.

3.2. Diahaline Volume Transport

Maps of the effective vertical diahaline velocity are shown in Figure 5. Note, that in all plots the effective vertical diahaline velocity is labeled diahaline velocity for brevity. All maps show the general picture of outgoing volume transport toward higher salinity classes in the south/southwestern, and incoming volume transport toward lower salinity classes in the northern/northeastern extent of the corresponding isohalines. This diahaline overturning circulation complements the classical picture of estuarine circulation with salty bottom inflow and brackish surface outflow sketched in Figure 2c.

To investigate this exchange flow further, we study the integrated incoming and outgoing diahaline transports:

$$\begin{aligned} Q_{dia}^{in}(S) &= - \int_{u_{dia,z}(x,y,S)<0} u_{dia,z}(x,y,S) dx dy \\ Q_{dia}^{out}(S) &= + \int_{u_{dia,z}(x,y,S)>0} u_{dia,z}(x,y,S) dx dy. \end{aligned} \quad (13)$$

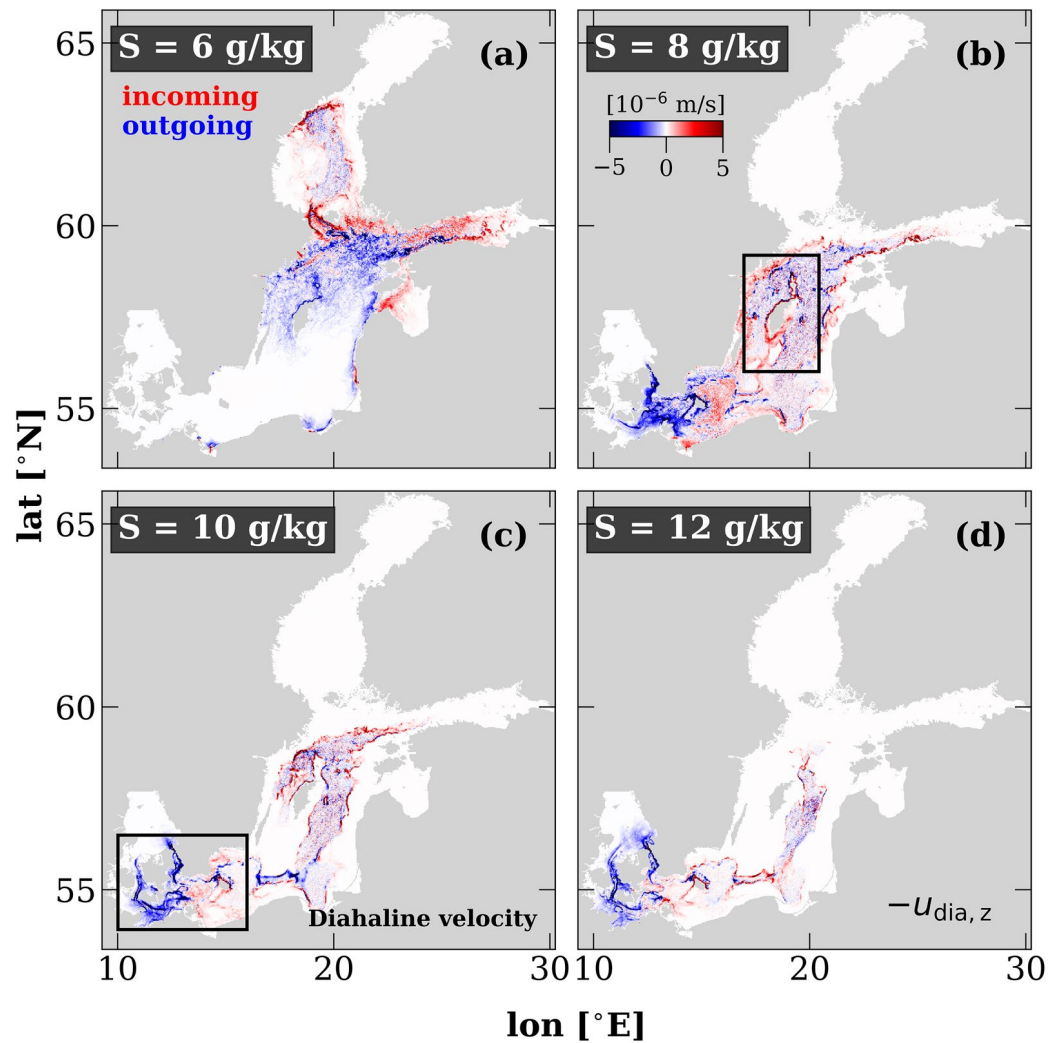


Figure 5. Maps of the effective vertical diahaline velocity, averaged over two years, across the isohalines of (a) 6, (b) 8, (c) 10, and (d) 12 g/kg. For the adopted sign convention, the reader is referred to Figure 2a. The black boxes in panels (b) and (c) show the location of the zoomed-in regions of Figures 12a and 12b, respectively.

The integrals in Equation 13 only integrate over areas with negative $u_{\text{dia},z}$ for $Q_{\text{dia}}^{\text{in}}$, and areas with positive $u_{\text{dia},z}$ for $Q_{\text{dia}}^{\text{out}}$, respectively. Similarly, we compute the areas of the isohalines where inflow and outflow are occurring:

$$\begin{aligned} A_{\text{in}}(S) &= \int_{u_{\text{dia},z}(x,y,S) < 0} dx dy \\ A_{\text{out}}(S) &= \int_{u_{\text{dia},z}(x,y,S) > 0} dx dy, \end{aligned} \quad (14)$$

The integrated diahaline transports are shown in Figure 6. The incoming as well as the outgoing diahaline transport show a symmetric spread with a net dominance of outgoing transports caused by the freshwater supply due to rivers and net precipitation. The strongest diahaline exchange flow with maximum in- and outflowing transports occurs across the isohaline with the largest area (salinity 7 g/kg, see Figure 4a).

This is different to many tidal estuaries where the strength of the exchange flow increases toward the highest salt classes, situated at the outlet of the estuary (see e.g., Figures 4c and 4d in Li et al. (2022) and Reese et al. (2023)). The incoming diahaline transport and the isohaline area where inflow occurs (see Figure 4a) disappear toward lower salinities, where the outflow due to freshwater river discharge dominates. The diahaline transport at higher salinities mainly depicts the near bottom inflow, and misses the near surface outflow across the portions of the

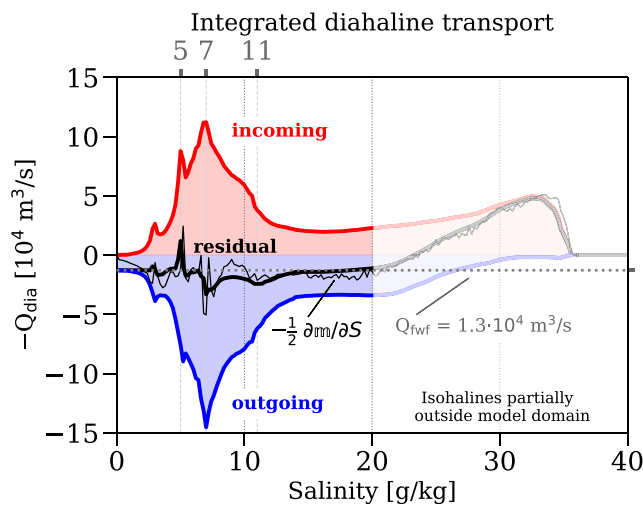


Figure 6. Integrated diahaline volumes transports. Incoming and outgoing contributions $Q_{dia}^{in/out}$ from Equation 13 are shown in red and blue, respectively. The residual transport (thick black line) is identical to Q_{dia} from Equation 10a. The dotted horizontal gray line is the net freshwater supply Q_{fw} due to river discharge, evaporation and precipitation. The thin black line displays the derivative of the integrated mixing per salinity class m with respect to salinity, with m from Equation 10c. It correlates with Q_{dia} (thick black line) with $R = 0.95$ and indicates the approximate validity of relation (11c). The paler patch shows the isohalines already extending outside the model domain, and thus do not account for all near surface outflow anymore. This is the intermediate case 2 in Figure 1.

isohaline area that are already outside the model domain (see paler patch in Figure 6 and reduced A_{out} in Figure 4a). Except for the missing outflow for high salinities and the diahaline exchange flow inside the non-tidal basins across isohalines of intermediate salinities, the residual integrated diahaline transport agrees very well with the net freshwater supply. This net outflow is associated with a generally dominating isohaline area across which outflow occurs (Figure 4a). Deviations between the mean freshwater supply and the residual integrated diahaline transport are expected, because time averaged results from our only 2 years long simulation period (including a Major Baltic inflow event) cannot represent a long-term balanced state of the Baltic.

In this study we have chosen to focus our analysis on three salt classes. The salt classes of 5, 7, and 11 g/kg were picked as they cover the most relevant domains for the exchange flow. Moreover, they follow as a natural choice from the results of the isohaline area, isohaline volume per salinity class and diahaline transport (respectively Figures 4 and 6). The salt class of 7 g/kg, in particular, proved to be the location of the maximum in these analyses.

3.3. Dihaline Diffusive Salt Transport

Maps of the effective vertical diahaline diffusive salt flux, averaged over 2 years, are shown in Figures 7a–7c for salt classes 5, 7, and 11 g/kg. Note, that in all plots the effective vertical diahaline diffusive salt flux is labeled diahaline diffusive salt flux for brevity. Mostly a down-gradient diffusive salt flux ($j_{dia,z} < 0$) is diagnosed across the three isohalines. In some areas very weak up-gradient diffusive salt fluxes are present, caused by the applied anti-diffusive advection schemes in the numerical model. The strongest effective diahaline diffusive salt fluxes occur across the isohaline of 11 g/kg

in the surface waters of the shallow Western Baltic Sea and in the Danish Straits toward the North Sea where wind and tidal mixing dominate. In addition, the diffusive salt flux is enhanced along certain coastlines and bathymetric features, where the isohalines are in contact with the bottom topography.

3.4. Dihaline Mixing

Maps for the time-averaged local mixing per salinity class $m = m_{phy} + m_{num}$ across the respective isohalines are shown in Figure 7d–7f. Mixing dominates over demixing for all three salt classes and leads to smoothed salinity gradients. Weak demixing tends to steepen the salinity gradients and occurs due to freshwater evaporation out of saline surface waters (counted as part of the physical mixing, see e.g., Figure 7h) and due to the numerical advection schemes (see negative numerical mixing in Figures 7k and 7l). The separation of the (total) mixing into physical and numerical contributions indicates that the simulation results are dominated by the physical mixing from the well-calibrated turbulence parameterization. The maps of physical and numerical mixing per salinity class (Figure 7g–7i, 7j–7l) resemble similar patterns since both contributions depend on the salinity gradient. The mixing contributions are highest in the shallow areas of the Western Baltic Sea and in the tidally influenced Danish straits toward the North Sea (7i, 7l). All salinity classes show hotspots of physical and numerical mixing at the rims of the Baltic basins where the isohalines touch the bottom topography.

The integrated mixing per salinity class is presented in Figure 8. This is the first time the integrated mixing per salinity class is shown for the Baltic Sea. A good agreement with the universal law of estuarine mixing $m(S) = 2SQ_{fw}$ is shown for smaller salinities up to 8 g/kg. For higher salinities, a deviation from the universal law is visible. This is because our temporal average of 2 years is not sufficiently long to remove the effects of varying volume and salt content on shorter time scales, which are not considered by the universal law. The turnover time of the Baltic Sea is around 25–30 years (Döös et al., 2004, and references therein), so a longer averaging period is expected to yield a better agreement with the universal law of estuarine mixing. Moreover, the deviation for salinities larger than 20 g/kg can be explained by the isohalines extending outside the model domain (intermediate case 2 in Figure 1). For most salinity classes inside the Baltic Sea, the integrated mixing is dominated by physical mixing due to turbulence parameterization.

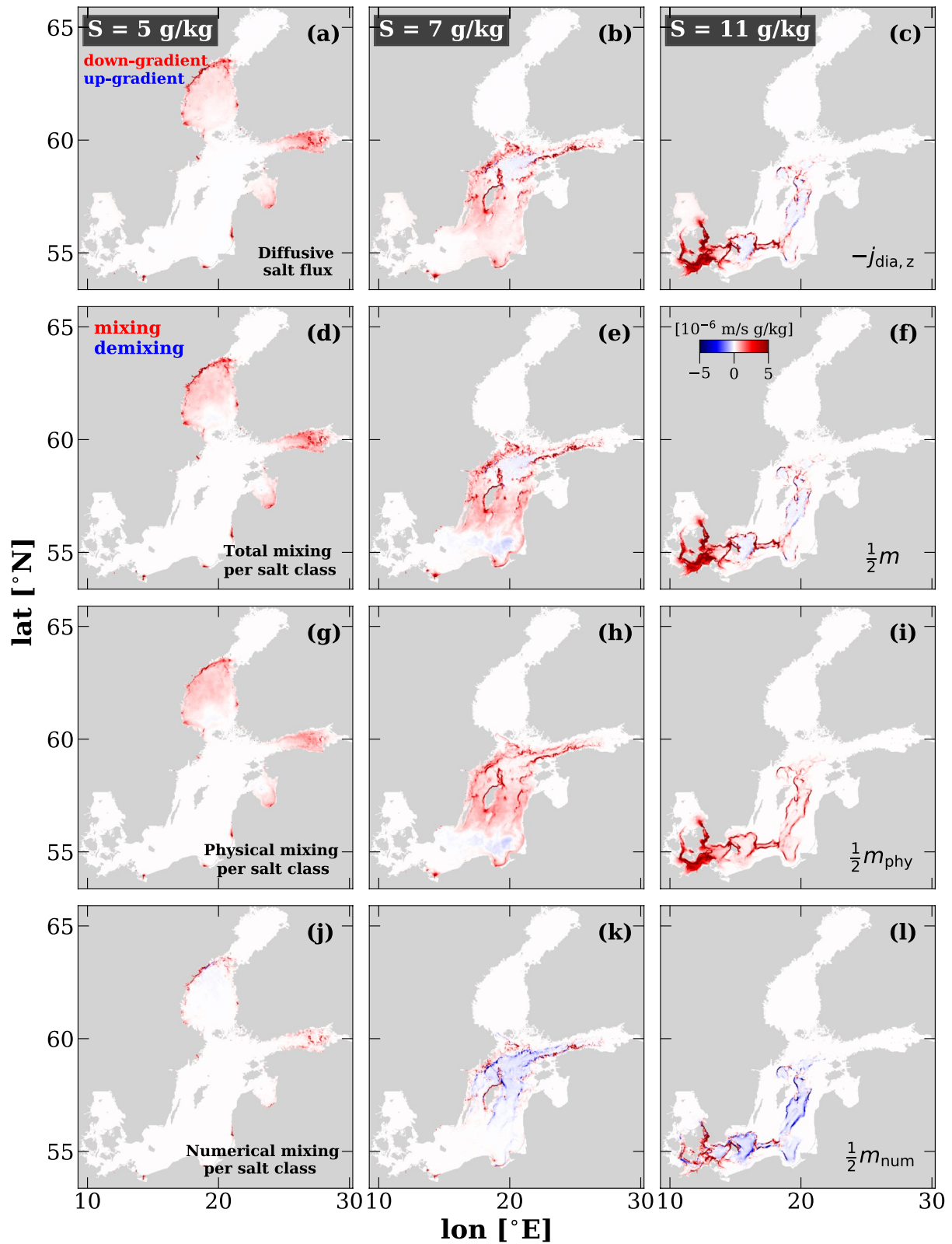


Figure 7. Maps of diahaline quantities averaged over 2 years. Column 1: salt class 5 g/kg; Column 2: 7 g/kg; Column 3: 11 g/kg. Row 1 (a–c): effective vertical diffusive salt flux; Row 2 (d–f): mixing per salinity class; Row 3 (g–i): physical mixing per salinity class; Row 4 (j–l): numerical mixing per salinity class. The almost identical patterns in panels (a)–(c) and (d)–(f) indicate the validity of Equation 9b.

