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Linking Local Salt Mixing and Exchange Flow in Tidal Estuaries

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“Another happy landing!”

— Obi-Wan Kenobi (Star Wars: Episode III – Revenge of the Sith)

Abstract

Estuaries are coastal water bodies where the density difference between terrestrial freshwater, e.g., from rivers, and salt water from the ocean classically drives a distinct circulation with a salty inflow and brackish outflow that emerges after tidal averaging: the estuarine circulation. Through mixing, the fresh and salty water masses entering the estuary are transformed into the brackish outflow towards the ocean. The interplay of mixing and estuarine circulation is therefore of key importance for the understanding of estuarine dynamics. Yet, while many studies have been dedicated to this topic, they often tend to rely on idealised conditions. Most real estuaries, however, are subject to spatially and temporally varying forcing from weather, tides, and freshwater discharge, which greatly impacts the timing and location of mixing. It is therefore unclear to which extent knowledge from the idealised studies can be transferred to realistic estuaries. Yet, as the estuarine circulation determines the transport of sediment, nutrients, plankton, and other floating material that is essential for the ecosystem and estuarine management such as dredging measures, it is important to understand the dynamics of realistic estuaries.

The aim of the present work was to thoroughly assess the interaction of mixing and estuarine circulation in realistic estuaries, covering the full chain of relations from estuary-wide, tidally averaged scales to local processes within a single tidal cycle. To this end, numerical simulations of the northwest German, partially mixed tidal Elbe estuary that had been validated with observational data were applied to resolve mixing and circulation dynamics in three-dimensional, Euclidean space as well as in salinity space on tidally resolving time scales. In three subsequent studies, it was found from the simulations that salt mixing in the Elbe estuary, defined as the decay of salinity variance, adjusted quickly to a changing freshwater discharge such that the discharge variability dominated the mixing signal. This applied even for extreme discharge conditions, implying a close balance between mixing, freshwater input, and estuarine circulation. Further, it was shown that local mixing on a single surface of constant salinity is closely linked to the water transport across said surface. This was then expanded to yield a direct, near-exact relation between the surface-integrated mixing and the estuarine circulation. From there, regions of enhanced mixing near the shoals of the navigational channel were identified to be of particular relevance to the estuarine circulation in the Elbe estuary. The underlying processes in these regions were mainly traced to the formation of salt plumes above the shoals throughout the tidal cycle as well as turbulent boundary layer mixing along the intersections of salt stratification with the channel topography.

In sum, the present work adds to our knowledge on how local, instantaneous processes of salt mixing underlie and interact with the tidally averaged patterns of estuarine circulation. It provides insight into the complex nature of these processes under realistic, highly variable conditions while simultaneously showing the robustness of the tidally averaged estuarine theory even for such conditions.

Kurzzusammenfassung

Ästuarie sind Küstengewässer, in denen der Dichteunterschied zwischen Süßwasser vom Land, wie z.B. aus Flüssen, und Salzwasser aus dem Meer eine Zirkulation antreibt, die klassischerweise aus einem salzigen Einstrom und einem brackigen Ausstrom besteht. Diese wird als ästuarine Zirkulation bezeichnet und erst nach einer Mittelung über die Gezeiten sichtbar. Vermischung transformiert die frischen und salzigen Einstrome im Ästuar zu dem brackigen Ausstrom zum Ozean, weshalb die Interaktion von Vermischung und Zirkulation eine Schlüsselrolle für das Verständnis der Dynamik in Ästuaren spielt. Zwar existieren zahlreiche Studien zu diesem Thema, doch diese betrachten typischerweise nur idealisierte Bedingungen im Ästuar. Im Gegensatz dazu weisen viele reale Ästuarie eine hohe Variabilität in Raum und Zeit auf. Diese Variabilität, z.B. durch Wetter, Gezeiten und Süßwasserzustrom, beeinflusst jedoch Zeit und Ort der Vermischung, weshalb es unklar ist, inwiefern sich die Ergebnisse idealisierter Studien auf reale Ästuarie übertragen lassen. Da aber die Zirkulation bestimmt, wie Sedimente, Nährstoffe, Plankton und anderes Material transportiert werden, die auch für das Ökosystem und Management-Maßnahmen wie die Instandhaltung der Fahrrinne wichtig sind, ist ein grundlegendes Verständnis der physikalischen Prozesse in realen Ästuaren unabdingbar.

Ziel dieser Arbeit war es, die Interaktion von Vermischung und ästuariner Zirkulation explizit in realistischen Gewässern zu untersuchen. Es sollten die Zusammenhänge von gewässerweiten, gezeitengemittelten Skalen bis hin zu lokalen Prozessen innerhalb eines einzelnen Gezeitenzyklus' abgedeckt werden. Dafür wurden numerische Simulationen des nordwestdeutschen, gezeitenbeeinflussten und partiell vermischten Elbeästuars durchgeführt, um die ästuarine Dynamik im dreidimensionalen euklidischen Raum sowie im Salzgehaltsraum auf gezeitenauflösenden Zeitskalen abzubilden. In insgesamt drei Studien wurde gezeigt, dass sich die Salzvermischung im Elbeästuar, hier definiert als der Abbau von Salzgehaltsvarianz, selbst unter extremen Bedingungen sehr schnell an Änderungen im Süßwasserzustrom anpasst, sodass dessen Signal die Vermischung dominiert. Dies impliziert eine feine Balance zwischen Vermischung, Süßwasserzustrom und ästuariner Zirkulation. Zusätzlich ist die lokale Vermischung auf einer einzelnen Oberfläche konstanten Salzgehalts eng mit dem Wassertransport durch diese Fläche hindurch verbunden. Dies wurde zu einer direkten, nahezu exakten Relation zwischen der oberflächenintegrierten Vermischung und der Stärke der ästuarinen Zirkulation ausgebaut. Von dieser Relation ausgehend, wurden Regionen verstärkter Vermischung nahe den Rändern der Elbfahrrinne ausgemacht, welche folglich von besonderer Bedeutung für die Zirkulation sind. Die zugrundeliegenden Prozesse in derartigen Regionen wurden in erster Linie auf zwei Mechanismen zurückgeführt: Die Entstehung salziger, bodennaher Wassermassen oberhalb des flachen Fahrrinnenrandes sowie Vermischung salzgeschichteten Wassers in der turbulenten Grenzschicht entlang der Fahrrinnenränder.

Die vorliegende Arbeit trägt maßgeblich zum Verständnis dazu bei, wie lokale, instantane Prozesse der Salzvermischung mit den großen, gezeitengemittelten Mustern der ästuarinen Zirkulation verknüpft sind. Sie offenbart, wie komplex solche Prozesse in realistischen, in Zeit und Raum äußerst variablen Ästuaren sein können, während sich die gezeitengemittelte Theorie selbst unter diesen Bedingungen als robust erweist.

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Publications

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Burchard, H., Klingbeil, K., Lange, X., Li, X., Lorenz, M., MacCready, P., and **Reese, L.** (2025). *The relation between exchange flow and diahaline mixing in estuaries*. Journal of Physical Oceanography, <https://doi.org/10.1175/JPO-D-24-0105.1>, in press.

Reese, L., Becker, M., Holtermann, P., Li, X., and Burchard, H. (2025). *The role of the shoal – salt mixing mechanisms in a partially mixed tidal estuary with channel-shoal geometry*. Continental Shelf Research, under review. Pre-print available at <http://ssrn.com/abstract=5133686>.

Other peer-reviewed publications:

Rummel, K., Gräwe, U., Klingbeil, K., Kolb, P., Li, X., **Reese, L.**, and Burchard, H. (2025). *Spatially resolved salt intrusion mechanisms in a tidal estuary and the impact of channel deepening*. Journal of Geophysical Research: Oceans, under review.

Conferences

- Physics of Estuaries and Coastal Seas (PECS), Bordeaux, France, 23rd–27th September 2024, oral presentation: *Lateral circulation and salt fronts determine mixing in a mesotidal estuary with tidal flats.*
- EGU General Assembly, Vienna, Austria, 14th–19th April 2024, poster presentation: *Stratification in non-tidal shallow coastal lagoons during extreme summer heatwaves.*
- Warnemünde Turbulence Days, Rostock, Germany, 17th–20th September 2023, oral presentation: *Local mixing determines spatial structure of diahaline exchange flow in a mesotidal estuary.*
- Virtual European Physical Oceanography and Shelf Seas Seminar Series (VEPOSSSS) in-person meeting, Bangor, UK, 12th–13th September 2023, oral presentation: *Local mixing and diahaline exchange flow under extreme runoff conditions.*
- IUGG Berlin, Germany, 11th–20th July 2023, oral presentation: *Local mixing intensity determines stratification in a mesotidal estuary – a study of extreme runoff conditions.*
- Physics of Estuaries and Coastal Seas (PECS), Perth, Australia, 24th–28th October 2022, oral presentation: *Salt Mixing in the Elbe Estuary.*

Abbreviations and Symbols

Abbreviations

ESCO: Eddy viscosity-Shear COvariance

GETM: General Estuarine Transport Model

GOTM: General Ocean Turbulence Model

SIPS: Strain-Induced Periodic Stratification

TEF: Total Exchange Flow

List of Used Physical Symbols

Symbol	Meaning	Physical Dimension
A_v	Vertical eddy viscosity	m^2s^{-1}
A_{est}	Surface area of the estuarine side of the dividing isohaline	m^2
A_T	Cross-sectional area with salinities $s > S$	m^2
A_z	Horizontal projection of the isohaline surface area	m^2
$A_{z,\text{est}}$	Horizontal projection of the surface area of the estuarine side of the dividing isohaline	m^2
b	Buoyancy	ms^{-2}
β	Haline contraction coefficient	kg/g
c	Arbitrary tracer concentration	1
χ	Local salt mixing	$(\text{g/kg})^2/\text{s}$
χ_v	Local vertical salt mixing	$(\text{g/kg})^2/\text{s}$
η	Surface elevation above $z = 0$	m
F_{in}	TEF bulk salt inflow	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
F_{out}	TEF bulk salt outflow	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
g	Gravitational acceleration	ms^{-2}
G_G	Subtidal along-channel barotropic pressure gradient per unit density due to gravitational circulation	ms^{-2}
G_R	Subtidal along-channel barotropic pressure gradient per unit density due to freshwater discharge	ms^{-2}
G_S	Subtidal along-channel barotropic pressure gradient per unit density due to tidal straining	ms^{-2}
H	Water depth below $z = 0$	m

K	Eddy diffusivity tensor	m^2s^{-1}
K_h	Horizontal eddy diffusivity	m^2s^{-1}
K_v	Vertical eddy diffusivity	m^2s^{-1}
m	Mixing per salinity class	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
m_{est}	Area-integrated local mixing on the estuarine section of the dividing isohaline surface	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
m_{num}	Numerical mixing per salinity class	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
m_{phy}	Physical mixing per salinity class	$(\text{g/kg})\text{m}^3\text{s}^{-1}$
m_{xy}	Local mixing on an isohaline surface	$(\text{g/kg})\text{m}\text{s}^{-1}$
$m_{xy,\text{num}}$	Local numerical mixing on an isohaline surface	$(\text{g/kg})\text{m}\text{s}^{-1}$
$m_{xy,\text{phy}}$	Local physical mixing on an isohaline surface	$(\text{g/kg})\text{m}\text{s}^{-1}$
M_S	Integrated mixing within an estuarine volume bounded by an isohaline surface	$(\text{g/kg})^2\text{m}^3\text{s}^{-1}$
M_T	Integrated mixing within an estuarine volume bounded by a vertical transect	$(\text{g/kg})^2\text{m}^3\text{s}^{-1}$
$M_{T,\text{num}}$	Integrated numerical mixing within an estuarine volume bounded by a vertical transect	$(\text{g/kg})^2\text{m}^3\text{s}^{-1}$
$M_{T,\text{phy}}$	Integrated physical mixing within an estuarine volume bounded by a vertical transect	$(\text{g/kg})^2\text{m}^3\text{s}^{-1}$
ν	Molecular diffusivity	m^2s^{-1}
q	TEF volume transport per salinity class	$\text{m}^3\text{s}^{-1}(\text{g/kg})^{-1}$
Q	TEF volume transport for salinity classes $s > S$	m^3s^{-1}
$Q_{\text{dia,est}}$	Diahaline volume transport on estuarine side of dividing isohaline	m^3s^{-1}
Q_{in}	TEF bulk volume inflow	m^3s^{-1}
Q_{out}	TEF bulk volume outflow	m^3s^{-1}
Q_r	Freshwater discharge	m^3s^{-1}
R	Pearson's correlation coefficient	1
ρ	Density	kg m^{-3}
ρ_0	Reference density	kg m^{-3}
S	Salinity (S -space)	g/kg
S_{bott}	Bottom salinity	g/kg
S_{div}	TEF dividing salinity	g/kg
S_{in}	TEF bulk inflow salinity	g/kg
S_o	Ocean salinity	g/kg
S_{out}	TEF bulk outflow salinity	g/kg
S_{surf}	Surface salinity	g/kg
s^z	Salinity (z -space)	g/kg
t	Time	s
u	Current velocity (vector)	m/s
u_{10}	Wind velocity 10 m above ground	m/s

u_{dia}^z	Diahaline velocity in z -space	m/s
$u_{\text{dia},z}^S$	Effective vertical diahaline velocity (S -space)	m/s
$u_{\text{dia},z}^z$	Vertical diahaline velocity (z -space)	m/s
$\mathbf{u}_h$	Horizontal velocity vector	m/s
u_G	Subtidal velocity due to gravitational circulation	m/s
u_R	Subtidal velocity due to freshwater discharge	m/s
u_S	Subtidal velocity due to tidal straining	m/s
$\mathbf{u}_s$	Velocity of the isohaline movement	m/s
u_x	Along-channel velocity	m/s
u_y	Cross-channel velocity	m/s
u_z	Vertical velocity	m/s
V	Volume	m ³
V_S	Estuarine volume bounded by an isohaline surface	m ³
V_T	Estuarine volume bounded by a vertical transect	m ³
W	Channel width	m
w_e	Entrainment velocity	m/s
x	Along-channel position	m
y	Cross-channel position	m
z	Vertical position	m

List of Used Mathematical Operators and Symbols

Symbol	Meaning
∂_i	Partial derivative with respect to i
∇	Nabla operator
∇_h	Horizontal gradient operator
Δ	Difference
$\text{diag}(\cdot, \cdot, \cdot)$	Diagonal matrix
$\langle \cdot \rangle$	Temporal averaging
$\hat{\cdot}$	Deviation from temporal average
$[\cdot]$	Reynolds averaging
$\tilde{\cdot}$	Deviation from Reynolds average
$\overline{\cdot}$	Vertical averaging
$\cdot'$	Deviation from vertical average
$\overline{\cdot}^A$	Area averaging
$ \cdot $	Magnitude (of a vector)
δ	Dirac function
ψ	Arbitrary function
n	Integer number

Chapter 1

Introduction

In coastal physics, the word estuary refers to transitional, coastal water bodies such as river mouths which are semi-enclosed, possess a free connection to the sea, and are subject to inflowing freshwater from one or more terrestrial sources (Cameron and Pritchard, 1963, Valle-Levinson, 2010). As such, estuaries are locations where (fresh) terrestrial and (salty) oceanic water masses meet and are mixed with each other. This leads to a characteristic circulation pattern of salty inflow from and brackish outflow toward the ocean – the *estuarine circulation* (see also Fig. 2.1). Salt mixing, here defined as the decay of salinity variance (Burchard and Rennau, 2008), is a fundamental requirement for the existence of this circulation, as it transports water across isohaline surfaces between the inflow and outflow layers, thus resulting in the brackish outflow. Simultaneously, the structure of the exchange flow influences in which locations intense mixing takes place. To improve our understanding of the physics of estuaries, it is therefore essential to decipher this interplay of salt mixing and the estuarine exchange flow.

In the past, important work towards such an understanding had been performed by Walin (1977), who introduced the use of isohaline coordinates to estuarine physics. Later, Wang et al. (2017), Li et al. (2022), and Klingbeil and Henell (2023) quantified the local link between mixing on an isohaline surface and the water transport across the same surface, providing a mixing–exchange flow relation for local, but not yet for bulk properties.

At the timing of the present work, the only relation that explicitly linked the intensity of the estuarine exchange flow, quantified here as the bulk volume inflow $Q_{\text{in}}(x)$ (Broatch and MacCready, 2022, MacCready and Geyer, 2024), to the mixing $M_{\text{T}}(x)$ within an estuary bounded by a transect at along-channel position x had been introduced by MacCready et al. (2018):

$$M_{\text{T}} \approx (S_{\text{in}} - S_{\text{out}})S_{\text{in}}Q_{\text{in}}. \quad (1.1)$$

This relation is a non-exact estimate that, with the bulk inflow and outflow salinities $S_{\text{in}}(x)$, $S_{\text{out}}(x)$ as additional variables, cannot provide a unique solution for the mixing as a function of the exchange flow intensity. An exact relation between the exchange flow intensity and estuarine mixing was therefore still missing.

Further, most of the estuarine exchange flow and mixing theory relies on the assumption of balanced conditions, i.e., conditions where sufficiently long temporal averaging removes any fluctuations in the form of salt or volume storage. Indeed, many studies on this topic make use of idealised estuaries (e.g., MacCready et al., 2018, Burchard et al., 2021) or idealised forcing conditions, in particular in the form of constant freshwater discharge (e.g., Wang et al., 2017, Li et al., 2022) or idealised tides (e.g., Wang et al., 2017, Wang and Geyer, 2018). Only a handful of recent studies such as Warner et al. (2020) and Broatch and MacCready (2022) use

fully realistic forcing to reveal the true temporal variability of estuarine mixing. Similarly, a realistic topography is known to result in a high spatial variability of mixing (Wang et al., 2017, Warner et al., 2020, Li et al., 2022, Henell et al., 2023). This spatial and temporal variability in realistic estuaries might lead to deviations from the idealised picture of past research.

With that in mind, the aim of this work is to improve our understanding of how mixing interacts with the exchange flow in realistic estuaries. To this end, it is necessary to understand how the estuarine exchange flow and mixing theory holds under highly variable, even extreme, realistic conditions, and to quantify how closely mixing and exchange flow are truly linked locally and estuary-wide. From this knowledge, underlying, local mechanisms of mixing and exchange flow may be identified and studied in detail.

There exists a large range of estuarine types as classified, e.g., by Geyer and MacCready (2014) based on the effectiveness of tidal mixing and the available freshwater input. Within the scope of the present work, not all types of estuaries could be covered. Instead, the focus is set on the northwest German Elbe estuary. It belongs to the common type of partially to well-mixed tidal estuaries which vary between vertically stratified and well-mixed conditions depending on the spring-neap cycle and the incoming freshwater discharge (see Geyer and MacCready, 2014). The Elbe estuary will be introduced in detail in Chapter 2. This chapter further summarises the theoretical framework required for the aims of this work, and introduces numerical simulations of the Elbe estuary that the theory has been applied to. In Chapter 3, each publication included in this cumulative thesis is summarised, highlighting the key findings from each study. Lastly, conclusions are drawn in Chapter 4.

Chapter 2

Methods

2.1 Physics of Estuaries

2.1.1 General Characteristics and Estuarine Circulation

In classical estuaries like the Elbe (see Burchard et al., 2004, Reese et al., 2024), the density structure $\rho(x, y, z, t)$ is typically dominated by salinity rather than temperature (see Knudsen, 1900, Walin, 1977, MacCready and Geyer, 2010). Under such conditions, the estuarine dynamics are highly influenced by salinity differences as will be seen throughout this section.

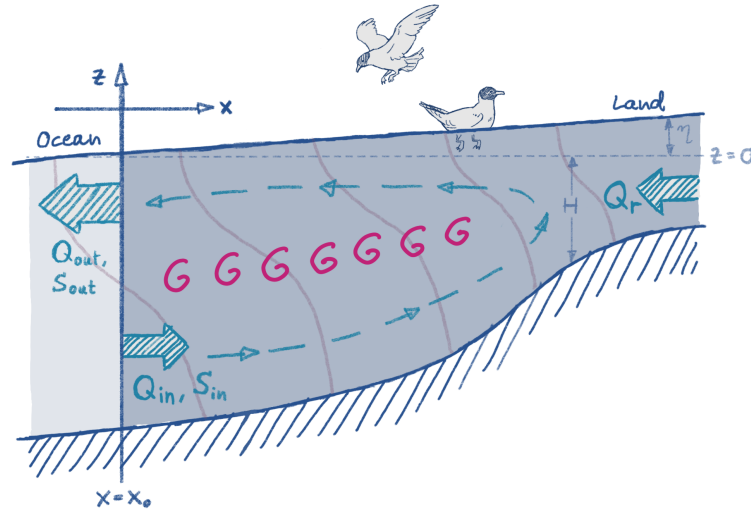


Figure 2.1: Schematic along-channel section of a classical estuary, illustrating the estuarine exchange flow with the freshwater inflow Q_r at salinity $S = 0$ and the saltwater inflow Q_{in} at $S = S_{in}$ as well as the brackish outflow Q_{out} at $S = S_{out}$ across a vertical cross-section at along-channel position $x = x_0$ that bounds the estuarine volume V_T (dark shading). Light purple lines indicate isohalines, and the pink spirals indicate mixing between the inflow and outflow layer. Additionally, the water depth H below $z = 0$ and the surface elevation η above $z = 0$ are shown.

In recent years, a multitude of mechanisms leading to or modifying the estuarine circulation have been found. The earliest known driver of the circulation was described by Hansen and Rattray (1965): the along-estuary density difference between freshwater on the terrestrial side and saltwater on the ocean side leads to a *baroclinic* pressure gradient that increases with depth and acts to drive saltwater in up-estuary (i.e., landward) direction. Simultaneously, a decrease of the surface elevation $\eta(x, y, t)$ towards the ocean yields a depth-independent, ocean-directed *barotropic* pressure gradient (see Fig. 2.1). In combination, the barotropic gradient dominates near the surface of the estuary and drives an outflow of brackish water in downstream (seaward)

direction, while the baroclinic gradient gains importance with depth, leading to a near-bottom, landward inflow of dense seawater into the estuary. This basic type of circulation occurs independently of tides and is known as the *gravitational circulation* (Hansen and Rattray, 1965).

Impact of Tides

If tides or another (periodic) variability are present, the estuarine circulation as described above will only become evident after sufficient temporal averaging, e.g., over several tidal cycles. It is therefore also referred to as a residual circulation (see, e.g., Geyer and MacCready, 2014).

Additionally, tides can play an essential role in driving their own type of residual circulation that adds to the estuarine pattern: a particularly important mechanism of tide-driven estuarine circulation in partially to well-mixed estuaries is the *tidal straining induced circulation* (Jay and Musiak, 1994, Burchard and Hetland, 2010, Burchard et al., 2011). Originally described as strain-induced periodic stratification (SIPS) by Simpson et al. (1990), some estuaries can vary between more well-mixed conditions at flood tide and more stratified conditions at ebb tide. Throughout flood, dense saltwater is pushed upstream, moving fastest near the free surface where the influence of bottom stress is lowest (see, e.g., Bowden and Fairbairn, 1952). Consequently, (faster) saltier water moves on top of (slower) fresher water, resulting in unstable stratification which is then mixed, leading to a more uniform water column at peak flood. During ebb, fresher water is moved downstream on top of saltier water, resulting in a stably stratified water column. While strain-induced periodic stratification specifically refers to conditions with a fully-mixed water column during flood tide, the general process of *tidal straining* may also occur in estuaries with a less extreme variability of stratification (explained, e.g., by MacCready and Geyer, 2010).

As stratification is known to stabilise a water column (Linden, 1979, 1980), turbulence will be suppressed during ebb such that a relatively higher portion of the ebb momentum is retained in the upper half of the water column and the current displays a more pronounced vertical shear. This is illustrated in Fig. 2.2b, where turbulence is represented by the vertical eddy viscosity $A_v(z, t)$. In contrast, under the well-mixed flood conditions, turbulence is stronger and allows the downward translation of a relatively higher portion of the flood momentum (see Fig. 2.2a). The resulting residual circulation consists of a near-bottom, upstream (flood-directed) transport of saltwater and a near-surface, downstream (ebb-directed) transport of freshwater (Jay and Musiak, 1994, Burchard and Hetland, 2010), named tidal straining induced circulation by Burchard et al. (2011).

Following Burchard and Hetland (2010), the tidally averaged, i.e., residual, along-channel velocity $\langle u_x \rangle(z)$ in a non-rotational estuarine water column with a constant along-channel salinity gradient $\partial_x S$ and periodic tidal forcing can be split into contributions from the river discharge (R), gravitational circulation (G), tidal straining (S), and wind straining. Using the notation from Geyer and MacCready (2014) and, like them, neglecting wind straining, this

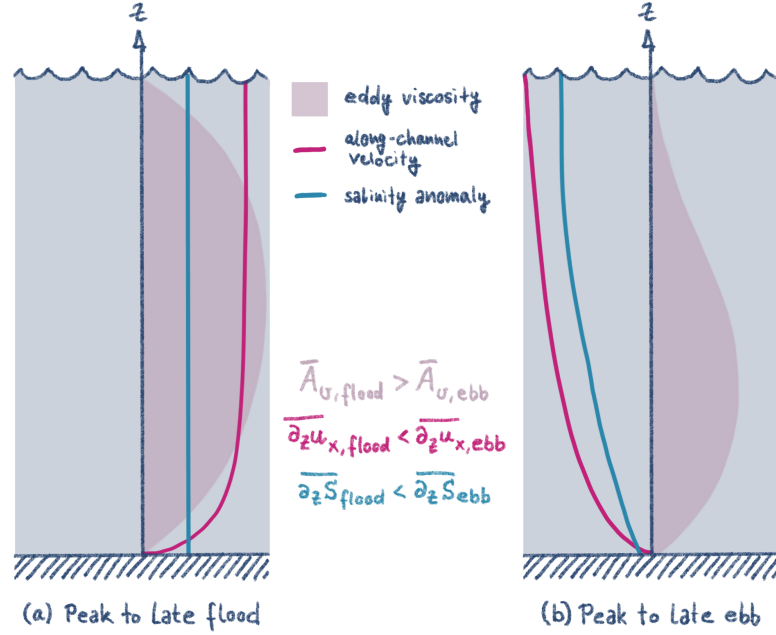


Figure 2.2: Qualitative vertical profiles of eddy viscosity $A_v(z, t)$, along-channel velocity $u_x(z, t)$, and the salinity anomaly (i.e., deviation from the tidal and vertical average) within an idealised estuarine water column at (a) peak to late flood and (b) peak to late ebb. Further, the vertically averaged quantities $\bar{\cdot}$ at flood and ebb are compared to explain the dynamics of tidal straining, where $S(z, t)$ is the salinity. Figure based on Fig. 2 from Geyer and MacCready (2014).

yields:

$$\langle u_x \rangle = u_R + u_G + u_S. \quad (2.1)$$

Temporal averaging of an arbitrary quantity ψ for a given time period Δt is here defined as

$$\langle \psi \rangle = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} \psi d\tau. \quad (2.2)$$

In (2.1), Δt equals the period of a sinusoidal tide. Additionally, the tidally averaged vertical shear stress $\langle A_v \partial_z u_x \rangle(z)$ can be decomposed into the covariance of the tidally varying vertical eddy viscosity $\hat{A}_v(z, t)$ and vertical shear $\partial_z \hat{u}_x(z, t)$ as well as their respective subtidal quantities $\langle A_v \rangle(z)$, $\langle \partial_z u_x \rangle(z)$:

$$\langle A_v \partial_z u_x \rangle = \langle \hat{A}_v \partial_z \hat{u}_x \rangle + \langle A_v \rangle \langle \partial_z u_x \rangle. \quad (2.3)$$

From this, Burchard and Hetland (2010) derived a velocity equation that can be decomposed into parts according to (2.1). As reviewed by Geyer and MacCready (2014), the resulting set of

equations for each component can be expressed as:

$$\begin{aligned}\frac{\partial u_R}{\partial z} &= \frac{G_R z}{\langle A_v \rangle}, \\ \frac{\partial u_G}{\partial z} &= \frac{G_G z}{\langle A_v \rangle} + \frac{z^2 \partial_x b}{2 \langle A_v \rangle}, \\ \frac{\partial u_S}{\partial z} &= \frac{G_S z}{\langle A_v \rangle} - \frac{\langle \hat{A}_v \partial_z \hat{u}_x \rangle}{\langle A_v \rangle},\end{aligned}\tag{2.4}$$

where a no-slip bottom boundary condition was applied and G_i is the subtidal along-channel barotropic pressure gradient per unit density caused by the surface elevation gradient associated with each respective component. The resulting velocity profiles for a weakly stratified estuary are shown in Fig. 2.3. As evident from (2.4), the river component $u_R(z)$ solely depends on the balance between the averaged bottom friction and the barotropic pressure gradient associated with the discharge. It is the discharge contribution to the residual velocity profile and always points in downstream direction, as the discharge alone cannot induce a circulation (see Fig 2.3). In the equation for the gravitational circulation $u_G(z)$ in (2.4), the baroclinic along-channel pressure gradient caused by the salinity difference is represented by the gradient of the buoyancy $b = -g(\rho - \rho_0)/\rho_0$, where g is the gravitational acceleration. The buoyancy $b(z)$ yields the relative gravitational forcing of a water mass of density $\rho(z)$ compared to a water mass of the reference density ρ_0 . It can be seen from (2.4) that for the gravitational circulation, the baroclinic pressure gradient competes with the barotropic pressure gradient as explained before. The resulting velocity profile for u_G (Fig. 2.3) shows the previously described pattern of a near-bottom inflow and a near-surface outflow. Lastly, the tidal straining component $u_S(z)$ is defined by the time-varying shear stress and has an inflow–outflow pattern similar to the gravitational circulation as seen in Fig. 2.3.

According to Burchard and Hetland (2010), the tidally driven circulation in weakly stratified estuaries can strongly exceed the gravitational circulation (see also Fig. 2.3). With increasing, more persistent stratification, the water column will remain partly stratified even at flood, eventually reducing the downward translation of flood momentum and the relative importance of the tidal straining induced circulation compared to the gravitational circulation (see also review by Geyer and MacCready, 2014). Later, Dijkstra et al. (2017) separated the interaction of the temporally varying eddy viscosity with the tidal and subtidal estuarine currents into several mechanisms beyond the tidal straining induced circulation, instead coining the term eddy viscosity-shear covariance (ESCO).

Lateral Effects

In estuaries with a channel-shoal geometry, the circulation contributions described above will affect the estuarine circulation in along-channel, or *longitudinal*, direction. Additionally, the interaction of the main, along-channel flow with the channel shoals will lead to a cross-channel circulation that can strengthen or weaken the along-channel estuarine circulation depending on its respective pattern (see review by Geyer and MacCready, 2014). This is referred to as

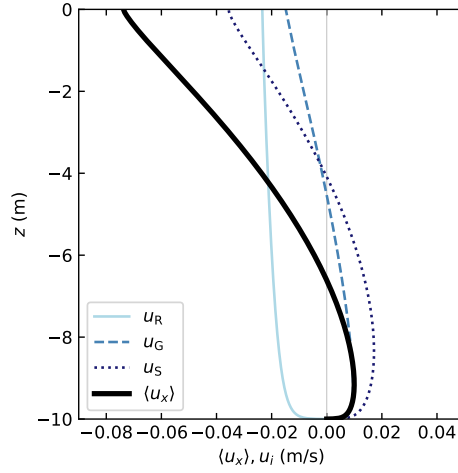


Figure 2.3: Exemplary profiles of the subtidal velocity components from (2.1) as given by (2.4), i.e., river discharge $u_R(z)$, gravitational circulation $u_G(z)$, and tidal straining induced circulation $u_S(z)$ as well as the total residual velocity profile $\langle u_x \rangle(z)$. The profiles were computed from a numerical, one-dimensional simulation of an estuarine water column with relatively weak vertical stratification, sinusoidal tidal forcing, and no surface stress. Figure adapted with permission from Burchard et al. (2023), Fig. 5a.

lateral circulation, and can be caused by several mechanisms as reviewed by MacCready and Geyer (2010) and Geyer and MacCready (2014). Depending on the underlying cause, such as differential advection (Smith, 1976, Nunes and Simpson, 1985), the influence of the Coriolis force (e.g., Kalkwijk and Booij, 1986, Johnson and Ohlsen, 1994), or channel curvature (e.g., Kalkwijk and Booij, 1986, Chant, 2002), the resulting lateral circulation pattern may differ (see also Lerczak and Geyer, 2004, MacCready and Geyer, 2010, Geyer and MacCready, 2014, and references therein).

Here, let us focus only on the effect of *differential advection*. This common process was originally described by Smith (1976) and first observed and further analysed by Nunes and Simpson (1985). Bottom stress above the shoals of the navigational channel of an estuary tends to reduce the along-channel current velocity compared to the channel center. This leads to differential advection of along-channel density gradients $\partial_x \rho$, resulting in their conversion to cross-channel gradients $\partial_y \rho$ and consequently the build-up of a cross-channel baroclinic pressure gradient, as illustrated in Fig. 2.4a,b. During flood, the incoming saltwater is advected faster along the channel center, such that the shoals become relatively fresher. The resulting baroclinic pressure gradient drives (salty) near-bottom water up the shoal and (fresher) near-surface water toward the channel center, typically leading to a symmetric two-cell circulation with surface convergence as depicted in Fig. 2.4c (Smith, 1976, Nunes and Simpson, 1985, Guymer and West, 1991). During ebb, the baroclinic pressure gradient and thus the resulting lateral circulation are inverted, as the shoals become saltier than the channel center (Fig. 2.4d).

Assuming a constant cross-channel density gradient $\partial_y \rho$ and a balance between the resulting pressure gradient and vertical stress divergence, analogous to the assumptions from Hansen and Rattray (1965) for the longitudinal gravitational circulation, Nunes and Simpson (1985) provided a simple solution for the cross-channel velocity $u_y(y, z)$ caused by differential

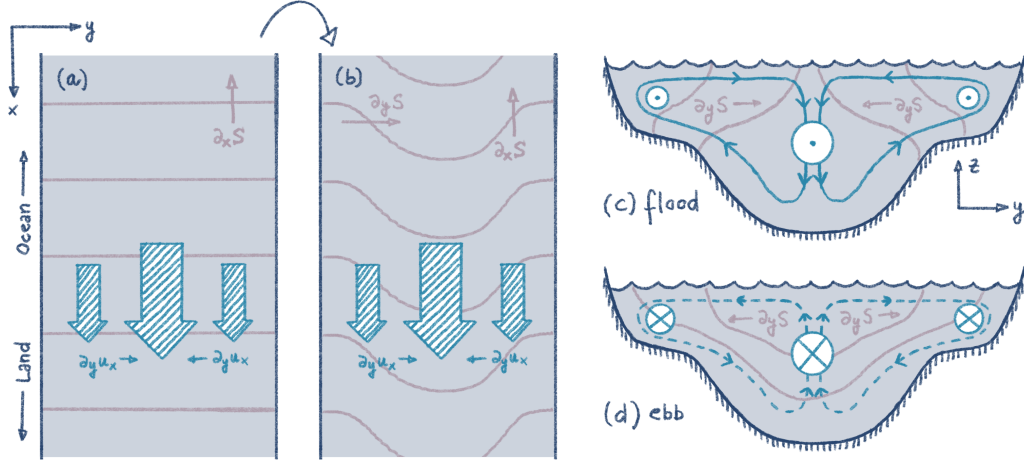


Figure 2.4: Schematic explaining the effect of differential advection and the resulting lateral circulation. Light purple lines indicate isohalines, blue arrows and symbols indicate current velocities. (a): Birds-eye view of an estuarine section during flood with an initial along-channel salinity gradient $\partial_x S$ and an along-channel current u_x that is slower above the shoals. In (b), the resulting, strained isohaline structure is shown which also includes a cross-channel salinity gradient $\partial_y S$. The lateral circulation that is driven by such a gradient is illustrated for an exemplary channel cross-section at (c) flood and (d) ebb. The size of the circles in (c) and (d) represents the relative magnitude of the along-channel velocity u_x . In (d), the dashed lines indicate the weaker lateral circulation compared to flood due to the reduced velocity difference between the shoals and channel center.

advection:

$$u_y = \frac{gH^3 \partial_y \rho}{48 \bar{\rho} A_v} \left\{ 9 \left(1 - \left(\frac{z}{H} \right)^2 \right) - 8 \left(1 + \left(\frac{z}{H} \right)^3 \right) \right\}. \quad (2.5)$$

In (2.5), $\bar{\rho}$ is the vertically averaged density, z is the vertical, and y is the cross-channel coordinate. From eq. (2.5) it becomes apparent that aside from the channel-shoal density difference $\partial_y \rho$ and the constant eddy viscosity A_v , the channel geometry as given by the water depth $H(y)$ and the channel-shoal distance (implicitly covered by the constant density gradient) plays an essential role for the establishment of a lateral circulation (see also Schulz et al., 2015).

For an upstream transect of the Elbe estuary, taken from data from Reese et al. (2025), a salinity difference $\Delta S \approx 6$ g/kg between channel and shoal at a transect width $W \approx 5$ km results in a mean density gradient of $\Delta \rho / (W/2) \approx \beta \Delta S \rho_0 / (W/2) = 0.002$ kg/m⁴. Here, the linear equation of state was used for the water density, neglecting temperature, with a haline contraction coefficient $\beta = 7.7 \cdot 10^{-4}$ kg/g (Millero and Poisson, 1981, Jackett and McDougall, 1985) and a reference density $\rho_0 = 1000$ g/kg. Further considering a mean transect depth $H = 10$ m, a vertically averaged salinity $\bar{S} \approx 7$ g/kg, and a vertical eddy viscosity $A_v \approx 10^{-4} \dots 5 \cdot 10^{-2}$ m²/s (see review by Geyer and MacCready, 2014), one can expect maximum lateral velocities ranging from $u_y \approx 0.0015$ m/s to $u_y \approx 0.7$ m/s. Compared to this, the tidal along-channel velocity in the Elbe estuary is usually of a greater magnitude of $u_x \approx 0.8 - 1.8$ m/s (Boehlich and Strotmann, 2008). This means that while the cross-channel velocity can play an important role in shaping the cross-channel density distribution and stratification, it is

predominantly the along-channel velocity that provides strong shear and therefore turbulence for salt mixing in estuaries.

As shown, e.g., by Lerczak and Geyer (2004), the lateral circulation caused by differential advection is often stronger during flood than ebb. They attributed this observation to a positive feedback between lateral circulation and momentum transport during flood and a negative feedback during ebb: through the flood-directed lateral circulation, low-momentum water is transported from the channel bottom onto the shoals of the estuary, which further slows the advection of water above the shoals. This reinforces the differential advection and consequently the flood-tide lateral circulation. During ebb, the circulation pattern is inverted and high-momentum water from the channel surface is advected onto the shoals where it accelerates the current and thus weakens the effect of differential advection (Lerczak and Geyer, 2004, see also Fig. 2.4c,d). As a result, the strong flood-directed lateral circulation with a surface convergence acts to distribute the high flood momentum further downward within the water column. During ebb, momentum is retained mostly within the fast-flowing surface layer due to the weaker lateral circulation with a surface divergence. This leads, again, to a reinforcement of the along-channel estuarine circulation pattern with a residual ebb-directed fresher surface layer and a flood-directed saltier bottom layer.

In sum, many different aspects can impact the along-channel estuarine circulation. Depending on the external forcing of the estuary, such as through wind (e.g., Lange and Burchard, 2019), surface heating (e.g., Lorenz et al., 2020), or ice coverage (e.g., Burchard et al., 2023), the resulting exchange flow can deviate from the above-described, classic two-layer case with brackish outflow and salty inflow. However, the Elbe estuary, which is the focus of the present work (see Section 2.2), displays the classic two-layer flow pattern (Reese et al., 2024, see Section 3.1.1).