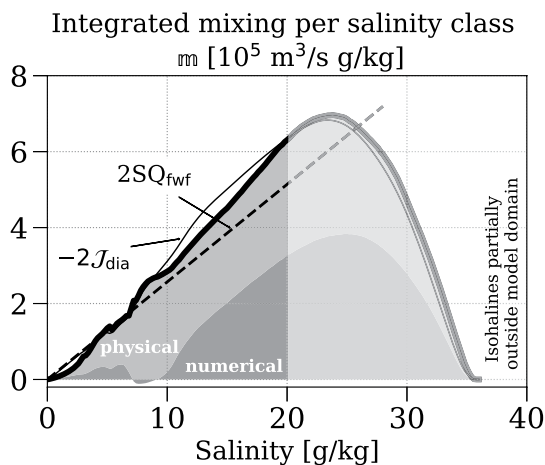


Figure 8. The integrated mixing per salinity class $m(S)$ from Equation 10c is shown by the solid black line. The physical and numerical contributions are displayed in light and dark gray, respectively. The thin black line shows the integrated diahaline diffusive salt transport from Equation 10b. It correlates with m with $R = 0.99$ and indicates the validity of Equation 11b. The dashed black line depicts the integrated mixing per salinity class following the universal law of estuarine mixing $m(S) = 2SQ_{fw}$. The paler patch shows the isohalines already extending outside the model domain, where most of the mixing predicted by the universal law would happen. This refers back to intermediate case 2 in Figure 1.

3.5. Relations Between Diahline Quantities

Here we analyze the validity of the relations in Equations 9a–9c. We do this by comparing the left and right hand side of each relation with each other.

Figure 9 directly compares the diagnosed effective vertical diahaline velocity $u_{dia,z}$ with the divergence of the diagnosed effective vertical diffusive salt flux in salinity space $\partial j_{dia,z}/\partial S$, and with the derivative of the diagnosed mixing per salinity class with respect to salinity $\partial m/\partial S$ for different isohalines. For each isohaline the different quantities show very similar results, with the directly diagnosed effective vertical diahaline velocity appearing more noisy and $\partial m/\partial S/2$ being more pronounced.

The direct comparison of the diagnosed effective vertical diahaline diffusive salt flux $j_{dia,z}$ with the mixing per salinity class m is presented in Figure 7. The dominating patterns of strong fluxes and mixing are very similar, except for small areas of demixing caused by freshwater evaporation out of saline surface waters without corresponding upgradient diffusive fluxes.

Overall, Figures 7 and 9 indicate that the analytical relations in Equations 9a–9c hold well in a realistic model for the estuary of the Baltic Sea. The smoother fields for the effective vertical diahaline diffusive salt flux and the mixing per salinity class could be explained by the fact that their reconstruction is based on the calculation of gradients with respect to S instead of a direct calculation. Another reason could be horizontal diffusive salt fluxes present in reality and our numerical model. However, horizontal diffusive salt fluxes have been neglected during the derivation of the idealized analytical relations in Equations 9a and 9c. Therefore, the directly diagnosed effective vertical diahaline velocity is less smooth and deviates from the analytical relations.

The maps of the diahaline quantities (Figures 7 and 9) give a useful general view and portray the relations to hold well. A more quantitative evaluation is given by the scatter plots in Figure 10. The correlations between the diahaline quantities are satisfying, because the deviations are caused by just a minority of data points. This is also confirmed by the excellent correlations between the integrated quantities. The relation in Equation 11a between the integrated diahaline transport and the integrated diahaline diffusive salt flux fits perfectly with a correlation coefficient of $R = 1.0$. The integrated diahaline diffusive salt flux and the integrated mixing per salinity class from Equation 11b are compared in Figure 8 and the correlation coefficient is $R = 0.99$. The relation in Equation 11c between the integrated diahaline transport and the integrated mixing per salinity class is shown in Figure 6. There, the derivative of the integrated mixing per salinity with respect to salinity is noisy, but it still correlates with $R = 0.95$. With this, also the integral relations have been verified in a realistic model for the estuary of the Baltic Sea.

3.6. Physically and Numerically Induced Diahline Exchange Flow

After having confirmed the validity of the relation in Equation 9c between the effective vertical diahaline velocity and the mixing per salinity class, this relation can be used to calculate separate estimates for the physically and numerically induced portions of the diahaline exchange flow in terms of the physical and numerical mixing contributions (see Section 3.4 and Figures 7g–7l).

Figure 11 compares the physically and numerically induced effective vertical diahaline velocities. In most areas the diahaline exchange flow across the presented isohalines is clearly dominated by physics, but it becomes clear that the role played by numerics is far from negligible. Both contributions show enhancement along the topographic boundaries.

By means of Equation 13, also the physically and numerically induced integrated incoming and outgoing diahaline transports can be obtained (Figures 11g and 11h). Interestingly, the resulting residual transports show opposite directions for the physical and numerical contributions across some isohalines, for example,

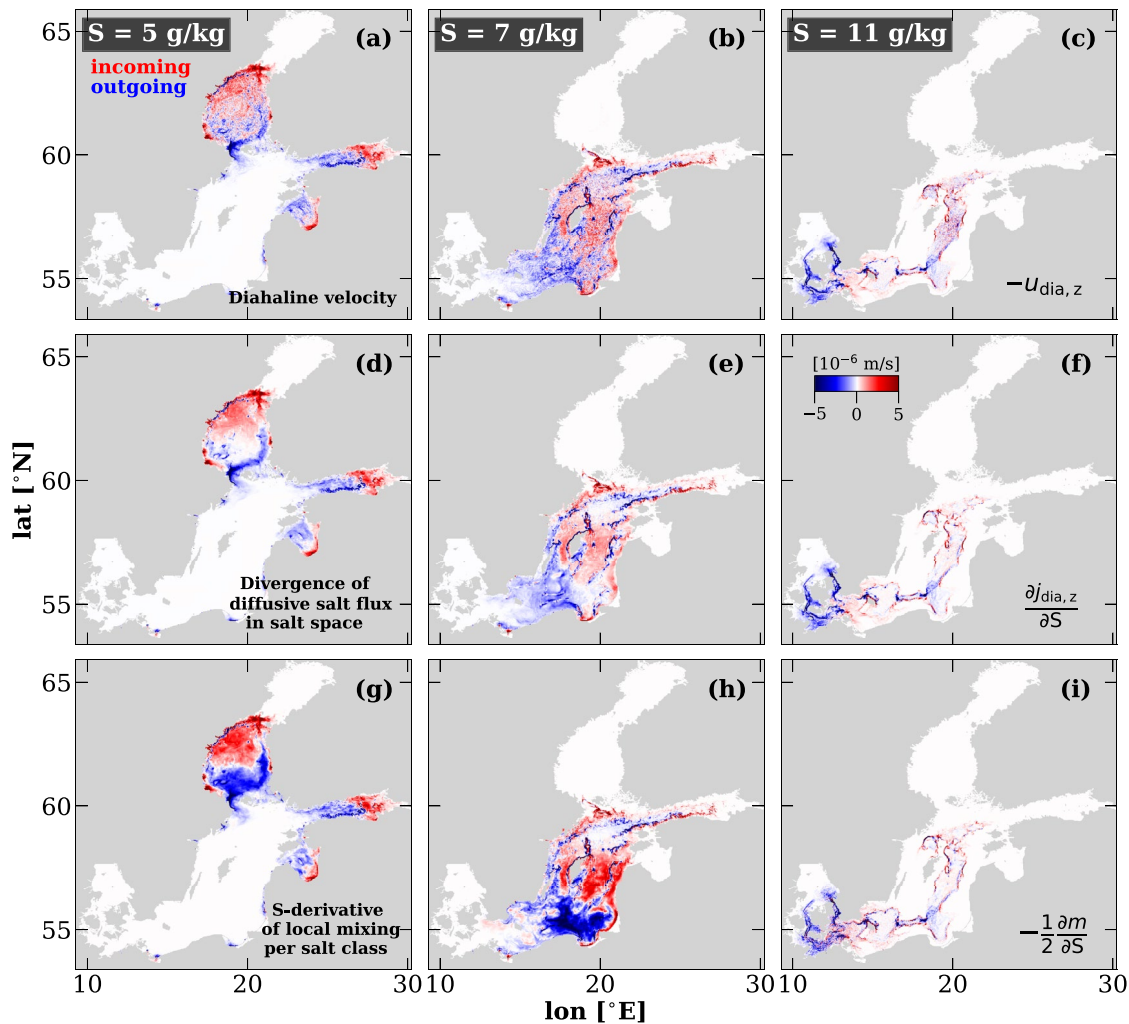


Figure 9. Maps of diahaline quantities averaged over 2 years. Column 1: 5 g/kg; Column 2: 7 g/kg; Column 3: 11 g/kg. Row 1 (a–c): effective vertical diahaline velocity; Row 2 (d–f): divergence of effective vertical diffusive salt flux in salt space; Row 3 (g–i): derivative of mixing per salinity class with respect to salinity. The similar patterns of the shown quantities for each isohaline indicate the approximate validity of Equations 9a–9c.

across 7 g/kg and 11 g/kg. Indeed, the integrated transports confirm that the physically induced contribution usually dominates the exchange flow across isohalines with salinities below 10 g/kg. However, for most isohalines the numerically induced transports contribute with up to 50% and more to the diahaline exchange flow (Figure 11i).

3.7. A More Detailed View on Boundary Mixing

Several of the Baltic Sea maps presented in this work, for example, Figure 9b, highlight hot spots for diahaline boundary mixing. Where the mixing is stronger, also the mixing gradient is increased. By means of Equation 9c also the diahaline velocity is stronger at mixing hot spots. Therefore, we can study the diahaline velocity when investigating the boundary mixing. Two mixing hot spots are zoomed in on in Figures 12a and 12b: the Gotland island in the former, and the Western Baltic Sea in the latter. Incoming velocities closest to land on an inner ring are shown along the north–western coastline of Gotland (Figure 12a). The inner ring with incoming $u_{dia,z}$ is followed by an outer ring with outgoing $u_{dia,z}$. The same structure is more clearly observable close to the Swedish coast north of Gotland and around the small island of Gotska Sandön to the north–east of Gotland. Furthermore, the seesaw pattern of an inner incoming velocity and outer outgoing velocity ring is present around the northern half of Bornholm island (Figure 12b).

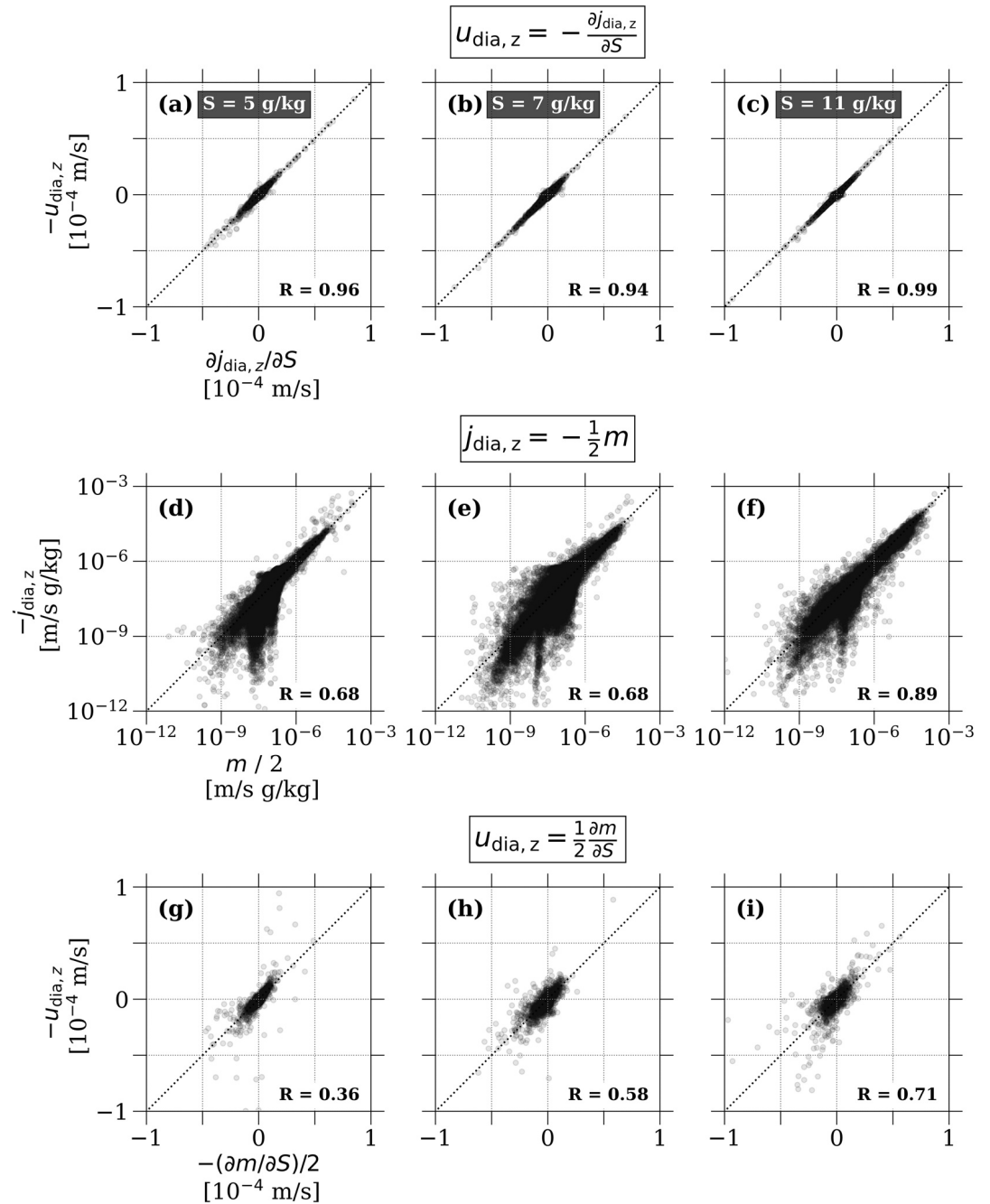


Figure 10. Scatter plots for the relations between the effective vertical diahaline velocity $u_{dia,z}$, the effective vertical diahaline diffusive salt flux $j_{dia,z}$ and the mixing per salinity class m . Left column: salinity class 5 g/kg; Middle column: salinity class 7 g/kg; Right column: salinity class 11 g/kg. First row: Equation 9a; Second row: Equation 9b; Third row: Equation 9c. For every scatter plot the corresponding correlation coefficient R is included.