2.1.2 Total Exchange Flow

The estuarine circulation was first quantified by Knudsen (1900) (see also translation by Burchard et al., 2018), who considered volume and salt conservation to derive a pair of equations yielding the bulk volume inflow and outflow across an arbitrary, cross-estuary transect at along-channel position x , $Q_{\text{in}}(x)$ and $Q_{\text{out}}(x)$, respectively, and their corresponding bulk inflow and outflow salinity $S_{\text{in}}(x)$ and $S_{\text{out}}(x)$:

$$Q_{\text{in}} + Q_{\text{out}} + Q_{\text{r}} = 0, \quad (2.6)$$

$$Q_{\text{in}}S_{\text{in}} + Q_{\text{out}}S_{\text{out}} = 0, \quad (2.7)$$

where (2.6) represents volume conservation and (2.7) represents salt conservation. The respective quantities are illustrated in Fig. 2.1. Note that a positive sign is here associated with an inflow into the estuarine volume, i.e., the freshwater discharge $Q_{\text{r}} \geq 0$ and the saltwater inflow $Q_{\text{in}} \geq 0$. The brackish water outflow is of negative sign, i.e., $Q_{\text{out}} \leq 0$. Combining both equations, the bulk volume inflow and outflow can be computed from their respective bulk

inflow and outflow salinity, S_{in} and S_{out} , and the freshwater discharge Q_r into the the estuary:

$$Q_{\text{in}} = \frac{S_{\text{out}}}{S_{\text{in}} - S_{\text{out}}} Q_r, \quad Q_{\text{out}} = -\frac{S_{\text{in}}}{S_{\text{in}} - S_{\text{out}}} Q_r. \quad (2.8)$$

Equations (2.8) are also known as the *Knudsen relations*. They are valid only for sufficiently long averaging periods where any effects of volume and salt storage vanish, although Burchard et al. (2018) provided a version of the relations that does include these storages. Further, the Knudsen relations neglect surface fluxes such as evaporation or precipitation and are based on the assumption that the freshwater discharge Q_r is of zero salinity whereas real rivers usually carry freshwater of low, but non-zero salinity. Nonetheless, because the related quantities are relatively easy to assess, the Knudsen relations make for a simple estimate of exchange flow in water bodies such as the Baltic Sea (Knudsen, 1900, Burchard et al., 2018).

More recently, MacCready (2011) introduced the Total Exchange Flow (TEF) framework which resolves the inflow and outflow across a given cross-estuary transect in salinity space. Due to the salinity-dominated density structure of classical estuaries, an isohaline framework that replaces the vertical coordinate with salinity classes S can be a useful tool for their analysis (see Walin, 1977). Instead of considering bulk values as in Knudsen (1900), each TEF transport is sorted into salinity classes S . The total volume transport $Q(S, x, t)$ for all salinity classes $s > S$ is then given as

$$Q = \int_{A_T} u_x dA, \quad (2.9)$$

where $A_T(S, x, t)$ is the fraction of the total cross-sectional area $A_T(S = 0, x, t)$ of the transect T at position x where salinities $s > S$ occur (see Fig. 2.5a). The velocity $u_x(x, y, z, t)$ is the component of the total current velocity $\mathbf{u}(x, y, z, t)$ that is orthogonal to the cross-section. Originally, MacCready (2011) applied tidal averaging $\langle \cdot \rangle$ already in (2.9). Here, this averaging will be applied at a later point without affecting the resulting quantities (see Wang et al., 2017, Klingbeil et al., 2019).

The derivative of $Q(S, x, t)$ with respect to S yields the cross-sectional volume transport $q(S, x, t)$ for a single salinity class S ,

$$q = -\frac{\partial Q}{\partial S}, \quad (2.10)$$

where the negative sign ensures that transports into the estuary are of positive sign as established above. Fig. 2.5b,c shows qualitative profiles for Q and q in discrete space.

Further, from the volume transport per salinity class, $q(S, x, t)$, bulk inflow and outflow values corresponding to $Q_{\text{in}}(x, t)$ and $Q_{\text{out}}(x, t)$ as in (2.6) can be found via integration of only the inflowing or outflowing transports, respectively (see also Fig. 2.5c):

$$Q_{\text{in}}(x, t) \equiv \int_0^{S_0} \langle q(x, S, t) \rangle|_{\text{in}} dS, \quad Q_{\text{out}}(x, t) \equiv \int_0^{S_0} \langle q(x, S, t) \rangle|_{\text{out}} dS, \quad (2.11)$$

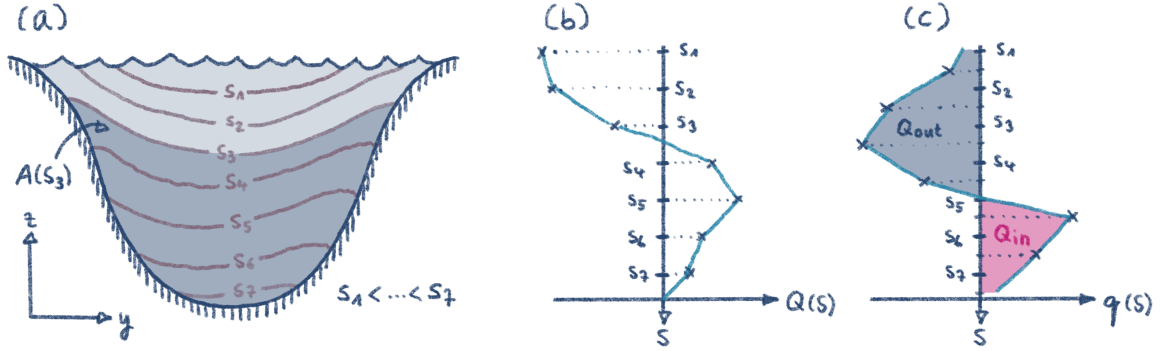


Figure 2.5: Explanatory sketch for the Total Exchange Flow in a discrete salinity space. (a): Cross-channel section with isohalines at salinity $S_1 < \dots < S_7$ with a regular spacing ΔS . The dark-shaded area shows the fraction of the cross-channel section that contains only salinities $S > S_3$, $A(S_3)$. (b): Discrete profile of the total volume transport $Q(S)$ for all salinity classes $s > S$, which is defined for each respective salinity class. (c) Respective inflow per salinity class, $q(S)$, which is defined at the interfaces between the salinity classes S . The shaded areas indicate the bulk inflow Q_{in} and outflow Q_{out} , respectively. Note that in (b) and (c), S_5 is the dividing salinity S_{div} . Figure based on Fig. 1.3 from Lorenz (2020).

where S_0 is the highest occurring salinity, i.e., ocean salinity. Additionally, tidal averaging $\langle \cdot \rangle$ has now been applied, but the time t dependency remains as a subtidal variability may exist. Likewise, the bulk incoming and outgoing salt transports are computed as

$$F_{in}(x, t) \equiv \int_0^{S_0} S \cdot \langle q(x, S, t) \rangle|_{in} dS, \quad F_{out}(x, t) \equiv \int_0^{S_0} S \cdot \langle q(x, S, t) \rangle|_{out} dS. \quad (2.12)$$

Instead of computing the bulk values as described above, however, Lorenz et al. (2019) introduced the numerically more robust *dividing salinity method* that locates the dividing salinity S_{div} between inflow and outflow layer from the maximum of $Q(S, x, t)$:

$$Q_{in}(x, t) = \max(\langle Q(S, x, t) \rangle) = \langle Q(S_{div}, x, t) \rangle, \quad Q_{out}(x, t) = -Q_{in}(x, t) - Q_r(t). \quad (2.13)$$

In Fig. 2.5b,c, the salinity class S_5 corresponds to the dividing salinity S_{div} . The dividing salinity method can easily be expanded for estuaries with more than one inflow or outflow layer by assigning a dividing salinity to each local maximum of $Q(S, x)$.

Lastly, the transport-weighted TEF inflow and outflow salinities $S_{in}(x, t)$, $S_{out}(x, t)$ follow from the bulk transports as

$$S_{in} \equiv \frac{F_{in}}{Q_{in}}, \quad S_{out} \equiv \frac{F_{out}}{Q_{out}}. \quad (2.14)$$

As shown by MacCready (2011), it is possible to derive the original Knudsen (1900) relations (2.8) from the Total Exchange Flow framework when sufficiently long averaging is applied such that storage effects vanish.

2.1.3 Estuarine Mixing

Tracer variance in a water body can be reduced through the mixing of water masses with different tracer properties. On the molecular scale, this happens via molecular tracer diffusion. With molecular diffusivities of the order of $\nu = 10^{-9} \text{ m}^2\text{s}^{-1}$, e.g., for salt (Mellor, 1996), this is a slow process that cannot alone explain the observed changes of tracers like salinity in oceanic water bodies, as reviewed by Gregg (1991). Instead, molecular diffusion acts in combination with turbulence: as explained in detail in the review by Villiermaux (2019), turbulent structures such as eddies can quickly increase local tracer gradients by warping existing tracer stratification from large to small scales. As a result, molecular diffusion, which depends on the tracer gradient, can reduce the variance much faster than under undisturbed conditions. Therefore, physical oceanography parameterises the impact of turbulence with an effective diffusivity, the eddy diffusivity (see review by Gregg, 1991), that tends to exceed the molecular diffusivity by several orders of magnitude in many water bodies. In the Elbe estuary, e.g., vertical eddy diffusivities of the order $K_v = 10^{-6} \dots 10^{-1} \text{ m}^2\text{s}^{-1}$ occurred in a numerical simulation by Burchard et al. (2004). The eddy diffusivity is directly related to the correlation between the fluctuations $\tilde{\cdot}$ of both the tracer concentration $c(x, y, z, t) = \bar{c}(x, y, z, t) + [\tilde{c}](x, y, z, t)$ and local velocity $u_i(x, y, z, t) = \bar{u}_i(x, y, z, t) + [\tilde{u}_i](x, y, z, t)$ in each spatial direction $i \in \{x, y, z\}$, respectively, from their respective Reynolds average $[\cdot]$ (see, e.g., Burchard and Rennau, 2008):

$$\begin{aligned} [\tilde{u}_x \tilde{c}] &\approx -K_h \partial_x [\tilde{c}] , \\ [\tilde{u}_y \tilde{c}] &\approx -K_h \partial_y [\tilde{c}] , \\ [\tilde{u}_z \tilde{c}] &\approx -K_v \partial_z [\tilde{c}] . \end{aligned} \tag{2.15}$$

Here, $K_h(x, y, z, t)$ is the horizontal and $K_v(x, y, z, t)$ is the vertical eddy diffusivity of the given tracer. A thorough explanation of Reynolds averaging can be found in Burchard (2002).

Often, *mixing* in oceanography is purely defined by means of local turbulence, e.g., in form of the local turbulent kinetic energy dissipation (as done, e.g., by Collignon and Stacey, 2013, Huguenard et al., 2015). However, such a definition would also imply high mixing rates for turbulent water masses that are already well-mixed, i.e., that do not contain a tracer gradient anymore. Thus, they are not suited for a proper quantification of water mass transformation, which explicitly refers to the water transport across isotracer surfaces (see review by Groeskamp et al., 2019). The estuarine circulation requires such a water transport between the inflow and outflow layers across *isohaline* surfaces (see also Walin, 1977).

In the present work, let us therefore follow Burchard and Rennau (2008) and define salt mixing as the destruction of mean salinity squared $[S]^2(x, y, z, t)$:

$$\chi(x, y, z, t) = 2K_h(\partial_x [S])^2 + 2K_h(\partial_y [S])^2 + \underbrace{2K_v(\partial_z [S])^2}_{\chi_v}, \tag{2.16}$$

where $\chi_v(x, y, z, t)$ is the vertical mixing. This definition equals the sink term of a budget equation for the mean salinity squared $[S]^2$ which in turn can be derived from the budget

equation for the mean salinity $[S](x, y, z, t)$ itself:

$$\frac{\partial [S]}{\partial t} + \mathbf{u} \nabla [S] - \nabla (\mathbf{K} \nabla [S]) = 0, \quad (2.17)$$

where $\mathbf{K} = \text{diag}(K_h, K_h, K_v)$ and internal sources or sinks of salinity have been neglected. The full derivation of (2.16) from (2.17) can be found in Burchard and Rennau (2008). With this definition, salt mixing acts to reduce salinity variance within a given water body.

Note that outside of eq. (2.15–2.17), only Reynolds-averaged quantities are considered in this work, but the $[\cdot]$ argument is dropped for convenience.

Variability of Mixing

Under the definition (2.16), salt mixing depends on both turbulence and the quantity that it acts on – salt stratification. By this definition, highest mixing occurs in places of ideal overlap between turbulence and stratification, as demonstrated, e.g., by Warner et al. (2020). As neither turbulence nor stratification tend to be uniform within estuaries, salt mixing is known to be highly variable in space and time: topographical irregularities and the interaction of the main flow with the estuarine topography may lead to the formation of local mixing hotspots (see, e.g., Wang et al., 2017, Warner et al., 2020) or broader regions of enhanced mixing as shown, e.g., in Li et al. (2022) and Henell et al. (2023), by influencing the isohaline structure (cf. Collignon and Stacey, 2013, Huguenard et al., 2015) or the local distribution of turbulence.

Throughout the spring-neap cycle, mixing in partially mixed estuaries is commonly known to be most intense at the transition from neap to spring: at neap tide, when the tidal energy available for mixing is low, excess stratification can be created which is mixed as soon as the tidal energy increases at the transition to spring (see, e.g., Wang et al., 2017, Li et al., 2018, Wang and Geyer, 2018). Similarly, mixing throughout the semidiurnal M_2 tidal cycle tends to be highest nearing peak ebb in partially mixed estuaries (e.g., Warner et al., 2020), as ebb stratification is usually higher than flood stratification (Simpson et al., 1990, see tidal straining in Section 2.1.1) and peak tidal velocities provide sufficient shear stress for mixing.

As expressed by Broatch and MacCready (2022) for the example of the Salish Sea (north-western USA), the energy required for mixing within a tidal estuary tends to be mainly provided by the tides themselves, but the variability of the available salinity variance (and resulting stratification) may far exceed the above described variability of the tidal energy. Although a variability of the conditions in the adjacent ocean may also impact the available salinity variance, it is the freshwater discharge that tends to be a major source of salinity variance and therefore of stratification in classical estuaries. Indeed, Broatch and MacCready (2022) reported a dominant control of the freshwater discharge on the timing of mixing in the Salish Sea (see also MacCready et al., 2018). The influence of the freshwater discharge will be further discussed in the following section, where a number of relations between estuarine salt mixing and the incoming discharge are introduced. Additionally, Broatch and MacCready (2022) found that the energy input through wind, rather than the tides, also impacts the timing of increased mixing in the Salish Sea.

Mixing Relations

In Euclidean space, (2.16) is the local mixing at any given position (x, y, z) within the estuary. If the estuarine volume $V_T(x, t)$ is bounded up-estuary by the end of salt intrusion (upstream of which no more mixing according to the definition (2.16) can occur because all salinity gradients vanish) and down-estuary by a vertical, cross-channel transect T at along-channel position x , the volume integral of $\chi(x, y, z, t)$ yields the total mixing $M_T(x, t)$ within the estuary:

$$M_T(x, t) = \left\langle \int_{V_T(x, t)} \chi(x, y, z, t) dV \right\rangle, \quad (2.18)$$

where, as before, $\langle \cdot \rangle$ indicates temporal (although not necessarily tidal) averaging.

Alternatively, the estuarine volume $V_S(S, t)$ can also be bounded by an isohaline surface of salinity S (Walsh, 1977, Burchard, 2020, see Fig. 2.6). In this case, the total mixing $M_S(S, t)$ is given as

$$M_S(S, t) = \left\langle \int_{V_S(S, t)} \chi(x, y, z, t) dV \right\rangle. \quad (2.19)$$

The mixing per salinity class $m(S, t)$ then yields the area integrated mixing on the selected isohaline surface:

$$m = \frac{\partial M_S}{\partial S} = \int_{A_z} m_{xy} dA_z, \quad (2.20)$$

where $A_z(S, t)$ is the horizontal projection of the isohaline surface area (see also Fig. 2.6). To yield maps of the local distribution of the mixing per salinity class, one can further compute the local mixing $m_{xy}(x, y, S, t)$ that occurs at a given horizontal location (x, y) on a single isohaline surface S , here following the definition from Klingbeil and Henell (2023):

$$m_{xy} = \left\langle \int_{-H}^{\eta} \delta(s^z - S) \chi dz \right\rangle, \quad (2.21)$$

where $s^z(x, y, z, t)$ is the salinity at a given spatial position (x, y, z) and $\delta(\psi)$ is the Dirac function applied to an arbitrary function ψ , which acts here to sample the mixing χ only in locations within the water column where the salinity S occurs.

As explained before, estuarine mixing is generally dependent on the incoming river discharge $Q_r(t)$. This was quantified for the total mixing $M_T(x, t)$ within a *transect-bounded* estuary by MacCready et al. (2018):

$$M_T \approx S_{in} S_{out} Q_r = (S_{in} - S_{out}) S_{in} Q_{in}. \quad (2.22)$$

According to (2.22), the volume-integrated mixing M_T can be estimated from the freshwater discharge Q_r into the estuary and the TEF bulk salinities $S_{in}(x, t)$, $S_{out}(x, t)$ across the transect at position x . In the second formulation, which was already shown in the Introduction (Section 1),

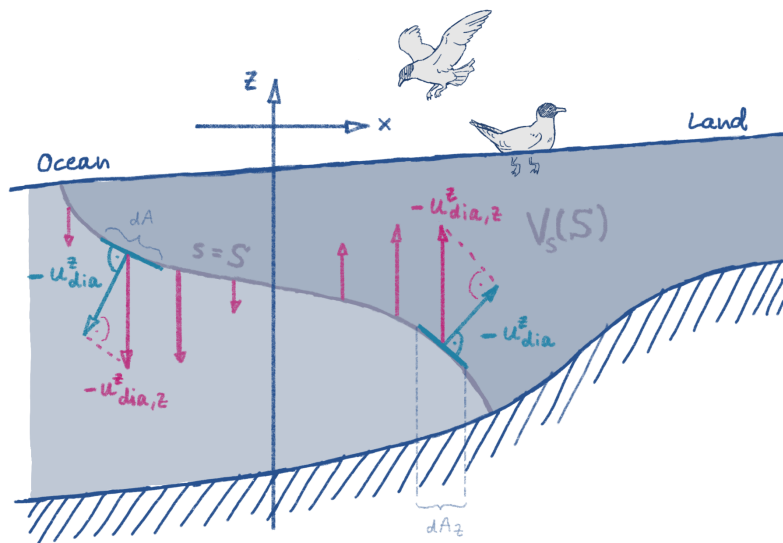


Figure 2.6: Schematic along-channel section of a classical estuary, illustrating the concept of an estuarine volume $V(S)$ (darker shading) bounded by an isohaline surface of salinity $s = S$. Additionally, the diahaline exchange flow on the bounding isohaline is shown in z -space using the vertical diahaline velocity $u_{\text{dia},z}^z$ (magenta). Its projection in the direction of the salinity gradient, u_{dia}^z , is added in light blue for two selected locations. To better illustrate the direction of the diahaline exchange flow, only the respective inverse directions of the diahaline velocities are depicted. Further, the definition of the isohaline surface element dA and its horizontal projection, dA_z , is shown.

eq. (2.22) further provides a direct relation between the estuarine exchange flow intensity $Q_{\text{in}}(x, t)$ and the estuary-wide mixing M_{T} .

For the total mixing $M_S(S, t)$ within an *isohaline-bounded* estuary, Burchard (2020) introduced a similar relation:

$$M_S = S^2 Q_r. \quad (2.23)$$

If derived with respect to the salinity class S , this yields a universal law of estuarine mixing (Burchard, 2020),

$$m = 2SQ_r, \quad (2.24)$$

stating that the salt mixing across an isohaline surface, $m(S, t)$, is determined exclusively by the salinity of the isohaline itself and the freshwater discharge entering the estuary.

Relations (2.23) and (2.24) are exact when surface fluxes are neglected and sufficiently long averaging, such that any effects of volume and salt storage vanish, is applied. Relation (2.22), on the other hand, is an approximation that, according to MacCready et al. (2018), typically has an error margin of about 10% when storage effects vanish.

2.1.4 Diahaline Circulation

Generally, a water transport across isohaline surfaces, i.e., a *diahaline* water transport, is enabled by processes such as salt mixing. It is a measure for water mass transformation (see Walin, 1977, 1982) and cannot occur through pure advection of salinity. This means that the diahaline water transport is of particular interest when trying to relate local mixing and the exchange flow.

To study diahaline dynamics, let us define the diahaline velocity, $u_{\text{dia}}^z(x, y, z, t)$, as the movement of an isohaline surface relative to the surrounding current velocity $\mathbf{u}(x, y, z, t)$. In z -space (i.e., Euclidean space), this can be expressed as follows:

$$u_{\text{dia}}^z = (\mathbf{u} - \mathbf{u}_s) \cdot \frac{\nabla s^z}{|\nabla s^z|}, \quad (2.25)$$

where $\mathbf{u}_s(x, y, z, t)$ is the total isohaline movement including advection by the current. As required, $u_{\text{dia}}^z(x, y, z, t)$ is defined orthogonal to the isohaline surface, i.e., in diahaline direction. It is of positive sign for flows in the direction of the salinity gradient $\nabla s^z(x, y, z, t)$ (i.e., in the direction of increasing salinity). For the purpose of numerical simulations, it is convenient to instead consider the *effective vertical diahaline velocity* in salinity space, $u_{\text{dia},z}^S(x, y, S, t)$ (Klingbeil and Henell, 2023):

$$u_{\text{dia},z}^S = \int_{-H}^{\eta} \delta(S - s^z) |\nabla s^z| u_{\text{dia}}^z dz, \quad (2.26)$$

where the Dirac function δ allows to compute $u_{\text{dia},z}^S$ as the effective sum of all locations in the water column where $s^z = S$ is given even when multiple salt intrusions are present. The equivalent of $u_{\text{dia},z}^S$ in z -space is denoted as $u_{\text{dia},z}^z$. In case of stable stratification, where $s^z = S$ occurs only once per water column, the two quantities are equal. One has to note here that with the definition (2.26), u_{dia}^z is the projection of $u_{\text{dia},z}^z$ in diahaline direction as illustrated in Fig. 2.6. Both quantities are positive in the direction of higher salinity. The quantity $u_{\text{dia},z}^S$ further corresponds to a local diahaline volume flux per unit horizontal area. In the case of stable stratification, it is equivalent to the entrainment velocity w_e from Wang et al. (2017) and Li et al. (2022).

In many estuaries, the vertical dimension (~ 10 m) is considerably smaller than the horizontal dimension ($\sim 10^2 - 10^3$ m), leading to near-horizontal isohaline surfaces even for weak stratification. Under such conditions, u_{dia}^z is nearly identical to $u_{\text{dia},z}^z$. At the same time, $u_{\text{dia},z}^S$ is less computationally expensive to diagnose than its projection in diahaline direction since it does not require the computation of the isohaline surface angle on a horizontal grid cell level. Instead, only the change of the vertical position of the isohaline surface needs to be known for each time step and grid cell. This makes $u_{\text{dia},z}^S$ the preferable choice of quantity in numerical simulations of estuaries with near-horizontal isohaline surfaces.

While the Total Exchange Flow framework (see Section 2.1.2) quantifies the circulation across a vertical, cross-estuary transect, it stands to reason that an analogous exchange flow

might exist across an isohaline surface, i.e., a single isohaline surface might show distinct regions of inflow towards lower salinity ($-u_{\text{dia},z}^S > 0$) and outflow towards higher salinity ($-u_{\text{dia},z}^S < 0$) as indicated in Fig. 2.6. In the present work, this will be referred to as the *diahaline exchange flow*.

As mentioned earlier, mixing is an important mechanism of diahaline water transport. Combining relations from Wang et al. (2017) and Li et al. (2022), Klingbeil and Henell (2023) quantitatively linked the diahaline exchange flow in terms of the effective vertical diahaline velocity, $u_{\text{dia},z}^S$, on a given isohaline surface to the local mixing per salinity class in the same location:

$$\langle u_{\text{dia},z}^S \rangle = \frac{1}{2} \frac{\partial m_{xy}}{\partial S}. \quad (2.27)$$

This relation neglects surface fluxes and horizontal mixing. In large-scale oceanography, a comparable relation for isopycnal surfaces has been known since the late 20th century (see McDougall, 1984, Marshall et al., 1999), while (2.27) is new to estuarine physics and the related isohaline instead of isopycnal framework.

2.1.5 Further Processes Driving Changes in Stratification

Aside from mixing, a number of mechanisms can affect stratification within a given estuarine water column. To identify the causes of local changes in stratification, a dynamic equation for the vertical salinity variance $(S')^2$ derived by Li et al. (2018) will be used:

$$\underbrace{\frac{\partial \int_{-H}^{\eta} (S')^2 dz}{\partial t}}_{\text{Tendency}} + \underbrace{\nabla_h \int_{-H}^{\eta} \mathbf{u}_h (S')^2 dz}_{\text{(A): Advection}} = \underbrace{-2 \int_{-H}^{\eta} \mathbf{u}'_h S' \cdot \nabla_h \bar{S} dz}_{\text{(B): Straining}} - \underbrace{\int_{-H}^{\eta} \chi_v dz}_{\text{(C): Vertical Mixing}}. \quad (2.28)$$

Here, ∇_h is the horizontal gradient operator and $S'(x, y, z, t)$ is the deviation of a vertical salinity profile $S(x, y, z, t)$ from its vertical average, i.e.,

$$S = \bar{S} + S', \quad (2.29)$$

with the vertically averaged salinity $\bar{S}(x, y, t)$. Analogously, the horizontal velocity vector $\mathbf{u}_h(x, y, z, t) = \bar{\mathbf{u}}_h(x, y, t) + \mathbf{u}'_h(x, y, z, t)$. Within (2.28), the tendency term yields the net rate of change of the integrated salinity variance within a given water column as the result of the remaining terms as explained in Fig. 2.7: advection (A) can carry in differently stratified water from the surroundings, while straining (B) acts to deform isohaline surfaces due to a vertical shear of horizontal velocities. A change of the isohaline shape corresponds to a change of stratification. Vertical mixing (C) transports water across the isohaline surfaces as explained in Sections 2.1.3 and 2.1.4 and generally acts to reduce gradients. In contrast to Li et al. (2018), let us explicitly differentiate here between longitudinal (along-channel; x -direction) and lateral (cross-channel; y -direction) straining B_x , B_y to assess the specific impact of longitudinal and lateral circulation each on the salinity distribution.

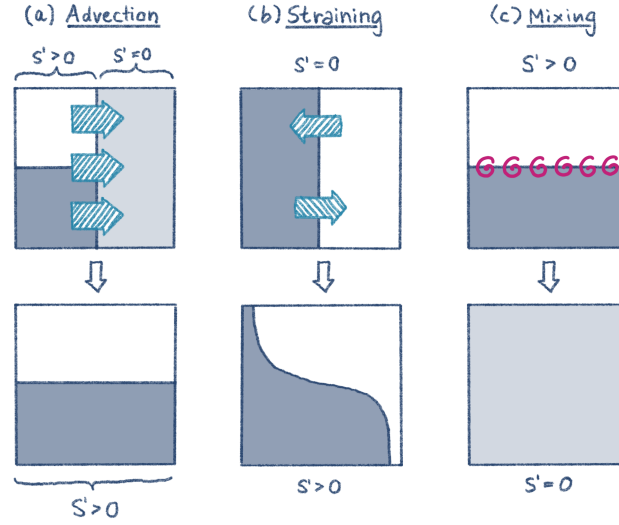


Figure 2.7: Illustration of the mechanisms described by the different terms in eq. (2.28), where white shading represents low, dark shading represents high, and light shading represents intermediate salinity. Light blue arrows give the current direction, and pink spirals represent turbulent mixing. The top panels show an exemplary initial state, while the bottom panels show the resulting state after each mechanism has acted. Sketch based on Fig. 1 from Burchard and Hofmeister (2008) and Fig. 1 from Li et al. (2018).

Eq. (2.28) neglects horizontal mixing, surface fluxes as well as inner sinks and sources of salinity. For the Elbe estuary considered in this work, however, the much larger horizontal than vertical scales result in negligible horizontal mixing compared to vertical mixing (see Reese et al., 2024).

It should further be noted that neither the tendency term in (2.28) nor the mixing definition (2.16) differentiate between stable (more dense water underneath less dense water) or unstable stratification (less dense water underneath more dense water). A reduction of either type of stratification will lead to a reduction of salinity variance. However, due to its energetically unfavourable state, an unstably stratified water column will mix without external energy input, while a stably stratified water column will require an external source of energy to become fully mixed on time scales shorter than that of molecular diffusion. In estuaries where unstable stratification does not widely occur, as is the case for the Elbe estuary that is the focus of the present dissertation (cf. Burchard et al., 2004, Reese et al., 2024, 2025), (2.28) is a good indicator for changes in stratification. In such a case, a positive rate of change represents an increase in stratification, while a negative rate of change represents de-stratification.

2.2 Numerical Simulations

The research aims of the present work required a high spatio-temporal data coverage to properly assess distributions of properties such as the Total Exchange Flow, local mixing, and diahaline velocity. In particular, the salinity space needed to be well-resolved in space and time. These requirements were best met by the use of numerical simulations. Across the studies presented

in the present work, two numerical setups of the Elbe estuary were used: a higher-resolved model run covering an analysis period of a single spring-neap cycle and a lower-resolved model run covering a longer analysis period of about one and a half years.

In the following, a description of the study region as well as the numerical model and used numerical setups will be given.

2.2.1 Study Region: The Elbe Estuary

The funnel-shaped Elbe estuary is located in northwest Germany adjacent to the German Bight, a part of the North Sea (see Fig. 2.8a,b). It connects the maritime trade port of Hamburg with the North Sea as well as, via the Kiel Canal, the Baltic Sea and is therefore of major economic importance (see, e.g., Boehlich and Strotmann, 2008).

Its dominant tidal constituent is the semidiurnal M_2 tide, modulated by a biweekly spring-neap cycle. With a tidal range from about 3.0 m at Cuxhaven, near the mouth of the estuary, up to > 3.5 m by Hamburg St. Pauli (see, e.g., Reese et al., 2024), it belongs to the group of mesotidal estuaries. The salt intrusion in the Elbe and thus the extent of the Elbe estuary usually ends near Lühort, near Elbe-km 60 in Fig 2.8a, while the tidal influence progresses further upstream, eventually limited by a weir in Geesthacht which marks the upstream end of the tidal Elbe (Boehlich and Strotmann, 2008). Stratification within the estuary varies between partially to well-mixed conditions depending on the tidal cycle, spring-neap cycle, and incoming freshwater discharge (Kappenberg and Fanger, 2007), which can range from $100 \text{ m}^3 \text{ s}^{-1}$ up to $> 4000 \text{ m}^3 \text{ s}^{-1}$, with a long-term average of $700 \text{ m}^3 \text{ s}^{-1}$ (Strotmann, 2015). In June 2013, an exceptional flooding occurred after intense rainfall in the southern regions of the Elbe catchment area (see, e.g., Grams et al., 2014). This resulted in the extreme discharge values of $> 4000 \text{ m}^3 \text{ s}^{-1}$, leading to a large amount of freshwater that entered the estuary. This freshwater was eventually exported to the German Bight, where it caused a significant increase in vertical density stratification (Kerimoglu et al., 2020, Chegini et al., 2020). Under the conditions studied within the present work, the Elbe estuary displayed varying degrees of vertical stratification, but no persistently vertically well-mixed salt distribution (cf. Reese et al., 2024, 2025). The vast majority of the freshwater discharge enters the tidal river through the weir in Geesthacht. Although numerous tributaries provide additional small, local freshwater sources throughout the entire length of the tidal river, they are of little importance for the overall estuarine mixing and exchange flow dynamics (Reese et al., 2024, see Fig. 2.8c for the average main and tributary discharge in 2012-2013).

The Elbe estuary is characterised by a channel-shoal geometry with a well-defined navigational channel (see Fig. 2.8a) that has been subject to major dredging activities since the 1930s (Boehlich and Strotmann, 2008) and that is surrounded by extensive tidal flats which are only flooded during high tide. The northeastern margin of the channel is adjacent to flat, permanently flooded shoals of up to 10 m depth, while the southwestern margin has a steep slope with no shoals (see Reese et al., 2025). Within the estuarine part of the river, and extending upstream to the city of Hamburg, the navigational channel has a largely uniform depth of 16 – 20 m that is constantly maintained by smaller dredging activities (Boehlich and Strotmann, 2008, see

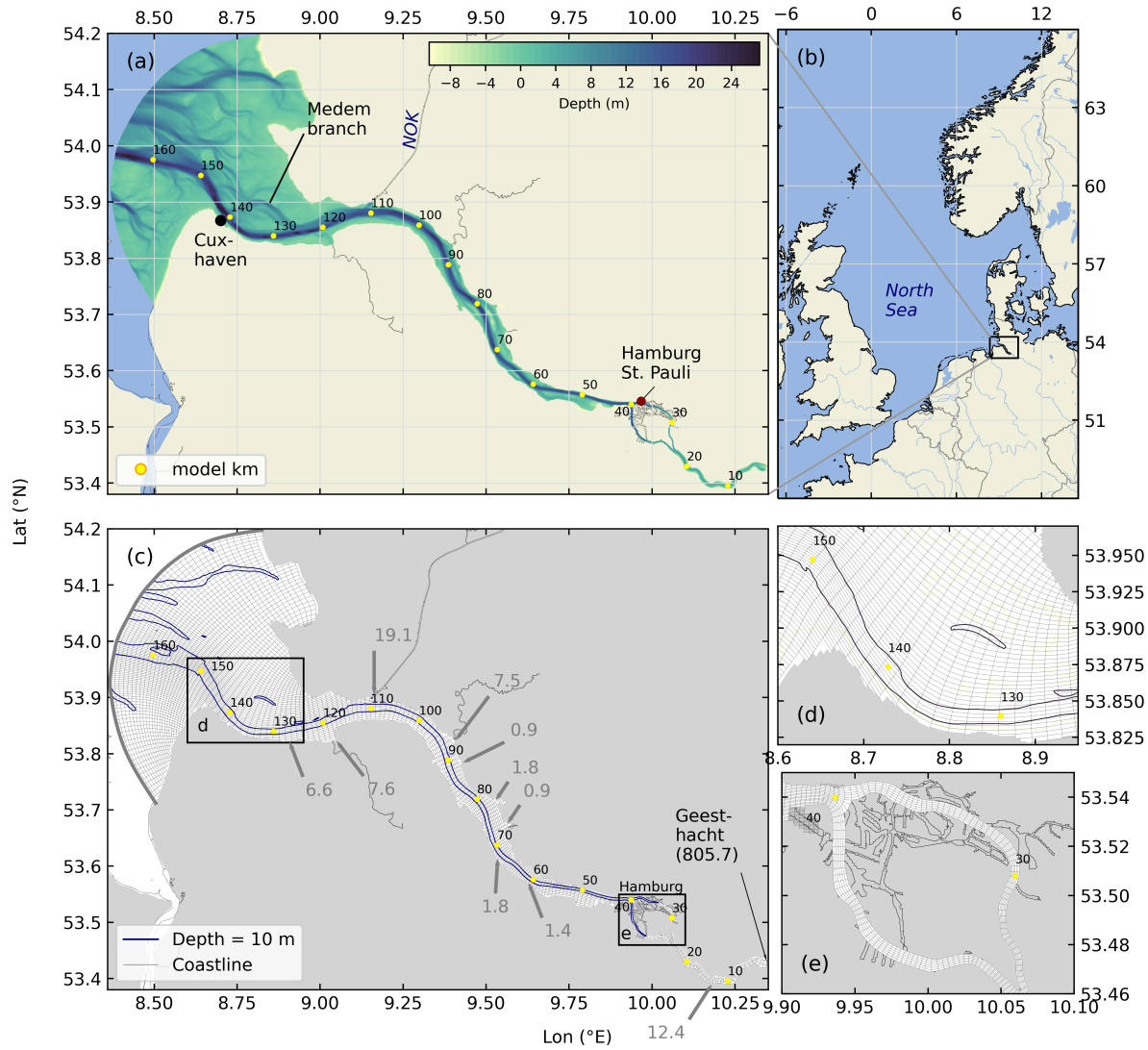


Figure 2.8: Model domain of the numerical tidal Elbe setup from Reese et al. (2024). (a) Setup topography showing the deep navigational channel, the city of Cuxhaven as well as the location of the Medem Branch and the gauge in Hamburg St. Pauli. Water outside of the model domain is coloured in light blue. The Kiel Canal is labelled “NOK”. (b) Location of the estuary at the North Sea shore. (c) Curvilinear grid used for the setup, with (d),(e) details from Cuxhaven and the City of Hamburg as indicated by the black rectangles. The bold grey line marks the open boundary of the setup. The main discharge into the estuary enters the model domain at Geesthacht, with the average discharge from August 2012 to December 2013 in parentheses (m^3/s). Grey arrows show the location of each tributary that is included in the setup, and their average discharge (m^3/s) for the same period as for Geesthacht. In (c) and (d), only every third grid line is shown. Yellow dots with numbers show the distance from the upstream end of the setup at cell centers between the 158th and 159th along-channel grid lines, here referred to as *model-km*. In (d), it can be seen that the complex channel system in the city of Hamburg is not covered by the model grid, which only includes the two main branches Norderelbe and Süderelbe. Figure taken from Reese et al. (2024), edited.

also Fig. 2.8a). As a result, the Elbe estuary shares its relatively simple channel-shoal geometry with many other medium-sized, tidal river estuaries that have been manipulated by humans for maritime traffic, such as the Hudson river estuary (see, e.g., Wang et al., 2017) or the Seine, Loire, and Weser estuaries (see, e.g., Grasso et al., 2025). This makes it a well-suited subject for the study of estuarine dynamics under realistic conditions: while its topography displays a local variability that would be missing in idealised setups, its overall shape is of a comparably simple nature, allowing to potentially generalise findings from the Elbe estuary also for similar estuaries as listed above. In particular, it has only one dominant freshwater source at the weir in Geesthacht (see previous paragraph) and consists, aside from the shallower Medem Branch near Cuxhaven (see Fig. 2.8a), of a single channel. Additionally, its recent past covers extreme events such as the previously mentioned 2013 flooding event, which can be of interest for the study of estuarine dynamics under unusual conditions. Yet, its mid-latitude location is associated with a moderate climate where surface fluxes such as precipitation and evaporation can be expected to be negligible compared to the incoming freshwater discharge, and where salinity clearly dominates the estuarine dynamics (see Burchard et al., 2004, Reese et al., 2024). For this reason, the Elbe was chosen as a suitable subject for the studies presented in this work.

2.2.2 Numerical Model

The setups used for the present work apply the hydrostatic kernel of the coastal ocean model GETM (General Estuarine Transport Model, Burchard and Bolding, 2002) in three-dimensional, realistic model runs. GETM provides a state-of-the-art drying and flooding algorithm which is well-suited for the tidal flats in the Elbe estuary as demonstrated previously by Burchard et al. (2004). It is a finite-volume model that works with baroclinic and barotropic mode splitting on structured C-grids, and its hydrostatic kernel includes the hydrostatic and Boussinesq assumption (Klingbeil and Burchard, 2013). GETM uses structured grids, which in the horizontal can be Cartesian or near-rectangular curvilinear. In the vertical, different coordinate types such as terrain-following sigma coordinates or adaptive coordinates that adjust to focus on stratified layers within the water column (Hofmeister et al., 2010) can be chosen.

For vertical turbulence closure, GETM was coupled to the General Ocean Turbulence Model (GOTM, Burchard et al., 1999, Li et al., 2021). This one-dimensional water column model was used here with a second-order algebraic closure (Canuto et al., 2001, Burchard and Bolding, 2001) of a k - ϵ two-equation model (Umlauf and Burchard, 2005). The horizontal eddy diffusivity and viscosity can be prescribed in GETM, e.g., as constant in space and time, or as a function of the local grid size (Smagorinsky eddy parameterisation, Smagorinsky, 1963). The latter is a convenient tool for curvilinear grids where the local grid size may vary strongly.

Using the method from Klingbeil et al. (2014), GETM allows for an output of the local mixing m_{xy} separated into a physical component $m_{xy,phy}$, based on real processes that are represented by the physical parameterisation of vertical turbulence in GOTM and of horizontal mixing in GETM, and a numerical component $m_{xy,num}$ related to truncation errors of the

Table 2.1: Differences between the coarser Elbe setup from Reese et al. (2024), Burchard et al. (2025) and the higher-resolved Elbe setup from Reese et al. (2025)

	Reese et al. (2024), Burchard et al. (2025)	Reese et al. (2025)
Simulation period	2012/02/01 – 2014/01/01	2024/01/01 – 2024/05/01
Analysis period	2012/08/01 – 2013/12/31	2024/04/16 – 2024/04/30
Horizontal grid (mean resolution)	616 × 305 (276 m along-channel; 151 m cross-channel)	2404 × 397 (80 m along-channel; 98 m cross-channel)
Vertical grid	30 sigma layers	40 adaptive coordinate layers (Hofmeister et al., 2010)
Main topography dataset	DGMW-z Elbe 2010 (Wasserstraßen- und Schifffahrtsamt Hamburg, 2011)	DGMW-z Elbe 2022 (Wasserstraßen- und Schifffahrtsamt Hamburg, 2024)
Initialisation and boundary forcing	600 m German Bight setup (Gräwe et al., 2015)	E.U. Copernicus Marine Service (2024)
Meteorological forcing	Operational Forecast Model ICON (Zängl et al., 2015) (≈ 7 km resolution)	MET Nordic operational archive (Norwegian Meteorological Institute, 2024) (≈ 1 km resolution)
Geesthacht discharge	Gauge Neu Darchau (Wasserstraßen- und Schifffahrtsamt Magdeburg, 2021)	Gauge Neu Darchau (Wasserstraßen- und Schifffahrtsamt Magdeburg, 2024) (multiplied by 1.3)
Discharge salinity	0 g/kg	0.5 g/kg
Tributaries included	yes	no
Horizontal eddy diffusivity	const. (20 m ² /s)	function of grid size (Smagorinsky, 1963)

numerical schemes used for the simulation (see also Burchard and Rennau, 2008):

$$m_{xy} = m_{xy,phy} + m_{xy,num} \cdot \quad (2.30)$$

As opposed to the strictly non-negative physical mixing, the second-order Superbee advection scheme applied in the present work (Mohammadi-Aragh et al., 2015) can lead to negative numerical mixing due to its tendency to amplify local gradients (see also Klingbeil et al., 2014).

For the analysis of mixing and exchange flow properties in salinity space, GETM uses salt bins of a prescribed, constant size ΔS , as described in detail in Burchard et al. (2021).

2.2.3 Numerical Setups

For the present work, two versions of a realistic numerical setup of the tidal Elbe were used that differ in their horizontal grid resolution, simulation period, and several other aspects as summarised in Table 2.1. The higher-resolved setup covering part of the year 2024 was derived from the original, coarser setup which covered the years 2012–2013. Both use a curvilinear grid that follows the thalweg of the navigational channel, as shown in Fig. 2.8c-e for the coarser setup from Reese et al. (2024). This allows for a convenient analysis of cross-channel transects along grid lines and the separation of along-channel and cross-channel velocity components, rather than needing to interpolate. It is further expected to reduce the numerical truncation error of the advection scheme as the grid lines follow the direction of the main current, thus reducing

the average number of grid cells that need to be crossed by a water parcel throughout a tidal cycle.

Both setup versions were further created to include a fully realistic topography and forcing. Due to the different simulation periods and the very active sediment dynamics that lead to fast changes of the estuarine topography (see Boehlich and Strotmann, 2008), different datasets had to be used for the coarse and higher-resolved setups, although the model domain shown in Fig. 2.8 for the coarse setup from Reese et al. (2024) remained almost identical. Most of the model domain for each setup version was covered by the 2010 (Wasserstraßen- und Schifffahrtsamt Hamburg, 2011) and 2022 (Wasserstraßen- und Schifffahrtsamt Hamburg, 2024) DGMW-z Elbe datasets, respectively. No major channel dredging was performed between the year of the datasets and the respective simulation periods. In the German Bight, some regions of the model domain had to be covered by interpolating additional datasets as listed in Reese et al. (2024) and Reese et al. (2025), respectively.

At the open boundary in the German Bight, realistic boundary forcing was prescribed from datasets as listed in Table 2.1. It included the sea surface elevation as well as vertical salinity and temperature profiles. The realistic meteorological forcing included precipitation, wind direction and magnitude 10 m above ground, dry air and dewpoint temperature 2 m above ground, as well as total cloud cover. Lastly, the freshwater discharge was prescribed at the upstream end of the model domain at Geesthacht. It consisted of daily averages from a gauge at Neu Darchau (see Table 2.1), which is located about 50 km upstream of Geesthacht. The coarse setup further included most of the small tributaries of the tidal Elbe (see Reese et al., 2024, for details and Fig. 2.8c for the location of the tributaries), but since their impact on the estuarine dynamics was found to be marginal in Reese et al. (2024), they were dropped in the high-resolution version.

Analyses in salinity space that required salinity binning were mainly performed with the setup from Reese et al. (2024), who used a bin size of $\Delta S = 0.2$ g/kg.

The calibration of the two setup versions varied with respect to the salinity: while in Reese et al. (2024), the originally too-high salt intrusion was countered by a high value of the constant horizontal eddy diffusivity $K_h = 20$ m²/s, Reese et al. (2025) multiplied the discharge intensity at Geesthacht by a constant factor of 1.3. For further details on the model calibration as well as for a validation of each setup, the reader is referred to Reese et al. (2024) and Reese et al. (2025), respectively.

Chapter 3

Key Results

3.1 Local Mixing Determines Spatial Structure of Diahaline Exchange Flow in a Mesotidal Estuary: A Study of Extreme Runoff Conditions

In general, the estuarine circulation and salt mixing are dependent on external forcing. A particularly important factor is the incoming freshwater discharge Q_r as has been explained in detail in Section 2.1.3. In theory, the estuarine circulation and mixing will adjust to a changing freshwater discharge until a new balance is established. However, as real estuaries may experience a high natural variability of forcing conditions, the system response time to adjust to changes might exceed the time scale of the variability. Then, no balance between discharge, exchange flow, and mixing would occur. To assess how closely all three aspects are linked to each other in a realistic mesotidal estuary, Reese et al. (2024) tested the validity of the mixing estimates (2.22) (MacCready et al., 2018) and (2.23) (Burchard, 2020) under highly variable and extreme discharge conditions. As explained in Section 2.1.3, these estimates rely on the assumption of long-term averaged conditions, meaning that storage effects within an estuary should vanish for the suggested averaging time such that a balance between mixing, circulation, and discharge is present. A convergence of the directly computed mixing and the mixing estimates would therefore reveal the time scales on which estuarine mixing adapts to changing freshwater forcing. If these time scales are sufficiently short to resolve extreme events, these estimates would further provide a convenient tool for an easy assessment of estuarine mixing under changing and even extreme discharge conditions.

Similarly to the mixing relations (2.22) and (2.23), the relation (2.27) presented by Klingbeil and Henell (2023) attests a theoretically close interdependence of estuarine mixing and the diahaline transport of water. Yet, as this relation neglects horizontal diffusion as mentioned in Section 2.1.4, further proof of its validity for realistic tidal estuaries is required. Additionally, the spatial pattern of the diahaline exchange flow within such estuaries had been still unknown at the timing of the publication.

In their study, Reese et al. (2024) considered two cases of extreme freshwater discharge for the example of the Elbe estuary: the exceptional high-discharge event from the month of June 2013 (Fig. 3.1b; see also Section 2.2), with a freshwater runoff that was characterized by a fast and strong increase of total discharge from about $1100 \text{ m}^3\text{s}^{-1}$ to about $4100 \text{ m}^3\text{s}^{-1}$ within less than two weeks and a subsequent, slower return to average conditions, and the dryer-than-average summer month of September 2012 (Fig. 3.1a) with consistently low discharge conditions of about $300 \text{ m}^3\text{s}^{-1}$ throughout the entire month. They further considered the

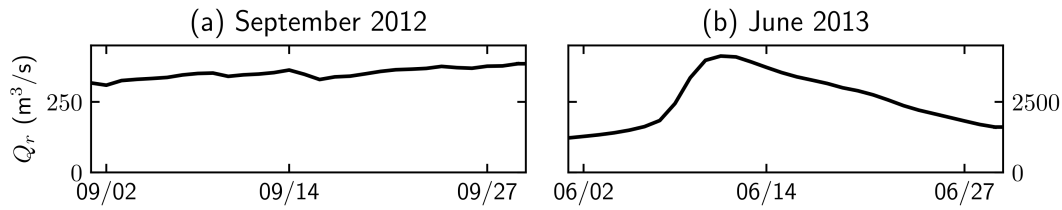


Figure 3.1: Time series of the daily averaged freshwater discharge $Q_r(t)$ in the Elbe estuary during (a) a low-discharge period in September 2012 and (b) an event of extremely high discharge in June 2013. Note that the y-axis in panel (b) is scaled by a factor of 10 compared to panel (a). Figure adapted from Reese et al. (2024).

sensitivity of mixing to changes of freshwater discharge throughout the entire study period from August 2012 to December 2013, and for the first time illustrated the spatial distribution of the diahaline exchange flow and its relation to the local mixing distribution for a tidal estuary. The study was based on model output from the lower resolved Elbe setup presented in Section 2.2.

3.1.1 General Conditions Within the Elbe Estuary

To put their findings into the context of the general estuarine conditions at the timing of the extreme discharge periods, Reese et al. (2024) first assessed the salinity distribution and Total Exchange Flow within the estuary.

As one would expect, the extreme discharge event from June 2013 lead to a considerable freshening of the Elbe estuary, while the low discharge from September 2012 resulted in reduced vertical stratification and a saltwater inflow reaching 30 km further upstream than in June 2013 (see Fig. 3.2). Regardless of the freshwater discharge intensity, the Total Exchange Flow $q(x, S)$ (see eq. (2.10)) within the Elbe estuary consisted of two layers – a salty inflow layer and a brackish outflow layer (see Fig. 3.3a,b). During the high-discharge event, the exchange flow was shifted in downstream direction due to the reduced salt intrusion length. In accordance with the increased stratification due to a higher freshwater input, the difference between the inflow and outflow layer salinities S_{in} , S_{out} was higher during high discharge than during low discharge (Fig. 3.3a,b).

3.1.2 Mixing Relations Under Varying Discharge Conditions

Reese et al. (2024) found that the volume-integrated mixing $M_T(x)$ within the estuarine volume upstream of a given transect at any along-channel position x can be reproduced by the MacCready et al. (2018) estimate (2.22) within an error margin of about 10 % when using a monthly average for both the low-discharge case of September 2012 and the high-discharge case of June 2013 (Fig. 3.4). This illustrates the close relation between the freshwater discharge and estuarine mixing, even under extreme conditions of fast change.

Further, the directly computed mixing per salinity class $m(S)$ was compared to the universal law of estuarine mixing (2.24) (Burchard, 2020) for three different choices of averaging periods:

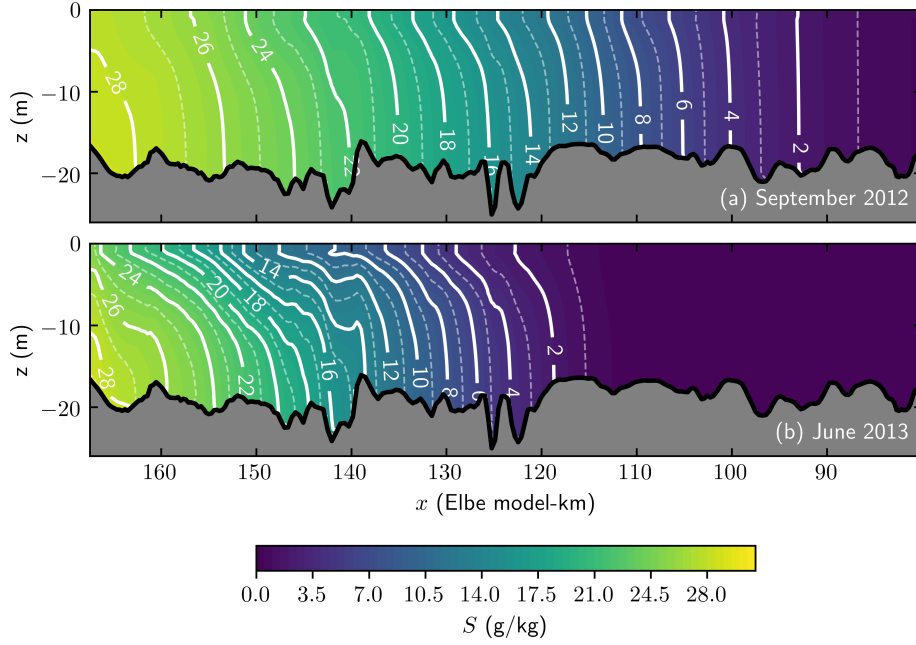


Figure 3.2: Distribution of the salinity S along the thalweg of the Elbe navigational channel, averaged for two spring-neap cycles during (a) the low discharge month of September 2012 and (b) the high discharge month of June 2013. The white lines indicate the salinity in steps of 1 g/kg, where dashed lines represent odd numbers. The bold black line and grey shading show the bottom topography. For the Elbe model-km locations, see Fig. 2.8. Figure adapted from Reese et al. (2024).

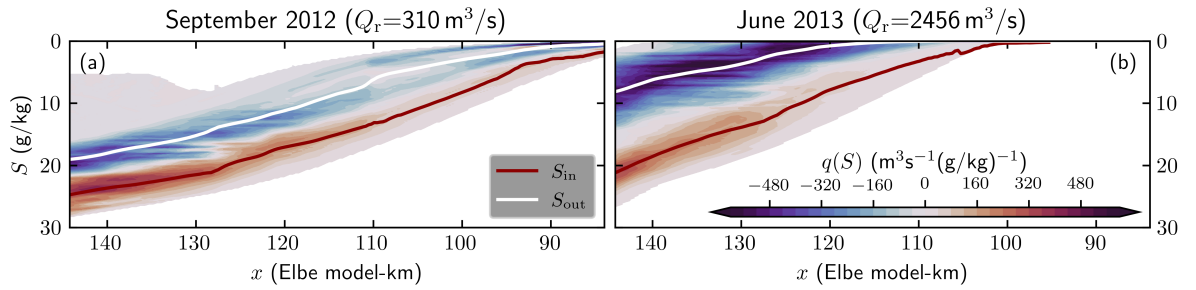


Figure 3.3: Volume transport per salinity class $q(x, S)$ from the Total Exchange Flow framework in the Elbe estuary, averaged for two spring-neap cycles during (a) a low discharge period in September 2012 and (b) an extreme high discharge period in June 2013, respectively, vs. along-channel position x and salinity class S . In the title of each panel, the average discharge Q_r of each month is given in brackets. The red and white lines indicate the TEF inflow and outflow salinities, $S_{in}(x)$ and $S_{out}(x)$. Figure adapted from Reese et al. (2024).

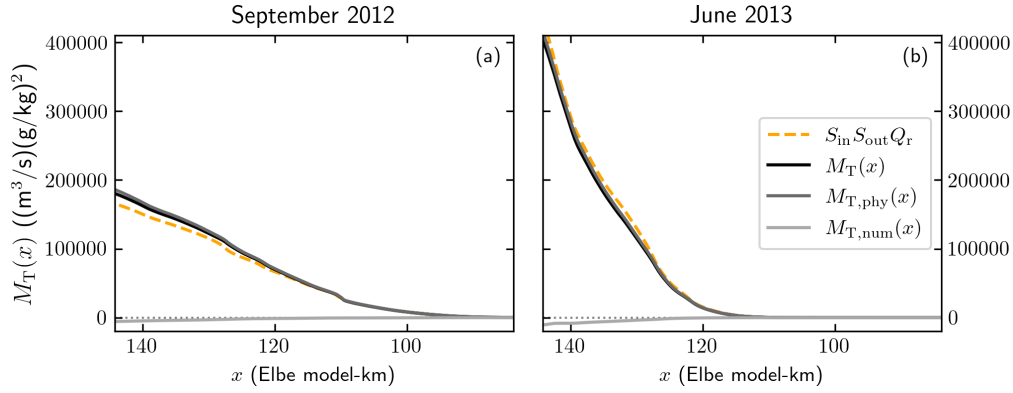


Figure 3.4: Mixing $M_T(x)$ (2.18) in the Elbe estuary within the estuarine volume bounded by a cross-channel transect at along-channel position x , averaged over two spring-neap cycles, respectively. The mixing is decomposed into numerical and physical mixing analogous to eq. (2.30). The dashed orange line indicates mixing as predicted by the estimate (2.22) from MacCready et al. (2018). Figure adapted from Reese et al. (2024).

two cycles of the dominant, semidiurnal M_2 tide (i.e., 24 hours), as well as one and two spring-neap cycles (i.e., two weeks and four weeks, respectively). Averaging periods of more than two M_2 tidal cycles that are not a multiple of the spring-neap period were considered unsuited for as they would inevitably introduce a bias caused by the incomplete spring-neap cycle. The results showed an increasing convergence of the directly computed mixing and the universal law with increasing averaging durations. Here, only the example of the longest averaging period of two spring-neap cycles is shown in Fig. 3.5. For the shorter averaging durations, the reader is referred to Reese et al. (2024). It was found that an averaging period of one to two spring-neap cycles was sufficient to reproduce the universal law while still properly resolving the increased mixing during the high discharge event in June 2013 due to intense freshwater input, as well as the reduced mixing during the low discharge period due to reduced freshwater input.

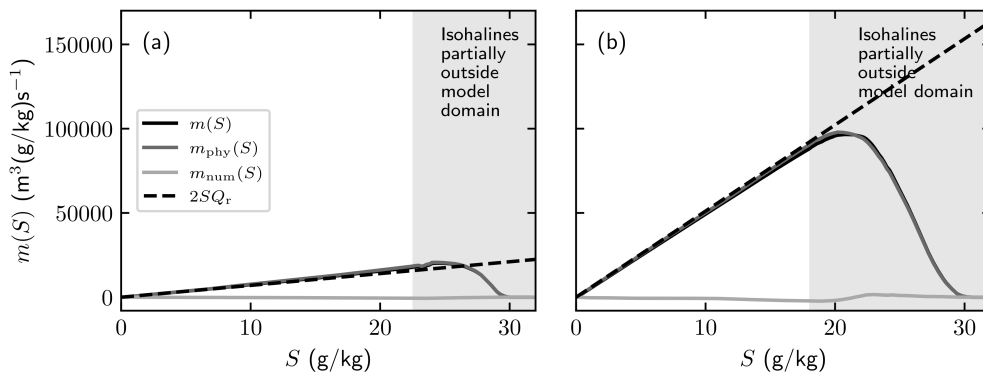


Figure 3.5: Performance of the universal law (2.24) in the Elbe estuary in (a) September 2012 and (b) June 2013 after an averaging period of two spring-neap cycles each. Bold lines show the simulated mixing per salinity class $m(S)$ as computed for the entire model domain of the tidal Elbe setup, dashed lines show the mixing as estimated from the universal law. Further, the physical (m_{phy}) and numerical (m_{num}) contributions to the total simulated mixing are depicted. The grey-shaded areas indicate salinities at which the isohalines partially left the model domain so that the universal law is no longer applicable to the model output. Figure taken from Reese et al. (2024).

Using an averaging period of only a single M_2 cycle, it was further shown that mixing in the Elbe estuary is greatly dominated by the freshwater discharge as predicted by the universal law (2.24) – even though a full convergence, as previously seen in Fig. 3.5, is not achieved for this shorter averaging period due to the influence of salt and volume fluctuations (i.e., storage). Yet, high-frequency variations of the wind as well as the spring-neap cycle had only a short-term, modifying impact on the instantly simulated mixing: fluctuations in discharge throughout the interval from August 2012 to December 2013 resulted in a considerably greater amplitude of mixing variability. This is shown for the 13 g/kg-isohaline in Fig. 3.6. A more thorough temporal analysis for the full salinity range of the Elbe estuary can be found in Reese et al. (2024). Their findings stand in contrast to many studies that solely focus on the impact of the spring-neap cycle on estuarine mixing, often using a constant discharge value as forcing (e.g., Wang et al., 2017, Li et al., 2022). Instead, the results agree well with the study by Broatch and MacCready (2022) performed on a realistic simulation of the Salish Sea, where a dominant influence of the freshwater discharge on the estuarine mixing intensity was identified. Adding to their findings, Reese et al. (2024) could clearly show that freshwater discharge from extreme events is no exception to this, and that such extreme events can be resolved and quantified with mixing estimates if the averaging period is chosen adequately.

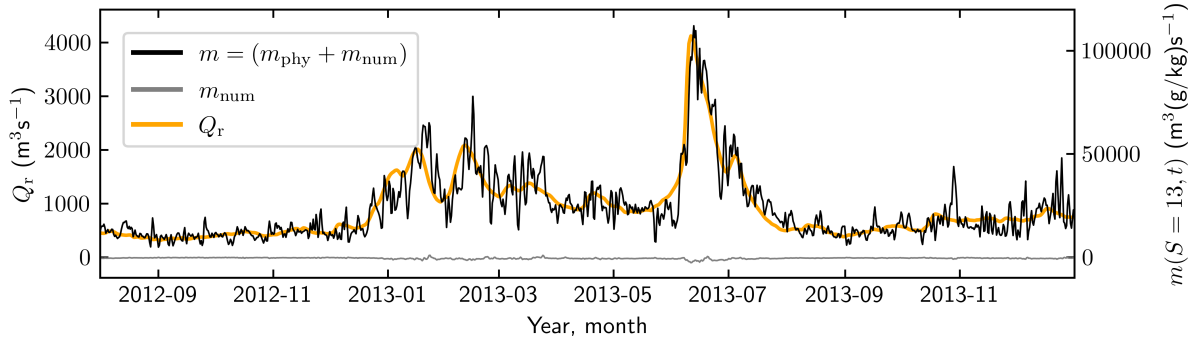


Figure 3.6: Time series of the M_2 -averaged mixing per salinity class, $m(S, t)$ (2.20), inside the Elbe estuary from August 2012 to December 2013 for a selected salinity class $S = 13$ g/kg. The figure shows the total mixing $m = m_{\text{phy}} + m_{\text{num}}$ and the numerical mixing m_{num} compared to the freshwater discharge $Q_r(t)$. The axis limits for the freshwater discharge were chosen to fit those of the mixing axis as given by the universal law (2.24), meaning that the discharge and mixing lines should align if mixing follows the universal law. Figure adapted from Reese et al. (2024).

Lastly, numerical mixing was low, as can be seen in Figs 3.4, 3.5, and 3.6. This was attributed to the thalweg-following curvilinear grid as explained in Section 2.2.3 as well as the high horizontal diffusivity of the setup that reduced gradients which would otherwise be acted on by numerical mixing. A control run with a strongly reduced horizontal diffusivity $K_h = 10^{-3} \text{ m}^2/\text{s}$ yielded qualitatively identical results for all key findings.

3.1.3 Relation Between Local Mixing and Diahaline Circulation

Lastly, while freshwater discharge impacts the mixing integrated over the estuarine volume or over the surfaces of single isohalines by providing a source of salinity variance required for

the mixing, it is local processes that define where in the estuary the mixing takes place: they interact with the local isohaline structure and consequently the local stratification as well as provide turbulence for the mixing to take place. Using the relation (2.27) derived by Klingbeil and Henell (2023), Reese et al. (2024) could show for the first time for a realistic tidal estuary that this local structure of estuarine mixing determines the structure of the diahaline exchange flow. As shown for the $S = 13$ g/kg isohaline in Fig. 3.7a for June 2013 (high discharge event), local mixing is most intense along steep topography, in particular at the shoals of the Elbe navigational channel. A similar pattern can be seen for the diahaline exchange flow (Fig. 3.7c), which has a well-defined two-layer structure with upstream inflow and downstream outflow of water across the isohaline surface, and hotspots in the same locations as mixing. If using the equation (2.27) from Klingbeil and Henell (2023) to compute $u_{\text{dia},z}^S$, the result (Fig. 3.7b) is almost identical to the direct computation (Fig. 3.7c), with the exception of a small amount of noise. In detail, a high spatial Pearson correlation between the distribution from equation (2.27) and the directly computed $u_{\text{dia},z}^S$ at $R^2 = 0.69$ (June 2013) and $R^2 = 0.76$ (September 2012; not shown) was found, demonstrating that horizontal diffusion can be neglected in the tidal Elbe even under realistic and extreme conditions.

The results for the low discharge period in September 2012 were qualitatively identical, but restricted to a smaller area per salinity class, since the estuary was more well-mixed and isohaline surfaces therefore smaller (not shown here; the reader is referred to Reese et al., 2024).

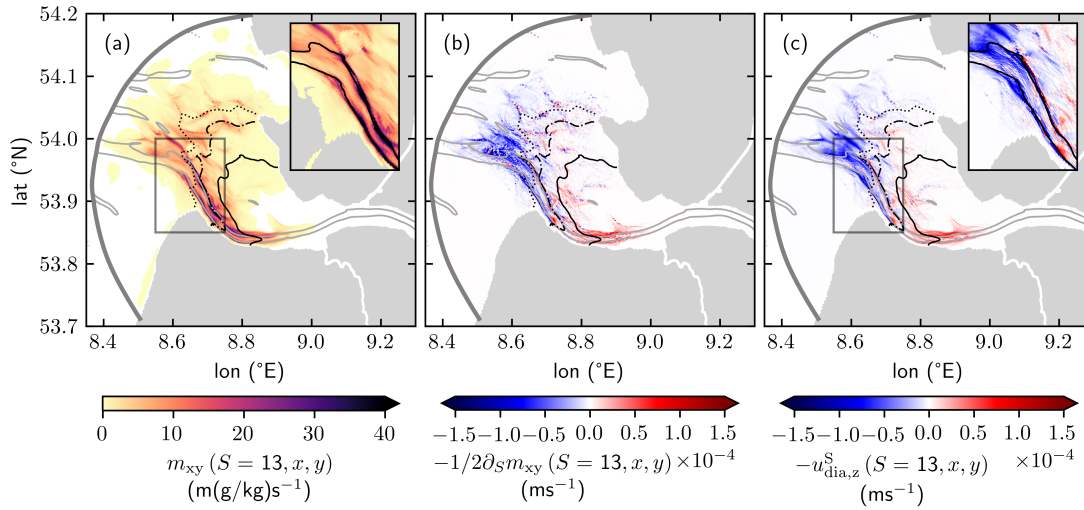


Figure 3.7: Local mixing and diahaline velocity in the Elbe estuary, shown for the isohaline surface at $S = 13$ g/kg and averaged over two spring-neap cycles in the high discharge month of June 2013. (a) Local mixing $m_{xy}(x, y)$ (2.21); (b) negative effective vertical diahaline velocity $-u_{\text{dia},z}^S(x, y)$ computed according to Klingbeil and Henell (2023) from the S -gradient of the local mixing as given in eq. (2.27); (c) $-u_{\text{dia},z}^S(x, y)$ as computed online with GETM. The negative sign for the diahaline velocity was chosen to depict the direction of the water transport, such that red shading implies an inflow into the estuary and blue shading implies an outflow toward the sea. Additionally, the 12 m-isobath (grey; black in the insets in a and c) as well as the mean isohaline height 20 % (solid black), 50 % (dash-dotted), and 80 % (dotted) above ground, normalised by the local mean water depth, are shown. Figure adapted from Reese et al. (2024).

3.2 The Relation Between Exchange Flow and Diahaline Mixing in Estuaries

In Reese et al. (2024), as summarised in Section 3.1.3, a key finding was the close relation of the diahaline exchange flow and local mixing, which was demonstrated to hold under realistic, even extreme conditions in a tidal estuary. Additionally, the structure of the diahaline exchange flow on an isohaline surface was found to consist of two well-defined layers. As a next step, it stands to reason that these results could be expanded by connecting the estuarine exchange flow to the diahaline exchange flow. This way, a quantitative, exact relation between the local mixing on an isohaline surface and the Total Exchange Flow intensity across a given vertical, cross-estuary transect could be provided. It was therefore the aim of the study by Burchard et al. (2025) to derive and validate such a relation for realistic estuaries.

3.2.1 Mixing–Total Exchange Flow Relation

The relation derived within the scope of this study can be retrieved directly from assumptions of volume conservation. For this purpose, let us consider a vertical, cross-estuary transect at along-channel position $x = x_0$ as shown in Fig. 3.8. In an estuary with a two-layer exchange flow, it is possible to identify a dividing isohaline surface $S_{\text{div}}(x)$ that separates the salty, usually near-bottom inflow from the brackish, near-surface outflow (MacCready, 2011, Lorenz et al., 2019). Assuming long-term averaged conditions where storage effects vanish, the Knudsen (1900) relations (2.8) are valid; i.e., from (2.6):

$$Q_{\text{out}} = -Q_{\text{in}} - Q_r. \quad (3.1)$$

Consequently, as apparent from Fig. 3.8, the volume transport $Q_{\text{dia,est}}(S_{\text{div}}(x))$ across the up-estuary section ($x > x_0$) of the dividing isohaline surface must equal the saltwater inflow $Q_{\text{in}}(x)$ across the transect:

$$Q_{\text{dia,est}} = Q_{\text{in}}, \quad (3.2)$$

where

$$Q_{\text{dia,est}} = \int_{A_{\text{est}}(S_{\text{div}})} \langle u_{\text{dia}}^z \rangle dA = \int_{A_{z,\text{est}}(S_{\text{div}})} \langle u_{\text{dia},z}^S \rangle dA_z. \quad (3.3)$$

Here, $A_{\text{est}}(S_{\text{div}}(x))$ is the area of the isohaline surface that is located on the up-estuary side ($x > x_0$) of the cross-channel transect at $x = x_0$, and $A_{z,\text{est}}(S_{\text{div}}(x))$ is its horizontal projection. The combination of equations (3.2) and (3.3) with relation (2.27) introduced in Section 2.1.4 and validated for the Elbe by Reese et al. (2024) then yields a direct, quantitative relation between the Total Exchange Flow, quantified here as Q_{in} (Broatch and MacCready, 2022, MacCready and Geyer, 2024), and the integrated mixing on the up-estuary section of the

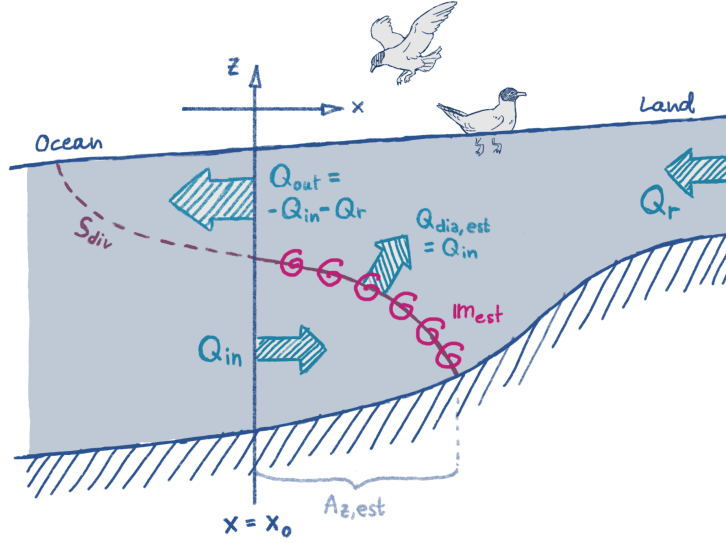


Figure 3.8: Schematic of an idealised estuarine cross-section, assuming long-term averaged conditions where salt and volume storage vanish and the Knudsen relations (2.8) are valid. The light blue arrows represent volume transports such as the bulk volume inflow Q_{in} and outflow Q_{out} across a vertical transect at $x = x_0$ which are separated by the dividing isohaline S_{div} , across which the inflowing diahaline volume transport $Q_{dia,est}$ occurs as a result of the surface-integrated mixing $m_{est}(S_{div})$ which takes place on the estuarine side of the transect, i.e., where $x > x_0$. From the land, a freshwater inflow Q_r enters the estuary. Additionally, the horizontal projection of the estuarine side of the dividing isohaline surface area, $A_{z,est}$, is shown.

dividing isohaline surface, m_{est} :

$$Q_{in}(x) = -\frac{1}{2} \frac{\partial m_{est}(S_{div}(x))}{\partial S}, \quad (3.4)$$

where

$$m_{est} = \int_{A_{z,est}(S_{div})} m_{xy} dA_z. \quad (3.5)$$

As introduced in eq. (2.21), the local mixing m_{xy} is a function of the salinity S . Relation (3.4) is exact within the bounds of accuracy of relation (2.27), meaning it only neglects horizontal diffusion and surface fluxes, which were found to be of little importance for the example of the Elbe estuary in Reese et al. (2024). A mathematically more thorough derivation of this relation, including the consideration of volume storage under conditions of insufficient averaging, can be found in Burchard et al. (2025).

It should be noted that relation (3.4) and its surrounding theory require a consistent use of isotracer coordinates (here: salinity) for both the mixing (see Klingbeil and Henell, 2023) and the exchange flow definition (TEF, see MacCready, 2011). Eulerian coordinates such as z -coordinates cannot be used for such a consistent mixing and exchange flow definition and cannot link mixing and exchange flow (cf. MacCready, 2011, Burchard et al., 2018). Hence, they do not satisfy (3.4).

3.2.2 Case 1: 2-Layer Exchange Flow in a Tidal Estuary

In Burchard et al. (2025), data from the same numerical Elbe simulation as presented and validated in Reese et al. (2024) was used. Again, the low (September 2012) and extremely high (June 2013) discharge months were considered with averaging times of two spring-neap cycles. As already shown by Reese et al. (2024), the Elbe estuary displays a classical 2-layer exchange flow in both months (see also Fig. 3.9c,d for a selected transect near Cuxhaven).

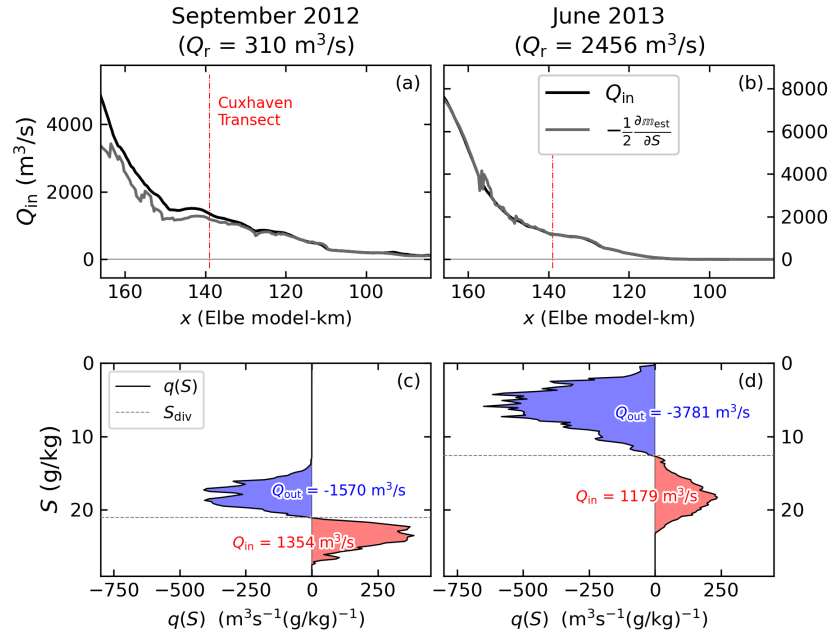


Figure 3.9: Mixing and exchange flow results for the Elbe estuary for low (September 2012, left) and high (July 2013, right) discharge situations, averaged over two spring-neap cycles, respectively. The average discharge Q_r for each month is given in the column titles. (a), (b): Left-hand side (black) and right-hand side (grey) of the exchange flow – mixing relation, (3.4), computed for cross-sections at position x along the Elbe estuary. The dashed red line indicates a cross-channel transect near Cuxhaven. (c), (d): Total Exchange Flow $q(S)$ across the Cuxhaven transect. The bulk inflow Q_{in} (red) and outflow Q_{out} (blue) intensity is indicated by the shaded areas as well as their respective numerical values. Further, the dividing salinity S_{div} is marked by a thin dashed line. Figure adapted from Burchard et al. (2025).

An evaluation of the key relation (3.4) for cross-channel transects along the full length of the estuary revealed that mixing and exchange flow were in balance along the entire estuary for the high discharge case (Fig. 3.9b) and almost in balance for low discharge, where a small contribution of a storage term was necessary to close the budget (Fig. 3.9a; for the inclusion of storage, the reader is referred to Fig. 3 from Burchard et al., 2025). This illustrates that the relation (3.4) can be a suitable analysis tool for a realistic tidal estuary under variable discharge conditions. Further, on the dividing isohaline S_{div} of the selected transect near Cuxhaven, shoal-enhanced mixing as in Reese et al. (2024) became apparent (not shown). This mixing, again, was directly linked to a two-layer diahaline exchange flow (analogous to that in Fig. 3.7) that was apparently separated into the respective inflow and outflow layers by the vertical transect (not shown; see Fig. 3 from Burchard et al., 2025). This division originates from the fact that inflow across the vertical transect occurs, by definition, mainly at salinities higher

than S_{div} , such that upstream of the transect, an inflow across S_{div} towards lower salinities must occur to close the budget and to allow for the outflow across the transect at salinities lower than S_{div} (see also Fig. 3.8).

3.2.3 Case 2: 3-Layer Exchange Flow in a Nontidal Estuary

Not all estuaries display a two-layer exchange flow. An example is the nontidal, northeast German Warnow estuary, which is located at the Baltic Sea coast. Its circulation is highly impacted by local wind forcing (Lange and Burchard, 2019). Further, the Baltic Sea salinity by the mouth of the estuary can change quickly in response to wind-driven upwelling or downwelling conditions, such that at times the estuary is saltier than the adjacent sea, which results in an inverted circulation. These aspects result in a highly variable estuarine circulation of the Warnow, and its long-term average has a three-layer pattern as shown and discussed in Burchard et al. (2025). Using similar assumptions as for the two-layer case, it is possible to expand the theory for n -layer estuaries, where consequently $n - 1$ dividing isohalines occur. For the three-layer Warnow, a respective pair of equations covering the high- and low-salinity dividing isohalines was derived in Burchard et al. (2025) and validated for the one-year averaged circulation across a transect by the river mouth (not shown). Similarly to the Elbe estuary, local mixing hotspots were found at the channel-shoal transition of the navigational channel and other locations of sloping topography (not shown).

Analogously to the two-layer case, additional storage terms could theoretically be derived also for multi-layer cases. Further, multi-entrance systems such as the Baltic Sea (see Henell et al., 2023, for a diahaline transport and mixing study of the Baltic Sea) would require TEF profiles across each opening which could then be added together for a single representative profile, which would likely result in a complex multi-layer case as mentioned above.

3.2.4 Implications of the Mixing–Total Exchange Flow Relation

The most important implication from Burchard et al. (2025) is that, under sufficiently long temporal averaging such that relation (3.4) is valid, mixing and the estuarine exchange flow are *in balance*. This contrasts the classical belief of a one-way relation according to which the exchange flow is a result of mixing (see MacCready et al., 2018). To some degree, this is already evident in the MacCready et al. (2018) relation (2.22). Yet, in contrast to (3.4), that relation is only an estimate and does not establish an unambiguous link between mixing and exchange flow as it contains the bulk inflow and outflow salinity S_{in} , S_{out} as additional variables.

Additionally, a guideline for the study of estuarine exchange flow dynamics was provided: by applying (3.4) to a numerical simulation that has been validated with observations to ensure a sufficient reproduction of real conditions, hotspot regions of mixing directly associated with the exchange flow can be identified and further studied to make out key processes of water

mass transformation. Such processes can then be further studied with numerical simulations, but could also motivate observational campaigns focussing on the identified key locations.

Lastly, the theory introduced by Burchard et al. (2025) uses time averaging and thus reproduces the average rather than the instantaneous conditions within an estuary; especially with respect to the residual circulation which usually only becomes apparent after tidal averaging. The shorter the averaging period, the larger the contributions from the storage term(s) will be. Nonetheless, Burchard et al. (2025) argue that it is generally possible to apply the theory to the study of selected conditions wherever sufficient temporal averaging is possible, such as certain discharge periods, neap, or spring tide. Still, the average dynamics are naturally the result of instantaneous dynamics, e.g., throughout a single tidal cycle, which need to be studied to fully understand the mechanisms of the Total Exchange Flow.

3.3 The Role of the Shoal – Salt Mixing Mechanisms in a Partially Mixed Tidal Estuary With Channel-shoal Geometry

As shown by Reese et al. (2024), the freshwater discharge into a partially mixed tidal estuary provides a source of salinity variance that the estuarine system can adapt to quickly through an adjusted mixing intensity. The processes leading to the adjusted mixing as predicted by the universal law (2.24) were traced to shoal-enhanced mixing, which, in turn, is of great importance for the estuarine exchange flow itself (Reese et al., 2024, Burchard et al., 2025). Within the final study of this thesis, Reese et al. (2025) therefore aimed to identify the exact mechanisms behind this shoal-enhanced mixing down to local scales on a tidal level to provide an understanding of the full chain of relations from local mixing to the estuary-wide residual circulation.

To this end, the higher-resolved version of the numerical Elbe setup as presented in Section 2.2.3 was validated with respect to an observational time series of near-shoal circulation and mixing processes from the outer Elbe estuary. For this process-oriented validation, the reader is referred to Reese et al. (2025). Next, regions and periods of elevated mixing were identified to be analysed for the underlying processes throughout a single M_2 tidal cycle. The analysis period consisted of a single spring-neap cycle from 16th to 30th April 2024 during which the freshwater discharge was nearly constant.