We investigate the pattern along two transects of local mixing per salinity class, derivative of mixing per salinity class and diahaline velocity (Figure 13). The velocity transect is shown in latitude–depth and latitude–salinity space, the mixing and mixing gradient transect only in latitude–depth space. Mixing is showcased for the sake of a direct display of boundary mixing, without passing by Equation 9c. A comparison of the mixing transects (Figures 13a and 13b) with the velocity transects (Figures 13e and 13f) confirms their appearance at the same locations. The similarity of the derivative of mixing per salinity class (Figures 13c and 13d) and the effective vertical diahaline velocity (Figures 13e and 13f) again confirm the validity of Equation 9c also in latitude–depth

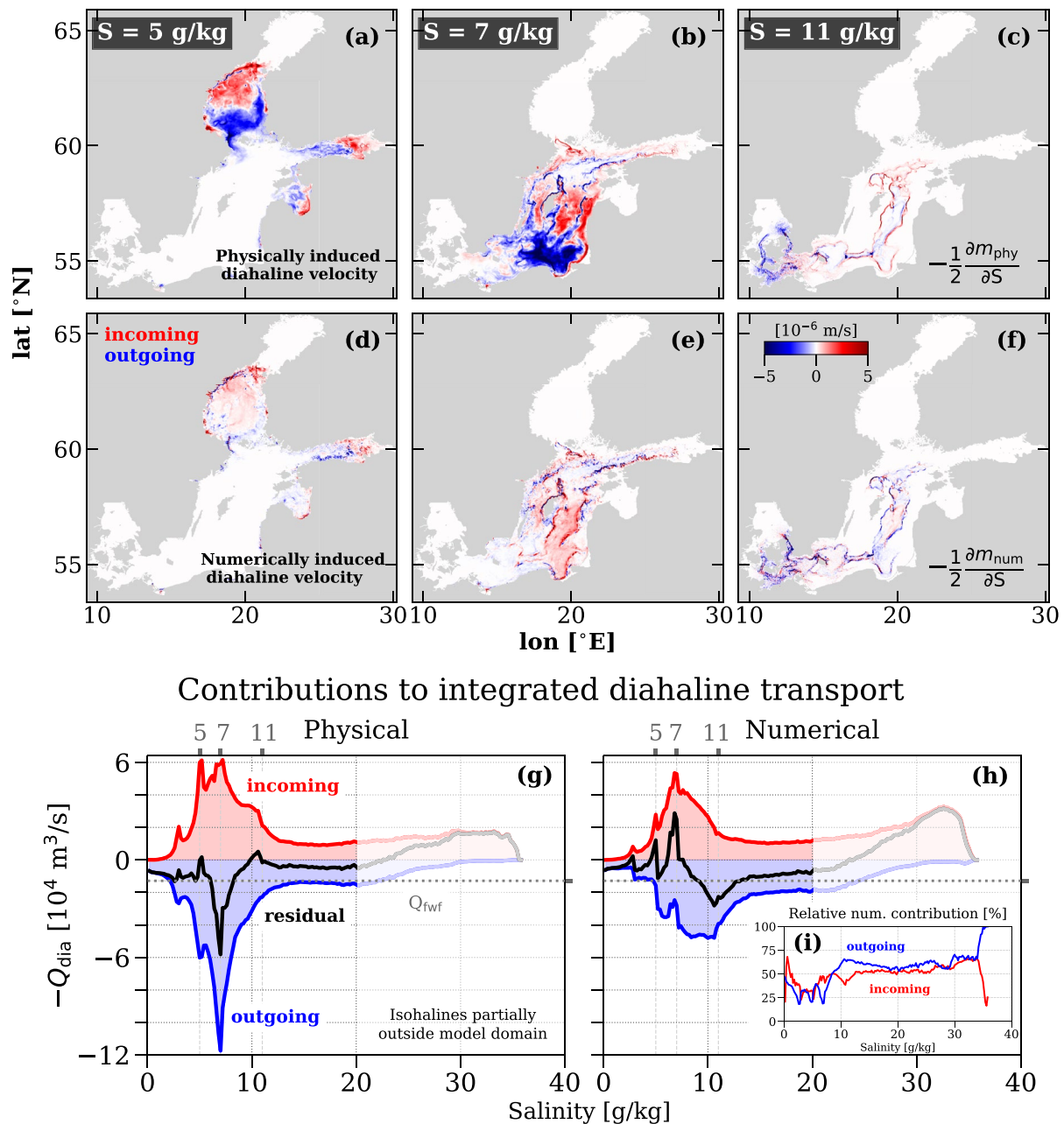


Figure 11. Maps of the physically (a–c) and numerically (d–f) induced effective vertical diahaline velocity, diagnosed by means of Equation 9c in terms of the 2-year averaged physical and numerical mixing per salinity class, m_{phy} and m_{num} , respectively. Left column: salinity class 5 g/kg; Middle column: salinity class 7 g/kg; Right column: salinity class 11 g/kg. Physical (g) and numerical (h) contributions to the integrated diahaline transport, individually separated into incoming and outgoing portions, calculated from Equation 9c. The relative contribution of the integrated numerical diahaline transport to the sum of the integrated physical and numerical diahaline transport is shown in (i).

space along these transects. Transect 1 spans from the Gotland island with steeper bathymetry to the Swedish coast with flatter bathymetry (Figures 13a, 13c, 13e, 13g). Transect 2 stretches from the Bornholm island to the southern Swedish coast (Figures 13b, 13d, 13f, 13h). The location of the transects is displayed in Figure 12. The isohalines included in z coordinates, and the isobaths included in S coordinates, connect the two spaces with each other, simplifying the interpretation and understanding of how they are connected. Regardless of the chosen space, the same structure is seen: a lower layer of incoming and an upper layer of outgoing velocities along the coasts. Consistent with the steep bathymetry of the Gotlandic coast, the observed structure is more spatially constrained. Off the flatter Swedish mainland coast, the two-layer structure is more spread out both horizontally

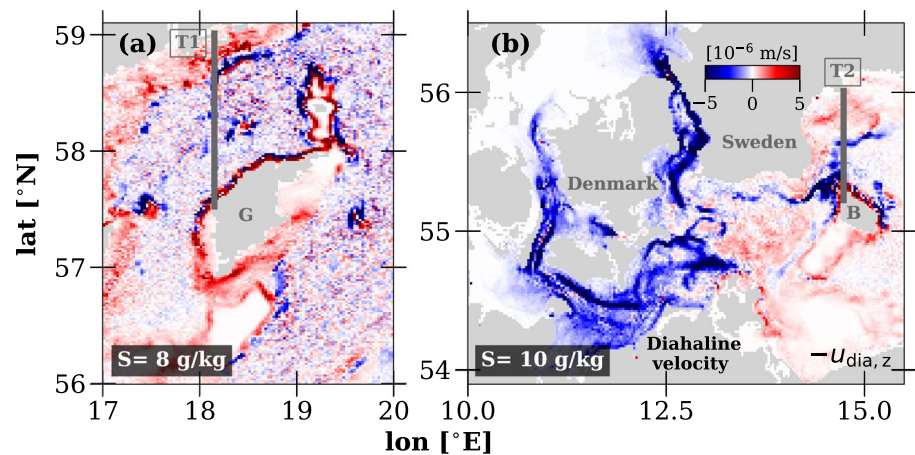


Figure 12. Zoom on the effective vertical diahaline velocity across the isohalines of 8 and 10 g/kg for (a) vicinity of Gotland island, and (b) Western Baltic Sea, respectively. For the location of the zoomed-in regions, see the rectangles in Figures 9b and 9c. G: Gotland island, B: Bornholm island. A temporal average is taken over 2 years. Details along the transects T1 and T2 are shown in Figure 13.

as well as vertically. The isobaths in Figure 13g reflect the different bathymetry in this region: they are denser off the Gotlandic coast with its steeper, and sparser off the Swedish mainland with its flatter topography. From transect 2, it is particularly visible how the S coordinates can be of use in visualizing and understanding the occurring processes: the incoming $u_{\text{dia},z}$ in S coordinates between latitudes of 55.3–55.4°N (Figure 13h) covers a larger area than the same structure in z coordinates (Figure 13f), and is thus easier to evaluate. Vertical integration of Equation 9c from minimum to maximum salinity, and noting that $m(S_{\text{min}}) = m(S_{\text{max}}) = 0$, shows that the vertical S -integral of $u_{\text{dia},z}(S)$ must vanish. This can also be estimated from Figures 13g and 13h. However, in fully physical space (Figures 13e and 13f) this is generally not the case.

4. Summary and Conclusions

In this paper we have investigated the relation between the local diahaline quantities of mixing per salinity class, salt flux and velocity in a numerical model of the fjord-type, non-tidal Baltic Sea. These quantities are connected with each other through newly derived, idealized relations in the earlier work by Klingbeil and Henell (2023). The bird's eye view in maps of local mixing per salinity class emphasizes the location of potential mixing hot spots. In these actively mixed regions the diffusive diahaline salt flux is also enhanced. The diahaline diffusive salt flux has the possibility to move water across the isohaline, and change the salinity of the transported water mass. Because the change in salinity is concurrent with mixing, the diahaline diffusive salt flux therefore gives information on where the mixing is occurring. The local diahaline velocity is a consequence of the diahaline diffusive salt flux, and the velocity itself determines the ensuing exchange flow. Thus goes the connection from local mixing per salinity class over diahaline diffusive salt flux to diahaline velocity: this is portrayed mathematically in Equations 9a–9c. A good agreement was shown between the local diahaline quantities, implying that the relations hold well.

Transects of local mixing per salinity class and diahaline velocity in latitude–depth and latitude–salinity space are studied for a closer look at diahaline boundary mixing. Also close-up views of mixing hot spots were shown. From the transects and close-up views an identical pattern was inferred in latitude–depth/salinity space in the former and latitudinal direction in the latter case. Its characteristics consists of a seesaw structure for (a) incoming diahaline velocity and (b) outgoing diahaline velocity: for the close-up maps in longitudinal direction an inner ring of (a), followed by an outer ring of (b) is observed; for the transect in longitude–depth space (a) appears in the deeper and (b) in the shallower layer; and for the transect in longitude–salinity space (a) occurs in the saltier and (b) in the fresher layer. An idealized sketch of the Baltic overturning circulation in longitude–depth space, including main processes, is shown in Figure 3e. A close-up view of the boundary processes is presented in Figure 14, which is adapted from earlier sketches in the works of Garrett (1990, his Figure 1b) and Ferrari et al. (2016, their Figure 2). The isohalines are impinging at a right angle on the bottom in the bottom boundary layer.

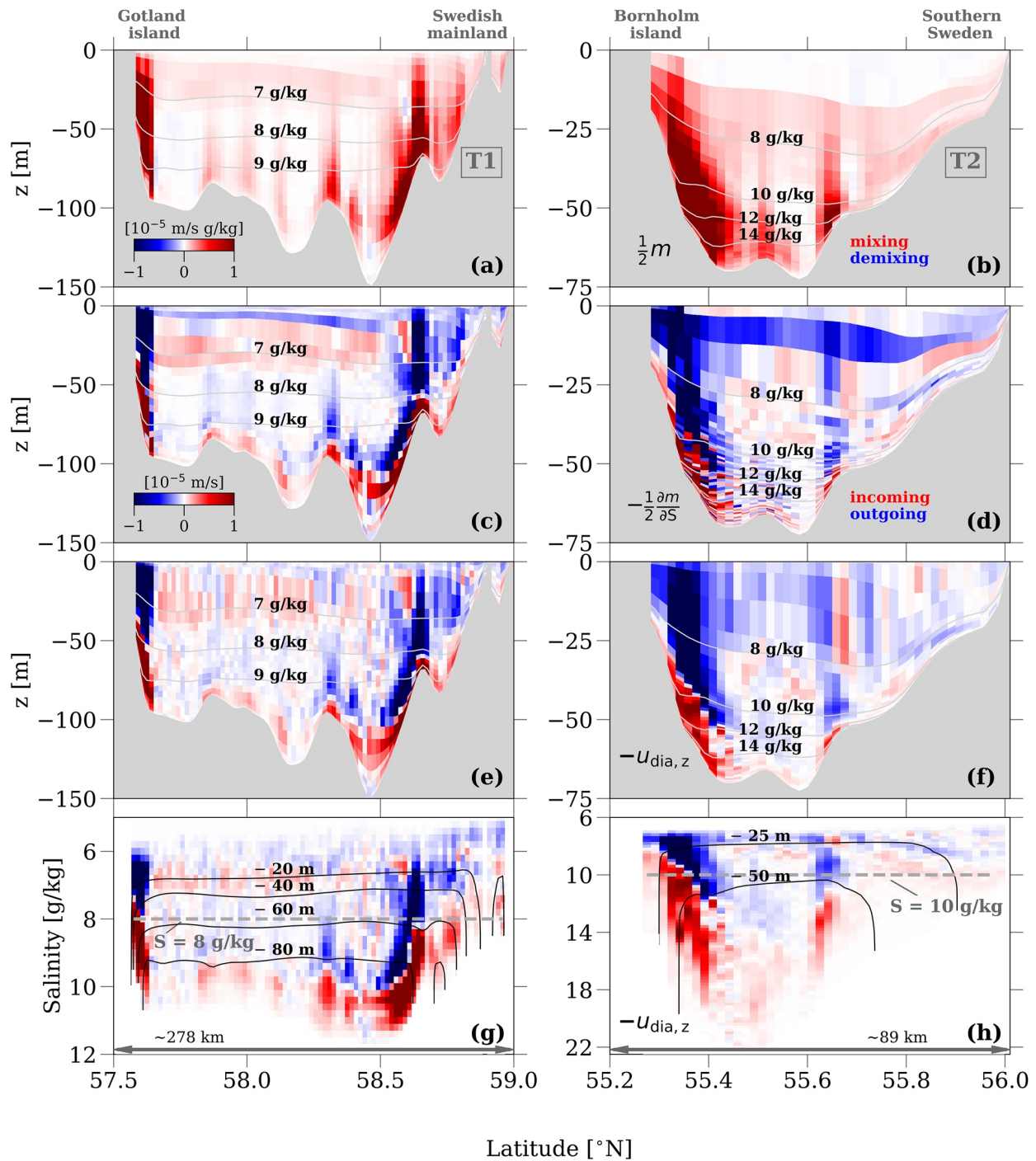


Figure 13. (a), (b) Local mixing per salinity class, (c), (d) derivative of the mixing per salinity class with respect to salinity, effective vertical diahaline velocity in (e), (f) geopotential and (g), (h) salinity space along the transects T1 and T2 shown in Figure 12. A temporal average is taken over 2 years. Isohaline contour lines are included in (a)–(f), and isobathic contour lines in (g), (h). Quantities in geopotential coordinates are obtained by consecutive arrangement of salt classes with their thicknesses, starting with lowest salinity at the ocean surface. The dashed gray lines in (g) and (h) correspond to the isohalines of 8 and 10 g/kg showcased in Figure 12.