3.3.1 Elevated Mixing in Time

Within the selected analysis period from Reese et al. (2025), no correlation was found between the mixing and near-constant freshwater discharge (not shown). Instead, strongest mixing coincided with the maximum of stratification at neap, i.e., at the timing of a generally reduced tidal amplitude (see Fig. 3.10b-d). In detail, the M_2 tidal cycle of strongest mixing was found to occur on the 17th to 18th of April. Such a timing of maximum mixing stands in contrast to the common notion that in partially mixed estuaries, most intense mixing occurs at the transition

from neap to spring, when the increased stratification from neap (i.e., $\partial_z S$) is combined with increasing tidal energy (i.e., higher K_v ; see, e.g., Wang et al., 2017, Li et al., 2018). This discrepancy could be explained by two aspects: first, a downwelling favourable wind event from westerly directions prematurely reduced the stratification within the estuary toward the end of neap (cf. Chen and Sanford, 2009, Lange and Burchard, 2019, for the destratifying tendencies of downwelling wind conditions), after which no further excess stratification could be created because the tidal energy was already too high (see Fig. 3.10a-c). Second, within the selected analysis period, neap tide coincided with a high diurnal asymmetry of the tidal amplitude (see Fig. 3.10b). This allowed for strong mixing already at neap tide whenever a diurnal maximum of the tidal amplitude (i.e., a higher K_v than would otherwise be available at neap) coincided with an M_2 ebb tide.

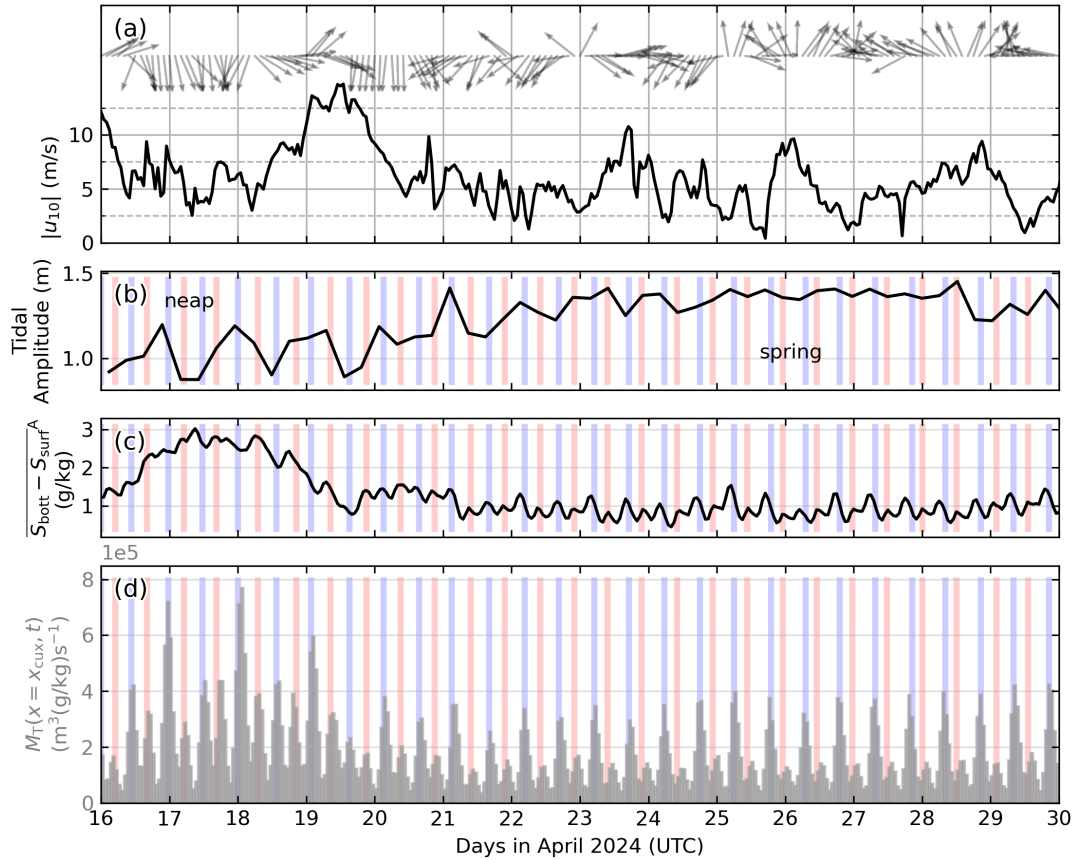


Figure 3.10: Simulated time series of salt mixing and related properties from the Elbe estuary throughout a full spring-neap cycle on 16th-30th April 2024. (a) Direction (arrows pointing in the direction in which the wind is blowing) and magnitude $|u_{10}(t)|$ (black line) of the wind 10 m above the surface; (b) tidal amplitude near Cuxhaven, computed as the difference between adjacent high and low tide water levels and vice versa; (c) area-averaged stratification $\bar{S}_{\text{bott}} - \bar{S}_{\text{surf}}^A(t)$ within the estuarine area $A(t)$ where the vertically averaged salinity $\bar{S}(x, y, t)$ is within the bounds $0.6 \text{ g/kg} \leq \bar{S} \leq 15 \text{ g/kg}$. $\bar{S}_{\text{bott}} - \bar{S}_{\text{surf}}$ is the difference between the salinity in the bottom and surface sigma layers of each horizontal model grid cell; (d) hourly averaged, volume-integrated mixing $M_T(x_{\text{cux}}, t)$ (2.18) within the estuarine volume $V_T(x_{\text{cux}}, t)$ bounded by a transect at an along-channel position x_{cux} near Cuxhaven. In (b)-(d), the vertical blue and red lines correspond to the timing of peak ebb and peak flood, respectively, defined as the timing of the highest vertically averaged ebb and flood current within a tidal cycle near Cuxhaven. Figure adapted from Reese et al. (2025).

With respect to the semidiurnal M_2 tidal cycle, mixing outside of neap clearly followed the timing of increased stratification, with a maximum at peak ebb and a secondary maximum at peak flood (see Fig. 3.10c,d), as also known from, e.g., Warner et al. (2020). At peak ebb and flood, the tidal energy and thus K_v are highest. Minima of stratification and mixing occurred at slack tides, where K_v is small due to the small tidal velocity.

3.3.2 Elevated Mixing in Space

Similar to the findings from Reese et al. (2024) and Burchard et al. (2025) on a single isohaline surface, also the integrated mixing per each horizontal grid cell of the Elbe setup was found to be intensified at the channel-shoal transition of the navigational channel (not shown). This tendency is even stronger at neap tide, as can be seen from Fig. 3.11: while mixing at the channel-shoal transition is stronger at neap tide than at spring tide, mixing within the channel itself is reduced, leading to an intensified overall contrast between channel and near-shoal mixing. The reason for the intensified shoal mixing at neap is the stabilising effect that increased stratification has on the water column within the channel such that channel mixing is suppressed. At the channel-shoal transition, on the other hand, the near-shoal mixing mechanisms as described in the following section become stronger with increasing stratification.

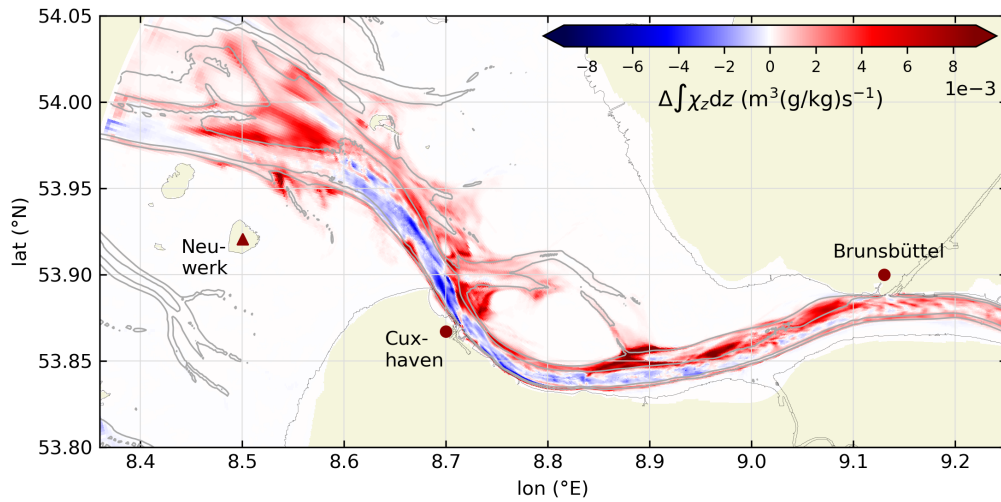


Figure 3.11: Difference between the simulated, vertically integrated local mixing $\int \chi_z dz$ in the Elbe estuary at the timing of maximum mixing as identified in Section 3.3.1 (neap tide; averaged from 17th April 12:00h UTC to 18th April 12:00h UTC) and $\int \chi_z dz$ at spring tide (averaged from 26th April 00:00h UTC to 27th April 00:00h UTC). Red shading means stronger mixing at neap, blue shading means stronger mixing at spring. Bold grey lines indicate the 12 m- and 6 m-isobaths. Figure adapted from Reese et al. (2025).

3.3.3 Mechanisms of Shoal-enhanced Mixing Throughout a Tidal Cycle

Analysing snapshots of different estuarine parameters such as mixing, vertical shear, and along- and cross-channel velocities (not shown) in conjunction with distribution maps of the terms of

the dynamic equation (2.28) for the vertical salinity variance from Li et al. (2018) throughout the M_2 tidal cycle (Fig. 3.12 and 3.13), Reese et al. (2025) identified two main mechanisms of near-shoal mixing in the Elbe estuary:

Mechanism 1 requires flat, channel adjacent shoals as shown on the right-hand side of the schematic cross-section in Fig. 3.14. During flood, differential advection drives a lateral current up the shoal as explained in Section 2.1.1. This leads to the formation of a salty bottom plume above the shoal as evident by the positive lateral straining $B_y > 0$ at the northern channel-shoal transition in the Elbe and the positive advection term $A > 0$ above the flat northern shoals themselves (Fig. 3.12a,d). Shear at the interface between the bottom plume and the fresher surface layer results in increased mixing, which during flood can reach into the navigational channel as well (see right-hand side of the cross-section in Fig. 3.14a). At slack, the isohaline structure becomes horizontally homogeneous (not shown). During ebb, incoming freshwater predominantly in the surface layer and above the shoal reinstates the plume shape as depicted in Fig. 3.14b. Here, this is a result of retained salt water above the shoal from flood as well as the faster turning of the tides above the shoals (i.e., fresher surface water above the shoals) and longitudinal tidal straining (see Section 2.1.1) rather than differential advection. This can be seen in the increased importance of the now mostly positive along-channel straining term $B_x > 0$ compared to flood (see Fig. 3.12c, 3.13c). Again, strong mixing results from high vertical shear at the plume-surface layer interface. Although of similar magnitude in its maximum intensity, ebb mixing at any given location tends to be more persistent compared to flood mixing, leading to the ebb-dominance of mixing as described in Section 3.3.1.

Mechanism 2 results from the intersection of isohaline surfaces with the channel topography, such that high stratification is confronted with the high turbulence generated in the bottom boundary layer (Garrett, 1990, Umlauf and Burchard, 2011, Henell et al., 2023, see zoom panel in Fig. 3.14). The intersection of the isohalines needs to be orthogonal due to a zero salt flux boundary condition, which causes a baroclinic pressure gradient along the topography. This can lead to an up-shoal boundary current (Wunsch, 1970, Phillips, 1970, Chen and Sanford, 2009), further allowing for shear and therefore mixing at the current-channel interface. Boundary layer mixing can occur on steeper shoals as well as along the head of the salt plume from mechanism 1 throughout both ebb and flood and is strongly dependent on the available amount of vertical stratification within the channel. In contrast to classical SIPS estuaries (see Section 2.1.1), along-channel straining in the Elbe estuary does not show a clearly destratifying tendency during flood (see Fig. 3.12c), which was attributed to a center- rather than surface-enhanced flood current (see schematic in Fig. 3.14a) which reduces the amount of saltier water that is moved on top of fresher water. Consequently, stratification was also available during flood, leading to a similar intensity of mechanism 2 as during ebb.

Additionally, topographical irregularities which can cause locally turbulent conditions were found to lead to local mixing hotspots if stratified water was advected from other regions. This can be seen in Fig. 3.12a,b near Cuxhaven and in Fig. 3.13a,b at the southeastern end of the Medem Branch, where the advection term $A > 0$ coincides with locally high values of the mixing term C .

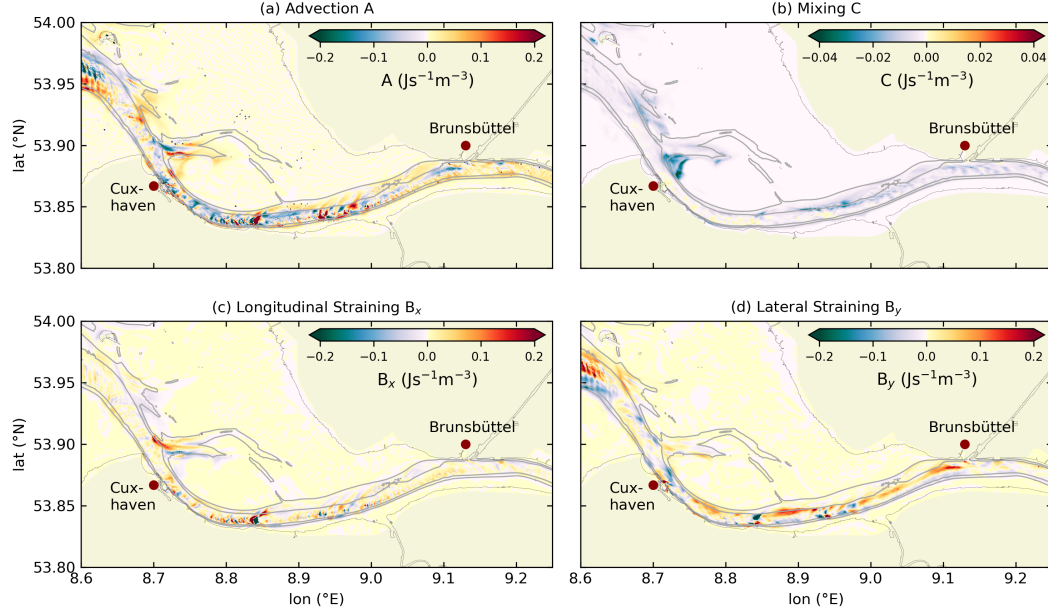


Figure 3.12: Selected terms from the dynamic equation for the vertical salinity variance (2.28), averaged over two hours around peak flood on 17th April 2024 (16:30h to 18:30h UTC). (a): Advection A , (b): vertical mixing C , (c): along-channel straining B_x , and (d): cross-channel straining B_y . For all terms, blue shading indicates destratification, and red shading indicates increasing stratification. The grey lines indicate the 12-m- and 6-m-isobaths. Note the different colourbar scale for the mixing term in (c) compared to the remaining panels. Figure taken from Reese et al. (2025).

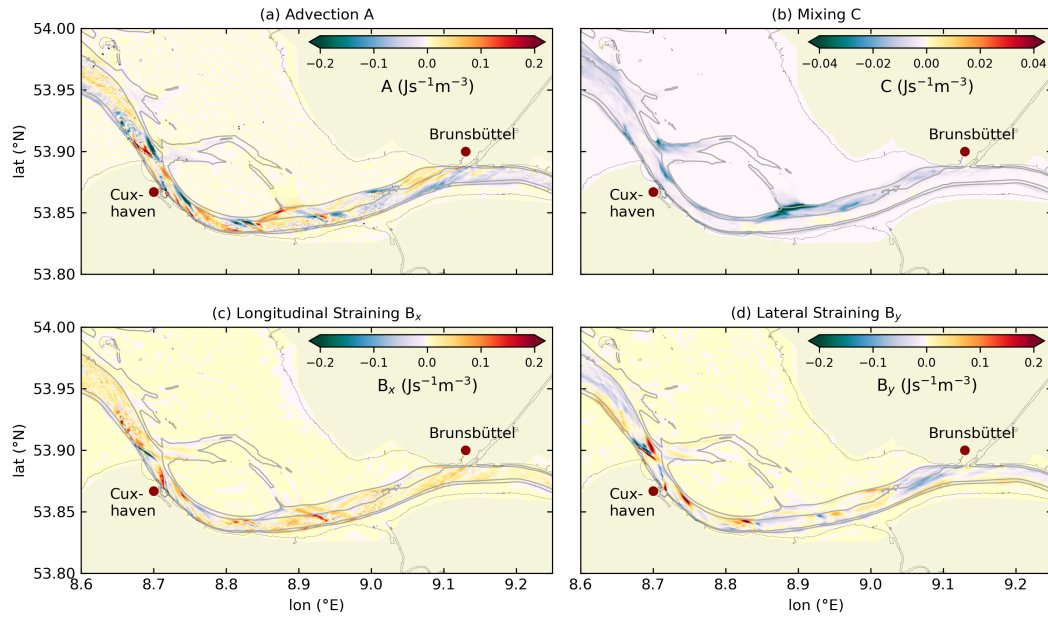


Figure 3.13: As in Fig. 3.12, but averaged around peak ebb on 17th to 18th April 2024 (22:30h to 00:30h UTC). Figure taken from Reese et al. (2025).

In total, Reese et al. (2025) could trace mixing in the Elbe estuary – and with that the estuarine exchange flow – to selected mechanisms that likely also occur in other partially mixed estuaries with a channel-shoal geometry (cf. Collignon and Stacey, 2013, Huguenard et al., 2015, Warner et al., 2020). Their findings underline the importance of lateral processes and channel-shoal interactions within such estuaries, indicating the complex nature of processes behind the well-known fact from studies such as Warner et al. (2020) that ebb mixing tends to exceed flood mixing.

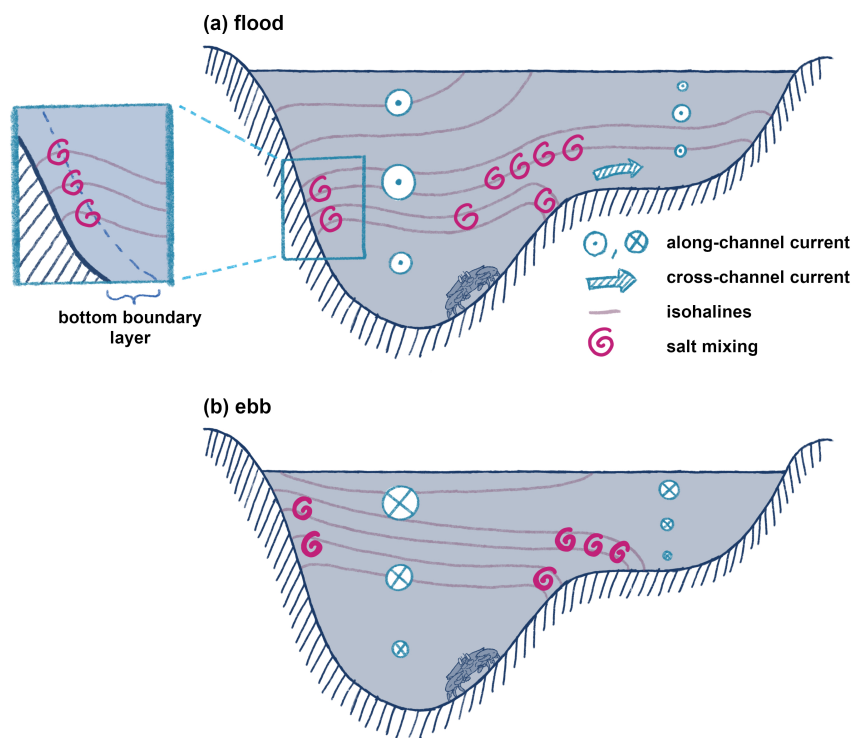


Figure 3.14: Schematic cross-section of an estuary with a flat shoal (right) and a steep slope (left), explaining the basic mechanisms of mixing at the channel-shoal transition as identified in Reese et al. (2025). (a) Flood: differential advection results in a baroclinic pressure gradient above the flat shoal that drives a shoal-ward lateral current (mechanism 1). As a result, a bottom salt plume is formed on the plateau. Mixing occurs at the interface between the bottom plume and fresher surface water, where the shear is high due to the center-enhanced flood current. It may also occur at the same interface further within the channel. Additional mixing is found where isohalines intersect with the turbulent bottom boundary layer (mechanism 2), as shown in detail in the zoom panel (adapted from Fig. 14 in Henell et al., 2023, and references therein). (b) Ebb: after slack after flood, the salt plume above the flat shoal is (partly) re-established due to incoming freshwater of the surface-enhanced ebb current (mechanism 1). Again, mixing rates occur at the plume interface due to vertical shear. Turbulent boundary layer mixing (mechanism 2) as explained in the zoom panel from (a) also occurs at ebb. The overall more persistent, but not necessarily more widespread mixing at ebb is indicated by the bold magenta spirals. Figure taken from Reese et al. (2025).

Chapter 4

Discussion and Conclusions

Here, salt mixing within partially mixed tidal estuaries has been assessed on local and estuary-wide scales for the example of the Elbe estuary, revealing the close interconnection between salt mixing and the estuarine exchange flow.

On local scales, mixing on a single isohaline surface could be linked to the water transport across this surface, and consequently to the diahaline exchange flow which displayed a distinct two-layer pattern (Reese et al., 2024), proving the applicability of the theoretically derived relation from Klingbeil and Henell (2023) for a realistic tidal estuary. Building on this result, the existing theory was combined to directly quantify the estuarine exchange flow in form of the TEF bulk inflow Q_{in} by means of the mixing on the estuarine side of the dividing isohaline surface of the Total Exchange Flow across a given vertical transect (Burchard et al., 2025). To achieve that result, volume conservation for sufficiently long temporal averaging such that storage effects vanish had to be applied. Using the derived relation, it was then possible to map the distribution of mixing and diahaline exchange flow on the dividing isohaline surface, making out regions of enhanced local mixing along the shoals of the navigational channel of the Elbe estuary that are of importance for the exchange flow. In another step, this knowledge was applied to identify the exact mechanisms related to salt mixing and the estuarine exchange flow. In case of the Elbe and similar estuaries, it was concluded that these mixing mechanisms were mainly the baroclinically-driven formation of a bottom salt plume that requires flat shoals, and turbulent boundary layer mixing at the intersection of stratification with the channel topography (Reese et al., 2025). The latter mechanism occurred on both, steep channel sidewalls and flat shoals, and depended strongly on the intensity of salt stratification within the channel. Simultaneously, deep-channel mixing decreased at the timing of strong stratification as stratification stabilises the water column, which further raises the importance of near-shoal mixing. In addition to the identified main mixing mechanisms, it was found that turbulence generated by local topographical irregularities can lead to mixing hotspots when stratification from other locations is carried in by advection.

In total, this work advances the understanding of the interplay between salt mixing and estuarine exchange flow on a holistic level by assessing the following, complete chain of relations: single mechanisms found throughout a tidal cycle make up for regions of enhanced estuarine salt mixing, which in turn are closely linked to regions of enhanced diahaline exchange flow across a single isohaline surface. Related regions can also be identified in the distribution of local mixing and diahaline exchange flow when averaged over longer time scales where storage effects vanish. Under such averaged conditions, the diahaline exchange flow then forms a closed circulation with the Total Exchange Flow, i.e., with the estuarine circulation. With respect to the integrated mixing on an isohaline surface, the link between exchange flow and mixing is strong even under extreme discharge conditions. Combining both ends of the

chain, it was shown here for the example of a partially mixed tidal estuary with a channel-shoal geometry how local processes along the channel shoals may act as the “basis” of the estuarine exchange flow.

In many details, this paints a more complex picture than what has previously been described from the study of more idealised estuaries: while past studies such as Wang et al. (2017), Wang and Geyer (2018), or Li et al. (2018) have put great emphasis on the spring-neap cycle as a modulator of salt mixing in partially mixed estuaries, it is the often considerable variability of the estuarine freshwater discharge that tends to dominate the temporal evolution of salt mixing. The respective time scales may even resolve extreme events, as shown here by Reese et al. (2024) in addition to an earlier study by Broatch and MacCready (2022) which did not include extreme events. Although the availability of stratification and tidal energy for mixing indeed also varies throughout the spring-neap cycle, it is not necessarily true that the highest mixing rates occur at the transition from neap to spring as commonly found in studies with idealised forcing (e.g., Wang and Geyer, 2018, Li et al., 2022, and others): a variability of external forcing, such as storm events, diurnal inequalities of the tidal amplitude, or freshwater floodings, can effectively obscure the spring-neap mixing signal by affecting the timing of available stratification and turbulent energy (Reese et al., 2024, 2025). Further, lateral processes resulting from a close channel-shoal interaction can be essential for mixing in partially mixed tidal estuaries with a channel-shoal geometry (Reese et al., 2025). This indicates that idealised estuaries that lack a lateral dimension, such as, e.g., in Burchard and Hetland (2010), may not properly reproduce realistic estuarine dynamics even when carefully calibrated, although they may still prove useful for the study of isolated longitudinal dynamics. The findings presented in this work further confirm the well-known ebb dominance of mixing (Warner et al., 2020), but emphasise that flood mixing cannot be neglected. In fact, in case of the formation of bottom salt plumes above flat shoals, it is implied that flood and ebb should not be considered independently of each other, as processes occurring during flood may well impact the salt distribution and stratification that are relevant during ebb (see Reese et al., 2025).

In light of such local and short-term complexity, it may seem astonishing that the estuary-wide, subtidal dynamics of mixing and exchange flow are well-reproduced even under highly variable forcing conditions. It was shown in the present work that mixing estimates such as (2.22) by MacCready et al. (2018) and (2.24) by Burchard (2020) generally tend to hold well (Reese et al., 2024) regardless of extreme discharge variability. Similarly, the Elbe estuary displays a well-defined two-layer Total Exchange Flow and diahaline exchange flow on monthly averages despite its variable topography (Reese et al., 2024), and mixing and exchange flow form a nearly closed budget on the same time scales (Burchard et al., 2025). This implies that the time-averaged theory of estuarine circulation is a robust framework well-suited for the study of realistic estuaries in a realistic environment. Going further, the results presented by Reese et al. (2024) and Burchard et al. (2025) even show that extreme discharge events can be resolved and analysed with this framework, which emphasises the potentially short adjustment times of estuarine dynamics to a changing external forcing. In detail, these adjustment times can be of the order of days to weeks.

Lastly, it nonetheless has to be noted that the findings presented in this thesis are mostly focussed on the Elbe estuary, a partially mixed tidal estuary. While they can likely be extended

for comparable estuaries that share the single-channel-shoal geometry and partially mixed, mesotidal characteristics, a multitude of other, distinctly different types of estuaries exist as classified, e.g., by Geyer and MacCready (2014). Future studies on estuarine mixing are necessary to understand how the processes and relations identified here may differ for such other types of estuaries. Yet, while the exact nature of local mixing mechanisms may vary with the estuarine configuration, the general chain of relations shown here may also hold for other types of estuaries. This is implied, e.g., by the findings for the non-tidal Warnow river estuary from Burchard et al. (2025) that yields a three-layer exchange flow when averaged, or by findings by Henell et al. (2023), who reported a high correlation between local mixing and diahaline exchange flow for the non-tidal Baltic Sea. Aside from the more specific findings, the present work can therefore also be seen as a guideline on how to identify local processes related to the mixing and exchange flow of a given estuary. The estuarine exchange flow is an important driver of estuarine transport processes – including sediment (e.g., Meade, 1969), pollutants (e.g., Pritchard, 1969), nutrients (e.g., Wei et al., 2022), and larvae of fish or other organisms (see review by Norcross and Shaw, 1984) – as well as water renewal or retention within the deeper sections of river channels, which may also affect the bottom water oxygen concentration (e.g., Sun et al., 2020). Therefore, the ability to trace the estuary-wide circulation to singular, local processes as well as the ability to estimate the impact of freshwater discharge on estuarine dynamics as shown in this thesis could act as a powerful tool also for the understanding of estuarine ecosystems and changes therein.

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Declaration of personal contributions to the publications

1 Local Mixing Determines Spatial Structure of Diahaline Exchange Flow in a Mesotidal Estuary: A Study of Extreme Runoff Conditions

For this study, the conceptualisation was mainly performed by me and my supervisor. I created, calibrated, and validated the Elbe setup by myself. Similarly, I created all plots and analysis scripts used in the study and performed the analyses myself. The paper was fully written by myself, and I also handled the revisions. Of course, all this would not have been possible without the ongoing, valuable input from my co-authors, in particular with respect to the model preparation, paper writing, and revision handling.

2 The Relation Between Exchange Flow and Diahaline Mixing in Estuaries

In the second study, it was mainly my supervisor who initiated the study concept. I was involved along with the other co-authors in the discussions and further development of the theory, in particular for the expansion of the three-layer case. This study re-used data from my Elbe setup from the first paper, and I created the Elbe and overview plots. The analysis for the Elbe estuary was also done by me, and I helped with the introduction of the study region. For the analysis of the three-layer Warnow case, I was involved in the planning and design of the analysis, but the setup and analysis itself were handled by Xaver Lange. The paper writing and review process were handled by my supervisor, although I and the other co-authors provided input throughout all stages and were involved in the discussion of the reviews.

3 The Role of the Shoal – Salt Mixing Mechanisms in a Partially Mixed Tidal Estuary With Channel-shoal Geometry

The final study of this thesis originated from a suggestion by my supervisor and was then almost exclusively designed by me. The numerical Elbe setup used here was a derivative of my own setup from the previous studies, heavily edited by Xiangyu Li, who most notably increased the setup resolution, updated the topography with more recent datasets, applied entirely new forcing and a new calibration, and provided the model runs. The process-oriented setup validation was done by myself with data from a measurement campaign that I planned, organised,

and performed with the help of my co-authors, in particular the priceless support by Peter Holtermann, who organised the measurement devices and provided his expertise throughout the planning, measurement, and analysis stages of the observed data. All analyses shown in the study were performed by myself, including the creation of all plots and schematics. The paper was written by myself aside from part of the methodology section for the observational data, which was covered by Peter Holtermann. As the paper is currently under review for the first time, no revisions have been handled yet. Again, I received valuable input from my co-authors throughout the creation of this study.

Publications

Local Mixing Determines Spatial Structure of Diahaline Exchange Flow in a Mesotidal Estuary: A Study of Extreme Runoff Conditions

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ABSTRACT: Salt mixing enables the transport of water between the inflow and outflow layers of estuarine circulation and therefore closes the circulation by driving a diahaline exchange flow. A recently derived universal law links the salt mixing inside an estuarine volume bounded by an isohaline surface to freshwater discharge: it states that on long-term average, the area-integrated mixing across the bounding isohaline is directly proportional to the freshwater discharge entering the estuary. However, even though numerous studies predict that periods of extreme discharge will become more frequent with climate change, the direct impact of such periods on estuarine mixing and circulation has yet to be investigated. Therefore, this numerical modeling study focuses on salinity mixing and diahaline exchange flows during a low-discharge and an extreme high-discharge period. To this end, we apply a realistic numerical setup of the Elbe estuary in northern Germany, using curvilinear coordinates that follow the navigational channel. This is the first time the direct relationship between diahaline exchange flow and salt mixing as well as the spatial distribution of the diahaline exchange flow is shown in a realistic tidal setup. The spatial distribution is highly correlated with the local mixing gradient for salinity, such that inflow occurs near the bottom at the upstream end of the isohaline. Meanwhile, outflow occurs near the surface at its downstream end. Last, increased vertical stratification occurs within the estuary during the high-discharge period, while estuarine-wide mixing strongly converges to the universal law for averaging periods of the discharge event time scale.

SIGNIFICANCE STATEMENT: Inside estuaries, such as river mouths, terrestrial freshwater is mixed with salty ocean water. This is accompanied by an estuarine circulation with inflow of saltwater into the estuary and outflow of brackish water toward the ocean. Here, we aim to better understand how salt mixing and estuarine circulation in a tidal estuary react to periods of extreme freshwater discharge. We find that even during extremely high or low discharge, salt mixing follows the freshwater discharge on time scales as short as days, and that estuarine circulation patterns are largely explained by the local distribution of mixing. As extreme runoff events are likely to occur more often with climate change, these findings may help to understand the dynamics inside future estuaries.

KEYWORDS: Ocean; Estuaries; Mixing; Numerical analysis/modeling

1. Introduction

Inside a classical estuary, salty ocean water is mixed with terrestrial freshwater. As a result, brackish water is exported from the estuary. Thus, sufficient temporal averaging reveals an inflow of salty water and an outflow of brackish water, known as classical estuarine circulation. This phenomenon was first quantified by Knudsen (1900) for the Baltic Sea. Later, Hansen and Rattray (1965) developed the first theoretical framework for a density-driven estuarine circulation. Further pioneer studies by Chatwin (1976) and Walin (1977) followed.

In recent years, it has become widely established to study estuarine dynamics within an isohaline framework (see, e.g., MacCready and Geyer 2001; Hetland 2005; MacCready 2011; Wang et al. 2017; Burchard et al. 2019). Such a framework had first been introduced to estuarine physics by Walin (1977). Using isohaline instead of vertical coordinates is often beneficial for estuarine studies because the classical estuarine circulation is largely salinity driven. Knowing at which salinities estuarine inflow and outflow occur, and how and where these water masses interact, is therefore of great help for the identification of key mechanisms. MacCready (2011) used such isohaline coordinates along a vertical, cross-channel transect to introduce the total exchange flow (TEF) framework. The TEF framework yields tidally averaged isohaline inflow and outflow per salinity class across this vertical transect. In contrast to an Eulerian (spatial) framework, it properly accounts for tidal salt fluxes. Therefore, when quantifying exchange flows in terms of Knudsen bulk values, the TEF transport-weighted inflow and outflow salinities are more representative of the exchange flow. Building on MacCready (2011), Sutherland et al. (2011) presented the temporal variability of the tidally averaged TEF across a transect in the

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fjord-like Puget Sound. Later, Wang et al. (2017) studied the along-channel variability of the TEF within the Hudson estuary. Further studies using the TEF framework have been conducted by Chen et al. (2012), Ganju et al. (2012), and many others.

A useful definition for salt mixing in estuaries is the destruction of salinity variance (see Burchard and Rennau 2008; Burchard et al. 2009). According to this definition, mixing is a function of the salinity gradient squared and the eddy diffusivity in each spatial direction. Therefore, it depends not only on turbulence but also on the availability of water masses of different salinities. Consequently, mixing may be strong in a stratified, but somewhat turbulent body of water and will vanish once the water body is homogeneous, i.e., once no further salinity gradients are found, even though turbulence is still present. So far, studies on estuarine mixing, such as Wang et al. (2017), Li et al. (2018), and MacCready et al. (2018), have mostly worked with constant freshwater runoff and focused on the spring–neap cycle as a modulator of salt mixing. However, Wang and Geyer (2018) found a dependence of mixing on the freshwater runoff for scenarios of different constant river discharges. They demonstrated that increased freshwater discharge entering an estuary leads to an increased salinity variance that outweighs the reduced salt intrusion. Additionally, sufficiently long time-averaged salt mixing M_T inside an estuarine volume bounded by a TEF transect can be estimated as the product of TEF inflow and outflow salinities S_{in} , S_{out} and freshwater runoff Q_r (MacCready et al. 2018):

$$M_T \approx S_{in} S_{out} Q_r. \quad (1)$$

Recently, Conroy et al. (2020) showed that the volume-integrated mixing in the relatively small Coos River estuary mostly follows the temporal evolution of the freshwater discharge. In accordance with these findings, Broatch and MacCready (2022) demonstrated that the mixing estimate by MacCready et al. (2018) works well in their realistic simulation of Puget Sound, even for tidal averaging only. Their study showed that mixing in Puget Sound is predominantly driven by freshwater runoff, indicating that the spring–neap variability found in the earlier studies may be of only secondary importance for at least some realistic estuaries.

Instead of a vertical transect, an estuarine volume can also be bounded by an isohaline surface (see MacCready and Geyer 2001; MacCready et al. 2002). Burchard (2020) considered estuarine volumes bounded by such isohaline surfaces to derive a universal law of estuarine mixing. Due to the different choice of the estuarine volume as compared to MacCready et al. (2018), this law yields an even more direct relation between mixing and freshwater runoff: it states that on long-term average and when neglecting surface fluxes, the mixing $M(S)$ inside the estuarine volume is determined from the respective bounding salinity S and average freshwater runoff Q_r alone:

$$M(S) = S^2 Q_r. \quad (2)$$

The importance of this law has since been demonstrated for an idealized estuary (Burchard et al. 2021) as well as for idealized conditions inside a complex estuary with multiple outlets (Li et al. 2022).

We summarize that freshwater runoff plays a vital role in the estuarine exchange flow, as predicted by the Knudsen (1900) relations, and in estuarine mixing. However, even though studies predict that periods of extremely high and low runoff will become more frequent with climate change (see, e.g., Christensen and Christensen 2004; van Vliet et al. 2013), the direct impact of such events on estuarine circulation and especially on mixing has not yet been studied. Most numerical studies that take extreme discharge values into account have only used idealized forcing, including idealized tides and a constant discharge, such as Wang et al. (2017) or Li et al. (2022). However, events of unusually high discharge are often driven by extreme rainfall events or human intervention such as weirs. They are therefore characterized by a strong variability of discharge in time, which cannot be represented by a choice of constant runoff. The few existing exchange flow and mixing studies using realistic forcing do not focus on extreme discharge events, and either do not include mixing at all (e.g., Sutherland et al. 2011), or do not include spatially resolved mixing or exchange flow analyses (e.g., Conroy et al. 2020; Broatch and MacCready 2022).

Furthermore, the mixing estimates from MacCready et al. (2018) and Burchard (2020) both assume “sufficiently long” averaging periods, which may differ between estuaries. For the aims of the present study, it could generally be said that an averaging period is sufficiently long when the computed total mixing converges to the respective mixing estimate. Even though Broatch and MacCready (2022) showed that the MacCready et al. (2018) estimate could generally perform well even for relatively short averaging periods of a single M_2 tidal cycle, neither estimate has yet been tested under realistic conditions of extreme runoff. The question remains whether choosing sufficiently short time spans to resolve such extreme events would reproduce these estimates correctly despite potentially rapid changes in discharge intensity. An exemplary event of extremely high runoff occurred in June 2013 in the Elbe estuary in the southeast of the German Bight. It consisted of a strong and fast increase of discharge from about $1000 \text{ m}^3 \text{ s}^{-1}$ to more than $4000 \text{ m}^3 \text{ s}^{-1}$ and occurred over the time scale of roughly 1 month. The Elbe estuary is a rather typical, funnel-shaped mesotidal estuary with a well-defined navigational channel surrounded by tidal flats. Previous studies showed that the high-discharge event led to temporally increased stratification in the German Bight, demonstrating the impact that such events can have on a coastal system (Voyanova et al. 2017; Kerimoglu et al. 2020; Chegini et al. 2020). In Kerimoglu et al. (2020), particularly strong mixing occurred in the shallow coastal waters, including the Elbe River mouth. In these regions, vertical mixing played an important role in destratification (Chegini et al. 2020). Even though these findings indicate that mixing is of great importance for coastal dynamics, none of the previous studies focused on the local influence of the high-runoff event on the circulation and mixing inside the Elbe estuary itself, leaving these questions open for future research.