This is a necessary condition to guarantee that no diffusive salt flux crosses the sloping boundary. In the bottom boundary layer an incoming, upward diahaline velocity is observed. Coherently, a negative mixing gradient is present. That is, the local mixing per salinity class increases with further distance from the bottom ($\partial m / \partial z > 0$), but salinity decreases, since it is highest directly at the bottom (if stably monotonic). Therefore, $\partial m / \partial S < 0$. The mixing gradient reaches a maximum, whereupon it decreases exponentially. The salinity continues to decrease

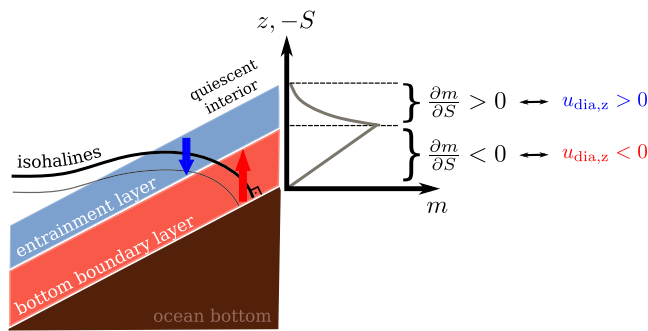


Figure 14. Sketch of the boundary mixing, adapted from Garrett (1990, his Figure 1b) and Ferrari et al. (2016, their Figure 2). The local link between mixing and exchange flow is visualized: they are connected through Equation 9c, which reads $u_{dia,z} = 1/2 \partial m / \partial S$. For information on the sign convention used for the effective vertical diahaline velocity, see Figure 2a.

since the water becomes fresher. From this results a positive mixing gradient, that is, an outgoing, downward diahaline velocity. A result consistent with these findings has been obtained by Umlauf and Burchard (2011), who applied an idealized one-dimensional model for the oscillating bottom boundary layer over sloping topography. In their Figure 5, they show profiles of up-slope velocity u and turbulent buoyancy flux b , both averaged over one oscillation period. The velocity profile shows an exchange flow with up-slope velocity near the bottom and down-slope velocity above. The location of the change in sign of velocity coincides exactly with the minimum of the turbulent buoyancy flux and is consistent with u being proportional to $-\partial b / \partial z$.

The mixing analysis by Klingbeil et al. (2014) and Equation 9c further render it possible to distinguish between the physically and numerically induced diahaline exchange flow. Despite the advanced numerical techniques of our coastal ocean model to reduce numerical mixing, the exchange flow across the majority of isohalines is associated up to 50% and more with numerical mixing. The maps of numerically induced, spurious diahaline salinity vari-

ance dissipation presented in this work, based on a column-by-column application of the WMT framework, add to earlier methods developed for diathermal fluxes in Holmes et al. (2021, their Figure 3).

Finally, this diahaline framework calls for its extension to the thermohaline overturning circulation of the World Ocean. Quantifying the contribution of the spurious numerically driven global circulation is of great interest for estimating the reliability of climate models.

Data Availability Statement

The model data used in this work are available from <https://doi.org/10.5281/zenodo.7754399> (Klingbeil, 2023).

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Highlights

Exploring the variability of a non-tidal marginal sea with a single-model ensemble

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- Ensemble reveals variability that cannot be covered by measurements or single model
- Inter-ensemble uncertainty of 4 days for the arrival time of a Major Baltic Inflow
- Ensemble model offers robust analyses of short-term dynamics in salinity space

Exploring the variability of a non-tidal marginal sea with a single-model ensemble

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Abstract

In this study we used single-model ensemble simulations, generated by perturbed initial conditions, to study the variability in the Baltic Sea. Each ensemble realization may be viewed as an additional outcome of the same stochastic process. The ensemble simulations reveal a high variability of the 2014/2015 Major Baltic Inflow event, which is not possible to cover with measurement data or an individual model realization. Furthermore, robust analyses of short-term dynamics up to daily temporal scales using the local Water Mass Transformation framework are rendered possible, when combined with single-model ensemble simulations.

Keywords: GETM, single-model ensemble, local Water Mass Transformation, Baltic Sea, Major Baltic Inflow, bottom gravity currents

1. Introduction

Lorenz (1963) discovered chaotic behavior when modeling weather systems, laying the foundation for the scientific domain of chaos theory, or deterministic chaos. Deterministic chaos combines two seemingly contradictory concepts: unpredictability and deterministic motion. A chaotic system can be defined in various ways. In this work, chaos is defined based on the system's sensitivity to initial conditions, which is one of the three defining properties of chaotic systems (Devaney, 2018).

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Physical processes in hydrodynamics are inherently turbulent and involve a stochastic component. This implies that for any given initial state and external forcing, the system does not follow a single determinable path (Büchmann and Söderkvist, 2016; Lamb, 1932). As Lorenz (1963) explained, this unpredictability does not negate the possibility of predicting statistical aspects of the system; rather, the system's precise physical state remains unpredictable. Büchmann and Söderkvist (2016) note that "the physical system may be seen as a stochastic process, which is executed only once." This stochastic nature is also inherent in numerical models of such systems, primarily arising from the non-linear coupled primitive equations upon which these models are built. Consequently, the outcome of a numerical model should be viewed as a single realization of a stochastic process. Perturbing the initial conditions of the model can lead to significantly different results. However, if the perturbation is sufficiently small, the additional simulation can be regarded as another realization of the same stochastic process, as the overarching stochastic characteristics of the model remain unaltered (Büchmann and Söderkvist, 2016). In this respect the variability of a single-model ensemble can be used to estimate the uncertainty of the model results, but also to explore the natural variability in a physical system.

In this work we applied single-model ensemble simulations to explore two key mechanisms in the Baltic Sea: i) the natural variability of a salt water inflow event, and (ii) local water mass transformation in the deep Baltic basins.

The Baltic Sea is a brackish semi-enclosed sea located in northeastern Europe. It is geographically highly constrained with only a smaller, shallow opening in its western reaches towards the North Sea (Fig. 1a). Large areas are today anoxic due to eutrophication, especially at depth. Therefore, the Baltic Sea is highly dependent on inflow events, originating from the North Sea, that mix the Baltic waters, and ventilate the deeper reaches (Reissmann et al., 2009). Such inflow events bring saline and oxygen-rich waters from the North Sea into the Baltic Sea. The combination of salt water inflows, freshwater discharge and water mass transformation in the deep basins sets up the large-scale estuarine circulation in the Baltic Sea.

The theoretical framework to investigate water mass transformation (WMT) and overturning circulation dates back to Walin (1977). Since then the framework has been applied in many studies. Maps of local water mass transformation rates, i.e., of diapycnal volume fluxes, have usually been analyzed on global and decadal scales (Lee et al., 2002; Maze et al., 2009; Megann, 2018).

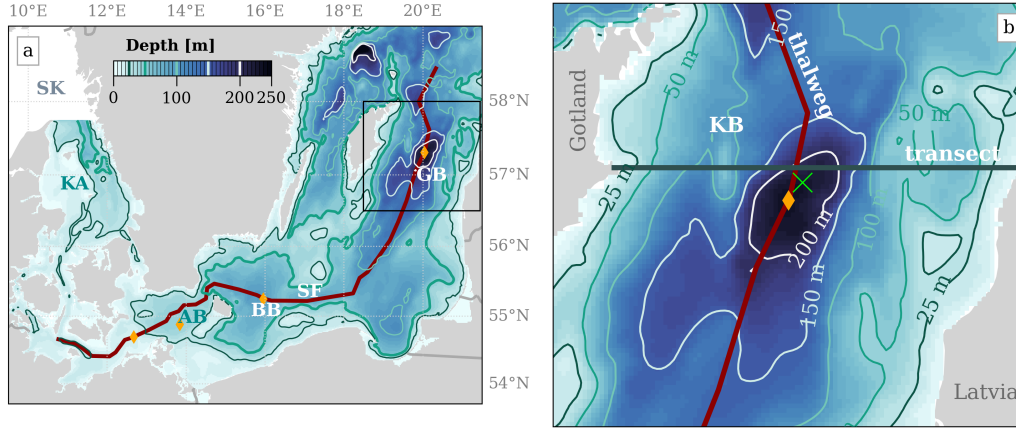


Figure 1: (a) Map of bathymetry in the region of interest: the western and central Baltic Sea. (b) Zoom on the eastern Gotland Basin. The isobaths of 25, 50, 100, 150 and 200 m are marked in different shades of green. The main basins or features of interest are denoted as SK - Skagerrak, KA - Kattegat, AB - Arkona Basin, BB - Bornholm Basin, SF - Slupsk Furrow and GB - eastern Gotland Basin in (a) and KB - Klintsbank in (b). Stretching through the different basins is the Baltic thalweg transect, shown in bordeaux. The orange markers show the location of the stations of Darss Sill, Arkona Basin, Bornholm Basin and Gotland Basin. The green cross in (b) marks the measurement location of the GODESS station. The transect corresponds to the transect in Fig. 11.

Recently, Henell et al. (2023) verified analytically derived relations between local WMT quantities (Klingbeil and Henell, 2023) in a one nautical mile simulation of the Baltic Sea. Despite being averaged over two years, the local WMT quantities contained a certain level of noise, and robust analyses on shorter time scales were not possible. The Baltic Sea is a large non-tidal estuary, so generating robust, averaged WMT quantities by extending a single simulation over dozens of tidal cycles, as is typically done in tidal estuaries, is not an option. Therefore, we will investigate to which extent single-model ensemble simulations can enable water mass transformation on shorter time scales.

This paper is structured as follows. First, the applied methods are introduced in Section 2. The numerical model and the generation of the single-model ensemble is described therein. The results and discussion section (Section 3) is divided into several subsections, where (i) a general overview sets the stage (Section 3.1), (ii) the internal variability in the single-model ensemble realizations is analyzed (Section 3.2), and, lastly, (iii) the integral

(Section 3.3) and local (Section 3.4) Water Mass Transformation is studied in the Bornholm and Gotland Basin. Concluding remarks are given in Section 4.

2. Methods

2.1. Numerical model

In this study we apply the numerical model for the Baltic Sea from Henell et al. (2023). It uses the coastal ocean model GETM (www.getm.eu), which is based on state-of-the-art numerical schemes and turbulence closure (Klingbeil et al., 2018). In recent years, the model code has been extended to provide accurate WMT diagnostics from an online binning procedure in salinity space, combined with conservative thickness-weighted averaging (Klingbeil et al., 2019). The model setup is well validated (Burchard et al., 2018; Gräwe et al., 2019) and will be used in this study to simulate the years 2014 and 2015, covering the 3rd largest major Baltic inflow (MBI) event from December 2014 to April 2015. Results will be analyzed from July 2014 to July 2015.

2.2. Generation of the single-model ensemble

The ensemble members are generated by perturbed initial conditions. Our model configuration uses prescribed open boundary conditions to prevent the system from escaping into a fundamentally different state. For the perturbation experiments, we utilized a hotstart file extracted from a simulation spanning 2012 to 2017, specifically on January 1, 2014. Following the methodology proposed by Büchmann and Söderkvist (2016), the initial fields were perturbed by adding a small value, $\varepsilon(x, y)$, to the salinity in each vertical column. This adjustment did not compromise the stability of the water column, since the changes involved only shifts in salinity profiles. The perturbation value, $\varepsilon(x, y)$, could take on positive or negative signs, ensuring that all resulting profiles retained positive salinity values. Random values for $\varepsilon(x, y)$ were drawn from a normal distribution with a mean of zero and a standard deviation of 10^{-10} g/kg, as recommended by Büchmann and Söderkvist (2016). It is important to note that our objective was not to target the most unstable modes to maximize the growth of disturbances, as discussed by (Polkova et al., 2019). Instead, the goal was to generate small-scale fluctuations that would produce an alternative realization of the dynamics.

97 The overall ensemble consists of 26 individual simulations. However, all
 98 analyses in this work are based on 18 members, while the remaining 8 mem-
 99 bers were only used to confirm the robust averages from the 18-member
 100 ensemble, in comparison to the averages obtained from the one with 26 en-
 101 semble members.

102 3. Results and Discussion

103 3.1. Evolution of the inflow event

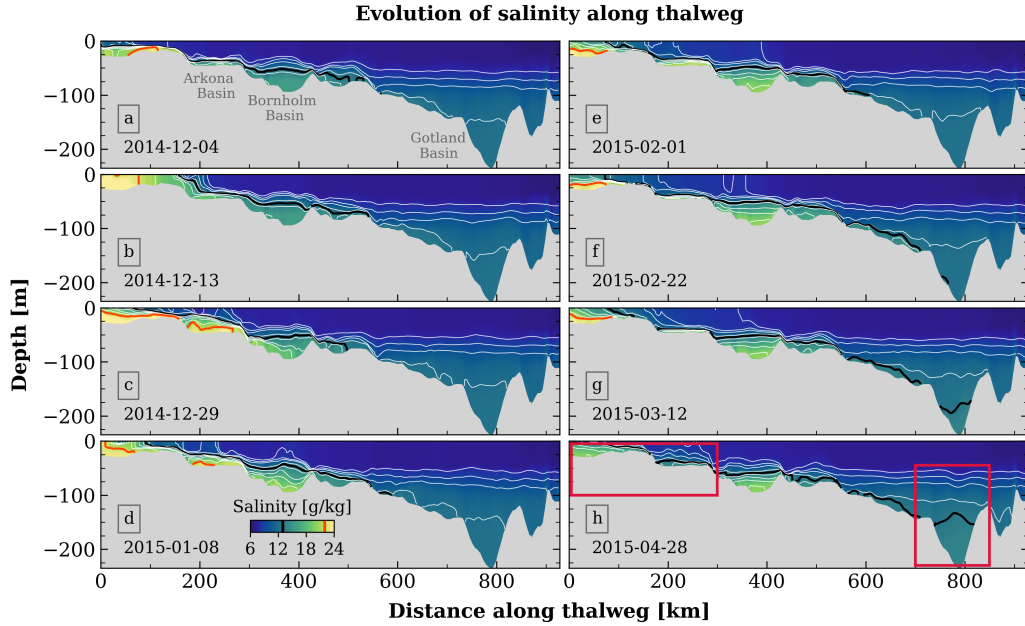


Figure 2: Ensemble-averaged salinity distribution along the Baltic Sea thalweg transect before and during the inflow event of 2014/2015. The thick black and orange lines show the 13 and 22 g/kg isohalines, respectively. See Fig. 1a for the path drawn by the Baltic thalweg transect. The red rectangles in (h) show the location of the regions studied in Fig. 3.

104 Fig. 2 shows the salinity along a section of the Baltic Sea thalweg, which
 105 stretches through all the deeper basins from the western Baltic Sea until
 106 slightly north of the eastern Gotland Basin (see Fig. 1a for the location).
 107 The arrival and evolution of the Major Baltic Inflow (MBI) of 2014/2015
 108 along the thalweg of the Baltic Sea is shown in Fig. 2. The inflow arrived on

109 13 December 2014 in the western Baltic Sea at the entrance of the thalweg,
 110 which agrees exactly with the observations described in Nausch et al. (2015).
 111 Gräwe et al. (2015) describe the main inflow phase to start on 15 December
 112 2014. The inflow arrives as a front of highly saline water (Fig. 2b), which
 113 then starts spreading throughout the Baltic basins, mixing the saline and
 114 oxygen-rich inflow water with the ambient waters until they overflow into
 115 the next basin, and eventually reach the Gotland Basin around the end of
 116 February (Fig. 2f). By 12 March (Fig. 2g), the Gotland Basin is filled with
 117 waters saltier than 13 g/kg. In April (Fig. 2h) the basin continues to fill
 up further with the MBI waters. The arrival of the MBI in the Arkona and

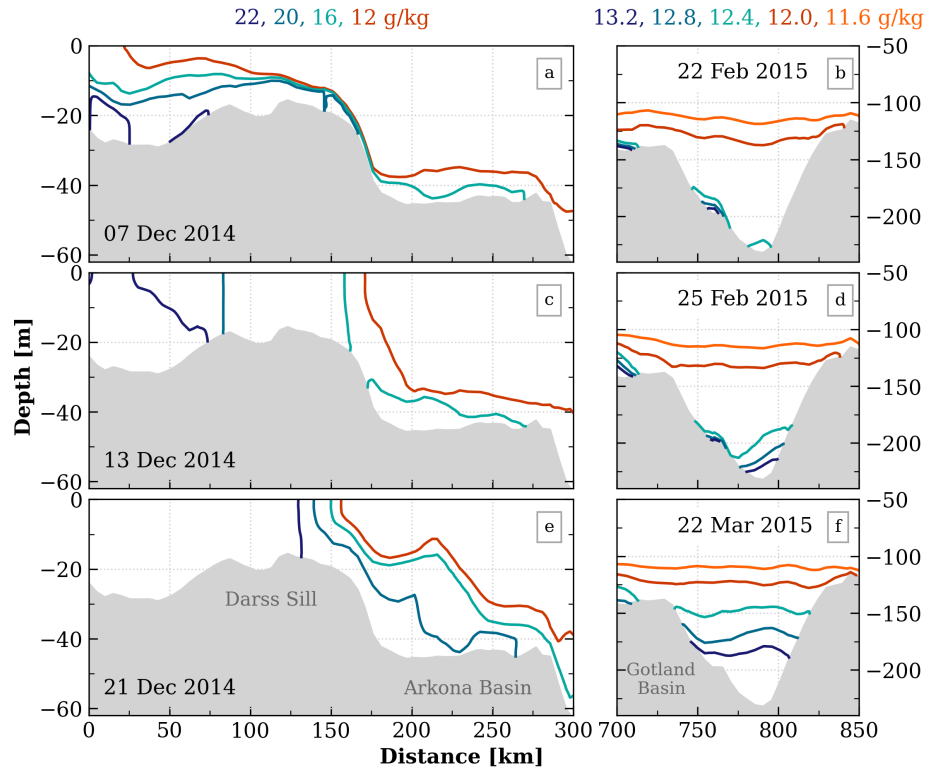


Figure 3: Column 1: Position of isohalines 12, 16, 20 and 22 g/kg at the Darss Sill on (a) 7 December 2014, (c) 13 December 2014, and (e) 21 December 2014. Column 2: Position of isohalines 11.6, 12.0, 12.4, 12.8 and 13.2 g/kg in the Gotland Basin on (b) 22 February 2015, (d) 25 February 2015, and (f) 22 March 2015.

118

119 Gotland Basin is also apparent in Fig. 3 from the changing isohalines at the
 120 Darss Sill in the western Baltic Sea, and in the Gotland Basin. This sill is

121 one of the major passages of the inflow water into the central basins of the
 122 Baltic Sea. The raising and tilting of the 12, 16, 20 and 22 g/kg isohalines,
 123 in response to the highly saline water masses of the MBI arriving in an area
 124 of lower salinity water, can be clearly observed in Fig. 3a,c,e for the Darss
 125 Sill. Also the filling of the Gotland Basin with saltier water from the inflow is
 126 apparent when examining Fig. 3b,d,f. On 22 February 2015 (Fig. 3b) waters
 127 with a salinity of above 13.2 g/kg have already descended into the basin, but
 128 not yet to its deepest reaches. However, by 25 February 2015 (Fig. 3d) the
 129 deepest parts are affected, and the entire basin has filled up with MBI waters
 130 by 22 March 2015 (Fig. 3f).

131 *3.2. Internal variability at key locations along the inflow path*

132 *3.2.1. Darss Sill station*

133 To begin analyzing the ensemble variability, we compare salinity and tem-
 134 perature profiles in Fig. 4a-l with measurements taken at the Darss Sill sta-
 135 tion (see location in Fig. 1). Generally, we can distinguish between periods
 136 with inflow into the Baltic Sea and outflow activity, respectively. During
 137 inflow conditions (e.g., 10 December 2014, 4 and 25 January 2015; Fig. 4a-c)
 138 a stratified water column with high salinities in the inflowing near bottom
 139 plume is observed. The ensemble variability is elevated, because inflows oc-
 140 cur in a pulse-like manner, making the exact location of the inflow fronts
 141 critical. Due to their inherently nonlinear character, the predictability of
 142 these fronts is, however, small, resulting in the observed larger variability.
 143 During outflow conditions (e.g., 15 February, 8 March, and 30 May; Fig. 4d-
 144 f) the salinity of the entire water column is low, and the ensemble variability
 145 is small. This is expected, as outflow conditions involve surface water masses
 146 with a narrow salinity range advecting from the Arkona Basin into the Belt
 147 Sea, and passing through the Darss Sill.

148 When examining the temperature profiles in Fig. 4g-l, only the profiles
 149 from 25 January show elevated ensemble variability. Since the profiles pre-
 150 sented are from winter, water masses in the Belt Sea are likely stratified
 151 in salinity but homogeneous in temperature. As a result, the temperature
 152 differences are minimal.

153 The time series of bottom salinity and temperature (Fig. 4m,n) show high
 154 temporal variability due to the pulse-like nature of the inflowing near-bottom
 155 plumes. All model runs show a systematic bias towards higher salinities, be-
 156 cause the model is not specifically calibrated for Darss Sill, but to reproduce
 157 the hydrography in the whole Baltic Sea, including the arrival of high-saline

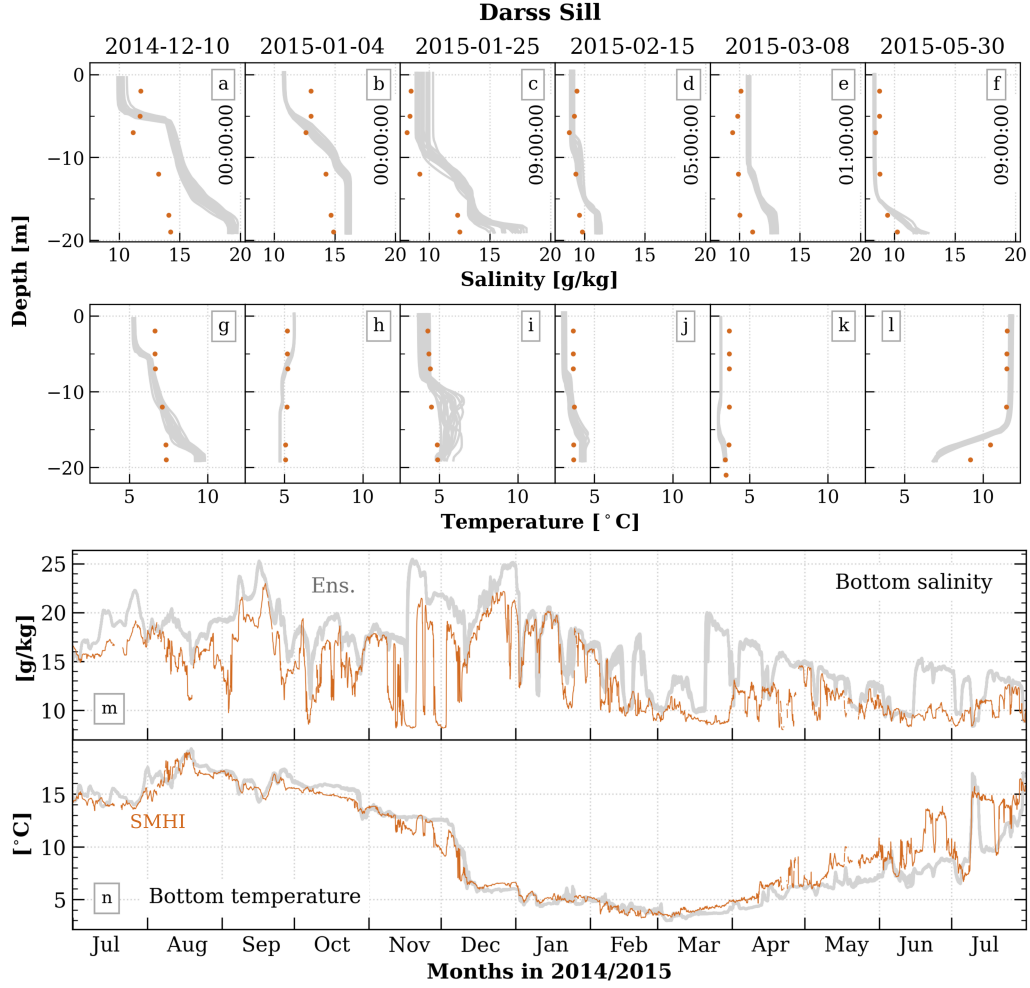


Figure 4: (a)-(l) Comparison of modelled salinity and temperature profiles from the ensemble simulations (gray lines) with measurement data (orange dots) at the station Darss Sill, see location in Fig. 1a. (m), (n) Comparison of modelled time series of bottom salinity and temperature (gray lines) with measurement data (orange lines) at the Darss Sill.

158 waters also in the, far downstream, deep Gotland Basin. Moreover, our nu-
 159 merical model with a resolution of one nautical mile cannot properly resolve
 160 all topographic features that impact the pathway of the inflowing plumes
 161 in reality. Compared to the temporal variability of the bottom salinity and
 162 temperature, the internal variability in the ensemble is low. This is due to

163 the well-constrained conditions of the near bottom water masses in the up-
 164 stream narrow and shallow Belt Sea, that limit the generation of ensemble
 165 spread in this part of the domain.

166 3.2.2. Arkona Basin station

167 At the Arkona Basin station (see location in Fig. 1), all profiles exhibit
 168 well-stratified water columns in terms of salinity, which are well reproduced
 169 by the model (Fig. 5a-n). Ensemble variability is low at the surface, as ob-
 170 served at the Darss Sill during outflow conditions. However, starting at the
 171 halocline and extending deeper, we observe a significant increase in ensemble
 172 variability. This can be explained similarly to the situation at Darss Sill:
 173 the total salt content in the Arkona Basin, and therefore the depth of the
 174 halocline, is highly sensitive to the timing of the inflow front, making it sub-
 175 ject to deterministic chaos. While the temperature ensemble variability at
 176 Darss Sill exhibited relatively small spreads, this is different in the Arkona
 177 Basin. As previously noted, the inflowing water masses are homogeneous in
 178 temperature, meaning that salinity primarily controls density. However, tem-
 179 perature in this context serves as a passive tracer, allowing us to track the
 180 movement of inflowing water masses. Ensemble variability is significantly
 181 elevated in the temperature profiles below the halocline (22–26 m depth).
 182 This indicates that water masses at these depths can have varying origins
 183 with different "release rates" (either from Darss Sill in the West or Drogden
 184 Sill, which is another possible inflow pathway from the Kattegat through the
 185 Sound between Denmark and Sweden north of the Arkona Basin). Conse-
 186 quently, the local water masses are a complex mixture of interleaving water
 187 masses from different sources.

188 As for the Darss Sill station, the time series of bottom salinity and tem-
 189 perature (Fig. 5o,p) show much higher temporal variability than internal
 190 variability in the ensemble. During late summer/fall 2014 the Arkona Basin
 191 was affected by minor baroclinic inflows (Nausch et al., 2015). Considering
 192 the challenges for numerical models mentioned before, the performance of
 193 our model to reproduce the resulting natural variability is state-of-the-art.

194 3.2.3. Bornholm Basin station

195 Except for late spring and summer 2015, the permanent halocline in the
 196 Bornholm Basin is well reproduced by the model simulations (Fig. 6a-g). As
 197 for salinity, also for temperature (Fig. 6h-n) the measurements are usually
 198 within the band given by the ensemble spread. With stratification mainly

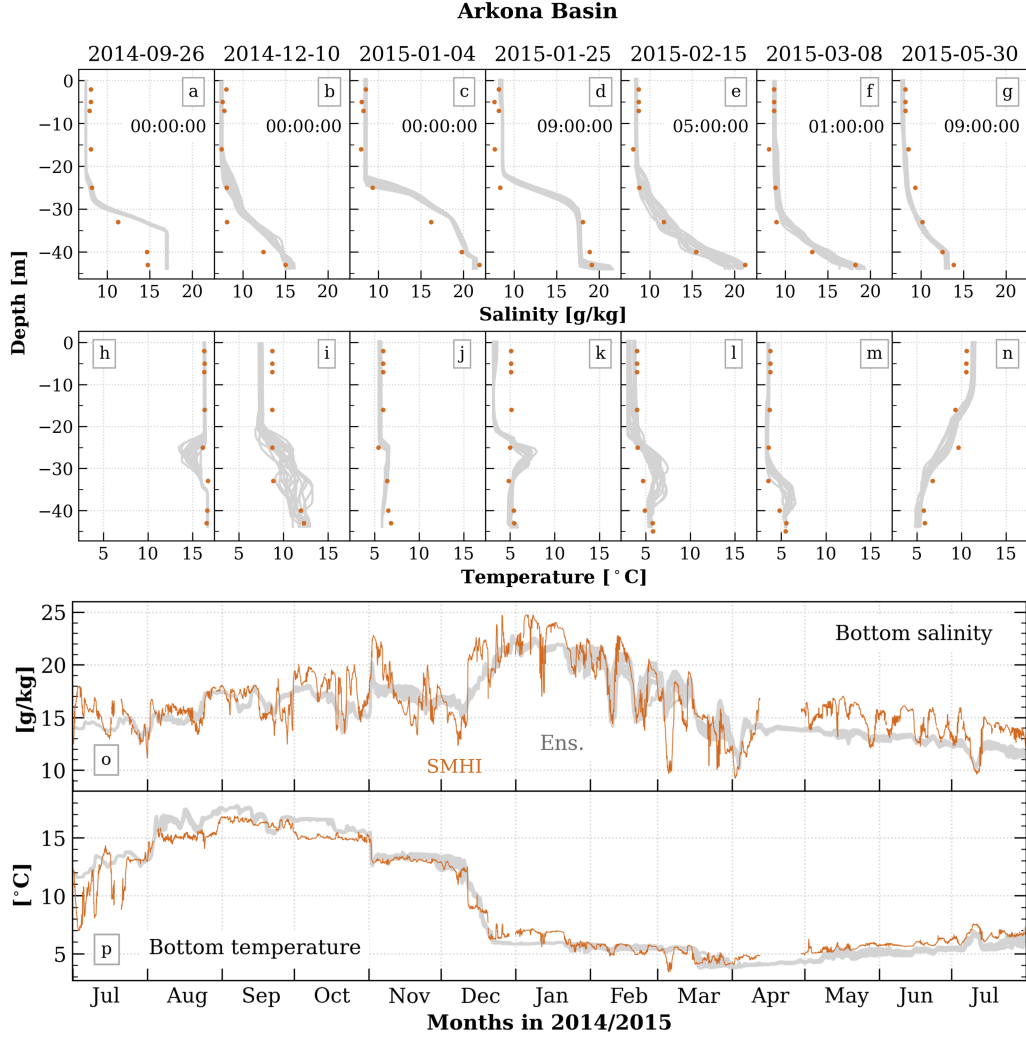


Figure 5: (a)-(n) Comparison of modelled salinity and temperature profiles from the ensemble simulations (gray lines) with measurement data (orange dots) at the station Arkona Basin, see location in Fig. 1a. (o), (p) Comparison of modelled time series of bottom salinity and temperature (gray lines) with measurement data (orange lines) at the Arkona Basin station.