Mixing can be related to the actual transport of water masses by considering a *diahaline velocity* relative to a moving isohaline that is directed in across-isohaline, i.e., diahaline,

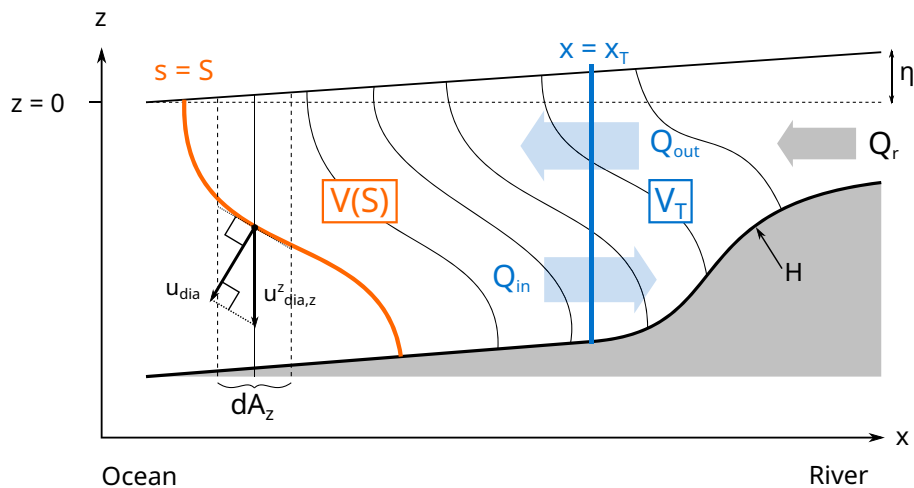


FIG. 1. Schematic along-channel section of a tidally averaged estuary, illustrating TEF and diahaline parameters. The bold black line and gray shading indicate the bottom topography, and the angled, bold black line indicates the water surface. The dashed horizontal line shows where $z = 0$; η is the surface elevation above $z = 0$, H is the depth of the bottom below $z = 0$, and Q_r is the freshwater runoff. The broad, semitransparent arrows indicate the tidally averaged flow directions. The thin, curved black lines represent isohalines. Blue: the vertical, cross-channel TEF transect at along-channel position $x = x_T$; the estuarine volume V_T is bounded by this transect, and the TEF bulk volume transport Q_{in} goes into and Q_{out} goes out of the estuarine volume. Orange: the estuarine volume bounded by the isohaline of salinity $s = S$. The dashed vertical lines bound a single, finite water column with horizontal area element dA_z . The arrows within the water column illustrate the difference between the diahaline velocity u_{dia} and the local diasurface volume flux per unit horizontal area in z coordinates, $u_{dia,z}^z$. Note that in most estuaries, the isohalines are almost horizontal so that u_{dia} and $u_{dia,z}^z$ are almost identical. In the stably stratified case illustrated here, the effective vertical diahaline velocity $u_{dia,z}^S$ equals $u_{dia,z}^z$. In a more general case, $u_{dia,z}^S$ has to be calculated from (18).

direction (see u_{dia} in Fig. 1). Such a diahaline transport per unit isohaline area (see Burchard et al. 2021) does not include advective motion because transport across an isohaline can only occur due to mixing. A related, vertically directed property is the local diahaline volume transport per unit horizontal area across an isohaline surface (see $u_{dia,z}^z$ in Fig. 1). Due to its definition as a velocity relative to the advective isohaline motion, the local diahaline volume transport per unit horizontal area has been described as entrainment velocity in previous studies by Wang et al. (2017) and Li et al. (2022). Wang et al. (2017) linked the entrainment velocity to the diahaline turbulent salt transport, i.e., the turbulent transport of salt across an isohaline. In Li et al. (2022), the diahaline salt transport was related to salt mixing. Recently, Klingbeil and Henell (2023) generalized the framework to support salinity inversions and, in this context, defined the *effective vertical diahaline velocity*. Moreover, they combined the relations from Wang et al. (2017) and Li et al. (2022), thus directly linking the effective vertical diahaline velocity to the gradient of mixing in isohaline coordinates. As this relation neglects the horizontal diffusion of salt, it has yet to be tested how well it holds for realistic estuaries, where horizontal diffusion might actually be of importance. While Henell et al. (2023) found a good agreement between the mixing gradient and effective vertical diahaline velocity within the microtidal Baltic Sea, it is still unclear how well

the estimate holds in a realistic tidal regime: the previously mentioned study by Wang et al. (2017) used only idealized forcing, including idealized tides and a constant, moderate freshwater discharge. Furthermore, it has not yet been shown for a tidal regime how well the estimate holds locally, i.e., for the *spatially resolved* diahaline exchange flow, and under temporally varying, extreme discharge conditions. So far, the studies by Wang et al. (2017), Li et al. (2022), and Henell et al. (2023) all have revealed a diahaline exchange flow with inflow toward lower salinities and outflow toward higher salinities, similar to the isohaline total exchange flow. The diahaline velocity may therefore provide insight into the spatial distribution of exchange flow under extreme conditions.

The present study aims to answer the open questions mentioned above for typical mesotidal estuaries. In detail, these questions are as follows:

- 1) Using averaging periods short enough to resolve extreme discharge events, will the mixing estimates by MacCready et al. (2018) and Burchard (2020) still be reproduced properly? Are these estimates therefore applicable to the study of extreme events?
- 2) How are extreme discharge events reflected in the total exchange flow (MacCready 2011), diahaline circulation, and salt mixing?

- 3) How closely is the two-dimensional distribution of the salinity gradient of mixing linked to the local diahaline exchange flow in a realistic hindcast simulation?

To address these questions, a realistic numerical setup of the Elbe estuary has been created for this study. The mathematical framework required for the TEF, estuarine salt mixing, and diahaline transport is introduced in [section 2](#), followed by the study region itself. Furthermore, the numerical setup is described and validated. In [section 3](#), the setup is applied to demonstrate the impact of the high-discharge event from June 2013 on local circulation and mixing. To this end, the high-discharge month of June 2013 is compared to the low-discharge month of September 2012. Additionally, the temporal evolution of mixing is considered. We draw some final conclusions in [section 4](#).

2. Methods

a. Mathematical framework

1) TOTAL EXCHANGE FLOW

This study applies the TEF framework introduced by [MacCready \(2011\)](#). It is used to analyze residual volume and salt transport across a vertical, cross-channel transect of an estuary (see transect at $x = x_T$ in [Fig. 1](#)). In addition to the original equations, the more general formulation by [Klingbeil and Henell \(2023\)](#) will be presented here.

With the along-channel velocity u normal to the vertical transect, the isohaline volume transport Q in all salinity classes $s > S$ (where S is the chosen salinity of an isohaline) is then given as

$$Q(x, S, t) = \int_{A_T} \mathcal{H}(s^z - S) u \, dA = \int_{A_S} u \, dA, \quad (3)$$

with the Heaviside step function,

$$\mathcal{H}(\psi) = \begin{cases} 0, & \psi \leq 0 \\ 1, & \psi > 0 \end{cases}, \quad (4)$$

for an arbitrary function ψ . In [\(3\)](#), t is the temporal argument, s^z is the salinity at a given spatial position (x, y, z) on the transect, A_T is the total cross-sectional area of the transect, and A_S is the cross-sectional area of the transect where $s > S$. The last term in [\(3\)](#) is the original definition by [MacCready \(2011\)](#). Note that in [MacCready \(2011\)](#), tidal averaging is applied here. However, following [Wang et al. \(2017\)](#) and [Klingbeil et al. \(2019\)](#), averaging can also be applied at a later point without changing the given properties.

To find the respective volume transport per salinity class, q , the derivative of Q with respect to salinity is computed:

$$q(x, S, t) \equiv -\frac{\partial Q(x, S, t)}{\partial S}. \quad (5)$$

Here, the negative sign is required such that q is positive for inflow and negative for outflow.

Integrating over the respective inflows and outflows per salinity class then yields the total inflow and outflow across the transect, namely,

$$\begin{aligned} Q_{\text{in}}(x, t) &\equiv \int_0^{S_o} \langle q(x, S, t) \rangle_{\text{in}} \, dS, \\ Q_{\text{out}}(x, t) &\equiv \int_0^{S_o} \langle q(x, S, t) \rangle_{\text{out}} \, dS, \end{aligned} \quad (6)$$

where S_o is the maximum salinity occurring along the transect and $\langle \cdot \rangle$ indicates temporal averaging, e.g., tidal averaging. This is the original definition for the bulk volume inflow and outflow as given by [MacCready \(2011\)](#). A numerically more robust method is the dividing salinity method ([MacCready et al. 2018](#); [Lorenz et al. 2019](#)), where, assuming a classical two-layer exchange flow,

$$Q_{\text{in}} = \max(\langle Q \rangle), \quad Q_{\text{out}} = -Q_{\text{in}} - Q_r. \quad (7)$$

Here, Q_r is the freshwater discharge entering the estuarine volume, averaged over the same period as the other properties. In this study, we use the dividing salinity method. Similarly, the ingoing and outgoing salt transport are defined as

$$\begin{aligned} F_{\text{in}}(x, t) &\equiv \int_0^{S_o} S \langle q(x, S, t) \rangle_{\text{in}} \, dS, \\ F_{\text{out}}(x, t) &\equiv \int_0^{S_o} S \langle q(x, S, t) \rangle_{\text{out}} \, dS, \end{aligned} \quad (8)$$

which can also be determined from the dividing salinity method, analogous to [\(7\)](#).

From these bulk values, transport-weighted inflow and outflow salinities can be computed:

$$S_{\text{in}}(x, t) \equiv \frac{F_{\text{in}}}{Q_{\text{in}}}, \quad S_{\text{out}}(x, t) \equiv \frac{F_{\text{out}}}{Q_{\text{out}}}. \quad (9)$$

The Q_{in} , Q_{out} , S_{in} , and S_{out} terms are the total exchange flow properties as given by [MacCready \(2011\)](#).

From these properties, the Knudsen relations ([Knudsen 1900](#)) can be obtained for sufficiently long temporal averaging ([MacCready 2011](#); [Burchard et al. 2018](#)).

2) SALT MIXING

Estuarine exchange flow is related to the mixing of water masses ([MacCready et al. 2018](#)). Following [Burchard and Rennau \(2008\)](#), mixing is defined here as the destruction of salinity variance:

$$\chi(x, y, z, t) = 2K_h(\partial_x s^z)^2 + 2K_h(\partial_y s^z)^2 + 2K_v(\partial_z s^z)^2. \quad (10)$$

This is the sink term of the salinity variance budget equation; see, e.g., [Burchard and Rennau \(2008\)](#). It therefore directly quantifies the decay rate of salinity variance. Here, K_h is the horizontal and K_v is the vertical eddy diffusivity of salt s , which may vary in space and time. The term ∂_i represents the partial derivative with respect to a coordinate x_i . Under this definition, mixing can only occur when the water body is not

fully mixed, and will increase quadratically with stratification for a given turbulent diffusivity.

The time-averaged total mixing M_T inside an estuarine volume bounded by a vertical TEF transect, V_T (see Fig. 1), can be found as the volume integral of χ :

$$M_T = \left\langle \int_{V_T} \chi dV \right\rangle. \quad (11)$$

Assuming long-term averaged conditions and neglecting surface volume fluxes, MacCready et al. (2018) approximated M_T as

$$M_T \approx S_{\text{in}} S_{\text{out}} Q_r. \quad (12)$$

The exact averaging period required for a convergence of the actual mixing with the estimate (12), and therefore the exact definition of what “long-term averaging” is, may vary between estuaries. Instead of considering a volume bounded by a vertical transect, we can also use an estuarine volume $V(S)$ that is bounded by an isohaline surface of salinity S (see Fig. 1). The total mixing inside $V(S)$ is found as a function of the bounding salinity S :

$$M(S) = \left\langle \int_{V(S)} \chi dV \right\rangle. \quad (13)$$

Using (13), Burchard (2020) showed that for long-term averaging (defined as above) and when neglecting surface volume fluxes, this property could also be computed from the bounding salinity and freshwater runoff:

$$M(S) = S^2 Q_r. \quad (14)$$

If formulated for the mixing per salinity class, $m(S) = \partial_S M(S)$, this is the universal law of estuarine mixing:

$$m(S) = 2S Q_r. \quad (15)$$

Again, this equation is valid only for long-term averaging.

The local mixing per salinity class inside a single water column, m_{xy} , is defined such that its area integral yields the mixing per salinity class for the full isohaline surface:

$$m(S) = \int_{A_z(S)} m_{xy}(x, y, S) dA_z, \quad (16)$$

where $A_z(S)$ is the horizontal projection of the isohaline surface $A(S)$ and dA_z is an infinitesimal horizontal area element. For the exact definition of m_{xy} , see Klingbeil and Henell (2023).

3) DIAHALINE TRANSPORT

While the TEF framework considers only isohaline properties, i.e., fluxes and transports *along* a given isohaline, it is also possible to consider the diahaline direction, i.e., *across* an isohaline. The diahaline velocity u_{dia} is the relative velocity of an isohaline to the three-dimensional flow velocity vector $\mathbf{u}$:

$$u_{\text{dia}}(x, y, z, t) = (\mathbf{u} - \mathbf{u}_s) \cdot \frac{\nabla S^z}{|\nabla S^z|}. \quad (17)$$

Here, $\mathbf{u}_s$ is the velocity of a given point on the isohaline surface and includes advective motion. For an illustration of u_{dia} , see Fig. 1.

For a single water column, the effective vertical diahaline velocity $u_{\text{dia},z}^S$,

$$u_{\text{dia},z}^S(x, y, S, t) = \int_{-H}^{\eta} \delta(S - s^z) |\nabla s^z| u_{\text{dia}} dz, \quad (18)$$

describes the diahaline volume transport per unit horizontal area across a given isohaline S (Klingbeil and Henell 2023). The $u_{\text{dia},z}^S$ is a vertically directed property and positive in the direction of higher salinity. For stable salt stratification, $u_{\text{dia},z}^S$ is identical to the negative entrainment velocity w_e used in Wang et al. (2017) and Li et al. (2022). The Dirac function $\delta(x)$ is introduced here as the derivative of the Heaviside step function. It is used to find an average value for $u_{\text{dia},z}^S$ in cases where the salinity S appears at multiple positions in the water column. We will refer to this as the term *effective*. From the effective vertical diahaline velocity, we can compute the integrated diahaline volume transport

$$Q_{\text{dia}}(S, t) = \int u_{\text{dia},z}^S dA_z, \quad (19)$$

which is equivalent to the entrainment flux Q_e from Wang et al. (2017).

Klingbeil and Henell (2023) linked the effective vertical diahaline velocity to the S derivative of the local mixing, as long as horizontal diffusive fluxes are neglected:

$$u_{\text{dia},z}^S = \frac{1}{2} \frac{\partial m_{xy}}{\partial S}. \quad (20)$$

Last, the local mixing m_{xy} computed from a numerical, hydrodynamic simulation can be split into a physical component $m_{xy,\text{phy}}$, originating from the turbulence parameterization, and a numerical component $m_{xy,\text{num}}$, caused by the discretization error of advection schemes (Burchard and Rennau 2008; Klingbeil et al. 2014):

$$m_{xy} = m_{xy,\text{phy}} + m_{xy,\text{num}}. \quad (21)$$

b. Study area

We have performed a hydrodynamic simulation of the Elbe estuary for this study. This partially to well-mixed, mesotidal estuary (see, e.g., Kappenberg and Fanger 2007; Stanev et al. 2019) is located in the southeast of the German Bight and consists of a well-defined, deep navigational channel widely surrounded by tidal flats (see Figs. 2a,b). The dominant tidal constituent is the M_2 tide. Inside the estuary, the tidal intrusion is limited by a weir at Geesthacht, marking the upstream end of the so-called tidal Elbe (see Fig. 2c). The end of the salt intrusion inside the tidal Elbe is usually located between Glückstadt and Stadersand (Boehlich and Strotmann 2008). However, it can extend almost as far upstream as Schulau (see Fig. 2a) for particularly low freshwater discharge (Bergemann 1995). Overall, the salt intrusion is strongly dependent on the freshwater discharge (see, e.g., Grabemann et al. 1995; Kappenberg and Grabemann 2001). Aside from its ecological function, the Elbe estuary is also of significant importance for

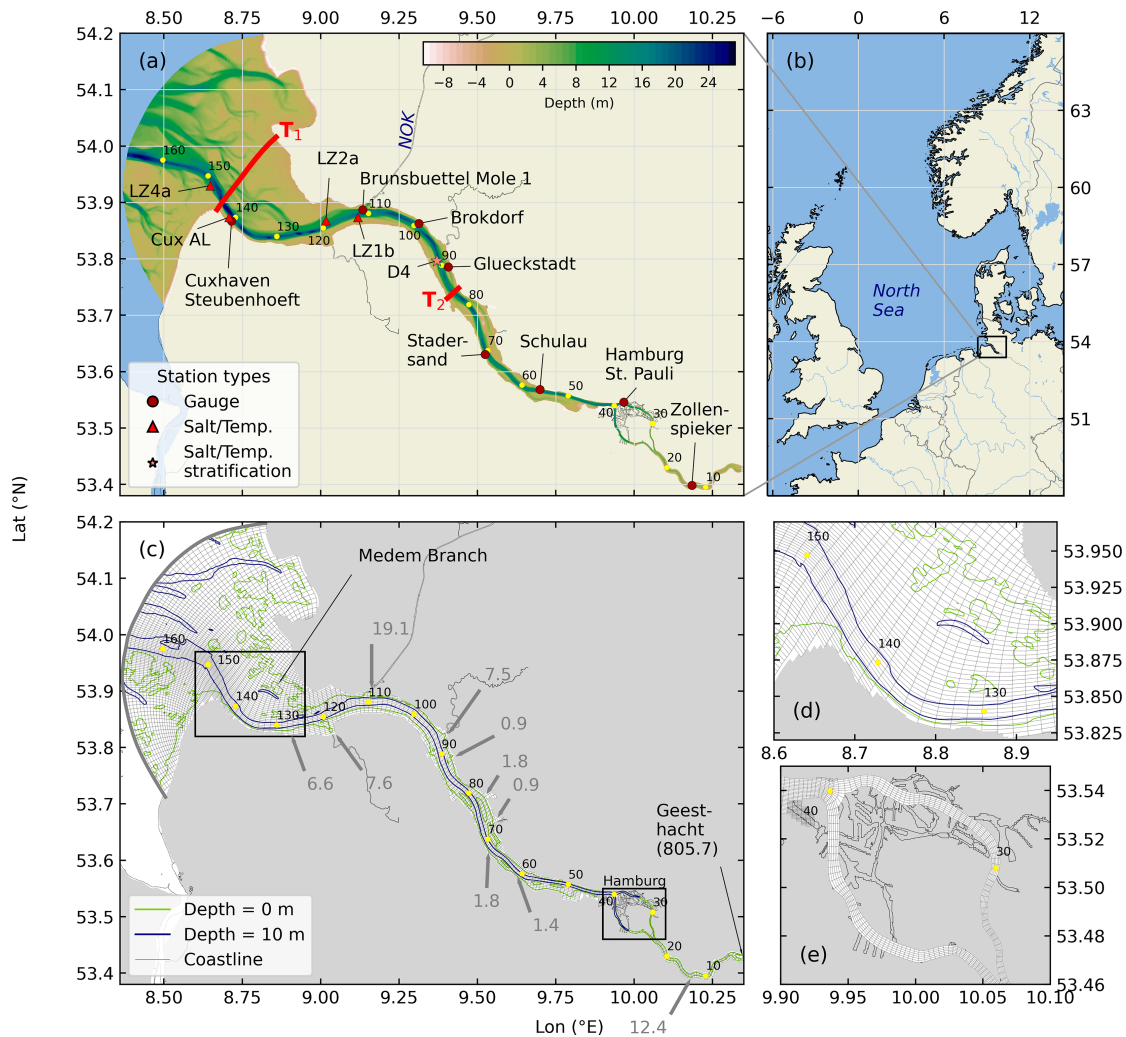


FIG. 2. Model domain of the numerical tidal Elbe setup. (a) Setup topography showing the deep navigational channel and locations of the observational stations used for calibration and validation. Gauges provide information for the tidal analysis. The full names of the salt and temperature stations are LZ4a Steinriff, Cuxhaven Alte Liebe, LZ2a Neufeldrede, and LZ1b Krummendeich. Station D4 (Rhinplate Nord) is the only station where stratification data for salinity and temperature were available. Water outside the model domain is colored in blue. The label “NOK” marks the Kiel Canal. The transects T_1 and T_2 bound the along-channel section that is studied in section 3b. (b) Location of the estuary on the North Sea coast. (c) Curvilinear grid used for the setup, with (d),(e) details shown as indicated by the black rectangles. The thick gray line marks the open boundary of the setup. The main discharge into the estuary enters the model domain at Geesthacht, with the average discharge from August 2012 to December 2013 in parentheses ($\text{m}^3 \text{s}^{-1}$). Gray arrows show the location of each tributary that is included in the model, and their average discharge ($\text{m}^3 \text{s}^{-1}$) for the same period as Geesthacht. In (c) and (d), only every third grid line is shown. Yellow dots with numbers show the distance from the upstream end of the setup at cell centers between the 158th and 159th along-channel grid lines, in the following referred to as “model-km”.

international maritime trade and shipping, with ports in Cuxhaven, Brunsbüttel, and the city of Hamburg (see, e.g., Boehlich and Strotmann 2008).

The freshwater runoff reaching the tidal Elbe via Geesthacht may vary strongly depending on conditions in its catchment area but averages around $700 \text{ m}^3 \text{s}^{-1}$ (Strotmann 2015). In June 2013, massive rainfalls in the Elbe catchment area (see, e.g., Grams et al. 2014) led to an extreme event with up to $4000 \text{ m}^3 \text{s}^{-1}$ of freshwater runoff passing a gauge in Neu Darchau, slightly upstream of Geesthacht. In comparison,

periods of particularly low runoff may occur predominantly in summer and early autumn (see Strotmann 2015). An exemplary runoff for a dry summer is the average of $300 \text{ m}^3 \text{s}^{-1}$ that occurred in the month of September 2012, which was more than $100 \text{ m}^3 \text{s}^{-1}$ below the average September runoff for the period from 1925 to 2012 (Strotmann 2014). In addition to the main runoff, the tidal Elbe has several small tributaries entering between Geesthacht and the German Bight. However, their runoff is small compared to the freshwater input from Geesthacht. The strong variability of the

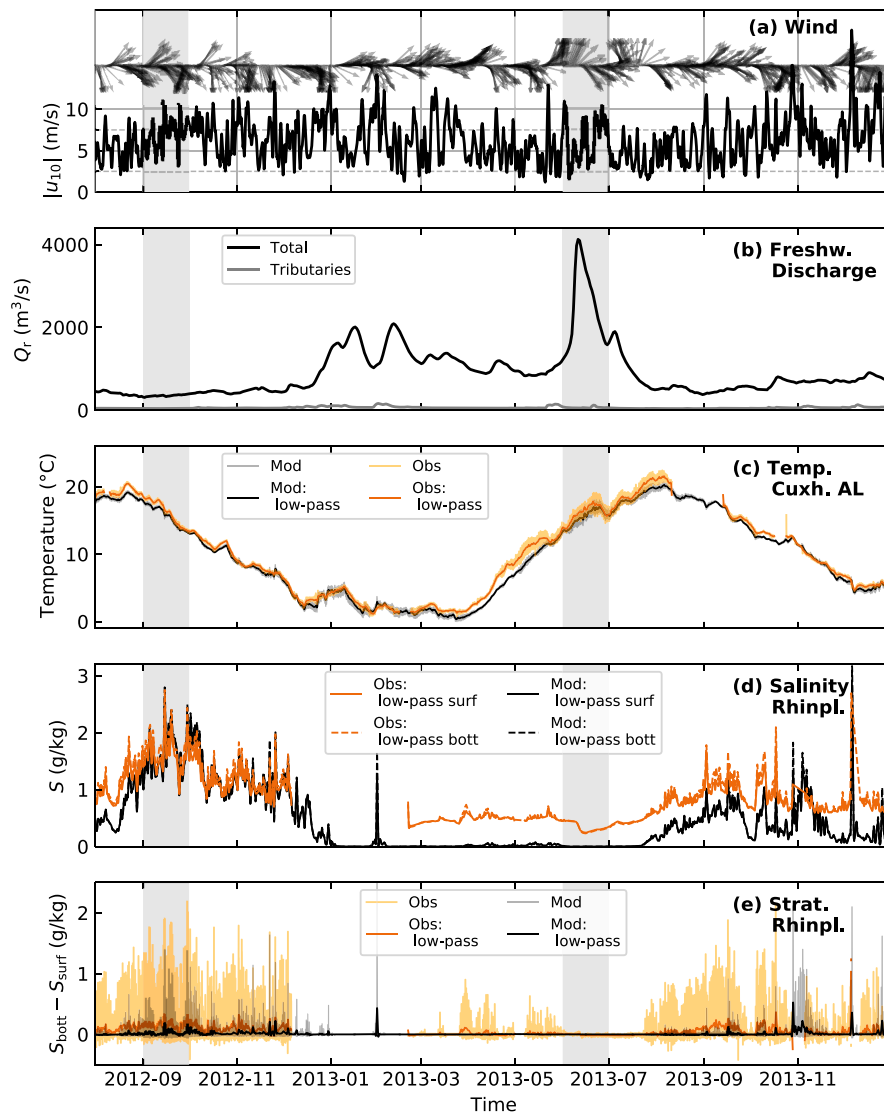


FIG. 3. Time series from August 2012 to December 2013 for different forcing and validation parameters. (a) Magnitude (black line) and oceanographic direction (arrows; point in the direction in which the wind is blowing) of the wind forcing used for the setup, spatially averaged over the Elbe River mouth region. The wind magnitude has been filtered with a 1-day running mean, while wind direction was filtered with a 7-day running mean and is shown with about one arrow per day. The wind forcing is given as the velocity vector at 10-m height. (b) Daily averaged runoff from all sources of freshwater discharge included in the setup, compared to the runoff of the tributaries only. (c) Modeled and observed water temperature 2.5 m above ground at Cuxhaven Alte Liebe. (d) Modeled and observed surface (bold; S_{surf}) and bottom (dashed; S_{bott}) salinity at D4 Rhinplate Nord. (e) Modeled and observed stratification $S_{bott} - S_{surf}$ at D4 Rhinplate Nord. In (c)–(e), the transparent colors (light orange, gray) represent tidally varying data and opaque colors (dark orange, black) represent 30-h low-pass-filtered, subtidal data. The gray-shaded areas in all panels mark the months of September 2012 and June 2013, which are the focus of this study.

total freshwater runoff is illustrated in Fig. 3b for the period from August 2012 to December 2013.

Due to the relatively simple, funnel-shaped topography of the estuary and its intermediate properties such as discharge intensity and tidal range, the tidal Elbe provides a good representation of realistic, medium to large tidal estuaries. We will therefore use it to compare the effects of low-runoff (September 2012) and extremely high-runoff events (June 2013)

on estuarine circulation, salt mixing, and diahaline properties in realistic mesotidal estuaries.

c. Numerical simulations

Our numerical setup uses the General Estuarine Transport Model (GETM; Burchard and Bolding 2002). The hydrostatic model kernel of GETM is used for the present study, which applies the hydrostatic and Boussinesq assumptions (Klingbeil

and Burchard 2013). GETM is designed explicitly for coastal ocean and estuarine applications (Klingbeil et al. 2018). It allows for an efficient splitting of the baroclinic and barotropic modes and includes a state-of-the-art drying-and-flooding algorithm. The latter is particularly suited for the Elbe estuary with its large tidal flats, as previously demonstrated by Burchard et al. (2004). Turbulence closure is provided through coupling with the General Ocean Turbulence Model (GOTM; Burchard et al. 1999; Li et al. 2021), using a k - ϵ two-equation model (Umlauf and Burchard 2005) with a second-order closure (Canuto et al. 2001; Burchard and Bolding 2001). The present study applies a second-order Superbee advection scheme with minimal numerical mixing (Mohammadi-Aragh et al. 2015) on a C-grid. The setup was run from February 2012 to December 2013 at a barotropic time step of 2 s and a baroclinic time step of 20 s. The first 2 months of 2012 were reserved for spinup, the period from April 2012 to December 2012 was used for calibration, and the analysis takes place for the period from August 2012 to December 2013.

The model domain used in this study reaches from the weir at Geesthacht to the southeastern German Bight, as shown in Fig. 2. The model topography shown in Fig. 2a consists of data for the year 2010 from the DGM-W 2010 tidal Elbe dataset (Wasserstraßen- und Schifffahrtsamt Hamburg 2011) as well as a German Bight dataset (Bundesamt für Seeschifffahrt und Hydrographie 2019; Heyer and Schrottke 2015). Between 2010 and 2013, no major dredgings were conducted along the navigational channel.

The weak curvature of the Elbe navigational channel allowed for the creation of a horizontal curvilinear grid that closely follows the thalweg (see Figs. 2c–e). This grants a convenient analysis of cross-channel transects along each respective, transversal grid line. Additionally, a thalweg-following grid will likely lead to reduced numerical mixing compared to a Cartesian grid since the main flow will, on average, cross fewer grid lines. The grid was created with the Delft3D curvilinear grid generation tool “rgfgrid” (Deltares 2020). The grid consists of 616 transversal (cross-channel) and 305 longitudinal (along-channel) grid lines of varying resolution with a focus on the navigational channel. On average, this leads to a horizontal grid resolution of 200–400 m in the along-channel direction. Across the navigational channel, where the grid is focused, the resulting cross-channel resolution ranges mostly between 50 and 100 m, while it becomes as coarse as 400 m away from the focus in the German Bight. Cell center line 158 closely follows the thalweg from the open boundary to transect T_2 in Fig. 2 and is therefore suited as a transect along the thalweg. In the vertical, 30 equidistant sigma layers have been prescribed, leading to a resolution finer than one meter, even in the deepest parts of the navigational channel.

Along the open boundary in the German Bight, we prescribe downscaled parameters from a 600-m German Bight setup (Gräwe et al. 2015) using the Flather boundary condition (Flather and Davies 1975). This boundary forcing includes a half-hourly resolved, realistic tidal forcing in the form of surface elevations and hourly resolved vertical salinity and temperature profiles. A sponge layer with a width of three grid cells provides a smooth transition from the open boundary to the interior of the model domain.

Meteorological forcing consists of downscaled, 3-h-resolved data from the operational forecast model ICON by the German Weather Service (Zängl et al. 2015). It has a resolution of about 7 km and includes precipitation, wind direction, and magnitude 10 m above ground, dry air and dewpoint temperature 2 m above ground, and total cloud cover. The area-averaged magnitude and direction of the included wind forcing are displayed in Fig. 3a.

The main freshwater runoff is prescribed at the upstream end of the setup. It consists of daily averaged observations from Neu Darchau (Wasserstraßen- und Schifffahrtsamt Magdeburg 2021) that have been shifted by 1 day, as the observed runoff from Neu Darchau passes the weir in Geesthacht with a delay of about that duration (see Boehlich and Strotmann 2008). Additionally, all Elbe tributaries downstream of Hamburg are included, as they may interfere with the area of salt intrusion despite their overall low discharge. The river Ilmenau upstream of Hamburg is also included because it is one of the largest tributaries of the tidal Elbe. For the daily averages used, see Strotmann (2014, 2015), Landesamt für Landwirtschaft, Umwelt und ländliche Räume Schleswig-Holstein (2022), and Niedersächsischer Landesbetrieb für Wasserwirtschaft, Küsten- und Naturschutz (2022). Additional data and weighting factors have been received via personal communication from the Bundesanstalt für Wasserbau (BAW). The weighting factors are required to estimate the runoff of each tributary at the point where they enter the tidal Elbe from the datasets mentioned above. For the Kiel Canal and Rhin, only constant discharge values of 19.1 and 0.9 m³ s^{−1}, respectively, were available, while the combined Medem and Hadelner Kanal discharge was given as monthly averages. All other tributaries were provided with daily averaged discharge. The locations and average discharge of all tributaries that are included in the setup are depicted in Fig. 2c. The summed-up discharge from all included sources is shown in Fig. 3b for the analysis period from August 2012 to December 2013. It can be seen that the contribution of the tributaries to the total discharge is small within our model. The discharge salinities are set to a constant 0 g kg^{−1} for a more convenient interpretation of the salt dynamics. In reality, the freshwater runoff at Geesthacht has a finite salinity of about 0.35 g kg^{−1} that may vary slightly with the runoff (see Strotmann 2015).

d. Observational data

Setup calibration and validation were performed by comparing model output and observational data. For the location, names, and types of the observational stations used, we refer to Fig. 2a. The gauge data used for a tidal analysis are provided at 1-min resolution, while salt and temperature measurements are given at 5-min resolution. Measurements of salt and temperature were located 2.5 m above ground. Only for station D4 Rhinplate, surface and bottom salt and temperature data were available from 2012 to 2013, allowing for additional analysis of vertical stratification. All data are freely available via Wasserstraßen- und Schifffahrtsamt Elbe-Nordsee and Hamburg Port Authority (2023) and Wasserstraßen- und Schifffahrtsamt Elbe-Nordsee (2023).

e. Validation of model performance

As previously stated, the full model run covers the period from February 2012 to December 2013. Within this period, the setup reaches a semibalanced state after about 1 month of spinup. The setup was calibrated with model output for April 2012 to December 2012. Calibration was performed with respect to the M_2 and M_4 tidal range and M_2 tidal phase as well as salinity and temperature 2.5 m above ground. The spatial distribution of the bottom roughness length z_0 was used as a calibration parameter for the tides. To this end, z_0 was set to be proportional to the water depth. This is based on the real bottom roughness distribution within the Elbe estuary. However, this alone did not sufficiently dissipate the tidal energy upstream of Brunsbüttel, where the river contracts. To counter this, an artificial, steep linear increase of z_0 upstream of Brunsbüttel was superimposed to the depth-dependent distribution. The resulting bottom roughness length ranges from 1×10^{-4} to 6×10^{-3} m. The salt intrusion was not found to be sensitive to the choice of z_0 and was instead calibrated by setting the constant parameter for horizontal physical diffusivity K_h to a value of $20 \text{ m}^2 \text{ s}^{-1}$. Temperature calibration was limited by the low resolution of forcing data; see below.

Model validation is performed for the period from August 2012 to December 2013, which is also used for our study in section 3. To quantify the performance of our model as compared to observational data, we apply a number of statistical parameters: for the tidal data, we use the relative deviation of the modeled tidal amplitude A_{mod} from the observed amplitude A_{obs} in percent,

$$\Delta A_{\text{rel}} = \frac{A_{\text{mod}} - A_{\text{obs}}}{A_{\text{obs}}} \times 100, \quad (22)$$

the difference between the modeled tidal phase ϕ_{mod} and the observed phase ϕ_{obs} in minutes,

$$\Delta \phi = (\phi_{\text{mod}} - \phi_{\text{obs}}) \times \frac{T_{\text{tide}}}{360^\circ}, \quad (23)$$

with the period T_{tide} of each respective tidal constituent in minutes, as well as the root-mean-square error (RMSE) of the 30-h low-pass-filtered (subtidal) surface elevation data:

$$\text{RMSE} = \left[\frac{1}{N} \sum_{i=1}^N (\eta_{\text{mod},i} - \eta_{\text{obs},i})^2 \right]^{1/2}. \quad (24)$$

Here, N is the total number of samples and $\eta_{\text{mod},i}$ and $\eta_{\text{obs},i}$ are the modeled and observed data at each point in time, respectively. To quantify the model reproduction of observed temperature, salinity, and stratification, we use the RMSE for the nonfiltered data as well as the Pearson R^2 , computed from the correlation coefficient R :

$$R = \frac{\sum_{i=1}^N (\eta_{\text{mod},i} - \bar{\eta}_{\text{mod}})(\eta_{\text{obs},i} - \bar{\eta}_{\text{obs}})}{\sqrt{\sum_{i=1}^N (\eta_{\text{mod},i} - \bar{\eta}_{\text{mod}})^2 \sum_{i=1}^N (\eta_{\text{obs},i} - \bar{\eta}_{\text{obs}})^2}}. \quad (25)$$

Here, $\bar{\eta}_{\text{mod}}$ and $\bar{\eta}_{\text{obs}}$ are the mean of the modeled and observed data, respectively.

The statistics of the calibrated model regarding tidal analysis, salinity, temperature, and stratification are summarized in Tables 1 and 2. Slightly larger deviations of the computed tidal M_2 and M_4 amplitudes from the observations, as well as an increased RMSE of the subtidal sea level variability, mostly occur in the less well-resolved setup region upstream of Glückstadt (Fig. 4, Table 1). For St. Pauli and Zollenspieker, this is accompanied by an underestimation of the M_2 , M_4 , and S_2 tidal phase. The S_2 tidal amplitude tends to be overestimated by the setup, with the strongest overestimation between Brunsbüttel and Schulau.

Salinity also tends to be overestimated by the setup, as can be seen for all stations shown in Fig. 5 as well as in Table 2. This overestimation increases in upstream direction. However, with a Pearson correlation coefficient of $R^2 \approx 0.8$ for each station, the overall agreement between simulated and observed salinity is still high. There is no notable difference between the correlation of salinity throughout the tidal cycle and low-pass-filtered salinity, meaning that tidal variability and subtidal changes in salinity are reproduced at a similar quality.

The simulated water temperature follows the observed annual cycle as well as short-term variability, such as the decrease in temperature in late June 2013 (see Fig. 3c). However, the setup underestimates temperatures, especially in spring and summer. This discrepancy increases in upstream direction, as can be seen from the increasing RMSE (see Table 2).

For the simulation period from 2012 to 2013, only the station “D4 Rhinplate Nord” was available to provide observational data for salt and temperature stratification (see Fig. 3e). This station is located close to the upstream end of the salt intrusion, where the salinity is low. Consequently, the M_2 -filtered salt stratification is weak and rarely exceeds 0.5 g kg^{-1} . The location of this station complicates the validation of the model performance with respect to stratification, as the model stratification at this point will strongly depend on the simulated end of the salt intrusion: slight differences in the location of the salt intrusion between the model and observations may lead to large deviations in stratification. Consequently, the correlation between modeled and observed salt stratification is low, with a Pearson R^2 of only about 0.3 (see Table 2). Overall, the setup underestimates the observed salt stratification at Rhinplate but performs slightly better at times where the low-pass-filtered salinity is closer to the observed salinity (Figs. 3d,e). During September 2012 and June 2013, which will be the focus of this study, the modeled stratification is relatively close to the observations. Temperature stratification (not shown) lacks some skill in the setup and is underestimated at station D4 (Rhinplate), with a low Pearson correlation of 0.2 (see Table 2). Despite the low correlation, the RMSE for temperature stratification is only at 0.1°C because temperature stratification is generally weak at Rhinplate: the observed top to bottom temperature difference rarely exceeds 1°C on tidal and 0.2°C on subtidal time scales.

Regarding the tidal analysis, the stations where the dominant M_2 tide is less well reproduced are located far outside the area of salt intrusion and are, therefore, of little interest to the present study. The model tendency to overestimate the S_2

TABLE 1. Statistical summary of the model performance from August 2012 to December 2013 regarding M_2 , M_4 , and S_2 tidal amplitude and phase compared to observations at different stations along the Elbe estuary. For the location of each station, see Fig. 2a. The full name of Cuxhaven Sth. is Cuxhaven Steubenhöft. The subtidal root-mean-square error (RMSE) between the simulated and observed subtidal range has been computed from the 30-h low-pass-filtered data.

Tidal gauge	M ₂			M ₄			S ₂			Subtidal RMSE (m)
	A _{mod.} , A _{obs.} (A _{rel})	φ _{mod.} , φ _{obs.} (Δφ)		A _{mod.} , A _{obs.} (A _{rel})	φ _{mod.} , φ _{obs.} (Δφ)		A _{mod.} , A _{obs.} (A _{rel})	φ _{mod.} , φ _{obs.} (Δφ)		
Cuxhaven Sth.	1.33, 1.35 (−1%)	340, 341 (−2 min)		0.09, 0.11 (−21%)	211, 208 (3 min)		0.36, 0.34 (5%)	52, 53 (−1 min)		0.119
Brunsbüttel	1.26, 1.24 (1%)	12, 13 (−1 min)		0.13, 0.13 (1%)	261, 255 (6 min)		0.32, 0.30 (8%)	85, 84 (1 min)		0.112
Brokdorf	1.25, 1.22 (3%)	28, 31 (−7 min)		0.12, 0.12 (3%)	282, 285 (−4 min)		0.31, 0.28 (12%)	102, 106 (−9 min)		0.120
Glückstadt	1.27, 1.22 (4%)	42, 41 (1 min)		0.11, 0.12 (−4%)	304, 301 (3 min)		0.31, 0.28 (10%)	116, 115 (4 min)		0.122
Stadersand	1.37, 1.30 (6%)	61, 61 (0 min)		0.11, 0.10 (12%)	361, 349 (12 min)		0.32, 0.29 (10%)	139, 137 (3 min)		0.126
Schulau	1.46, 1.41 (4%)	71, 71 (0 min)		0.15, 0.10 (46%)	32, 28 (5 min)		0.34, 0.32 (7%)	151, 149 (3 min)		0.129
St. Pauli	1.55, 1.57 (−1%)	80, 83 (−6 min)		0.19, 0.17 (15%)	48, 65 (−17 min)		0.36, 0.36 (1%)	161, 162 (−2 min)		0.135
Zollenspieker	1.13, 1.10 (3%)	116, 121 (−9 min)		0.15, 0.17 (−11%)	152, 165 (−14 min)		0.26, 0.25 (4%)	199, 203 (−8 min)		0.275

tide is apparently countered in upstream direction by increasing tidal dissipation. The remaining differences between the model and observations can be explained by local topography and bottom roughness differences due to the limited model resolution.