199 determined by salinity, temperature can exhibit significant variability at each
 200 depth level, which is also shown by the ensemble simulations.

201 The arrival of the MBI in the deepest part of the Bornholm Basin is
 202 observed around 26 December 2014 (Fig. 6o). All ensemble members agree

203 closely on this arrival date. Before this event, bottom salinity remained
 204 constant, as the water masses were stagnant and had an age exceeding one
 205 year (see Fig. 9 in Gräwe et al., 2015). However, the ensemble variability
 206 in temperature tells a different story (Fig. 6p). Starting in mid-September,
 207 the temperature spread increases significantly. As discussed for the Arkona
 208 Basin station, the temperature can be treated, in a first-order approximation,
 209 as a passive tracer, which serves as a proxy for different origins and release
 210 rates of specific water masses. The pool of Arkona bottom waters, fed by
 211 several minor baroclinic inflows until late autumn, was intermittently par-
 212 tially flushed into the Bornholm Basin, where the newly arrived water masses
 213 either interleaved or directly mixed into the bottom waters. The increased
 214 ensemble variability in temperature (Fig. 6h,p) indicates a high sensitivity
 215 to these flushing or overspilling events. Contrary to the ensemble simula-
 216 tions, the sparse observational data could not resolve this variability. With
 217 the MBI’s arrival, variability in both salinity and temperature dissipated,
 218 and temperature stabilized with minimal ensemble variability. This inflow,
 219 ranked third-largest over the past 100 years (Mohrholz et al., 2015), compre-
 220 hensively flushed the Bornholm Basin, displacing its water masses into the
 221 Gotland Basin.

222 3.2.4. *Gotland Basin station*

223 Compared to the range between surface and bottom values, the ensemble
 224 variability is rather low and also compares well with the variability of differ-
 225 ent measurements (Fig. 7a-n). The near bottom profiles clearly indicate an
 226 overestimation of salt and temperature by all modelled inflows. This likely
 227 suggests insufficient plume mixing as it travels from the Bornholm Basin to
 228 the Gotland Basin. Nonetheless, considering the large error margins observed
 229 in model intercomparison projects for the Baltic Sea (Placke et al., 2018),
 230 the deviations of approximately 0.5 g/kg in salinity and 1 K in temperature
 231 can be regarded as relatively small.

232 The time evolution of bottom salinity and temperature in the Gotland
 233 Basin, shown in Fig. 7o,p, highlights the arrival of the inflow to this dynam-
 234 ically significant basin. The ensemble-wide spread of the arrival date for the
 235 saltier water masses spans four days, from 19 to 23 February 2015 (see inset
 236 axis in Fig. 7o). This is an increase compared to the single-day spread ob-
 237 served in the Bornholm Basin (Fig. 6o). This demonstrates that the general
 238 predictability of the arrival of MBIs is limited. Focusing on the arrival of the
 239 inflow, we can identify distinct modes. Some ensemble members depict the

240 inflow as a massive, abrupt front (upper ensemble members), while others
 241 show a more gradual arrival, spread out over time (lower ensemble members).
 242 Interestingly, a slight perturbation in some ensemble members becomes ap-
 243 parent in mid-April, forming two distinct branches of equilibrium states from
 244 May onward. This split encompasses a range of approximately 0.25 g/kg in
 245 salinity.

246 Similar to the Bornholm Basin, the time series of bottom temperatures in
 247 the Gotland Basin again reveal periods of large ensemble variability before
 248 the arrival of the inflow (Fig. 7p). This variability can be attributed to two
 249 mechanisms. The first mechanism can be described as a "shortcut." The ad-
 250 vancing major inflow pushed water from the bottom pool of the Arkona Basin
 251 into the Bornholm Basin. Since these water masses were not overly dense,
 252 they slid on top of the dense, stagnant bottom water in the Bornholm Basin
 253 (but remained below the halocline). They moved toward the Gotland Basin,
 254 effectively mimicking a pre-inflow. The second mechanism involves uplifting
 255 the old, stagnant bottom water in the Bornholm Basin by the denser major
 256 inflow. The newly arrived, denser water masses displaced the older water
 257 masses, pushing them into the Gotland Basin and generating a second peak
 258 in the pre-inflow. Since the density of the water masses was similar in both
 259 mechanisms (due to similar salinity), temperature can provide insight into
 260 the different pathways. Observations indicate that the temperature spread of
 261 the pre-inflow can reach up to 1.5 K (Fig. 7p), suggesting that the ensemble
 262 members are still too conservative in capturing this variability. Investigating
 263 the oxygen concentration could prove beneficial in gaining a better under-
 264 standing of these mechanisms. This approach would allow for a distinction
 265 between old stagnant bottom water, oxygen-rich major inflow water masses,
 266 and intermediate water masses (Holtermann et al., 2017).

267 *3.3. Integral Water Mass Transformation in deep Baltic basins*

268 Since salinity is key for the stratification and estuarine circulation in the
 269 Baltic Sea, we now continue our analyses in salinity space. During model run-
 270 time, we binned volume and fluxes into salinity classes and stored these di-
 271 agnostics as daily averages for each simulation. From the ensemble-averaged
 272 data, we analyze the water mass composition and transformation in the deep
 273 Baltic basins. Figs. 8 and 9 show the evolution of the water masses, and
 274 the integrated fluxes across isohalines, in the Bornholm and Gotland Basin,
 275 respectively.

276 3.3.1. Bornholm Basin

277 The Bornholm Basin, with its maximum depth of 92 m, is closed up to
 278 the depth of the Slupsk Sill at about 60 m, across which waters can spill over
 279 into Slupsk Furrow and flow further towards the Gotland Basin (see map in
 280 Fig. 1a). The water mass composition of the deep Bornholm Basin below
 281 $z=-61$ m is provided in Fig. 8a. At the beginning of December 2014, the
 282 basin was filled with water masses with salinities between 13 and 16 g/kg.
 283 From mid of December 2014 until the beginning of January 2015, the inflow
 284 with high salinity waters reached the deep Bornholm Basin and increased
 285 the volumes in all salinity classes between 16 and 22 g/kg (red area in Fig.
 286 8b). The early arriving water masses with 16 g/kg represent the original
 287 bottom waters from the Arkona Basin that were pushed out by the inflowing
 288 MBI there (see Fig. 5o). The water masses with 20 g/kg and more, arriving
 289 end of December 2014, are finally the MBI waters. The increased volume
 290 below high salinity isohalines lifts low salinity waters, and the corresponding
 291 low salinity isohalines, across the virtual lid at $z=-61$ m, and out of the
 292 deep basin (Fig. 8a). In addition to these volume changes due to fluxes
 293 across the lateral and vertical basin boundary, the volume in salinity classes
 294 changed due to the convergence and divergence of diahaline volume fluxes
 295 $\partial Q_{\text{dia}}/\partial S$ (Fig. 8c). The substantial decrease of the inflowing high salinity
 296 volumes due to diahaline volume flux divergence (strong blue area in Fig.
 297 8c) is the reason why, in particular, the isohalines of 21 and 22 g/kg do
 298 not show up in Fig. 8a. The underlying diahaline volume flux Q_{dia} (Fig.
 299 8d) is a measure for the water mass transformation between salinity classes
 300 associated with diahaline diffusive fluxes J_{dia} (Fig. 8e). The latter are caused
 301 by turbulent mixing (Burchard, 2020) and the relation $Q_{\text{dia}} = -\partial J_{\text{dia}}/\partial S$
 302 holds (Walín, 1977). The diahaline diffusive salt flux is naturally directed
 303 from higher to lower salinity classes (red "upward" in Fig. 8e). However,
 304 due to discretization errors in advection schemes, numerical models can also
 305 cause slight anti-diffusive fluxes (Klingbeil et al., 2014; Mohammadi-Aragh
 306 et al., 2015), which explain the blue "downward" fluxes in Fig. 8e. Due
 307 to the strong diahaline diffusive flux between inflowing high salinity waters,
 308 and the initial low salinity waters, water volume is moved from both – the
 309 high salinity classes (red "upward" fluxes in Fig. 8d) and the low salinity
 310 classes (blue "downward" fluxes in Fig. 8d) – towards intermediate classes
 311 (red "convergence" in Fig. 8c). Fig. 8b indicates an additional smaller inflow
 312 of high salinity waters at the end of January 2015 (expanding red volumes

313 between 17 and 20 g/kg in Fig. 8b). Because the inflowing volumes did not
 314 have a higher salinity than the water mass at the bottom of the basin, this
 315 inflow cannot be detected in the evolution of the bottom salinity (Fig. 6o).
 316 From February to July 2015, the volumes below the 15 g/kg isohaline shrank,
 317 and low salinity isohalines sank down across the virtual lid back into the deep
 318 basin (Fig. 8a). This volume change can be explained by persistent mixing
 319 (Fig. 8e), and the resulting diahaline volume flux divergence, in the donating
 320 higher salinity classes (blue area in Fig. 8c), and the convergence in the
 321 accepting lower salinity classes (red area above).

322 The evolution of the water mass composition in Fig. 8a also offers an
 323 estimate of the total volume of inflowing high saline waters into the deep
 324 part of the Bornholm Basin. At the beginning of the inflow in December
 325 2014, the 16 g/kg isohaline was already present in the basin, but with almost
 326 no volume below it. This isohaline was lifted up until February 2015 by an
 327 inflowing volume of approximately 125 km³ below it. Subsequent waters –
 328 flowing from the Arkona Basin into the Bornholm Basin during February and
 329 March 2015, with salinities lower than 16 g/kg (in particular the remaining
 330 15 g/kg waters counted by Gräwe et al. (2015) as part of his estimate of a
 331 total inflow volume of 298 km³ into the Arkona Basin) – are not considered
 332 in our estimate. These water masses interleaved above the virtual lid, and
 333 slid directly towards Slupsk Sill, and further on into the Gotland Basin.

334 Of course, the water mass composition in Fig. 8a, calculated from the
 335 integrated volume below the virtual lid, cannot represent the complex shape
 336 and varying vertical position of the isohalines in 3D space. In particular,
 337 isohalines, that seem to be sufficiently below the virtual lid in Fig. 8a, will
 338 indeed cross the virtual lid in some areas of the basin, which explains the
 339 wide band of strong non-diahaline volume changes in lower salinity classes in
 340 Fig. 8b. Therefore, during the inflow from end of December 2014 to January
 341 2015, also water masses with salinities higher than 15 g/kg were pushed out
 342 towards the Gotland Basin. As we will show below in Sec. 3.3.2, with our
 343 analyses in salinity space, we can indeed detect two distinct inflow periods in
 344 the Gotland Basin: the first caused by the pushed out, old Bornholm waters,
 345 and the second by late inflow waters from the Arkona Basin, sliding over the
 346 early inflow waters that filled the deep Bornholm Basin.

347 3.3.2. *Gotland Basin*

348 The Gotland Basin has a maximum depth of 248 m. In the following, we
 349 analyze the water masses below a virtual lid at a depth of $z=-150$ m. The

350 water mass composition of the deep Gotland Basin is provided in Fig. 9a.
 351 At the beginning of January 2015, the basin was filled with water masses of
 352 salinities between 12.0 and 12.4 g/kg. Over a long time, from February to
 353 April 2015, two distinct inflow periods substantially filled the basin with high
 354 saline waters (red area Fig. 9b). The first period, from mid-February to the
 355 end of March 2015, represents the inflow of the old waters from the Bornholm
 356 Basin, pushed out there by the early MBI waters, while the second period in
 357 April 2015 represents the inflowing, later MBI waters, sliding over the deep
 358 Bornholm Basin filled with saltier MBI waters (see Sec. 3.3.1). During the
 359 first period, the volume between 12.4 and 14.8 g/kg is increased (Fig. 9b), but
 360 the volume in salinity classes higher than 13.8 g/kg is rapidly transformed
 361 into lower salinity waters (Figs. 9c,d). The second inflow period increased
 362 the volumes between 12.8 and 14.6 g/kg, with volumes higher than 14.0 g/kg
 363 subsequently being transformed into lower salinity waters as well. After the
 364 inflow, the deep basin was filled with water masses from 13.0 to 14.0 g/kg.

365 In the stagnation period after the inflow, a slight volume increase of the
 366 highest salinity waters between 13.4 and 14.0 g/kg was simulated (Fig. 9a,c).
 367 The underlying "downward" volume fluxes (blue in Fig. 9d) and upgradi-
 368 ent diffusive fluxes (blue in Fig. 9e) are unphysical and caused by the anti-
 369 diffusive advection schemes in the numerical model.

370 The analyses in salinity space revealed two distinct inflow periods. The
 371 second one cannot be detected from the evolution of the bottom salinity in
 372 Fig. 7o. Moreover, Fig. 9a indicates that later inflow waters even pushed out
 373 the just arrived earlier inflow water. With the 12.4 g/kg isohaline lifted out,
 374 above the virtual lid, at the end of March 2015, the first inflow period com-
 375 pletely filled the deep Gotland Basin with approximately 125 km³. The ad-
 376 ditional filling during the second period, with approximately another 50 km³
 377 high saline waters (estimated by the lift of the 12.8 g/kg isohaline), confirms
 378 the superposition of old Bornholm waters (also approximately 125 km³; see
 379 Sec. 3.3.1) and later MBI waters. More inflowing water masses into the
 380 Gotland Basin with lower salinities can be assumed above the virtual lid.

381 *3.4. Local Water Mass Transformation within the Gotland Basin*

382 In Sec. 3.3.2 and Fig. 9, we discussed the integral diahaline volume fluxes
 383 Q_{dia} as a metric for the water mass transformation in the Gotland Basin.
 384 Here, we refine the analysis by studying the spatial distribution of the di-
 385 ahaline volume fluxes within the basin. For this purpose, we focus on the
 386 isohalines of salinities 12.4 g/kg, 13.2 g/kg and 13.8 g/kg. Here, the smallest

387 and largest salinities include the range of salinity classes that is substan-
 388 tially filled during the inflow (Fig. 9a). The intermediate isohaline shows
 389 interesting features because of its vicinity to the virtual lid after the inflow.
 390 Fig. 10 shows the ensemble-averaged local diahaline volume fluxes per unit
 391 horizontal area $u_{\text{dia},z}$ across the three isohalines, and averaged over different
 392 periods.