The discrepancies between the modeled and observed salinity seem to be of a more complex origin. While the increasing overestimation of salinity in upstream direction indicates that the simulated salt intrusion is not sufficiently mixed with freshwater, the underestimation of stratification at Rhinplate implies that mixing is too strong. We conclude that vertical mixing might be overestimated in our simulation, leading to potentially reduced stratification. However, without observational data further downstream of the end of the salt intrusion, it is impossible to properly quantify the true extent of stratification underestimation. To explain the too-strong salt intrusion, it is consequently possible that horizontal fronts experience too little mixing in the simulation, despite our calibration with a rather high horizontal diffusivity of $K_h = 20 \text{ m}^2 \text{ s}^{-1}$. A comparative model run with a strongly reduced diffusivity $K_h = 0.001 \text{ m}^2 \text{ s}^{-1}$ yielded an unrealistically strong salt intrusion within the estuary and increased numerical mixing due to increased stratification, while the qualitative nature of our results regarding mixing and estuarine and diahaline circulation presented in section 3 was not changed. The respective versions of Figs. 5 and 3 as well as all figures from section 3 for the low-diffusivity case are included as Figs. S1–S8 in the online supplemental material. These results imply that our choice of K_h does not directly impact the dynamics discussed in section 3, which are dominantly driven by vertical stratification and mixing.

The station D4 Rhinplate Nord differs from the other stations in that it shows a tendency of salinity underestimation instead of overestimation: due to the finite salinity of the real Elbe freshwater, the observed salinities at this station do not fall below about 0.25 g kg^{-1} , while our simulation uses a freshwater runoff of 0 g kg^{-1} . This explains the underestimation of salinity from February 2013 to August 2013 (see Fig. 3d) despite the model tendency to overestimate the salt intrusion: during this phase, the runoff was relatively high (Fig. 3b), and stratification was low, so the observed salinity $> 0 \text{ g kg}^{-1}$ can likely be attributed to the real freshwater runoff. In phases where the simulated salt intrusion is slightly too strong, but the freshwater influence is still present, this may result in a seemingly correct reproduction of observed salinities, such as in September–December 2012.

To explain the temperature discrepancy between the model and observations, the $7 \text{ km} \times 7 \text{ km}$ resolved DWD weather forcing data were compared to a different dataset from a $1 \text{ km} \times 1 \text{ km}$ resolved atmospheric model (Norwegian Meteorological Institute 2022). The comparison indicated that the 7-km data resolution cannot correctly reproduce air temperatures directly above the Elbe River. While both datasets agreed above land, significant differences could be observed above the river, where the 7-km data tended to prescribe temperatures closer to those found on land. Unfortunately, the high-resolution data were not available for the period from 2012 to 2013. The underestimation of temperature stratification may

TABLE 2. Statistical summary of the model performance from August 2012 to December 2013 regarding salinity S , salt stratification $S_{\text{bott}} - S_{\text{surf}}$, temperature T , and temperature stratification $T_{\text{bott}} - T_{\text{surf}}$ compared to observations at different stations along the Elbe estuary. The full names of Cuxhaven AL, LZ2a, LZ1b, and D4 are Cuxhaven Alte Liebe, LZ2a Neufeldreede, LZ1b Krummendeich, and D4 Rhinplate Nord, respectively. All values shown are for the nonfiltered (i.e., tidal) data. Temperature and salt stratification have been computed as the difference between surface and bottom values. Note that stratification data were available only for station D4 Rhinplate Nord, where bottom, surface, and stratification values are shown in separate rows.

Salt/temp station	R^2 (RMSE)			
	S	$S_{\text{bott}} - S_{\text{surf}}$	T	$T_{\text{bott}} - T_{\text{surf}}$
LZ4a Steinriff	0.834 (2.0 g kg ⁻¹)	—	0.993 (0.7°C)	—
Cuxhaven AL	0.823 (3.5 g kg ⁻¹)	—	0.992 (0.8°C)	—
LZ2a	0.853 (3.1 g kg ⁻¹)	—	0.992 (1.3°C)	—
LZ1b	0.857 (2.4 g kg ⁻¹)	—	0.994 (1.4°C)	—
D4 (surface)	0.858 (0.5 g kg ⁻¹)	—	0.995 (1.5°C)	—
D4 (bottom)	0.857 (0.5 g kg ⁻¹)	—	0.995 (1.5°C)	—
D4 (stratification)	—	0.293 (0.2 g kg ⁻¹)	—	0.203 (0.1°C)

have the same cause. However, due to the generally low subtidal stratification, temperature is considered here to be only of minor importance for the estuarine dynamics inside the tidal Elbe.

Despite the overlap of the calibration and analysis periods, no clear bias in the model performance was found between the end of 2012 (analysis and calibration) and the year 2013 (only analysis).

From the above-presented performance of our numerical setup, we conclude that our simulation is suited for the aims of this study. Nonetheless, it should be kept in mind that the strength of vertical stratification might be slightly

underestimated, while horizontal salinity gradients may be overestimated.

3. Results and discussion

In the following, TEF, mixing, and diahaline properties will be compared for the high-runoff month of June 2013 and the low-runoff month of September 2012. Unless mentioned otherwise, these properties have been averaged over two spring-neap cycles, i.e., over the first 29.5 days of each month. This will be referred to as spring-neap *averaged*. In section 3c,

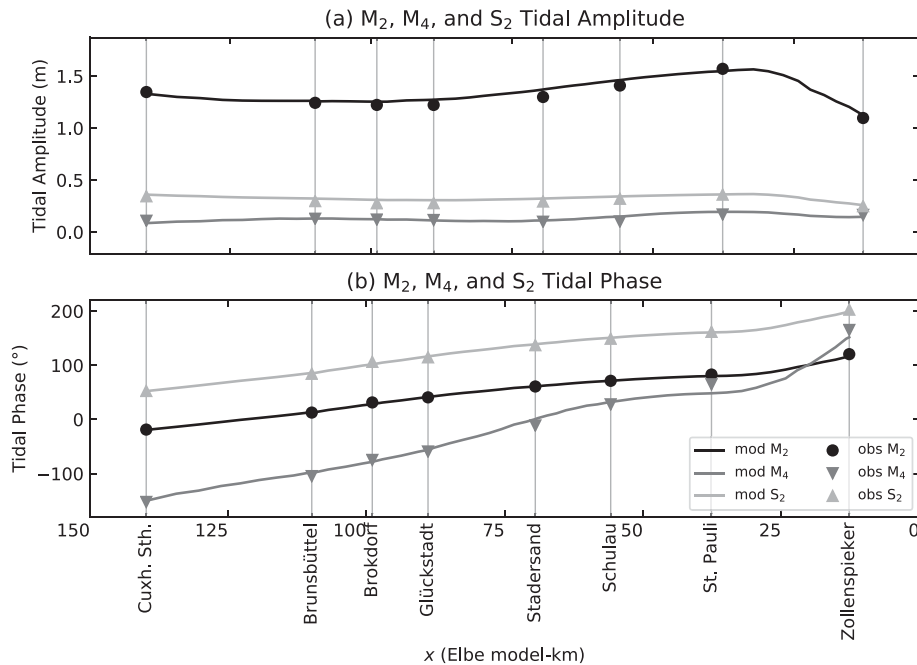


FIG. 4. Comparison of M_2 , M_4 , and S_2 (a) tidal amplitude and (b) tidal phase from the tidal Elbe setup with observational data from different gauges along the channel, which are located at the vertical lines and named along the x axis. For the model data, the tidal amplitude and phase have been computed along the navigational channel. The full name of the leftmost gauge is Cuxhaven Steubenhöft. The tidal analysis has been performed for the analysis period from August 2012 to December 2013.

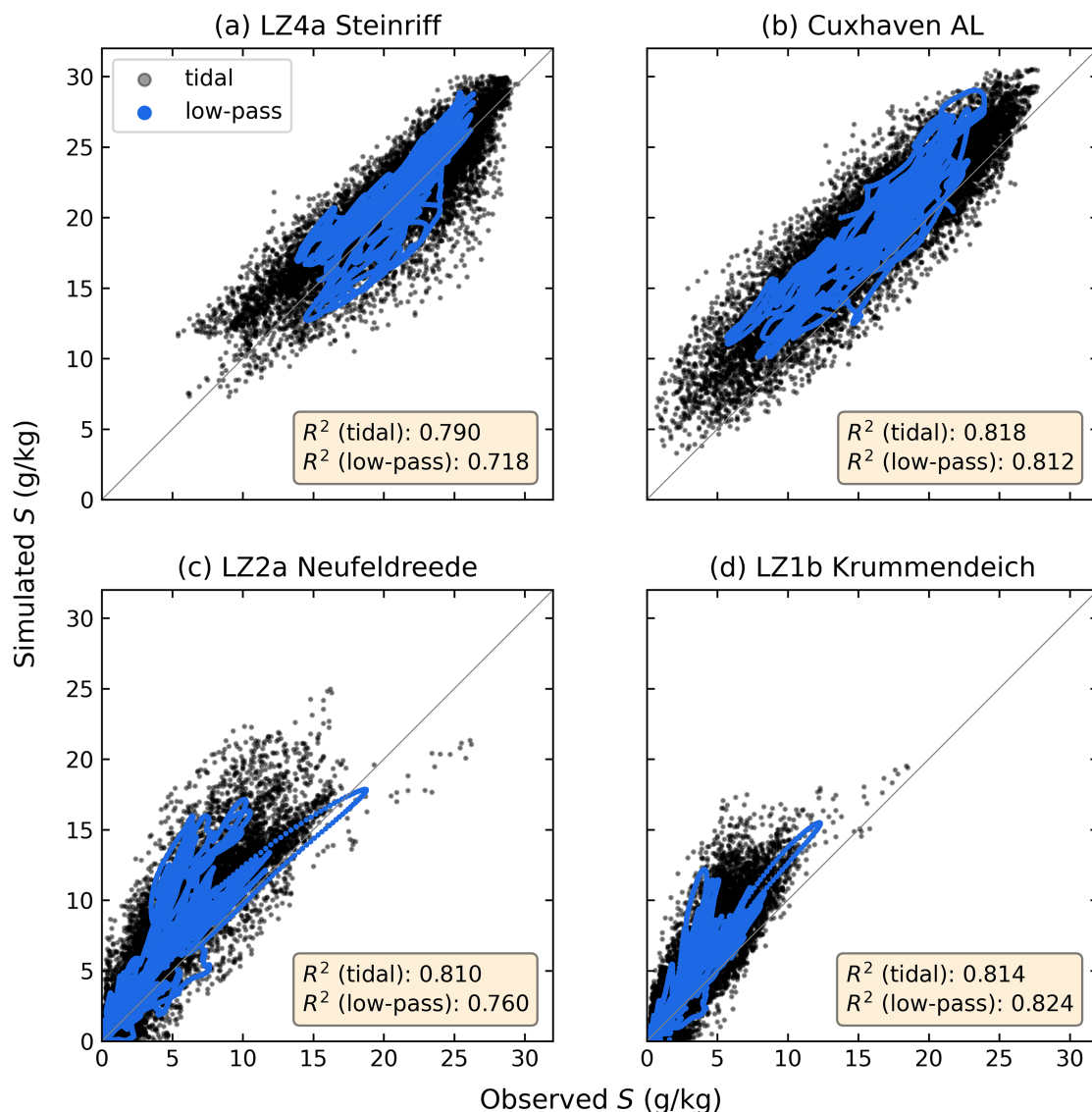


FIG. 5. Correlation of observed and simulated salinity 2.5 m above ground at the stations (a) LZ4a Steinriff, (b) Cuxhaven Alte Liebe, (c) LZ2a Neufeldreede, and (d) LZ1b Krummendeich for the analysis period from August 2012 to December 2013. Gray dots represent tidally varying salinity data, while the blue dots represent data that have been low-pass-filtered to remove M_2 tidal variability. The stations are given in an order of increasingly upstream positions.

this choice of averaging period is motivated and tested in more detail. Mixing will additionally be analyzed as an M_2 -averaged, temporally varying property from August 2012 to December 2013.

a. Salt distribution

To illustrate the general situation regarding salinity and stratification inside the Elbe estuary for each month, we first introduce the salinity distribution in September 2012 and June 2013, shown in Fig. 6. Since the spring-neap variability of salt intrusion within each month was found to be much smaller than the differences between both months, we only consider the spring-neap averaged distributions here. We find that the high-runoff event in June 2013 has resulted in a significant freshening of the estuary compared to the low-runoff

period in September 2012. This is true for both the surface salinity and the vertical salt distribution along the thalweg. In June, the salt intrusion has moved about 30 km downstream compared to September (see Figs. 6c,d). Furthermore, increased isohaline areas and increased vertical stratification are found in June. A time-resolved analysis of stratification at Cuxhaven Steubenhöft (see Fig. 2a), defined as the difference between bottom and surface salinity as before in Fig. 3e, revealed that in our simulation, this vertical stratification is persistent throughout the entire tidal cycle from 4 to 24 June 2013 (not shown). During low tide, stratification reaches up to 10 g kg^{-1} , while a reduction of up to 8 g kg^{-1} occurs during high tide. In September 2012, persistent stratification only occurred for two 3-day periods after neap tide and is generally much weaker than in June 2013.

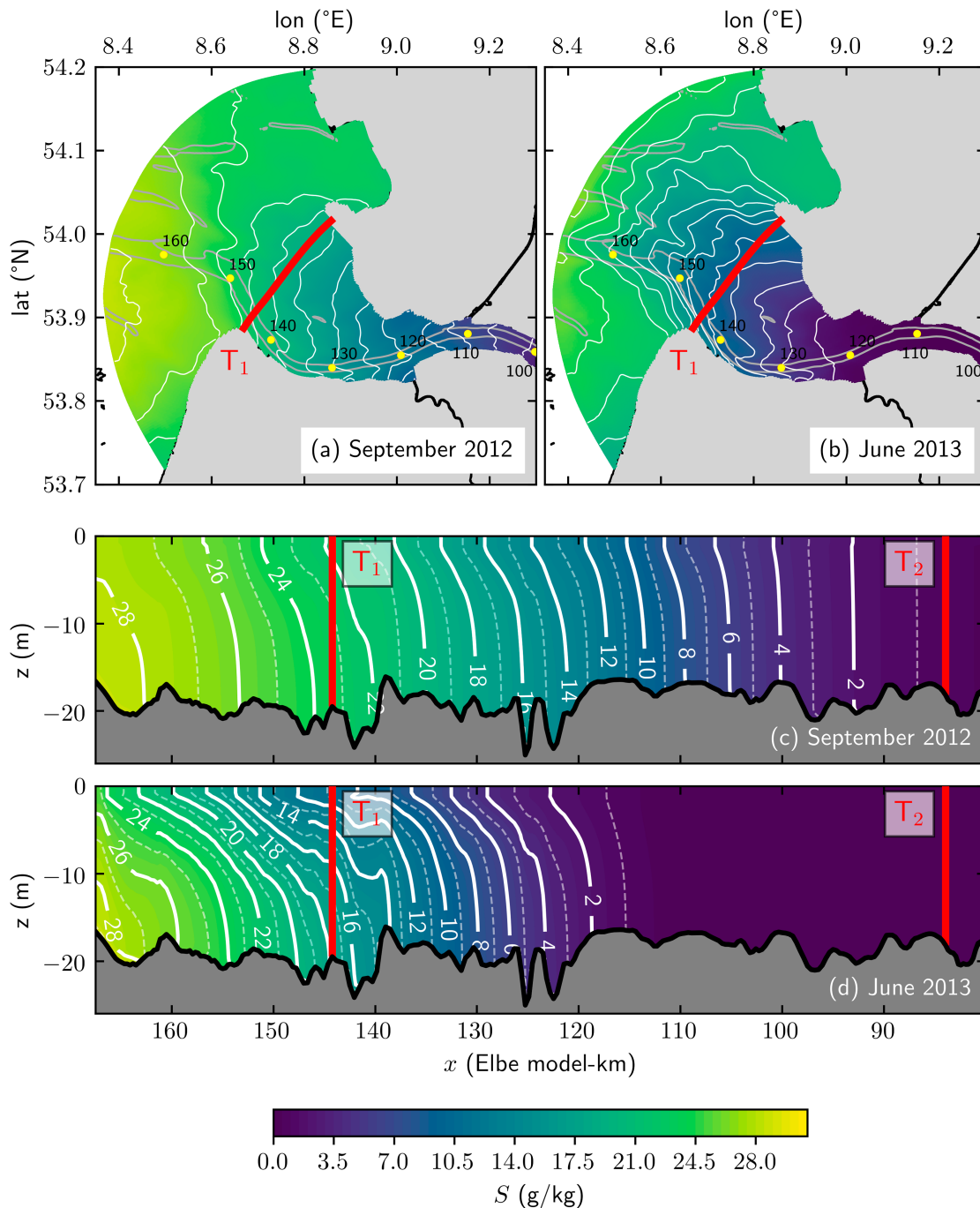


FIG. 6. Simulated, spring-neap averaged salinity distribution inside the Elbe estuary. (a),(b) Surface salinity in September 2012 and June 2013, respectively. (c),(d) Vertical salinity distribution along the navigational channel in September 2012 and June 2013, respectively. Bold white lines are isohalines at even salinities, and dashed white lines are isohalines at odd salinities. In (a) and (b), the gray outline corresponds to the 12-m isobath. The black outline in (c) and (d) indicates the bottom topography. Transects T_1 and T_2 enclose the estuarine volume discussed in section 3b.

The freshening of the estuary and coastal waters during the extreme runoff event in June 2013 is consistent with earlier studies of this event, including observational data presented by Voynova et al. (2017) as well as numerical simulations of the German Bight by Kerimoglu et al. (2020) and Chegini et al. (2020). However, the increased stratification found in our simulation for June 2013 contrasts the findings by

Kerimoglu et al. (2020) and Chegini et al. (2020). These studies reported an increased vertical stratification in the deeper parts of the German Bight, but no persistent stratification was found within the estuary itself. It is likely that the comparatively large-scale setups of the German Bight used for these studies could not resolve important processes within the Elbe estuary, as mentioned by Chegini et al. (2020) themselves.

Furthermore, it should be noted that both [Kerimoglu et al. \(2020\)](#) and [Chegini et al. \(2020\)](#) found that the stratification dynamics in the German Bight were not only runoff-driven but also strongly dependent on wind direction and magnitude. Within the area corresponding to the model domain of the present study, however, the results by [Kerimoglu et al. \(2020\)](#) showed that the distribution of surface salinity depended almost exclusively on freshwater runoff instead of wind, meaning that our model domain only includes the discharge dominated section of the river mouth. Additionally, the wind magnitude and direction above the Elbe River mouth were similar in September 2012 and June 2013 and the magnitude did not reach the strength of the autumn and winter storms from 2013 (see [Fig. 3a](#)). In the following, we will therefore compare September 2012 and June 2013 without discussing wind conditions. As shown in the following paragraphs, this is reasonable with respect to spring–neap averaged mixing dynamics, which can primarily be attributed to freshwater discharge.

b. Influence of freshwater discharge on the estuarine circulation

To analyze differences in the estuarine circulation between September 2012 and June 2013, we consider the along-channel (x -) variability of TEF properties, mixing, and effective vertical diahaline velocity between the transects T_1 and T_2 from [Fig. 2a](#). We find that all properties become nonzero further downstream in June than in September, which can be attributed to the reduced salt intrusion in June. In both months, the sum of inflow and outflow is close to the spring–neap averaged freshwater runoff; see [Figs. 7a](#) and [7b](#). The sum slightly underestimates the magnitude of the runoff in September, while it is overestimated in June. These deviations are due to slow mean water level variations in the German Bight which are included in the boundary conditions. At the same time, the bulk inflow and outflow salinities are considerably fresher in June, accompanied by a strongly increased difference $\Delta s = s_{\text{in}} - s_{\text{out}}$ toward the downstream end of the channel section ([Figs. 7c,d](#)). This is consistent with the findings from the previous section as well as the broader salinity range covered by the TEF inflow and outflow ([Figs. 8c,d](#)). The longitudinal distribution of $Q(x, S)$ shown in [Figs. 8a](#) and [8b](#) can be interpreted as a streamfunction for water transport in salinity space. It is of similar shape in both months.

Next, we compare the volume-integrated mixing inside the estuarine volume bounded by a TEF transect at position x to the mixing estimate (12) from [MacCready et al. \(2018\)](#) (see [Figs. 7e,f](#)). In September, the simulated mixing is underestimated by the estimate (12) by up to 10%, which is within the range of accuracy presented by [Burchard et al. \(2019\)](#) for idealized estuaries. In June, the estimate and total mixing agree even better, with only a small overestimation. Numerical mixing is small in both months so that the total mixing M_T closely represents physical mixing. The numerical mixing is weakly negative due to the choice of advection scheme; see [Klingbeil et al. \(2014\)](#) for an in-depth discussion of the negative mixing tendencies of the Superbee advection scheme. Most notably,

however, mixing increases much faster with volume in June than in September. A similar behavior is found for the cross-channel integrated local mixing per salinity class,

$$m_x(x, S) = \int_{y_{\min}}^{y_{\max}} m_{xy}(x, y, S) dy, \quad (26)$$

shown in [Figs. 8e](#) and [8f](#). In (26), $y_{\min}(x)$ and $y_{\max}(x)$ are the bounding cross-channel coordinates of the river section. Here, the overall mixing intensity is strongly increased in June. In both months, local maxima of mixing can be found at model-km 122, 127, and 140. In September, an additional maximum occurs at model-km 110, which in June is in the freshwater range and therefore not visible. Mixing is strongest for salinity classes between the inflow and outflow layers. It tends to span a broader salinity range in places where local maxima occur, particularly at the 110-km maximum.

The cross-channel integrated estimate (20) for the effective vertical diahaline velocity from [Klingbeil and Henell \(2023\)](#), by definition, yields local extrema in the same x -locations as the cross-channel integrated local mixing; see [Figs. 8g](#) and [8h](#). Results are very similar to the directly computed distribution of $\int u_{\text{dia},z}^S dy$ shown in [Figs. 8i](#) and [8j](#). In particular, we can see a layer of outward-directed diahaline transport at low salinities and a layer of inward-directed diahaline transport at high salinities. The separation of the two layers closely follows the average of the flux-weighted TEF (isohaline) bulk salinities, $(S_{\text{in}} + S_{\text{out}})/2$. Overall, the effective vertical diahaline velocity is of greater magnitude in June than in September.

In a modeling study of the Hudson River estuary with idealized external forcing, [Wang et al. \(2017\)](#) focused on the along-channel variability of the isohaline transport $q(x, S)$, entrainment velocity (here, $-u_{\text{dia},z}^S$), and diffusive salt flux (i.e., salt mixing) within a single spring–neap cycle. The spring–neap averaged along-channel profiles yielded results similar to the ones found in this study, with a two-layer total exchange flow. [Wang et al. \(2017\)](#) also located the strongest mixing in between the inflow and outflow layers, with local extrema due to topography effects. The mechanisms causing such local extrema were studied in detail by [Warner et al. \(2020\)](#). Most notably, they showed that the locations and mechanisms of strong mixing vary between flood and ebb. As in our study, the entrainment velocity in [Wang et al. \(2017\)](#) displayed local extrema in the same along-channel locations as mixing. Here, we find a similar causality with topography: At model-km 110, the Kiel Canal connects with the estuary (see [Fig. 2a](#)), providing a topographical irregularity as well as an additional inflow of freshwater. The mixing of this new freshwater source explains the wide salinity range of this extremum, occurring at lower salinity classes than the remaining extrema. The extrema at 122 and 127 km coincide with the location of two particularly deep sections of the navigational channel (see [Figs. 6c,d](#)) as well as the upstream end of a side branch of the navigational channel, the so-called Medem branch (see [Fig. 2c](#)). At 140 km, this branch reconnects with the navigational channel, explaining the last of the occurring extrema.

Whereas the study by [Wang et al. \(2017\)](#) focused on the along-channel variability of estuarine circulation within a

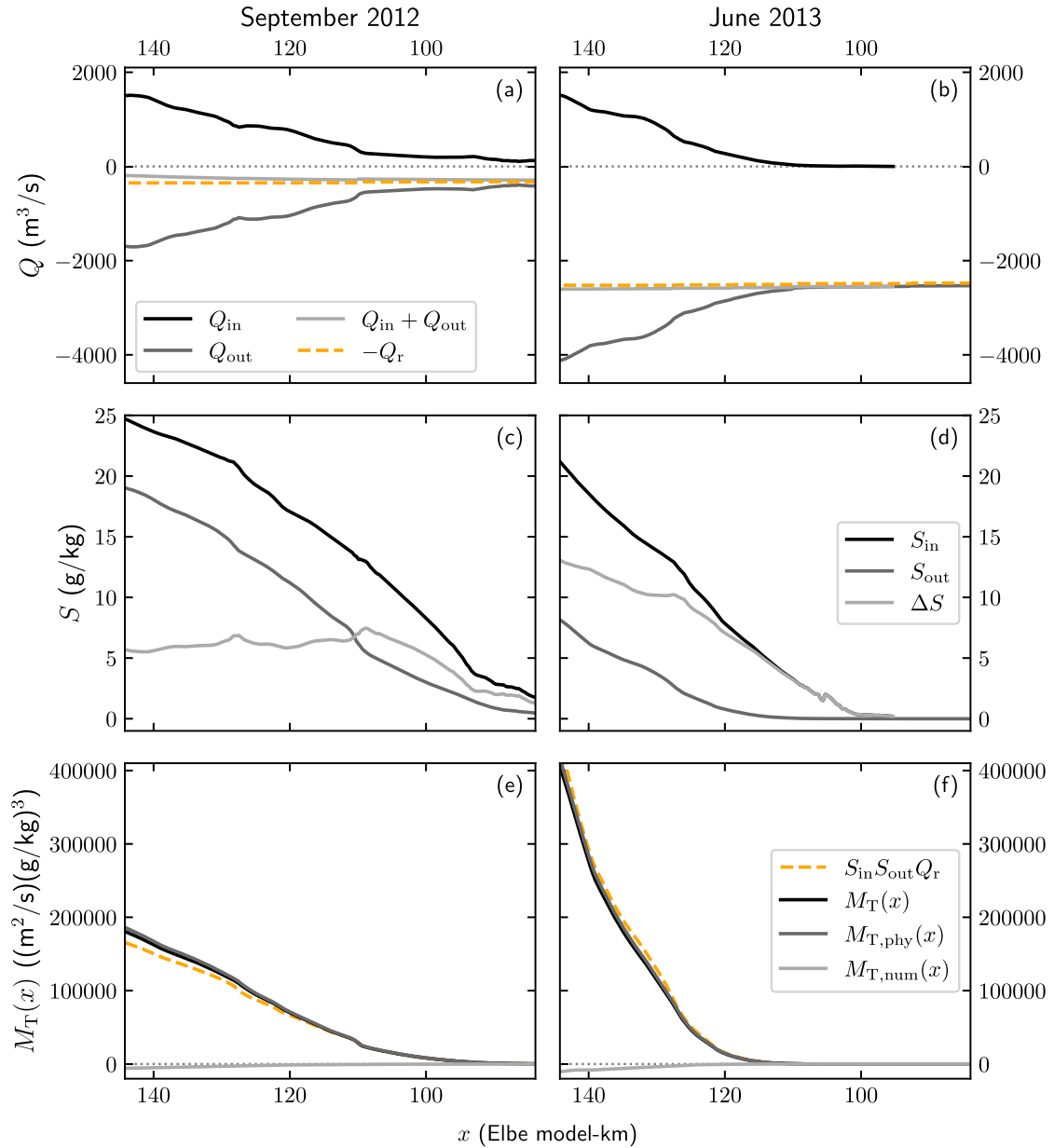


FIG. 7. Along-channel variability of spring-neap averaged TEF properties in (left) September 2012 and (right) June 2013. (a),(b) TEF inflow and outflow and their sum $Q_{in} + Q_{out}$, and spring-neap averaged freshwater runoff Q_r . (c),(d) Respective TEF inflow and outflow salinities and their difference $\Delta S = S_{in} - S_{out}$. (e),(f) Total mixing M_T (11) inside the estuarine volume bounded by a vertical transect at each respective model-km, its numerical and physical contributions $M_{T,num}$ and $M_{T,phy}$, and the mixing estimate (12) from MacCready et al. (2018). The runoff Q_r is a step-like function of the along-channel distance x , as tributaries are added in downstream direction starting at the position x where they enter the estuary.

single spring-neap cycle and at constant runoff, we focus here on the impact of extreme runoff. From our results, it is evident that the freshening of the estuary in June 2013 applies to all TEF, mixing, and diahaline parameters. Additionally, the broader salinity range of $Q(x, S)$ and $q(x, S)$ in June directly results from the increased vertical salt stratification. The estuarine circulation, therefore, reacts strongly to the increased runoff but without changing the basic shape of its streamfunction $Q(x, S)$ and its two-layer structure. Regarding the TEF bulk values, such a runoff dependency has, e.g., also been

found for the Hudson and Merrimack estuaries (Chen et al. 2012).

Our results show that the strengthened isohaline outflow $q(x, S)$ during high runoff is accompanied by increased mixing intensity. The increase in effective vertical diahaline velocity links this increased mixing with the diahaline circulation: The excellent agreement between relation (20) and the directly computed diahaline velocity in both months (see Figs. 8g–j) implies that horizontal diffusion is of minor importance in the Elbe estuary. The S gradient of the local mixing per

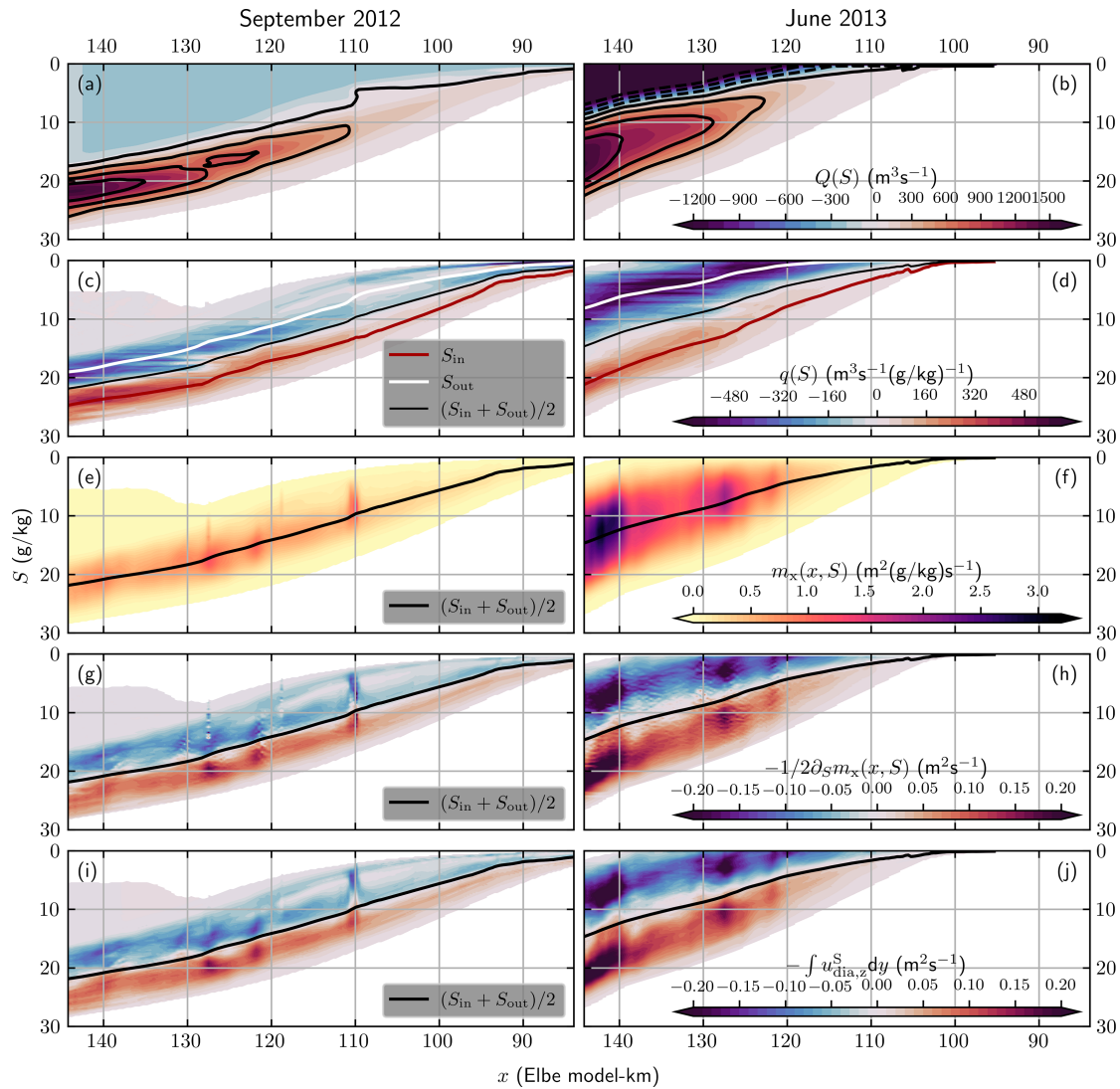


FIG. 8. Spring-neap averaged TEF, mixing, and diahaline properties vs along-channel position x and salinity class S in (left) September 2012 and (right) June 2013. (a),(b) Volume transport $Q(S)$ for salinities $s > S$. (c),(d) Volume transport per salinity class $q(S)$. The red and white lines indicate the TEF inflow and outflow salinities, respectively. The black line represents the average of TEF inflow and outflow salinity, i.e., $\bar{S} = (1/2)(S_{\text{in}} + S_{\text{out}})$. (e),(f) Local mixing per salinity class, integrated in cross-channel direction. (g),(h) Negative effective vertical diahaline velocity as estimated from (20) (Klingbeil and Henell 2023). (i),(j) Negative effective vertical diahaline velocity as computed online with GETM.

salinity class (here, m_x) therefore directly forces the diahaline circulation.

Last, from Figs. 7e and 7f, it follows that the mixing estimate (12) holds well for the high-runoff event in June 2013, while slightly larger deviations occur in September 2012. In a numerical study of mixing in the fjord-like Puget Sound, Broatch and MacCready (2022) found an excellent agreement between the estimate and actual mixing even for only tidally averaged properties. They argued that in their study, mixing was mostly limited to the river mouths far inside the estuary, while salinity variance from the seaward boundary only played a minor role. In our study, mixing appears to be strongly runoff-dependent for the high-runoff period in June 2013. Short estuarine turnover times would be expected for such periods,

with only short-lived volume and salt storage along the seaward estuarine boundary. Under such conditions, the estimate should indeed perform similarly well as in Broatch and MacCready (2022). In September, however, when runoff is low, storage effects may gain some importance due to increased turnover times.

c. Universal law of estuarine mixing

In contrast to the mixing estimate (12) from MacCready et al. (2018), the universal law (15), which describes the mixing across a single isohaline surface, depends only on the freshwater runoff and is independent of the TEF inflow and outflow salinities, which were found to vary strongly between September 2012 and June 2013. Because the universal law

refers to an estuarine volume bounded by isohalines instead of a vertical transect, it is also independent of the spatial location of the salt intrusion. A good agreement between the universal law and the simulated mixing after sufficiently long averaging therefore directly illustrates the dependence of mixing within such a volume on freshwater runoff. As mentioned by Burchard (2020), it may depend on different factors, such as the type of estuary, how long exactly a “sufficiently long” averaging period would be. In the case of the extreme runoff events considered in this study, we try to find averaging periods that properly cover the extent of each event while still allowing for a convergence of the simulated mixing with the universal law. To this end, only a limited number of averaging periods are suited in the first place: To properly resolve the extreme event, averaging should at maximum be performed for the time span of the event. In the case of the Elbe high-runoff event, this is about 1 month. Shorter averaging periods should not consist of incomplete cycles of the dominant M_2 or spring–neap tides. Otherwise, it would not be possible to distinguish between effects of the respective tidal cycle and effects of the extreme event. Consequently, we here compare the conformance of simulated mixing to the universal law for averaging periods of two M_2 cycles (about 1 day), one spring–neap cycle (about 2 weeks), and two spring–neap cycles (about 4 weeks). For better compatibility of the 1-day and 2-week averaging periods to the 1-month period, we choose time frames at different stages of each event. For the low-runoff period in September, the runoff is relatively constant, so that the 1-day averaging periods are about equally spaced throughout the month. Placement has been chosen to cover phases of increasing (S-M2-3) and right after decreasing (S-M2-1) runoff as well as the day of greatest change (S-M2-2); see Fig. 9a. For the June event, the spread of different runoff situations is much greater (Fig. 9b), so an additional fourth 1-day window was chosen. The four windows cover the comparatively low, but increasing runoff in the beginning of June (J-M2-1), the day of strongest runoff increase (J-M2-2), the day of maximum runoff (J-M2-3), and a day of decreasing runoff toward the end of the month (J-M2-4). For the 2-week averaging periods, we chose time frames covering the first two weeks (SN-1), center two weeks (SN-2), and last two weeks of each month (SN-3), respectively.

The universal law yields mixing across isohalines completely inside the model domain. In our numerical simulation, isohalines at higher salinity classes will leave parts of the model domain, reducing the integration surface and thus leading to a deviation of the simulated mixing from the universal law. To quantify which salinity classes leave the model domain to a significant amount, we consider the averaged, integrated diahaline volume transport (19). For isohalines fully inside the model domain, this quantity should be close to Q_r . Consequently, all salinity classes where the integrated diahaline volume transport diverges from Q_r leave the domain to such a degree that the simulated mixing can no longer be compared to the universal law. In the case of the funnel-shaped Elbe estuary, this is identical to the salinity classes where the average isohaline surface area does not increase monotonously toward higher salinity classes anymore. In the

following, we will only compare the universal law to the mixing in salinity classes that are fully inside the model domain.

The results displayed in Figs. 9c–h show that in September, where the runoff is mostly uniform, the computed mixing is similar to the universal law almost independently of the averaging period. Only for the 1-day averaging periods S-M2-2 and S-M2-3, some deviation from the universal law occurs at higher salinity classes, which implies storage effects. For the remaining 1-day period S-M2-1, as well as all longer averaging periods, the simulated mixing is very close to the universal law. In contrast to September, the computed mixing in June only converges toward the universal law with an increasing length of the averaging period. During periods of greatest change, the deviation from the universal law is greater than during periods of smaller change, as can be seen for the 1-day averaging J-M2-2 as well as the 2-week averaging during the first half of the month J-SN-1. For the 1-month averaging period, the computed total mixing per salinity class is close to the universal law for both months for isohalines fully contained inside the setup volume (see Figs. 9g,h). The absolute deviation from the universal law is found to be about the same in both months. In September, the actual mixing is slightly underestimated, while in June, it is slightly overestimated.