393 Since the dynamics during the arrival of the inflow in February 2015 oc-
 394 cur on short time scales, fluxes averaged over a single day are presented in
 395 column 1 of Fig. 10. Despite using averaged data from a large ensemble sim-
 396 ulation, daily data of $u_{\text{dia},z}$ are still noisy. Nevertheless, while the inflowing
 397 plume was reaching the center of the basin on 21 February 2015, coher-
 398 ent signatures of up-gradient diahaline volume fluxes toward higher salinity
 399 classes (blue "downward" areas) and down-gradient ones toward lower salin-
 400 ity classes (red "upward" patterns) can already be diagnosed (Fig. 10a). The
 401 inflowing plume consists of various layers of different salinities. As can be
 402 seen from the deviation between the isobath of $z=-150$ m and the green
 403 contour line (enclosing the area in the basin, where the isohalines are below
 404 the virtual lid at $z=-150$ m), the shown layers are not the ones closest to
 405 the bottom. But, due to the Coriolis force the plume is attached to the east-
 406 ern slope of the basin and the layers are exposed to the bottom boundary
 407 layer on the eastern side (Umlauf and Arneborg, 2010a,b). Due to this, and
 408 the entrainment with surrounding waters at the front and at the other side,
 409 the margins of the plume show the highest water mass transformation rates
 410 (Fig. 10a1–c1). Between the high saline bottom, and the less saline top, lay-
 411 ers of the plume, water is transformed towards intermediate salinities (red
 412 areas with "upward" fluxes towards lower salinities for isohalines of 13.2 and
 413 13.6 g/kg in Fig. 10b1,c1, and blue areas with "downward" fluxes towards
 414 higher salinities for isohalines of 12.4 and 13.2 g/kg in Fig. 10a1,b1). Averag-
 415 ing over longer time scales creates a slightly clearer picture of some features
 416 (Fig. 10a2–c3), but also removes relevant short-term hotspots induced by the
 417 passage of the inflowing plume.

418 After the inflow, the isohaline of 12.4 g/kg is above the virtual lid, outside
 419 of the deep basin (Fig. 9a). It indicates some elevated water mass transfor-
 420 mation at some boundaries and in the basin's interior (Fig. 10a4–a6). The
 421 isohaline of 13.2 g/kg is partly below, and above, the virtual lid (Fig. 10b4–
 422 b6). The dome above, in the center of the basin, is caused by rim currents
 423 as described by Holtermann et al. (2014), and shown in their Fig. 9a. These
 424 rim currents are also expected to induce the water mass transformations in

425 the center of the basin. The isohaline of 13.8 g/kg within the deep basin
426 shows low levels of increased water mass transformations at the boundaries,
427 in addition to the unphysical slight downward volume fluxes in the remain-
428 ing parts, due to the anti-diffusive advection schemes in the numerical model
429 (Fig. 10c4–c6).

430 Except for some locations (e.g., 10b3), the typical red/blue pattern of
431 the secondary circulation closed to sloping topography, consisting of down-
432 gradient fluxes in the bottom boundary layer and up-gradient fluxes in the
433 entrainment layer above (Garrett, 1990; Ferrari et al., 2016; Henell et al.,
434 2023), could not clearly be observed in the deep Gotland Basin. We assume
435 that this is due to the steep topographic slopes and the coarse resolution in
436 the numerical model.

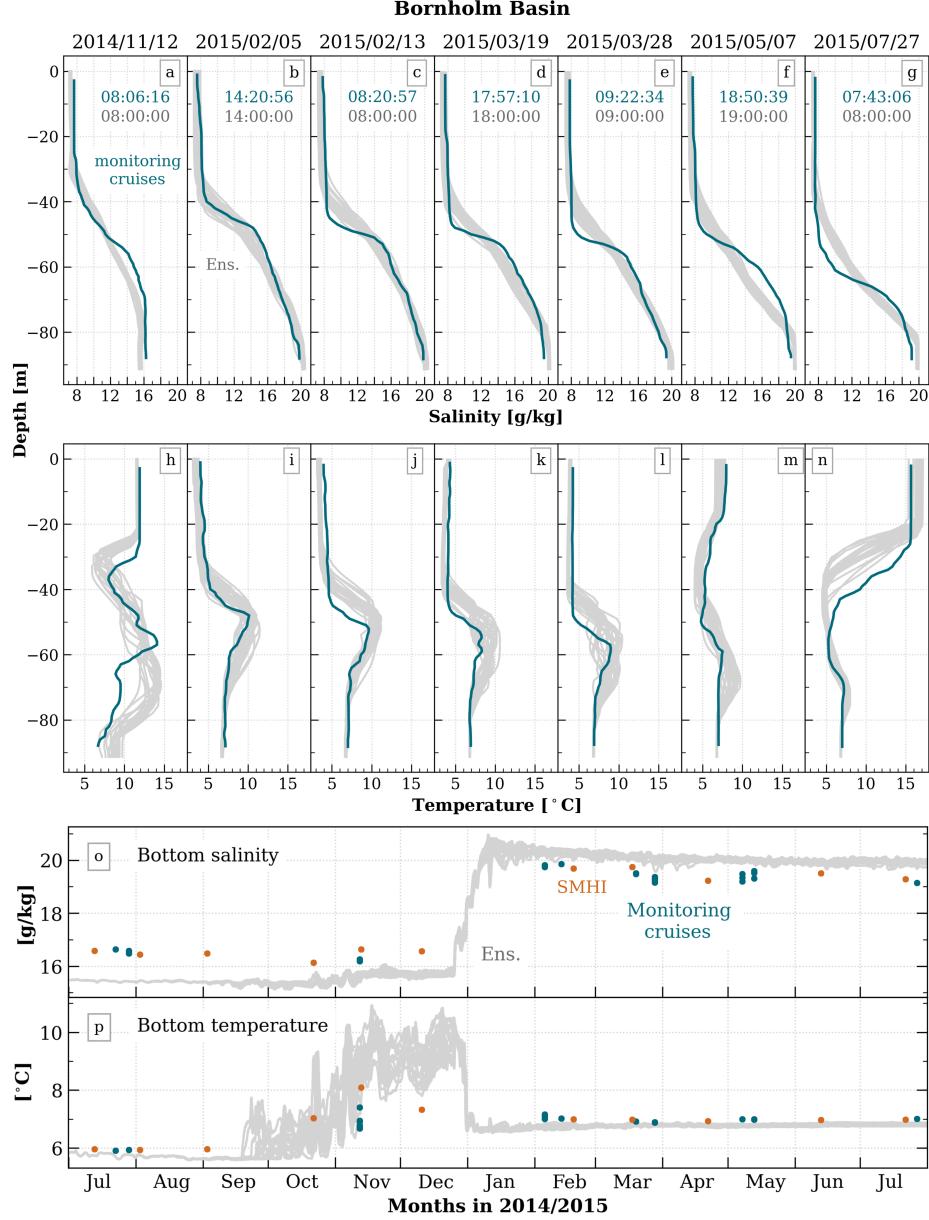


Figure 6: (a)-(n) Comparison of modelled salinity and temperature profiles from the ensemble simulations (gray lines) with measurement data (turquoise lines) at the station Bornholm Basin, see location in Fig. 1a. (o), (p) Comparison of modelled time series of bottom salinity and temperature (gray lines) with measurement data (turquoise and orange dots) at the Bornholm Basin station.

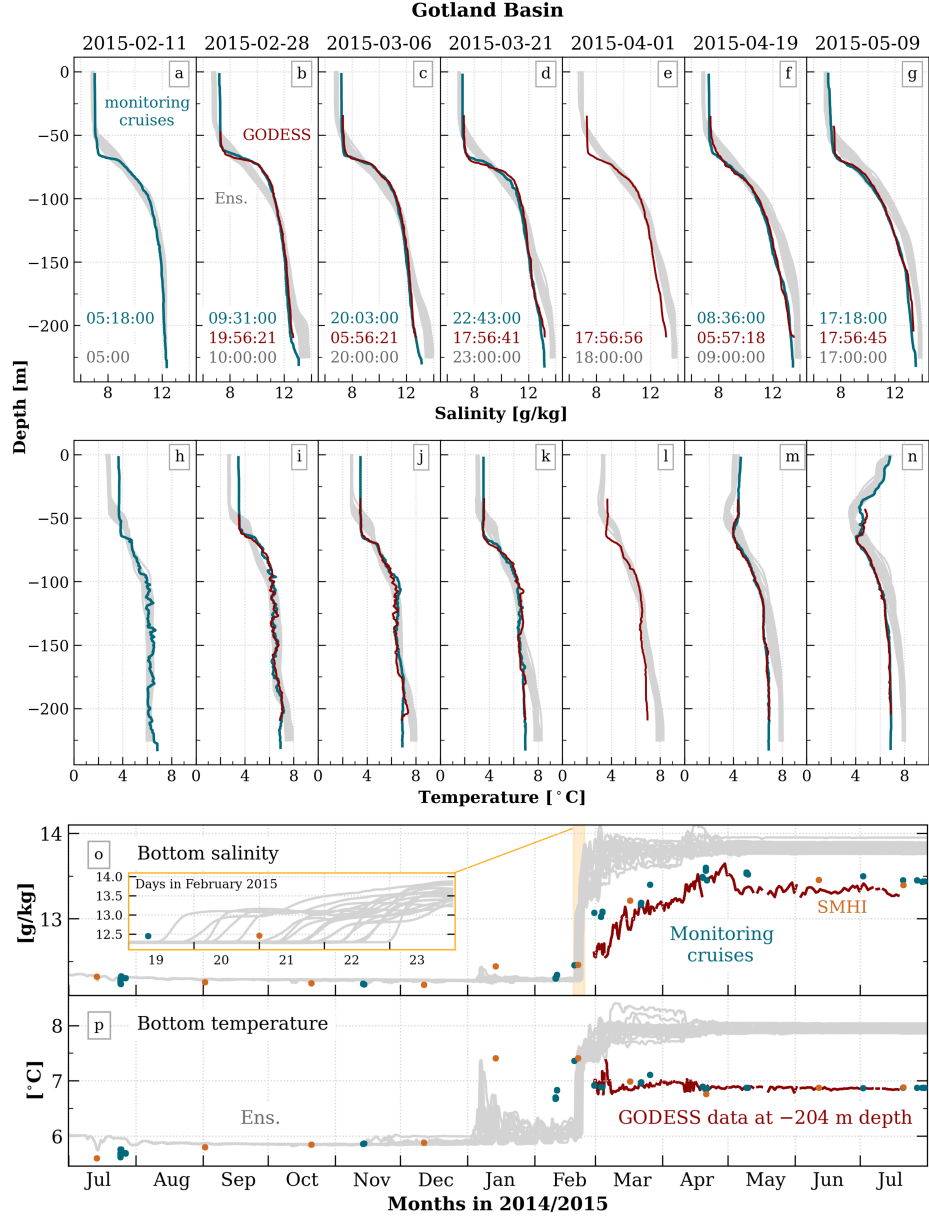


Figure 7: (a)-(n) Comparison of modelled salinity and temperature profiles from the individual ensemble realizations (gray lines) with measurement data (turquoise lines) at the station Gotland Basin, see location in Fig. 1a. (o), (p) Comparison of modelled time series of bottom salinity and temperature (gray lines) with measurement data (turquoise and orange dots) at the Gotland Basin station.

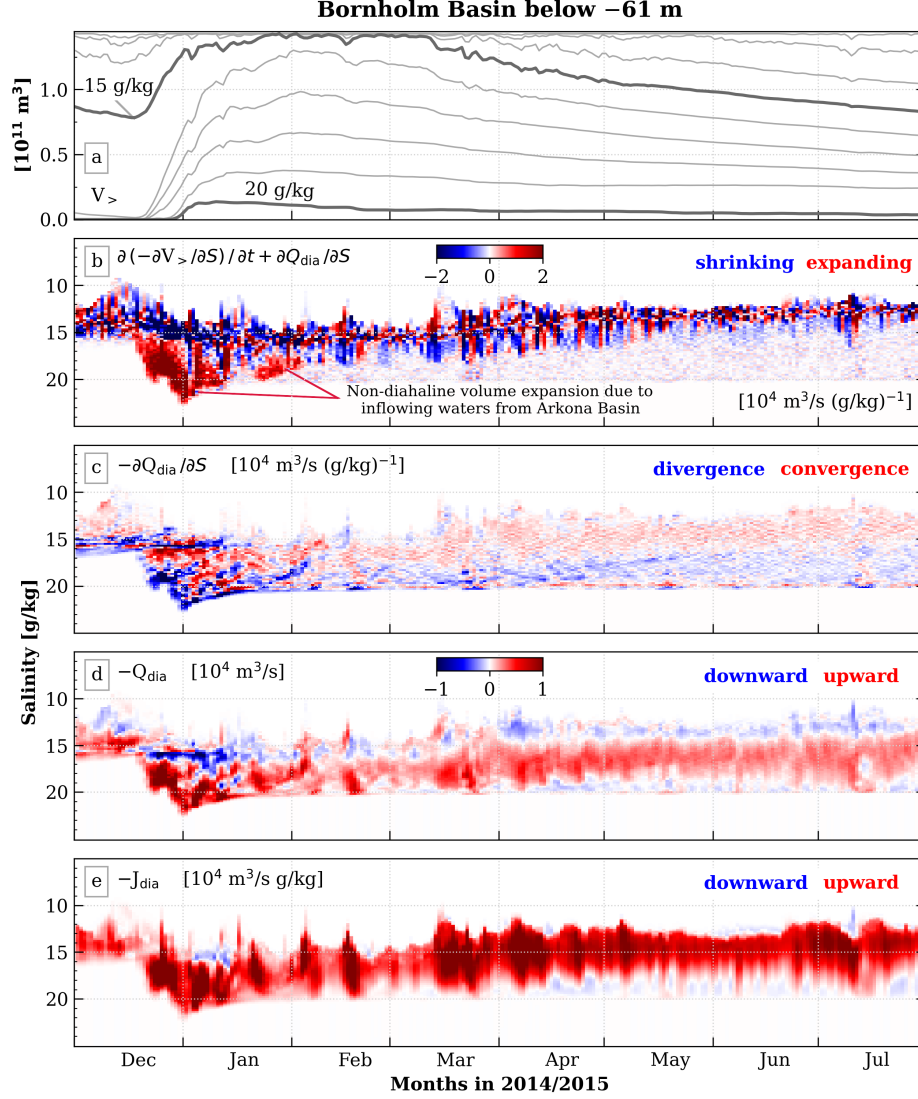


Figure 8: Time series of ensemble-averaged quantities in salinity space in the Bornholm Basin below a virtual lid at $z=-61$ m: (a) stacked volume in salinity classes with the height of an isohaline representing the cumulative volume $V_{>}$ below it, (b) non-diahaline volume change per salinity class $\partial(-\partial V_{>}/\partial S)/\partial t + \partial Q_{\text{dia}}/\partial S$ due to lateral fluxes and fluxes across the virtual lid, (c) volume change per salinity class due to the convergence of diahaline volume fluxes $-\partial Q_{\text{dia}}/\partial S$, (d) diahaline volume flux Q_{dia} , and (e) diahaline diffusive salt flux J_{dia} . Fluxes towards lower salt classes are labeled "upward". Panels (a) and (b), as well as (c) and (d) share the same colorbars, respectively.

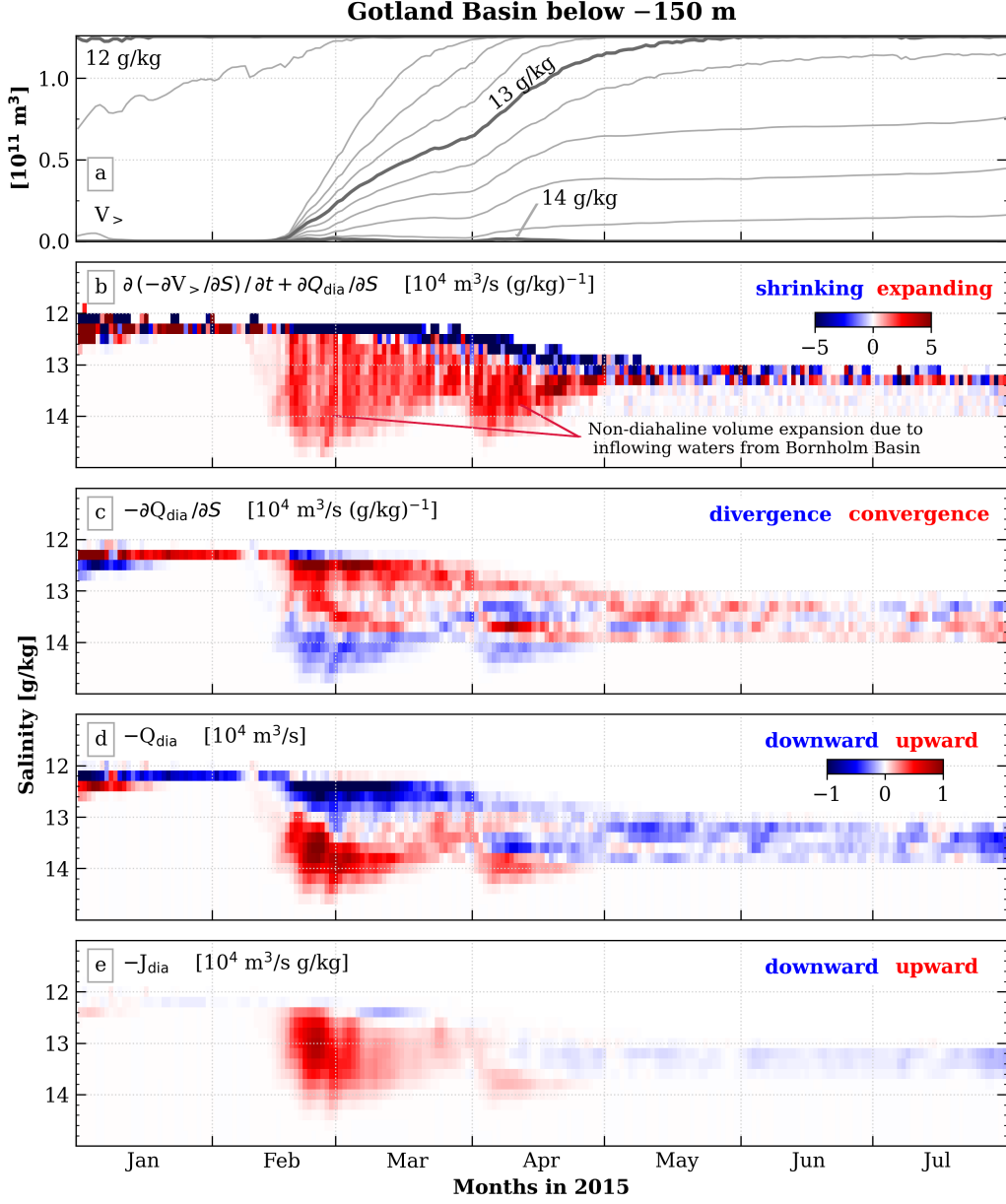


Figure 9: Same as in Fig. 8 but for the Gotland Basin and below a virtual lid at $z=-150$ m. The spatial distribution of the diahaline volume fluxes Q_{dia} within the basin for selected isohalines is shown in Fig. 10.

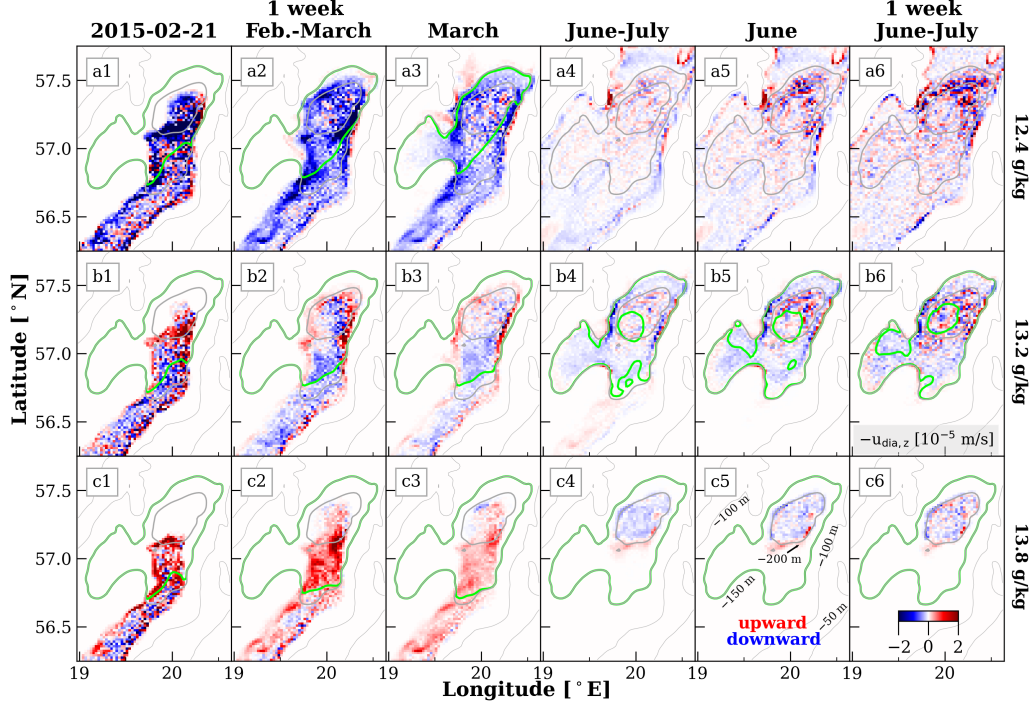


Figure 10: Maps of ensemble-averaged local water mass transformation rates (diahaline volume flux per unit horizontal area $u_{\text{dia},z}$) across the isohaline surfaces of salinities 12.4 g/kg (row a), 13.2 g/kg (row b) and 13.8 g/kg (row c) in the Gotland Basin, averaged over different periods (columns 1 to 6). The first three columns cover the first inflow period with the plume approaching the center of the basin from Southwest on 21 February 2015, while the last three columns cover the stagnation period after the inflow. Fluxes towards lower salt classes are labeled "upward". Gray contour lines depict isobaths, while the green contour lines enclose the parts in the basin where the isohalines are below the virtual lid at $z = -150$ m. Areas above the virtual lid are not considered in the integrated diahaline volume fluxes Q_{dia} below the lid shown in Fig. 9d.

437 4. Conclusions

438 In this study we applied single-model ensemble simulations to the Baltic
439 Sea. We generated multiple realizations of the major Baltic inflow event
440 from December 2014 to April 2015 and analyzed the simulated variability.
441 Our analyses revealed interesting aspects such as (i) large variability in the
442 bottom temperatures of the deep Baltic basins before the inflow, which can
443 hardly be detected from sparse measurement data from monitoring cruises,
444 (ii) an uncertainty of 4 days for the arrival time of the inflow in the deep
445 Gotland basin.

446 The ensemble data also enabled the analysis of local water mass trans-
447 formation rates down to daily scales, in other works usually done on multi-
448 annual or multi-decadal time scales. The analysis in salinity space clearly
449 revealed two distinct inflow periods in the deep Gotland Basin, which cannot
450 be detected from time series of bottom salinity.

451 In this paper we focused on a Major Baltic Inflow event. In Fig. 11 we
452 outline the analysis of daily water mass transformation ensemble data from
453 a local, short wind event. Indeed the data provide a rather clear picture
454 of hotspots of water mass transformation rates at the surface and in the
455 bottom boundary layers at the topographic slopes. While the former is only
456 pronounced during storm events, the latter lasts longer due to generated
457 currents and is ubiquitous during the winter season with regular strong winds.
458 This indicates the feasibility to investigate water mass transformations on
459 very local and short time scales in future high-resolution simulations with
460 single-model ensembles.

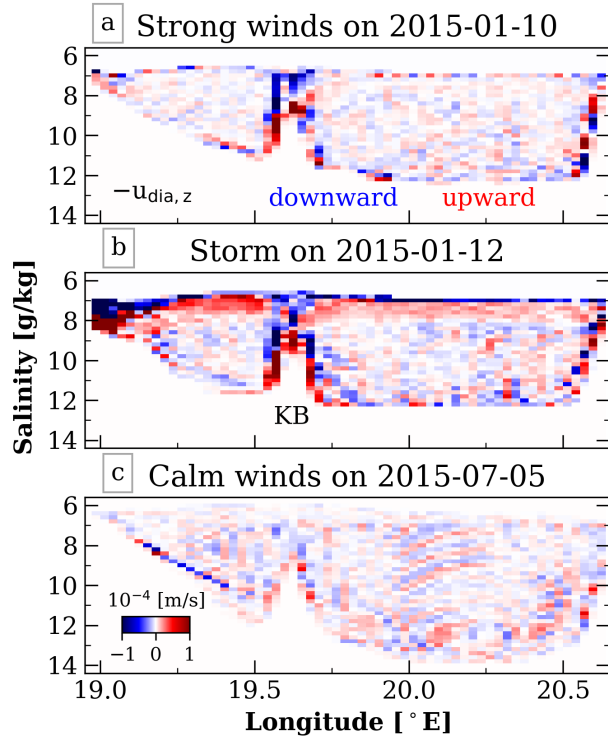


Figure 11: Ensemble-averaged local water mass transformation rates (diahline volume flux per unit horizontal area $u_{\text{dia},z}$) along a transect through the Gotland Basin across the Klintsbank under the influence of (a) strong wind conditions during winter, (b) storm two days later, and (c) calm wind conditions during summer. See Fig. 1b for location of the transect and of Klintsbank.

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Resume

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- 03/2016 – 08/2019  **Polyglot Museum Guide**
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Publications in peer-reviewed journals

Journal Articles

- 1 E. Henell, H. Burchard, U. Gräwe, *et al.*, “Exploring the variability of a non-tidal marginal sea with a single-model ensemble,” *Ocean Modelling*, vol. 198, p. 102 615, 2025, ISSN: 1463-5003.  DOI: 10.1016/j.ocemod.2025.102615.

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Conferences

- | | |
|----------------|--|
| September 2023 | <ul style="list-style-type: none"> 📖 Warnemünde Turbulence Days (WTD), Warnemünde (Germany), talk,
<i>Application of a local diahaline Water Mass Transformation framework to the Baltic Sea</i> 📖 Virtual European Physical Oceanography and Shelf Sea Seminar Series (VEPOSSSS), Menai Bridge (Wales, UK), talk,
<i>Applying a local diahaline Water Mass Transformation framework to a fjord-type, non-tidal estuarine system to investigate diahaline mixing and exchange flow</i> |
| July 2023 | <ul style="list-style-type: none"> 📖 International Union of Geodesy and Geophysics General Assembly (IUGG), Berlin (Germany), talk,
<i>How local diahaline mixing drives the overturning circulation in the Baltic Sea</i> |
| June 2023 | <ul style="list-style-type: none"> 📖 Gordon Research Conference Coastal Ocean Dynamics (GRC), Smithfield (USA), poster,
<i>Spatial composition of the diahaline overturning circulation in a fjord-type, non-tidal estuarine system</i> |
| May 2022 | <ul style="list-style-type: none"> 📖 European Geophysical Union General Assembly (EGU), Vienna (Austria), talk,
<i>Analyzing Diahline Exchange and Mixing in the Baltic Sea</i> |

Skills

- | | |
|---------------------|--|
| Coding | <ul style="list-style-type: none"> 📖 Python – Advanced level (xarray, matplotlib, numpy, scipy, pandas) 📖 R, MATLAB, Fortran, bash, git – Intermediate or beginner level |
| Scientific programs | <ul style="list-style-type: none"> 📖 ncview, ncdump, L^AT_EX, ArcGis |
| Other | <ul style="list-style-type: none"> 📖 MS Office, Jupyter Lab, Visual Studio Code, InkScape, Obsidian, Content Management Systems |

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- | | |
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| English | 📖 Fluent |
| French | 📖 Fluent (C1) |
| Korean | 📖 Beginner |

Teaching

- | | |
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| 2022/12 | 📖 Workshop on nonverbal oral communication |
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Meetings, Courses and Workshops

Winter and Spring Schools

- 05/2024  TRR181 RTG Spring School
- 05/2023  TRR181 RTG Spring School
- 03/2023  International Baltic Earth Winter School for Young Scientists on “Earth System Science for the Baltic Sea Region”
- 05/2022  TRR181 RTG Spring School
- 02/2022  TRR181 RTG Winter School
- 06/2021  TRR181 RTG Spring School
- 03/2021  TRR181 RTG Winter School

TRR181 meetings

- 09/2024  Annual Retreat.
- 09/2023  Annual Retreat, *poster*.
- 12/2022  M-Day (Mathematics Area Meeting)
- 09/2022  Collaboration meeting
-  Annual Retreat, *poster*.
- 09/2021  Annual Retreat, *poster*.

TRR181 RTG school

- 09/2021, 01/2022  Introduction to Numerics
- 11-12/2021  Fundamentals of Meteorology
- 10/2021  Fundamentals of Oceanography
- 06/2021  Introductory course on second-moment turbulence closure

Career development workshops for female scientists

- 06/2024  Advancing Academic Career and Leadership Perspectives
- 06/2023  Networking & Impostor Syndrome
- 11/2022  Resilience in Academia - Dealing with Success and Failure
- 06/2022  Gender Equality in Academia
- 11/2021  Academic Career Assessment – Visions, Aims and Perspectives

University of Rostock courses

- WS 2021/2  Coastal Ocean Processes, winter term
- SS 2021  Ocean Modeling, summer term
-  Marine Turbulence, summer term

Other courses

- 05/2021  A film studio in your pocket – Creating scientific short films with a smartphone (Marum)
- 02/2021  Advanced Ocean Modeling (Marum)
- 01/2021  Skills week with workshop “Self-presentation and Networking” (IOW)

References

Available on Request

Rostock, 15 August 2025