The comparison of the different averaging periods demonstrates that even in a single estuary, the period required for conformance to the universal law may vary strongly depending on the state of the estuary. For periods of uniform freshwater discharge, even an averaging period as short as a day may lead to an excellent estimation of the actual mixing. However, we note that our setup was forced with daily-averaged freshwater discharge, so shorter-scale changes of discharge are not included. Inside a real estuary, the required averaging period might therefore be slightly longer than a day. For sudden discharge events such as in June, daily averages yield a rough estimation of the actual mixing, but longer averaging of at least one spring–neap cycle (2 weeks) is necessary for a more accurate prediction. However, for 2-week averaging, the exact quality of the estimate still depends on the placement of the period within the event. A 1-month averaging period removes this dependency, as it covers the full event and reproduces the universal law well. We therefore consider the averaging period of 1 month to be a good choice for the analysis of the high-discharge event and for the comparison to the low-discharge period in September 2012. The results for 1-month averaging demonstrate that the universal law (15), just as the mixing estimate (12) before, holds well under the extreme runoff conditions in June. It also holds well in September, demonstrating that mixing in the Elbe estuary is indeed strongly runoff-dependent on spring–neap averaged time scales. As before for the estimate (12), deviations from the universal law can most likely be explained with storage effects.

d. Temporal variability of mixing

So far, we have demonstrated that the spring–neap averaged mixing is stronger in June than in September and

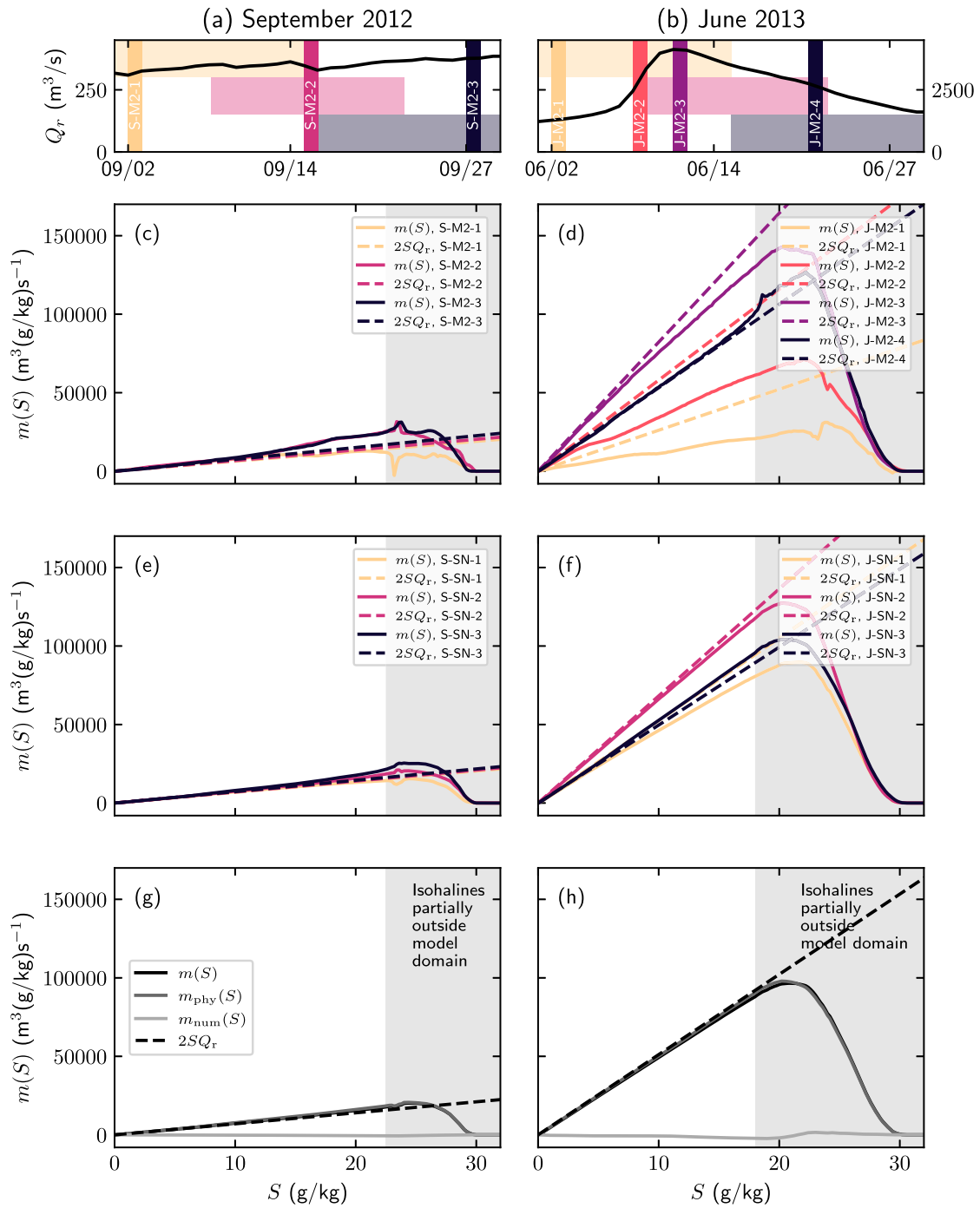


FIG. 9. Performance of the universal law (15) in the Elbe estuary in (left) September 2012 and (right) June 2013. (a),(b) Daily-averaged freshwater discharge. Vertical lines show the placement of the 1-day averaging periods displayed in (c) and (d). Colored bars show the placement of the single spring-neap cycle averaging periods displayed in (e) and (f). From top to bottom, these averaging periods cover the first two weeks (SN-1), center two weeks (SN-2), and last two weeks (SN-3) of the first 29.5 days of each month. Note that the y axis in (b) has been scaled with a factor 10 compared to (a). (c)–(h) Simulated mixing per salinity class $m(S)$ as computed for the entire model domain of the tidal Elbe setup (bold lines) compared to the universal law (dashed lines) for averaging periods of two M_2 cycles in (c) and (d), one spring-neap cycle in (e) and (f), and two spring-neap cycles in (g) and (h). In (g) and (h), the physical and numerical fractions m_{phy} and m_{num} of the total simulated mixing are also shown. The gray-shaded areas indicate salinities where the isohalines are not fully inside the model domain, computed for the 1-month averaging period.

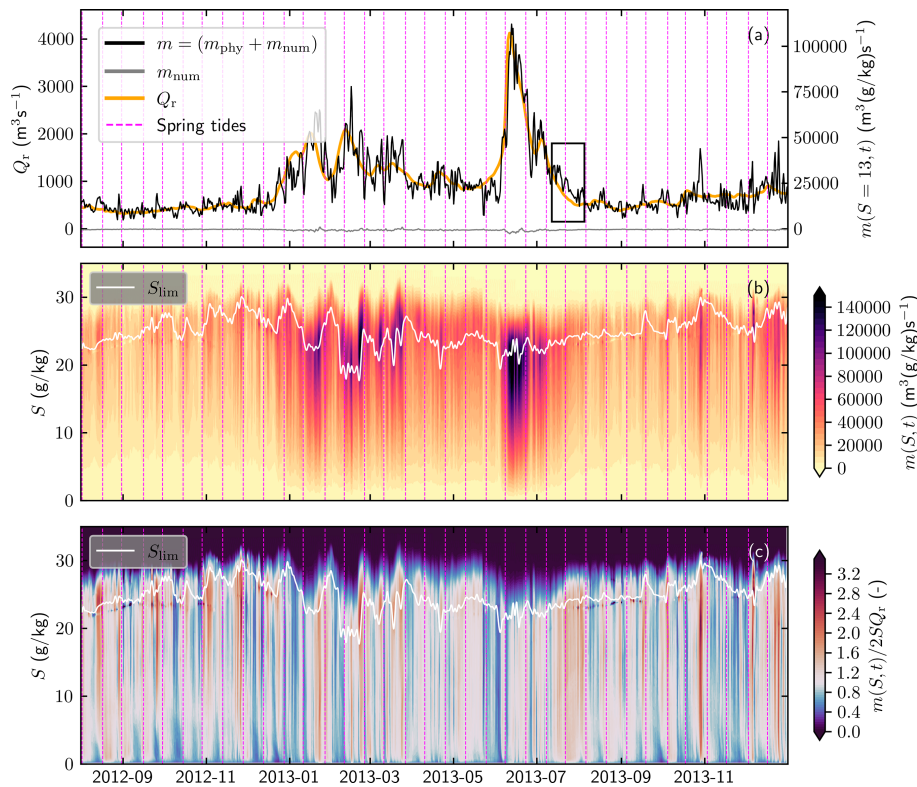


FIG. 10. Temporal evolution of M_2 -averaged mixing inside the Elbe estuary from August 2012 to December 2013. (a) Mixing at a salinity $S = 13 \text{ g kg}^{-1}$, showing numerical mixing and total mixing $m = m_{\text{phy}} + m_{\text{num}}$, and freshwater runoff Q_r . The freshwater runoff has been linearly interpolated from daily averages to the M_2 -cycle data points of mixing. The axis for the freshwater runoff has been scaled with the universal law (15) to fit the proportions of the mixing axis. The black rectangle marks the period of prolonged mixing underestimation by the universal law seen also in (c). (b) Total mixing per salinity class $m(S, t)$ for all salinity classes. (c) Total mixing per salinity class $m(S, t)$ normalized with the universal law (15). The dashed magenta lines indicate spring tides. The white line in (b) and (c) is the maximum salinity S_{lim} still fully inside the model domain for the area surrounding the navigational channel. The northeastern and southwestern parts of the open boundary have not been considered for S_{lim} because there, negligible amounts of freshwater enter the model domain without notably influencing mixing and circulation inside the estuary.

strongly runoff-dependent in both months. To put these findings into further context, we now consider the temporal evolution of total mixing per salinity class and of the universal law. We find that even the tidally averaged mixing adjusts to changes of the discharge, but with an overlying variation on shorter time scales of several days that was found to coincide with variations of wind magnitude (see Figs. 3a and 10a). Periods of increased mixing can be found from January to April 2013 and in June 2013 and coincide with increased runoff. The extreme runoff event in June is accompanied by the strongest mixing within the entire considered time period, meaning it is also an extreme mixing event. The periods of generally increased mixing occur throughout all salinity classes (Fig. 10b). During weaker runoff in September and October 2013, an additional signal of increased mixing becomes visible around the transition from neap to spring tides. This apparent spring-neap signal is more pronounced when mixing per salinity class is normalized with the universal law (15); see Fig. 10c. There, the signal occurs during low runoff

as brief periods of strong underprediction by the universal law, i.e., $m(S, t)/(2SQ_r) > 1$. A comparative model run with a reduced constant horizontal diffusivity $K_h = 0.001 \text{ m}^2 \text{ s}^{-1}$ yielded a more pronounced spring-neap signal due to the presence of stronger vertical stratification, but the freshwater discharge still remained the source of strongest modulation of salt mixing (see Fig. S7). Additional periods of strong underprediction in Fig. 10c were found to coincide with storms, especially from January to April 2013; see also Fig. 3a. During periods of increased mixing associated with high runoff, on the other hand, $m(S, t)/(2SQ_r)$ mainly varies between values of 0.8 and 1.4, meaning that mixing roughly follows the universal law. The river flood is immediately succeeded by a prolonged period of relatively strong and consistent underestimation in late July and early August 2013 (see Figs. 10a,c).

In consistency with Fig. 9, the results from Figs. 10a and 10c show that the universal law is a reasonably good, first approximation even for the temporal evolution of mixing with a varying freshwater runoff. This underlines the key role of

freshwater runoff with respect to mixing in the Elbe estuary. For Puget Sound, Broatch and MacCready (2022) demonstrated that the spring–neap cycle and wind forcing are clearly of secondary importance. Here, we find a similar situation for the Elbe, where wind mostly has a modulating effect. However, we also see that the universal law tends to fail for strong wind events, i.e., periods of increased wind amplitude that last only up to a few days. An example is the strong underestimation of mixing by the universal law in late October 2013. During such periods, previously built-up stratification can be degraded, volume storage changed, and salt storage can be increased due to large-scale effects in the German Bight. Such processes are not represented in the freshwater runoff and thus the universal law, leading to the reported mismatch.

Earlier studies that used idealized, constant runoff scenarios found a strong spring–neap dependence of mixing, such as Wang et al. (2017), MacCready et al. (2018), Wang and Geyer (2018), and Li et al. (2022). For the Changjiang estuary, which has a powerful tidal spring–neap signal, a spring–neap variability of mixing was found even for a realistic runoff scenario (Li et al. 2018). However, the study focused on a relatively short period of three spring–neap cycles and did not put mixing into the context of the freshwater runoff. To study a high- and a low-runoff scenario in the Pearl River estuary, Li et al. (2022) used idealized spring–neap modulated tidal forcing. Similar to the present study, they found an increased spring–neap variability of the conformity of mixing to the universal law during the low-runoff scenario. The magnitude of the spring–neap variability of mixing is expected to be similar throughout the year. When normalized with the universal law, it becomes more visible during low runoff, when the relative deviation with respect to the magnitude of the runoff is largest.

Last, the period of increased underestimation by the universal law in July and August 2013, after the extreme event in June, possibly results from the destruction left over of stratification that was built up during the high-runoff period. It supports our assumption that the slight overestimation of mixing by the universal law in June, as found in Fig. 9h, coincided with a decrease in salt storage, which could also be interpreted as a relative increase in freshwater storage. Such a freshwater storage would lead to additional mixing as the system returns to normal. As the mixing overestimation occurs throughout all salinity classes, it is unlikely that it is solely caused by open boundary forcing. Nonetheless, the increased stratification in the German Bight reported by Voynova et al. (2017) until the end of August 2013 may still have played some part in the overestimation via open boundary forcing.

In addition to the findings from Broatch and MacCready (2022) and earlier studies, we conclude that the accuracy of mixing estimates in the Elbe estuary is not independent of freshwater runoff: for phases of low runoff, the choice of the averaging period can strongly impact the accuracy of an estimate, e.g., due to increased visibility of the spring–neap cycle. Nonetheless, on time scales of weeks to months, freshwater runoff is the dominant driver of the temporal evolution of mixing in the Elbe estuary.

e. Horizontal dynamics

In the previous sections, we have shown that during the extreme runoff event in June 2013, water is mixed as predicted by the universal law. To better understand the nature and location of underlying mechanisms, the following section will focus on the horizontal distribution of mixing and diahaline velocity in September 2012 and June 2013. The isohaline $S = 13 \text{ g kg}^{-1}$ is chosen as a representative salinity class because it covers the area of the river mouth without leaving the model domain in either month. Therefore, dynamics are covered within the deep navigational channel as well as on the surrounding tidal flats.

Due to the increased stratification in June, the isohaline surface and local mixing m_{xy} are distributed over a significantly increased area compared to September (Figs. 11a,b). The overall magnitude of local mixing is greater in June than in September. For both months, but especially in June, mixing is mostly confined to the river channel since little stratification, and therefore little mixing and entrainment, occurs on the tidal flats. In detail, the strongest mixing m_{xy} occurs along the banks of the navigational channel and in other locations where the topography gradient is enhanced.

Regarding the effective vertical diahaline velocity, we also find that the estimate (20) by Klingbeil and Henell (2023) holds well, aside from a slightly noisy quality due to the computation of the salinity gradient (Figs. 11c–f). In fact, the estimated and directly computed $u_{\text{dia},z}^S$ correlate with a Pearson correlation coefficient R^2 of 0.76 and 0.69 in September 2012 and June 2013, respectively. Like with mixing, the magnitude of the diahaline velocity is increased along strong topography gradients and, aside from the steep sidewalls, low inside the navigational channel itself. This is particularly obvious in the detail panels in Figs. 11e and 11f. It can generally be seen that $-u_{\text{dia},z}^S$ is negative in the downstream region of the isohaline surface (outflow toward higher salinities) and positive in the upstream region (inflow toward lower salinities).

The relatively clear separation of positive and negative diahaline velocities suggests a well-defined two-layer exchange flow with a downstream, near-surface export of freshwater toward the North Sea and an upstream, near-bottom import of ocean water into the estuary. This diahaline exchange flow is strongly topography-dependent and mostly confined to the navigational channel. This is consistent with findings by Li et al. (2022) for the Pearl River estuary during a low-runoff scenario where the river plume did not reach any offshore islands. However, in their study, the diahaline velocity did not appear to be quite as strongly limited to channels, and there was no clear pattern of increased mixing along channel sidewalls. The topography dependence of mixing can be related to lateral differential advection, which is associated with a lateral shear between the inner channel and shoals. This is possibly caused by a process similar to the one described in Warner et al. (2020). They explained increased mixing near the channel shoals of the Hudson estuary during ebb tide with the build-up of salinity fronts in such locations. Since the diahaline velocity indeed correlates well with the local mixing

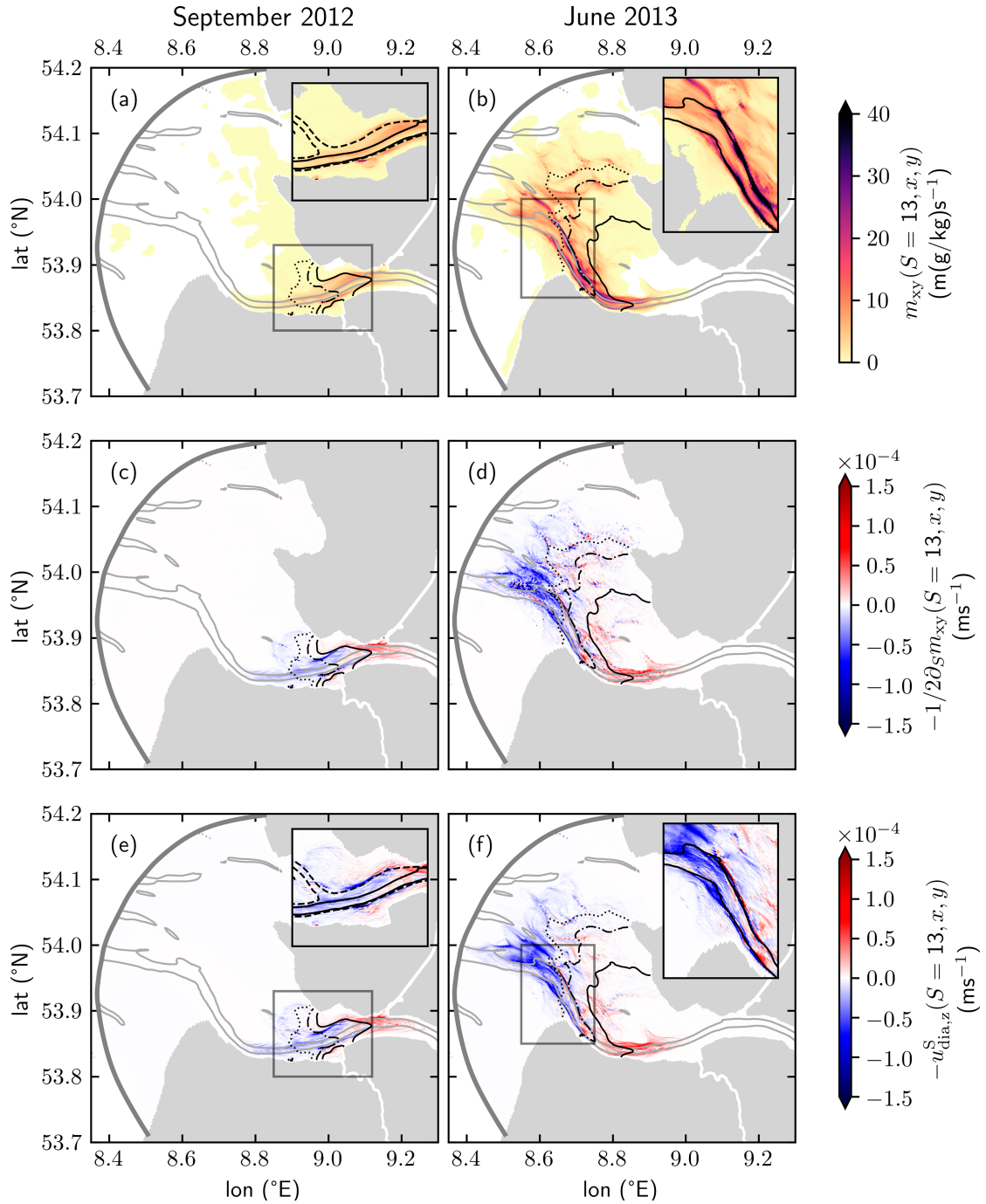


FIG. 11. (a),(b) Horizontal distribution of local mixing $m_{xy}(S, x, y)$. (c),(d) Negative effective vertical diahaline velocity as estimated from the local mixing gradient from (20). (e),(f) Negative effective vertical diahaline velocity as computed online with GETM. All properties are shown for $S = 13 \text{ g kg}^{-1}$ and have been spring-neap averaged for (left) September 2012 and (right) June 2013, respectively. The bold gray line marks the open boundary of the setup, thin gray lines represent the 12-m isobath, and the black lines represent the relative height of the $S = 13 \text{ g kg}^{-1}$ isohaline above ground at intervals of 0.2 (bold), 0.5 (dash-dot), and 0.8 (dotted). The inset figures in (a), (b), (e), and (f) show details as indicated by the black rectangles, with the 12-m isobath as a bold black line. In the insets in (a) and (e), an additional 6-m isobath was added as a dashed line.

gradient, we can conclude from relation (20) that high diahaline velocities occur where the local mixing varies strongly throughout the salinity classes. Consequently, the diahaline exchange flow is mainly confined to the channel shoals and

other strong topography gradients as described above. Therefore, only a small part of the total estuarine area is responsible for the majority of the water exchange across salinity classes.

Last, various potential mechanisms exist that adjust volume- or isohaline surface-integrated mixing to increased runoff inside an estuary. Namely, isohaline surfaces can be increased by moving them to areas with larger cross sections or entirely out of the river, or local mixing can be increased due to higher eddy diffusivities (Burchard 2020). In our study, the strongly increased isohaline area during high runoff in combination with increased local mixing intensity indicates that both mechanisms may be of importance.

4. Summary and conclusions

In this study, we have analyzed the impact of extreme discharge conditions on estuarine circulation, diahaline exchange flow, and salt mixing inside the Elbe estuary. Relatively short averaging periods from two M_2 tidal cycles up to two spring-neap cycles allowed the comparison of dynamics during a period of low and extremely high runoff, respectively. It was shown that the simulated mixing converges toward the estimate by Burchard (2020) with the length of the averaging period. An averaging period of two spring-neap cycles was found to properly reproduce the total exchange flow (TEF) as well as the mixing estimates from MacCready et al. (2018) and Burchard (2020). At the same time, each extreme event was still clearly represented in the resulting parameters. With our results, we have demonstrated that the estuarine system of the Elbe River adjusts relatively fast to changes of the freshwater discharge. Consequently, the TEF framework and the mixing estimates from MacCready et al. (2018) and Burchard (2020) can be suitable tools for the study of estuarine dynamics even under extreme discharge conditions. In addition to earlier findings by Voynova et al. (2017), Kerimoglu et al. (2020), and Chegini et al. (2020) for the German Bight, we have further found that the high-runoff event in June also led to increased stratification within the Elbe estuary itself. We have shown that the estuarine circulation within the Elbe estuary consists of a classic two-layer flow with high-salinity inflow and low-salinity outflow. All parameters of the isohaline exchange flow, i.e., the TEF, were found to be freshened during the high-runoff event in June 2013 compared to the low-runoff period of September 2012. As a result, salt intrusion varied strongly between low- and high-runoff periods. As demonstrated before by Broatch and MacCready (2022) for the Salish Sea, we have found here that freshwater runoff strongly drives mixing in the Elbe estuary. For periods of lower runoff, we could additionally identify a potential weak modulation of mixing by the spring-neap cycle which gained relevance in a comparative scenario where horizontal diffusivity was reduced. The diahaline exchange flow, quantified by the effective vertical diahaline velocity $u_{dia,z}^S$, was shown here for the first time in a spatially resolved manner and under realistic conditions for a tidal estuary. It is well defined within the Elbe estuary and consists of a near-surface outflow near the downstream end of the isohaline surface and a near-bottom inflow near the upstream end. The spatial distribution of the diahaline exchange flow follows the salinity gradient of local mixing, as given by the estimate from Klingbeil and Henell (2023). It could therefore be concluded that horizontal diffusion is of

minor importance for mixing in the Elbe estuary, even under extreme discharge conditions. This means that the diahaline exchange flow is driven by vertical rather than horizontal mixing. Our results further show that due to its relation to the local mixing, the majority of the diahaline exchange flow is confined to regions of strong topography gradients. This provides a first insight into potential mechanisms behind the spatial structure of the diahaline exchange flow and estuarine salt mixing inside mesotidal estuaries, which are possibly related to the mixing due to the build-up of salinity fronts described by Warner et al. (2020). As a next step, finding a link between the diahaline exchange flow and the (isohaline) total exchange flow could directly quantify the connection between salt mixing and estuarine circulation.

Last, with the expected increased frequency of both high- and low-runoff events (see, e.g., Christensen and Christensen 2004; van Vliet et al. 2013), we conclude that typical mesotidal estuaries such as the tidal Elbe will likely be subject to more frequent changes between periods of freshening and temporary stratification and well-mixed periods of high salt intrusion. It might be of interest for future studies to investigate the impact that such changes may have on the estuarine sediment dynamics and ecosystem.

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Data availability statement. The GETM source code used for this work is archived on Zenodo (<https://doi.org/10.5281/zenodo.7741730>). Boundary forcing as well as initial salt and temperature distributions was retrieved from the numerical setup presented in Gräwe et al. (2015). Meteorological forcing was provided from the ICON model by the German Weather Service (Zängl et al. 2015), which cannot be made public due to its proprietary nature. Therefore, the numerical setup cannot be made public in a fully functional state. Instead, the full tidal Elbe setup used in this study, including forcing and initial distributions, is available on request via the corresponding author of this study. The numerical data from the tidal Elbe setup that have been used for this study are archived at

<https://doi.org/10.5281/zenodo.10230005> and <https://doi.org/10.5281/zenodo.10230235>. The setup topography as well as freshwater runoff of the main river and tributaries as used in this study is available through <https://doi.org/10.5281/zenodo.10222958>. For rivers where daily-averaged data were available, the data were retrieved from the following public domain resources: <http://www.portal-tideelbe.de> (Wasserstraßen- und Schiff-fahrtsamt Magdeburg 2021), <https://hsi-sh.de/pegelsuche.html> (Landesamt für Landwirtschaft, Umwelt und ländliche Räume Schleswig-Holstein 2022), and <http://www.wasserdaten.niedersachsen.de/cadenza/pages/home/welcome.xhtml> (Niedersächsischer Landesbetrieb für Wasserwirtschaft, Küsten- und Naturschutz 2022). Constant and monthly averaged freshwater runoff data from the remaining tributaries as well as weighting factors for gauge data were provided by the Bundesanstalt für Wasserbau via personal communication. Observational data used for the calibration and validation of the numerical setup are freely available through <http://www.portal-tideelbe.de> (Wasserstraßen- und Schiff-fahrtsamt Elbe-Nordsee and Hamburg Port Authority 2023; Wasserstraßen- und Schiff-fahrtsamt Elbe-Nordsee 2023). For the creation of the numerical grid of our setup, the Delft3D rgfgrid GUI (Deltares 2020) was used. The software is available through <https://oss.deltares.nl/web/delft3d/home> and requires a license that can be freely requested on the same website. All figures in this study have been created with Matplotlib version 3.3.4 (Hunter 2007; Caswell et al. 2021), freely available through <https://matplotlib.org>. The respective Python scripts are available through <https://doi.org/10.5281/zenodo.10222958>. The map in Fig. 2b was created with cartopy v0.17.0 (Met Office 2015; Elson et al. 2018), available through <http://scitools.org.uk/cartopy>, and using the NaturalEarthFeature function (made with Natural Earth. Free vector and raster map data at natural-earthdata.com). A tidal analysis was performed using the pytides package (Cox 2018), available through <https://github.com/sahitono/pytides>. TEF bulk values were computed with pyTEF (Lorenz and Boergel 2021), available through <https://florianboergel.github.io/pyTEF>.

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The relation between exchange flow and diahaline mixing in estuaries

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ABSTRACT: Estuaries with excess freshwater discharge are characterized by inflow of saline water from the ocean and outflow of brackish water towards the ocean. The intensity of this so-called estuarine circulation is known to be connected to salinity mixing inside the estuary. Here, the water mass transformation process of mixing is conveniently defined as the destruction of salinity variance within the estuarine volume. In the present study, we derive a new relation that shows how the estuarine exchange flow and the mixing inside the estuary determine each other. The result is a quantitative relation between the inflow volume at a fixed transect across the estuary and the distribution of the diahaline mixing inside the estuary. The concept of dividing salinities between inflowing and outflowing transports is used here. More specifically, the estuarine exchange flow equals the derivative of the mixing (with respect to salinity) on the estuarine part of the dividing salinity isohaline. We show for two realistic example estuaries how the exchange flow and the mixing are spatially distributed on the dividing salinity isohaline. Those estuaries include a channelized tidal estuary and a non-tidal industrialized estuary. While the former shows a basic two-layer division between inflow and outflow, the latter has a more complex three-layer structure, due to offshore upwelling and downwelling dynamics. The new theory provides the recipe for analyzing the relation between mixing and exchange flow in any estuary and helps to identify the regions where the mixing occurs that is consistent with the exchange flow.

Significance Statement

Estuaries are coastal water bodies connecting rivers to the ocean by mixing riverine freshwater with inflowing saline ocean water such that outflowing brackish water is generated. This is the key water mass transformation process that characterizes estuaries. To provide the upper parts of estuaries with salt from the ocean, a landward salt transport against the river flow is required, the so-called estuarine circulation. Our study derives a time-averaged relation that quantitatively connects the estuarine mixing and the estuarine circulation in a two-way manner as opposed to the common notion of circulation depending on mixing. This relation is demonstrated for numerical models of two estuaries, a tidal estuary with a simple two-layer circulation and a non-tidal estuary with a three-layer circulation driven by high temporal variability of offshore salinity.

1. Introduction

This study connects two concepts of estuarine dynamics quantitatively, (i) the exchange flow through a fixed transect across the estuary and (ii) the exchange flow across and mixing on an isohaline surface. Both concepts are based on temporal averaging of the estuarine dynamics. Often, the averaging period is chosen long enough to allow neglecting storage effects in the sense that the average temporal changes of volume and salt content in the estuary are sufficiently small. For tidal flow, averaging over one spring-neap cycle is often sufficient to neglect the storage terms (e.g., Li et al. 2022). For convenience, within this study, the storage terms are neglected by analyzing long-term averaged conditions, but for completeness all formulations including storage terms are given in the appendix. Non-linear effects of temporal variability (e.g., spring-neap cycle, variations in run-off, changes in offshore conditions, MacCready et al. 2018; Geyer et al. 2020; Lange et al. 2020; Reese et al. 2024; MacCready and Geyer 2024) are included but not explicitly investigated here. The two estuarine concepts are briefly reviewed here:

(i) Exchange flow across fixed estuarine transects has already been described by Knudsen (1900), see also a review and a translation of Knudsen's paper (Burchard et al. 2018b). Volume and salt conservation for long-term averaged estuarine conditions can be formulated as

$$Q_{\text{in}} + Q_{\text{out}} + Q_r = 0, \quad Q_{\text{in}} s_{\text{in}} + Q_{\text{out}} s_{\text{out}} = 0, \quad (1)$$

with the inflow volume transport $Q_{\text{in}} \geq 0$ across a fixed transect at salt water inflow salinity s_{in} , the outflow transport volume $Q_{\text{out}} \leq 0$ at brackish water outflow salinity s_{out} , and the freshwater river discharge $Q_r \geq 0$ into the estuarine volume (assuming to be of zero salinity), see also the sketch in Fig. 1b. The Knudsen relations can also be formulated including storage terms for water and salt (Burchard et al. 2018b). With this, an estuary can be regarded as a *mixing machine* (Wang et al. 2017) that mixes fresh riverine and salty ocean water to generate brackish estuarine water. The fundamental function of estuarine mixing has already been mentioned by Knudsen (1900) who stated: *As the freshwater spreads out over the seawater it mixes with it so that the salinity of the surface increases seawards* (translation by Burchard et al. 2018b). As a measure for estuarine mixing, the decay rate of salinity variance per unit volume, $\chi_s = 2K_h (\partial s / \partial x)^2 + 2K_h (\partial s / \partial y)^2 + 2K_v (\partial s / \partial z)^2$ had been proposed (Burchard and Rennau 2008, with K_h and K_v being the horizontal and the vertical eddy diffusivity, respectively). In numerical models numerical mixing due to truncation errors in the tracer advection schemes occurs in addition to this physical mixing. It can be exactly quantified using the methods by Burchard and Rennau (2008) or Klingbeil et al. (2014). Mixing inside estuaries bounded by a fixed transect could be quantified by MacCready et al. (2018) as

$$\mathbb{M} = s_{\text{in}} s_{\text{out}} Q_r = (s_{\text{in}} - s_{\text{out}}) s_{\text{in}} Q_{\text{in}}, \quad (2)$$

where $\mathbb{M} = \langle \int_V \chi_s dV \rangle$ is the long-term averaged decay rate of salinity variance inside the estuarine volume V (with $\langle \cdot \rangle$ denoting time-averaging). The last equality in (2) is using (1). A mixing formulation including storage terms can be derived (Burchard et al. 2019).

For the present study, it is convenient defining Q_{in} as a measure for estuarine exchange flow intensity (Broatch and MacCready 2022; MacCready and Geyer 2024). With this, using (2), zero estuarine mixing $\mathbb{M}$ is consistent with zero exchange flow Q_{in} , which can be referred to as the extreme fjord case, where the riverine water entering the fjord is leaving the fjord as fresh water towards the ocean ($s_{\text{out}} = 0$). For given values of s_{in} and Q_r , the first part of (2) shows that $s_{\text{out}} \rightarrow s_{\text{in}}$ would maximize the mixing $\mathbb{M} \leq s_{\text{in}}^2 Q_r$, while the second part indicates that in that limiting case $Q_{\text{in}} \gg Q_r$ is possible. An example of this is low river discharge strong-tide basins in the Wadden Sea of the German Bight (Gräwe et al. 2016). A comparable exchange flow estimate had been introduced as the average of the inflow and outflow transports (Geyer et al. 2020; MacCready et al.

2021): $Q_e = \frac{1}{2}(Q_{\text{in}} - Q_{\text{out}}) = Q_{\text{in}} + \frac{1}{2}Q_r$, where the latter equality is using (1). By neglecting the influence of Q_r on Q_e , again Q_{in} is obtained as a measure for the exchange flow.

To consistently calculate the inflow and outflow volume transports and salinities, MacCready (2011) proposed the Total Exchange Flow (TEF) framework, which resolves inflows and outflows as a function of salinity class. Note that Walin (1977) already laid the foundations for TEF in his Eq. 2. For simple exchange flow situations where inflows occur at higher salinities than outflows, a unique dividing salinity s_{div} exists that separates inflows and outflows in salinity space (Lorenz et al. 2019). More complex exchange flows with multiple inflows or outflows consequently have more dividing salinities.

(ii) The concept of analyzing estuarine dynamics on isohaline surfaces has been introduced in the visionary paper by Walin (1977). Similarly to the present study, he considered volume and salt conservation below an isohaline surface of a long-term averaged estuary bounded by a fixed transect. The major relation derived by Walin (1977) is (using our notation)

$$Q(S, x) = Q_{\text{dia}}(S, x) = -\frac{\partial J_{\text{est}}(S, x)}{\partial S}, \quad (3)$$

where $Q(S, x)$ is the volume transport into the estuary across this fixed transect at position x for all salinities larger than S , $Q_{\text{dia}}(S, x)$ is the diahaline transport through the isohaline surface of salinity S that is situated on the estuarine side from the transect and $J_{\text{est}}(S, x)$ is the upward diffusive salt transport across this part of the isohaline. Walin (1977) stated about this relation (his Eq. 7): *Equation (3) represents in the most simple way how the deep water supply is related to the overall vertical (i.e. cross-isohaline) mixing properties in the basin.* The key relation of our study will be similar to (3) for the special case of $S = s_{\text{div}}$, giving

$$Q(S = s_{\text{div}}(x), x) = Q_{\text{in}}(x). \quad (4)$$

Based on the pioneering work of Walin (1977), a Water Mass Transformation (WMT) framework for mostly larger oceanic scales has been constructed by several authors (see, e.g., Zika et al. 2012; Hieronymus et al. 2014; Pemberton et al. 2015; Groeskamp et al. 2019).

The nucleus of the estuarine mixing theory presented here is the local relation between the diahaline volume transport per unit horizontal area, $u_{\text{dia},z}(S, x, y)$, see Fig. 1a, and the local mixing

per salinity class, $m(S, x, y)$:

$$u_{\text{dia},z} = \frac{1}{2} \frac{\partial m}{\partial S}, \quad (5)$$

which establishes the dependence of residual estuarine circulation on estuarine mixing on the local scale (Klingbeil and Henell 2023). The diahaline volume transport per unit horizontal area $u_{\text{dia},z}(S, x, y)$ is defined as the time-averaged local contribution to the diahaline transport $Q_{\text{dia}}(S, x) = -\int_{A_{\text{est}}(S,x)} u_{\text{dia},z}(S, x, y) dA$, where $A_{\text{est}}(S, x)$ is the horizontal area covered by the isohaline inside the estuary (Fig. 1c). Similarly, the local mixing per salinity class $m(S, x, y)$ is defined as the local distribution of the mixing per salinity class, $\mathbb{m}_{\text{est}}(S, x) = -\partial \left\langle \int_{V_{\text{est}}(S,x)} \chi_s(x, y, z, t) dV \right\rangle / \partial S = \int_{A_{\text{est}}(S,x)} m(S, x, y) dA$ with the estuarine volume $V_{\text{est}}(S, x)$ for all salinities $s \geq S$ (see Fig. 1b,c and Klingbeil and Henell 2023, for details).

For a stable and monotone salinity stratification, the relation (5) can be directly derived from the one-dimensional vertical salinity equation

$$\frac{\partial s}{\partial t} + w \frac{\partial s}{\partial z} - \frac{\partial}{\partial z} \left(K_v \frac{\partial s}{\partial z} \right) = 0, \quad (6)$$

with the physical vertical velocity w by transformation into salinity coordinates. Under those conditions, after time-averaging,

$$u_{\text{dia},z}(S) = - \left\langle \frac{\partial z}{\partial S} \frac{\partial S}{\partial t} + w \right\rangle = - \frac{\partial}{\partial S} \left\langle K_v \frac{\partial S}{\partial z} \right\rangle = \frac{1}{2} \frac{\partial m}{\partial S} \quad (7)$$

results (Wang et al. 2017; Klingbeil and Henell 2023). In this monotone case and for long-term averages, $u_{\text{dia},z}$ can be simply calculated from the divergence of the time-averaged vertically integrated transport under the isohaline, see Fig. 1a for an explanatory sketch and (A1). For a rigorous derivation for the general three-dimensional case with non-monotone salinity distribution in three dimensions, see Klingbeil and Henell (2023). Note that a relation similar to (5) has been derived (McDougall 1984; Marshall et al. 1999) and has been used in several ocean modelling studies (see, e.g., Ferrari et al. 2016; McDougall and Ferrari 2017). It can be shown that the mixing per salinity class equals twice the upward diffusive salt transport across the isohaline (Burchard et al. 2021):

$$\mathbb{m}_{\text{est}}(S) = 2J_{\text{est}}(S). \quad (8)$$

The isohaline framework has been used by several authors to investigate mixing and exchange flow processes in tidal estuaries, such as the role of turbulent diahaline salt fluxes for maintaining estuarine salt intrusions (MacCready and Geyer 2001), the role of advective and diffusive diahaline transports for explaining the long-term isohaline structure of tidal estuaries (MacCready et al. 2002) and turbulent mixing in river plumes (Hetland 2005). Based on the work of Walin (1977), Burchard (2020) derived a universal law of estuarine mixing, postulating that the long-term averaged mixing per salinity class is twice the salinity of the respective salinity class times the river run-off. This relation has been reproduced by a number of numerical model experiments in several tidal estuaries, showing that typically monthly averaging is sufficient to reproduce the law (Burchard et al. 2021; Li et al. 2022; Reese et al. 2024).

The local relation (5) between diahaline exchange flow and the derivative of mixing with respect to salinity has been investigated for estuarine segments by Wang et al. (2017). Two-dimensional fields of diahaline exchange flow and local diahaline mixing have been computed (Li et al. 2022; Henell et al. 2023; Reese et al. 2024). Across a given isohaline surface, water generally leaves an estuarine volume further downstream the estuary near the surface, and enters further upstream close to the bottom. Large differences occur between different estuaries.

The research gap that we intend to fill with the present theory is to derive relations which explicitly equate exchange flow and mixing in estuarine systems and show their applicability to different estuarine systems. Such a framework can then be used to identify mixing hotspots that are consistent with the estuarine circulation and to further investigate those critical regions and processes that explain the water mass transformations and overturning circulation in estuarine systems. The mixing relation (2) by MacCready et al. (2018) has been an important step towards such a quantification, but it still contains the bulk inflowing and outflowing TEF salinities as parameters. We are here combining the mixing and exchange flow concepts for fixed transects and specified isohalines laid out above in (i) and (ii) to derive such a relation.

The paper is organized as follows: After this introduction, the numerical model applied for this study is described (Sec. 2a) and the estuarine model set-ups are explained (Sec. 2b). Afterwards, the key relations between mixing and exchange flow, (9) for estuaries with two-layer exchange flow and (10) for estuaries with three-layer exchange flow are presented in Sec. 3. The accuracy of these relations is then demonstrated for the two-layered tidal Elbe estuary (Sec. 3a) and the three-layered

non-tidal Warnow estuary (Sec. 3b). Implications of the results are discussed in Sec. 4. A detailed derivation of (9) and (10) including storage terms can be found in the appendix at the end of the paper. The appendix also contains a table (Tab. A1) with all variables used throughout the paper.

2. Methods

a. Numerical model

For all simulations, the General Estuarine Transport Model (GETM, www.getm.eu, Burchard and Bolding 2002) is applied, which is a finite-volume, structured-grid model with explicit mode splitting and vertically adaptive coordinates (Hofmeister et al. 2010; Gräwe et al. 2015a; Klingbeil et al. 2018). Vertical turbulent mixing which plays an essential role in this study is parameterized by means of a k - ε turbulence closure model with an algebraic second-moment closure (Umlauf and Burchard 2005), using the turbulence module of the General Ocean Turbulence Model (GOTM, www.gotm.net, Burchard et al. 1999; Umlauf et al. 2005). The properties on isohaline surfaces are diagnosed by a binning in salinity classes using a prescribed constant ΔS (see Burchard et al. 2021, for details).

b. Estuarine model set-ups

The model simulations for the two estuaries are using realistic bathymetry, lateral boundary conditions, atmospheric forcing and river run-off. For both model simulations, surface freshwater fluxes due to precipitation and evaporation were applied, but did not play a significant role in the freshwater budget of the estuaries. Both temperature and salinity fields were calculated in these simulations.

For the Elbe estuary simulations, a bathymetry has been used that is representative for the year 2010, and since no major dredgings have been carried out in the three subsequent years, it is also representative for the analyzed months September 2012 and June 2013. These bathymetry data have then been interpolated onto a curvilinear grid that is following the navigational channel, resulting in a horizontal resolution of 200-400 m in along-channel direction and 50-100 m in cross-channel direction. In the vertical, 30 equidistant σ levels were used. Lateral boundary conditions have been extracted from a 600 m resolution simulation of the Southern North Sea (Gräwe et al. 2015a). Atmospheric forcing has been provided by the German Weather Service with a horizontal

resolution of about 7 km and a temporal resolution of 3 hours. For further details of the Elbe estuary model setup, see Reese et al. (2024).

For the Warnow estuary simulations, a Cartesian grid with a constant resolution of $20 \text{ m} \times 20 \text{ m}$ has been used. Lateral boundary conditions are downscaled from a 600 m resolution model of the Western Baltic Sea (Gräwe et al. 2015a) via a 200 m model resolution intermediate model. In the vertical, 25 equidistant σ levels were used. For the atmospheric forcing, the same data source as for the Elbe model was used. The model simulations were initialized at the beginning of 2013, such that sufficient spin-off time was provided for this analysis of the year 2014. Daily averaged river-runoff from the Warnow river in the south was the only lateral freshwater source to the model. For further details of the Warnow estuary model setup, see Lange et al. (2020).

3. Results

The key relation that is derived for this study is a direct quantitative relation between the inflow transport Q_{in} across a fixed cross-section and the S -derivative of the diahaline mixing integrated over the horizontal area covered by the estuarine part of the dividing salinity isohaline, $\mathbb{m}_{\text{est}}(s_{\text{div}})$:

$$Q_{\text{in}}(x) = -\frac{1}{2} \frac{\partial \mathbb{m}_{\text{est}}(s_{\text{div}}(x), x)}{\partial S}, \quad (9)$$

see Fig. 1b (in vertical Cartesian coordinates) and Fig. 1c (in salinity coordinates). Eq. (9) is directly obtained by inserting $S = s_{\text{div}}$ into (3), derived by Walin (1977) and combining it with (8). Eq. (9) can also be derived by lateral integration of the local mixing relation (5) over the area of the dividing salinity isohaline that is located upstream of the transect, see Fig. 1b,c and in the appendix, where (A14) shows a version of the key relation (9) including the storage term.

With (9), we have derived for the first time a direct relation between estuarine mixing and exchange flow intensity for two-layer estuaries. This convenient relation can easily be extended to estuaries with a multi-layer flow through multiple channels. In some situations, substantial deviations from the two-layer Knudsen-type of flow shown in Fig. 1b,c can occur (Lorenz et al. 2019). In Fig. 1d, a situation is shown for a three-layer exchange flow with inflow at high and low salinities, $Q_{\text{in,high}}$ and $Q_{\text{in,low}}$, respectively, and one outflow Q_{out} at intermediate salinities. Now, two dividing salinities occur, $s_{\text{div,high}}$ and $s_{\text{div,low}}$. The transports across the isohalines of these dividing salinities on the estuarine side are given by $Q_{\text{dia,high}} = Q_{\text{in,high}}$ and $Q_{\text{dia,low}} = -(Q_{\text{in,low}} + Q_r)$,

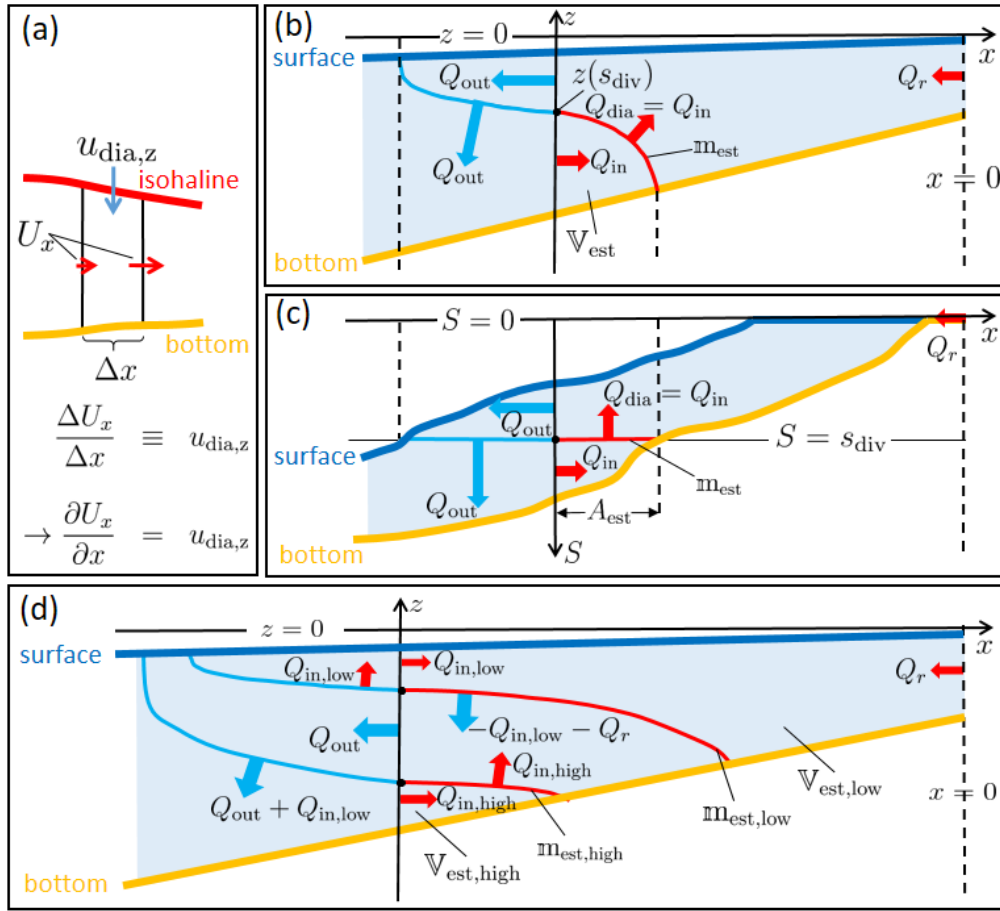


FIG. 1. Sketch explaining the connection between exchange flow and diahaline mixing. a: Dependence of the diahaline volume transport per unit horizontal area $u_{dia,z}$ on the divergence of horizontal transport U_x , for simplicity only shown for the x -direction, b: two-layer flow in x - z coordinates, c: two-layer flow in x - S coordinates, d: three-layer flow in x - z coordinates. The inner part of the isohalines are shown as bold red lines, and the outer part is shown as bold blue lines. Inflowing transports (> 0) are shown as red arrows and outflowing transports (< 0) as blue arrows. In panels b-d, the water volume is marked by light blue shading.

respectively. The mixing integrated over the estuarine parts of each of these isohalines are denoted as $m_{est,high} = m_{est}(s_{div,high})$ and $m_{est,low} = m_{est}(s_{div,low})$. Given the previous relation (9) and assuming the geometry as shown in Fig. 1d as well as long-term averaging (negligible storage terms), we obtain the following relations between exchange flow and mixing for the three-layer

flow:

$$\begin{aligned}
 Q_{\text{in,high}} &= -\frac{1}{2} \frac{\partial m_{\text{est,high}}}{\partial S}, \\
 -(Q_{\text{in,low}} + Q_r) &= -\frac{1}{2} \frac{\partial m_{\text{est,low}}}{\partial S},
 \end{aligned} \tag{10}$$

where we dropped the explicit dependence on x for convenience. Based on this geometrical principle, relations between exchange flow and mixing can be constructed also for situations with more than three layers. A version of (10) including storage terms is given in (A15).

In the following sections, we explore high-resolution model results for a tidal estuary with two-layer exchange flow (Elbe estuary, see Sec. 3a) and a non-tidal estuary with three-layer exchange flow (Warnow estuary, see Sec. 3b). The locations and bathymetries of the estuaries are shown in Fig. 2. For all simulations, the General Estuarine Transport Model (GETM, getm.eu, Burchard and Bolding 2002) is applied. The simulations are realistic and validated, using both salinity and temperature as active tracers (see details in Sec. 2).

a. Tidal two-layer estuary

The Elbe estuary is investigated here as a typical two-layer estuary with inflow at high salinities and outflow at low salinities (Reese et al. 2024). It is a mesotidal estuary with a pronounced navigational channel (Fig. 2c), and is characterized by a dominant semi-diurnal tide and a pronounced spring-neap cycle. The tidal influence has an upstream limit that is given by a weir in Geesthacht located about 150 km upstream of the mouth. The salt intrusion is highly dependent on the river discharge which can vary by more than one order of magnitude between $< 100 \text{ m}^3\text{s}^{-1}$ and $> 2000 \text{ m}^3\text{s}^{-1}$ (Kappenberg and Grabemann 2001). At the upstream limit of the salt intrusion, a pronounced estuarine turbidity maximum typically occurs (Postma and Kalle 1955; Kappenberg et al. 1995; Burchard et al. 2004, 2018a). The mixing in the Elbe estuary is dominated by the strongly variable river run-off rather than by the spring-neap cycle (Reese et al. 2024).

With its elongated structure, the Elbe estuary is highly suitable for an analysis of mixing and exchange flow at all cross-sections along its longitudinal axis. The results for the Elbe estuary have been extracted from the model study by Reese et al. (2024) who carried out numerical simulations with a curvi-linear grid that follows the navigational channel. Results for the two-layer mixing relation (9) along the estuary and mixing and exchange flow analysis with respect to a transect

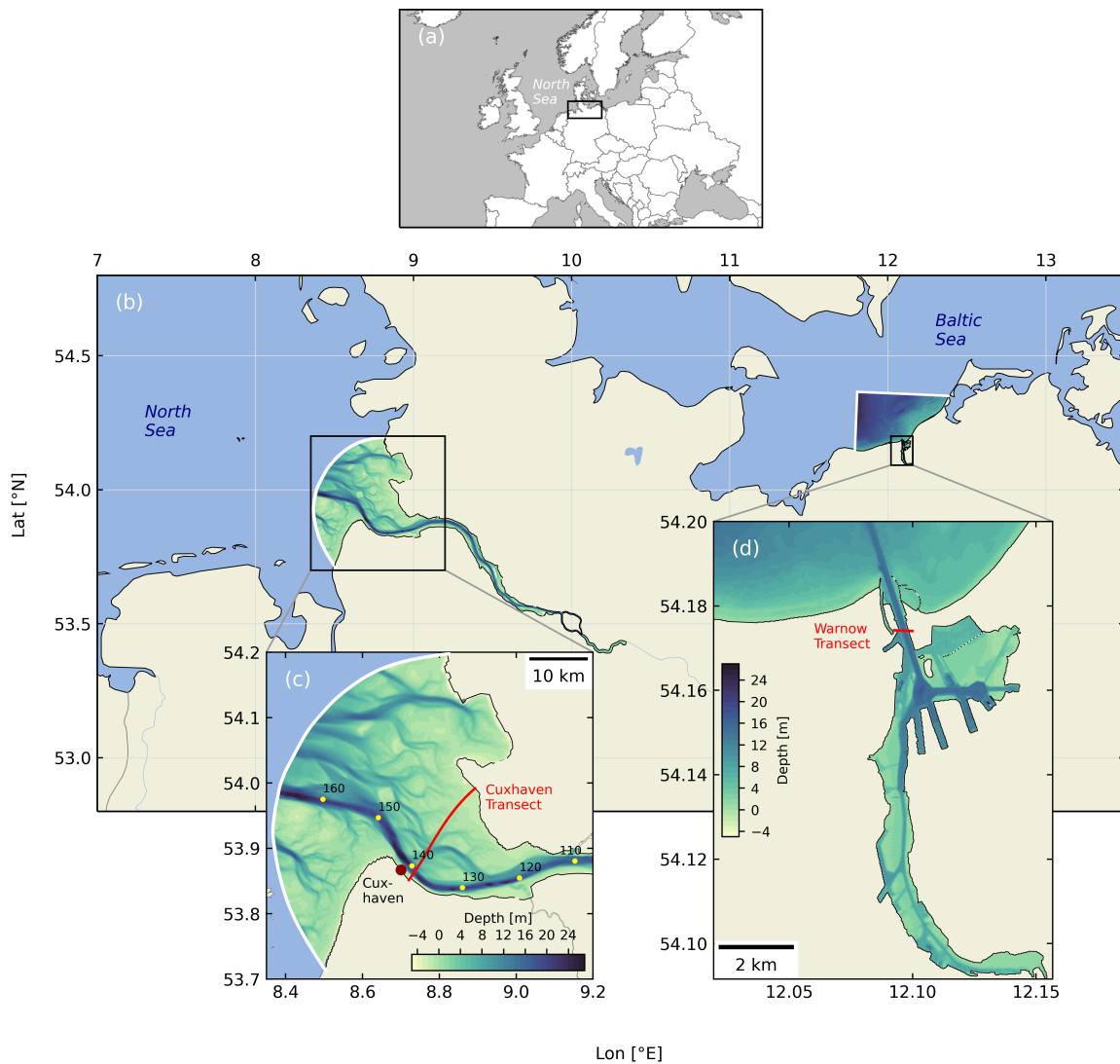


FIG. 2. Locations and bathymetries of the two estuaries investigated in the present study. a: Map of Europe with an outline of the map area of panel b indicated; b: Map of northern Germany with the complete model domains for the two estuaries; white lines indicate the open boundaries; c: Bathymetry of the lower Elbe estuary, with a white line marking the open boundary and a red line marking the Cuxhaven transect; d: Bathymetry of the Warnow estuary, with a red line marking the Warnow transect.

at the mouth of the estuary (Cuxhaven transect) are shown in Fig. 3 with averaging intervals ΔT being two spring-neap cycles for comparably low ($Q_r \approx 350 \text{ m}^3\text{s}^{-1}$ in September 2012) and exceptionally high ($Q_r \approx 2500 \text{ m}^3\text{s}^{-1}$ in June 2013) monthly-mean river run-off. For both months, the numerically calculated budget of (9) is largely closed along the range of more than 70 km along the estuary (Fig. 3a,b). For the low runoff month (Fig. 3a), the storage term makes a small

contribution to the budget at some locations, but for the high run-off (Fig. 3b) the storage term is negligible all over the estuary. For both months, the estuarine circulation across the Cuxhaven transect is a classical two-layer circulation, as shown by the TEF profiles in Fig. 3c,d. The dividing salinity is much higher for the low-runoff month ($s_{\text{div}} = 21.0$ g/kg) than for the high-runoff month ($s_{\text{div}} = 12.6$ g/kg), because the salt intrusion has propagated farther into the estuary for low runoff. Interestingly, the exchange flow intensity across the Cuxhaven transect as quantified by Q_{in} is slightly higher for the low run-off ($Q_{\text{in}} = 1354 \text{ m}^3\text{s}^{-1}$) than for high run-off ($Q_{\text{in}} = 1179 \text{ m}^3\text{s}^{-1}$), probably due to the much lower run-off velocity in September 2012. During high discharge, the entire circulation cell is shifted downstream, such that in June 2013 the position of the transect relative to the along-channel development of the circulation is further upstream as in September 2012. There, the salt intrusion reaches farther upstream such that the circulation is already quite strong in the region of the transect. In June 2013, however, the transect is close to the end of the salt intrusion such that the estuarine circulation is not fully developed. For both months, the distribution of the local mixing per salinity class m is spread over the entire area covered by the isohaline of the dividing salinity, but highest values are above steep bathymetry at the edges of the navigational channel (Fig. 3e,f). Generally, the level of mixing is higher for the high-runoff month June 2013, which is in accordance with the universal law of estuarine mixing (Burchard 2020), as shown for this Elbe simulation (Reese et al. 2024). Seemingly, the Cuxhaven transect divides the $u_{\text{dia},z}$ distribution into inflow towards lower salinities near the bottom ($-u_{\text{dia},z} > 0$) landwards of the transect and outflow towards higher salinities near the surface ($-u_{\text{dia},z} < 0$) seawards of the transect (Fig. 3g,h). This can be explained by the fact that cross-transect inflows occur for salinities higher than the dividing salinity and therefore inflows should dominate the estuarine part of the dividing salinity isohaline as sketched in Fig. 1b,c.

b. Non-tidal three-layer estuary

The Warnow estuary is a small industrialized estuary of the essentially non-tidal and brackish Western Baltic Sea (Fig. 2d). The Baltic Sea itself is strongly salinity-stratified all year around, such that its coasts are characterized by regular wind-driven upwelling events during all seasons (Lehmann and Myrberg 2008). Since the Western Baltic Sea is strongly stratified in salinity, wind-driven upwelling (during easterly winds) and downwelling (during westerly winds) dynamics

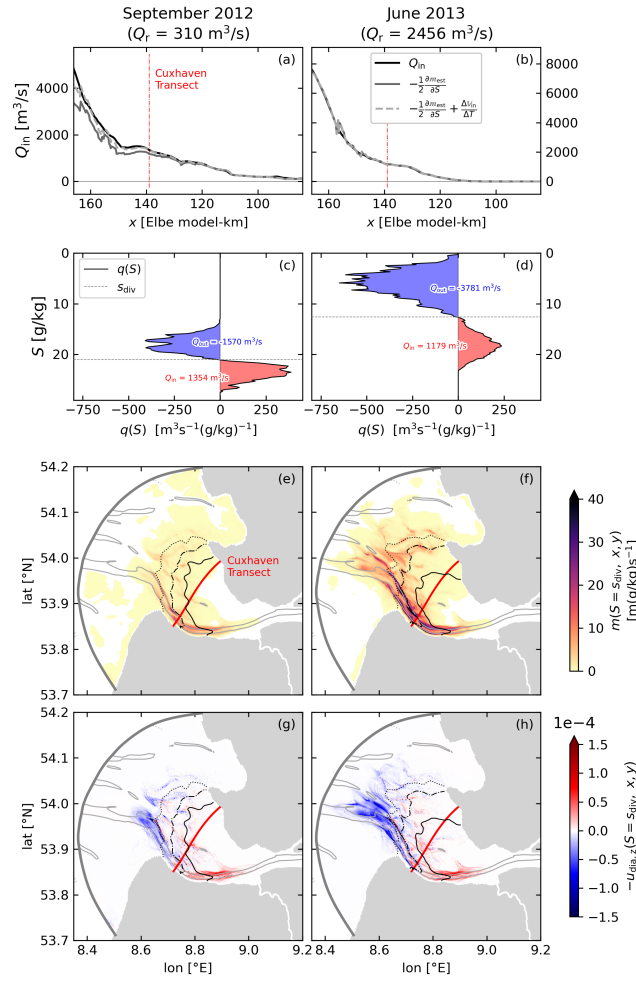


FIG. 3. Mixing and exchange flow results for the Elbe estuary for low (September 2012, panels a, c, e, g) and high (July 2013, panels b, d, f, h) run-off situations. The average discharge Q_r for each month is given in the axis titles. a,b: Left-hand side (black line) and right-hand side (solid gray line) of exchange flow - mixing relation, see (9), taken along the Elbe estuary; dashed grey lines represent the right-hand side of relation (9) corrected by the storage term $\Delta V_{\text{est}}/\Delta T$ (ΔT denoting the averaging period); the Cuxhaven transect (see panels e-h for its location) at km 139 is indicated as dashed red line; c,d: Total Exchange Flow $q(S) = -\partial Q/\partial S$ across the Cuxhaven transect; the amounts of Q_{in} (red) and Q_{out} (blue) are indicated as numbers and graphically as shaded areas. The dividing salinity is marked as a thin dashed line; e,f: diahaline mixing per salinity class, m on the s_{div} isohaline of the Cuxhaven transect (bold red line); the mean relative isohaline heights above ground of $\sigma = -0.8$ (solid), $\sigma = -0.5$ (dash-dotted) and $\sigma = -0.2$ (dotted); g,h: as in panels e,f but for the diahaline volume transport per unit horizontal area $u_{\text{dia},z}$ across the s_{div} isohaline of the Cuxhaven transect; incoming (positive) transports are marked in red, and outflowing (negative) transports are marked in blue.

drive a high variability of surface salinity at its southern coast (Fennel and Sturm 1992). At the mouth of the Warnow estuary, salinity ranges between 10 g/kg during downwelling and 20 g/kg during upwelling. In addition, upwelling waters can be 5 - 10 °C colder than the downwelling waters. Therefore, during upwelling the salinity outside the estuary is higher than inside, driving an estuarine circulation with inflows at high salinities and outflows at low salinities. During downwelling, the salinity outside the estuary can drop by more than 10 g/kg within less than one day to values below inside the estuary, supported by a temperature increase, such that a density-driven anti-estuarine circulation is occurring (Lange et al. 2020). In addition, during so-called Major Baltic Inflows (MBIs), huge amounts of high-salinity waters pass through the Western Baltic Sea (Gräwe et al. 2015b), such that during the MBI occurring at the end of 2014, salinity in the Warnow estuary increased considerably (Lange et al. 2020).

Based on a TEF analysis of the entire year 2014 using the simulations by Lange et al. (2020), the three-layer circulation of the Warnow can be clearly seen in Fig. 4a. The upper circulation cell for low salinities is formed during downwelling, and the lower cell with high salinities is formed during upwelling (Fig. 4b). The two dividing salinities are $s_{\text{div,high}} = 16.8$ g/kg and $s_{\text{div,low}} = 11.2$ g/kg. Other than in the Elbe scenario (Sec. 3a), the isohalines of the dividing salinities extend far beyond the limits of the model domain (Fig. 4c,d). On both isohalines, there is considerable mixing also visible in the Western Baltic Sea adjacent to the Warnow estuary. In fact, the isohaline of $s_{\text{div,low}}$ covers large parts of the central Baltic Sea (Wüst 1957; Henell et al. 2023). The spatial distribution of the local mixing per salinity class m inside the estuary is clearly focused above steep topography along the edge of the dredged navigational channel. For the $s_{\text{div,low}}$ isohaline, mixing levels are generally higher. The spatial distribution of $u_{\text{dia,z}}$ is clearly distinct across the two isohalines (Fig. 4e,f). For the $s_{\text{div,high}}$ isohaline, inflow dominates, such that $-u_{\text{dia,z}} > 0$ in most locations, meaning that volume flows into the estuary from high to low salinities (Fig. 4f). For the $s_{\text{div,low}}$ isohaline, a diahaline exchange flow is visible (Fig. 4e) inside the estuary. At the southern part of the estuary, inflow towards low salinities dominates, and at the northward part, outflow towards high salinities dominates.

Despite the complex patterns of mixing, inflow and outflow inside the estuary, the numerical calculation of the transport budgets according to (10) averaged over the year 2014 shows that it is nearly closed, see Tab. 1. The difference between the discrete evaluations of the left-hand side

TABLE 1. Volume transports across the Warnow transect shown in Fig. 4c-f in $[\text{m}^3\text{s}^{-1}]$ through interfaces for the three-layer estuarine circulation in the Warnow estuary averaged over the year 2014. The numbers in columns 2 and 3 reflect the left-hand side and those in column 4 reflect the right-hand side of (10). The numbers in column 5 give the difference between the left-hand and the right-hand sides of this equation as the numerical calculation error. The second and third rows show the values for high and low dividing salinity isohalines, respectively.

$[\text{m}^3\text{s}^{-1}]$	$Q_{\text{in},x}$	Q_r	$-0.5\partial\text{mest},x/\partial S$	error
x: high	35.03		36.08	-1.03
x: low	11.12	10.91	21.65	0.38

and the right-hand side are about 3% for the high-salinity isohaline of $s_{\text{div},\text{high}}$ and about 2% for the isohaline of $s_{\text{div},\text{low}}$. Calculations show that storage terms are largely negligible due to the long averaging interval of one year.

4. Discussion and Conclusions

The key result of this study is the first derivation of an exact quantitative relation between exchange flow and mixing in estuaries, highlighting how essential water mass transformations are for understanding estuaries. Estuarine exchange flow is defined here relative to fixed transects across the estuary. Since the generally continuous transition between estuary and river plume prohibits the specification of a distinct seaward limit of an estuary, the theory is formulated for an arbitrary estuarine transect. In this formulation, the estuarine circulation in simple estuaries with a two-layer circulation equals the S -derivative of the mixing integrated over the dividing salinity isohaline landwards of the transect, as shown in (9). This emphasizes the importance of the dividing salinity s_{div} for each transect. So far, s_{div} has only been used for the interpretation of Total Exchange Flow profiles and the accurate calculation of Q_{in} and Q_{out} as well as s_{in} and s_{out} (MacCready et al. 2018; Lorenz et al. 2019; Broatch and MacCready 2022). For the mixing - exchange flow relation (9), *estuarine circulation* needs to be quantified as the inflowing volume transport calculated in salinity coordinates, following the Total Exchange Flow (TEF) analysis framework established by MacCready (2011). *Mixing* needs to be quantified for the same quantity (salinity) that defines the coordinate of the circulation analysis to obtain this simple key relation (Klingbeil and Henell 2023). Using other coordinate systems as reference for the inflowing volume transport such as Eulerian (e.g., z or σ coordinates) would give different results (MacCready 2011; Burchard et al. 2018b)

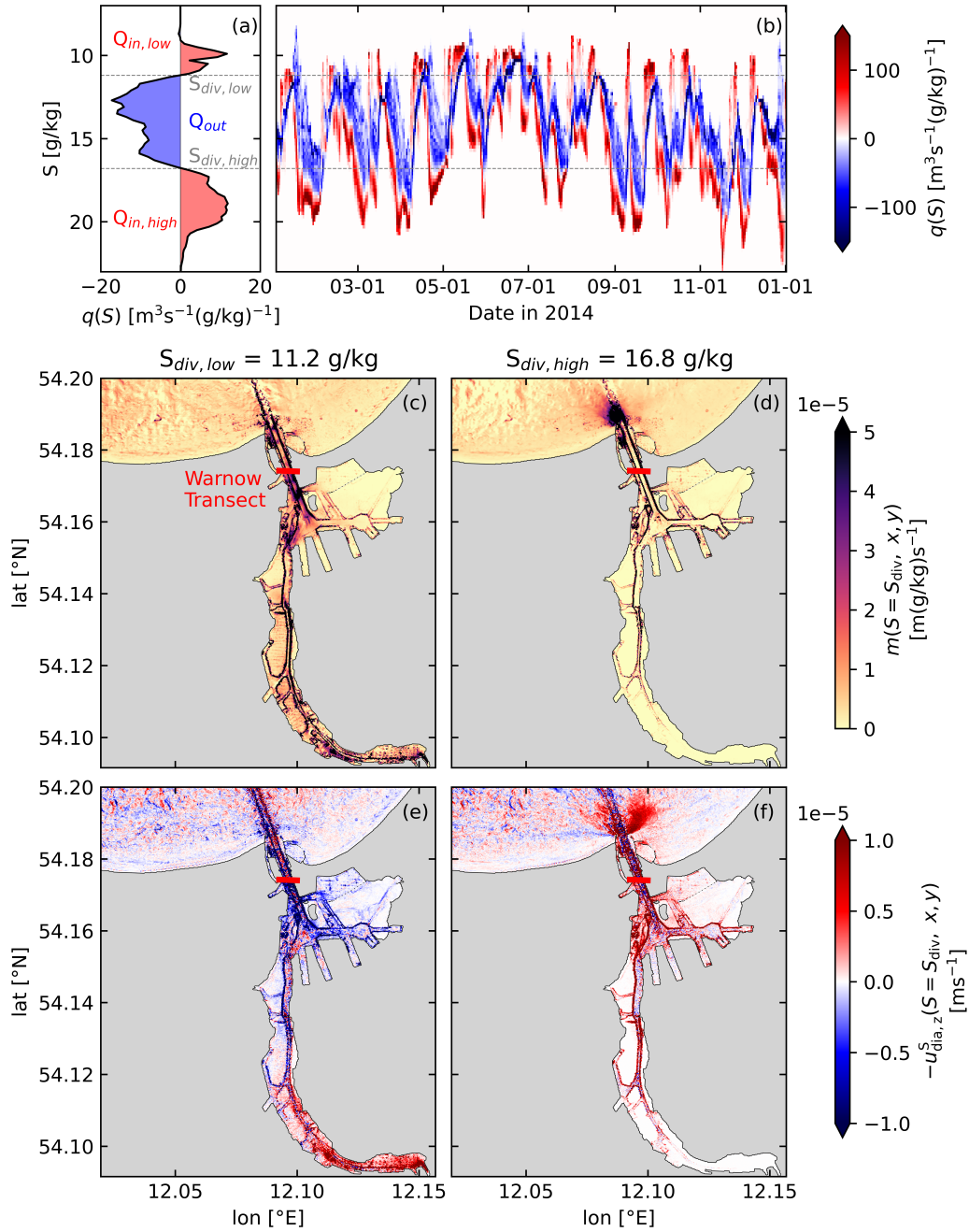


FIG. 4. Mixing and exchange flow results for the Warnow estuary during the year 2014. a: Total Exchange Flow (TEF) across the Warnow transect shown in panels c-f averaged over the entire year; b: Temporally resolved TEF; c,d: local mixing per salinity class m on the dividing salinity isohalines for $s_{div,low}$ (c) and $s_{div,high}$ (d); e,f: diahaline volume transport per unit horizontal area $u_{dia,z}$ on the dividing salinity isohalines for $s_{div,low}$ (e) and $s_{div,high}$ (f). In panels a and b, the horizontal lines indicate the two dividing salinities.

and violate the relation (9). Such an Eulerian exchange flow analysis is common (Hansen and Rattray 1965; Geyer and MacCready 2014; Lange et al. 2020), but does not establish any relation to estuarine water mass transformation processes. While for the two-layer estuarine exchange flow, mixing gradients are analyzed on the isohaline with the unique dividing salinity, more complicated multi-layer exchange flow requires analysis of mixing gradients on multiple dividing isohalines as shown in relation (10).

Going back to the example of the two-layer circulation, it is remarkable that the time-averaged exchange flow across a fixed transect is quantified by the S -derivative of mixing on only one single isohaline surface, ignoring the mixing occurring at other salinities in the estuary. However, it could be argued that mixing and other hydrodynamic processes at all salinities inside the estuary (i.e., landward of the transect) contribute to adjusting the time-averaged mixing and position of the dividing salinity isohaline in a way that relation (9) is fulfilled. Similar arguments hold for the more complex multi-layer estuaries following relation (10) for three layers or similarly derived multi-layer relations.

It is evident in both estuaries that the mixing is substantially elevated over sloping bathymetry along navigational channels. This has been described before for tidal estuaries as the effect of lateral differential advection (Lacy et al. 2003; Geyer et al. 2020): cross-flow lateral shear in combination with an along-flow salinity gradient leads to a cross-flow salinity gradient being much stronger than the along-flow gradient. The cross-flow salinity gradient induces a cross-flow density gradient leading to lateral exchange flow generating a vertical salinity gradient. Along-flow tidally induced turbulence (high K_v) in conjunction with the vertical salinity gradient over the slopes (high $|\partial s/\partial z|$) leads to substantially enhanced mixing $\chi_s \approx 2K_v (\partial s/\partial z)^2$. In non-tidal estuaries such as the Warnow estuary, this process has not yet been investigated, but similar processes might be at work there as well.

Our findings give the picture of a subtle balance between mixing and exchange flow in estuaries. The common notion that *Estuarine exchange flow is related to mixing* (MacCready et al. 2018) which implies a one-way relation should be reformulated to *Mixing and estuarine exchange flow are in balance for sufficiently long time averaging*. The bulk mixing relation (2) derived by MacCready et al. (2018) supports this latter argument, but still contains the inflowing and outflowing salinities s_{in} and s_{out} as variables in the mixing (M) - exchange flow (Q_{in}) relation. Furthermore, relation (2)

is only approximate, whereas relation (9) is exact (for long-term averaging and negligible surface freshwater fluxes).

The examples presented in this paper are limited to two-layer and three-layer estuaries with only one connection to the ocean. In the real world many other types exist. Estuaries might, for example, have a circulation with more than three layers. By cutting a transect through the Central Baltic Sea, Lorenz et al. (2019) obtained an exchange flow with four layers and three dividing salinities that were accurately identifiable using their numerical methods. The S -derivatives of mixing can now be quantified on those isohalines and mixing hotspot locations can be identified. A straight-forward extension of the three-layer key relation (10) could then be applied to check for consistency with the intensities of the volume transports (i.e., the complex exchange flow) in the four layers.

Many estuarine systems have more than one connection to the ocean such as the Baltic Sea (with the Sound, the Great Belt and the Little Belt as connections, see, e.g., Burchard et al. 2018b) or the Gulf of St. Lawrence with the major connection through the Cabot Strait and a minor connection through the Belle Isle Strait (Dickie and Trites 1983). Also those multi-entrance estuarine systems can be investigated by means of the relations derived here. In a model set-up for such a system, transects would be chosen across each of the entrances, individual TEF profiles for each entrance would be calculated and then these TEF profiles would be added to each other. In a simple case, a two-layer exchange flow would result, such that (9) could be applied for analysis. However, it would be more likely that the combined TEF profile has more layers, such that the three-layer relation (10) or a derived more complex relation would have to be applied. In cases where one of the entrances dominates (such as in the case of the Gulf of St. Lawrence), however, only a small disturbance of the dominating TEF profile would be expected. In case of the Baltic Sea, a diahaline exchange flow and mixing analysis has recently been conducted by Henell et al. (2023) for selected isohalines. It would be straight-forward to repeat that analysis for the dividing isohalines identified by a combined TEF analysis for all three entrance channels. The caveat of the Henell et al. (2023) study was, however, the relatively short averaging period of two years which is much shorter than the overturning time scale of the Baltic Sea of a decade or more (Reissmann et al. 2009), such that storage terms might dominate the balance.

The required length of the averaging periods to fulfill relations (9) and (10) depends on the time scales of mixing and exchange flow processes in the estuaries under investigation. The monthly

averages (essentially two spring-neap cycles) for the Elbe estuary show that for the low-runoff scenario (Fig. 3a) storage terms still contribute slightly to the volume transport budgets at some locations, showing that the adjustment time scales for this case are longer than one month. In contrast, in the high-runoff scenario (Fig. 3b) storage terms are sufficiently small.

The time-averaged theory developed here characterizes the average dynamic state of an estuary, as contrasted to a typical state. For example, for the tidal estuary (Sec. 3a), the two-layer flow situation is not present during ebb or flood, and is only weakly detectable during short times of flow reversal during slack tides (Schulz et al. 2020). It requires at least tidal averaging to obtain the two-layer exchange flow. Substantial differences in exchange flow occur between neap and spring tides (Chen et al. 2012), as well as between high and low run-off (Fig. 3c,d). The three-layer flow (Sec. 3b) in the non-tidal estuary is only occurring for short times in between the upwelling and downwelling dominated periods. Otherwise, there are mainly characteristic estuarine (upwelling) and anti-estuarine (downwelling) exchange flow situations present. The analysis method presented here is suitable to analyze these different states of the estuaries (spring, neap, upwelling, downwelling) separately. The more unsteady these states are, the more relevant storage effects would be. Storage terms can easily be added to the analysis method (as indicated for the low run-off case in the tidal estuary, see Fig. 3a), such that it is suitable for in-depth investigations of transient estuarine states.

The theory derived here provides the fundamental recipe for analyzing the relation between mixing and exchange flow in any estuary. It helps to identify the regions where the mixing occurs that is consistent with the exchange flow. Although only the mixing on the dividing salinity isohaline is included in the mixing - exchange flow relation (9), mixing elsewhere in the estuary indirectly influences the distribution of all isohalines and as such feeds back to the mixing of the dividing salinity isohaline.

Generally, observations are intrinsically prone to undersampling, such that mixing or overturning circulation are hard to observe directly. The sampling requirements for TEF profiles directly derived from mooring observations across transects have been presented by Lemagie et al. (2022) for three different tidal estuaries. However, in most estuarine systems such observations would be too demanding due to the complexity of the estuaries or limitations in equipment and personnel. Mixing observations covering the estuaries would be even more demanding. Instead of purely observational approaches, a numerical model for the estuarine system under investigation needs

to be constrained by critical observations, e.g. of water levels, temperature, salinity and velocity profiles. If available, turbulence and mixing observations should be added. Once the numerical model is sufficiently calibrated against the observations, e.g. by adjusting bed roughness, boundary conditions and by reducing numerical errors, the model results can be considered as a sufficient representation of reality (in the sense of a digital twin). In that way it becomes clear that observations are essential for setting up a representative numerical model. Specifically observations close to the key processes are important such as those representing water mass transformation processes or overturning circulation. Tracer release experiments as they have, for example, been carried out for the Baltic Sea (Holtermann et al. 2012, 2014) or for the Gulf of St. Lawrence (Stevens et al. 2024) are such critical experimental observations that have been successfully reproduced by numerical models, although the reproduction of tracer spreading depends on available numerical resolution and accuracy. Once a sufficient numerical model simulation is available, model results will be analyzed using the new mixing relation to motivate identifying the temporally and spatially varying mixing. In a next step, suitable transects need to be chosen, dividing salinities to be identified and exchange flow and mixing on those critical isohalines to be quantified. Once mixing hotspots are identified, the model results can in turn motivate research cruises to such potentially critical areas to verify the processes causing high mixing rates.

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Data availability statement. The model simulations that are analyzed here have been described in detail by Lange et al. (2020) and Reese et al. (2024), see the data availability statements in those publications.

APPENDIX

Calculating exchange flow intensity from estuarine mixing

For the present study we consider the long-term averaged state of an estuarine system which is stably stratified in salinity, i.e., the time-averaged salinity decreases with distance from the bottom. For an arbitrary water column in this system located at a fixed horizontal position (x, y) , integration of the continuity equation from the bottom to an isohaline of salinity S reads as (assuming incompressibility)

$$\frac{\Delta H(S, x, y)}{\Delta T} + \frac{\partial U_x(S, x, y)}{\partial x} + \frac{\partial U_y(S, x, y)}{\partial y} = u_{\text{dia},z}(S, x, y), \quad (\text{A1})$$

with the time-averaged horizontal transports in x and y direction, $U_x(S, x, y)$ and $U_y(S, x, y)$, respectively, vertically integrated from the bottom to the isohaline height, the change in isohaline height $\Delta H(S, x, y)$ divided by the averaging duration ΔT , and the time-averaged diahaline volume transport per unit horizontal area $u_{\text{dia},z}(S, x, y)$ (defined positive downward, towards increasing salinity), see Fig. 1a. We call an estuarine system *long-term averaged* when ΔH is negligibly small everywhere, i.e., when $|\Delta H|/\Delta T \ll |\partial U_x/\partial x + \partial U_y/\partial y|$ for all positions (x, y) . Note that the x -axis is pointing into the estuary, see Fig. 1.

To develop the present theory, (A1) and (5) will be integrated along the part of isohaline surfaces that is situated on the estuarine side of an arbitrary transect across the estuary.

Lateral integration of (A1) along constant S over constant width W results in

$$\frac{\Delta A(S, x)}{\Delta T} + \frac{\partial Q(S, x)}{\partial x} - U_{\text{dia}}(S, x) = 0 \quad (\text{A2})$$

with the accumulated volume transport across the transect at location x for all salinities larger than S ,

$$Q(S, x) = \int_W U_x(S, x, y) dy, \quad (\text{A3})$$

the laterally integrated diahaline transport across a line with constant x and S ,

$$U_{\text{dia}}(S, x) = \int_W u_{\text{dia},z}(S, x, y) dy \quad (\text{A4})$$

and the cross-sectional area for all $s \geq S$,

$$A(S, x) = \int_W H(S, x, y) dy. \quad (\text{A5})$$

Note that the assumption of a constant width W is no restriction, since practically W could be taken as the maximum width such that for locations with smaller width velocities and mixing rates are assumed to be zero outside the estuary (Burchard et al. 2018a). With the volume transport per salinity class across a fixed transect located at position x ,

$$q(S, x) = -\frac{\partial Q(S, x)}{\partial S} \quad (\text{A6})$$

being the Total Exchange Flow (TEF) as introduced by MacCready (2011) and (A2) it becomes clear that for long-term averaging ($\Delta A/\Delta T \rightarrow 0$), Q is the streamfunction of the estuarine overturning circulation in (S, x) -space (MacCready 2011) established by $(-\partial Q/\partial S, \partial Q/\partial x) = (q, U_{\text{dia}})$.

Integration of (A2) from an arbitrary transect location $x < 0$ to $x = 0$ with $Q(S, 0) = 0$ for all S (freshwater range of the estuary) leads to

$$Q(S, x) = -\int_x^0 U_{\text{dia}}(S, \xi) d\xi + \frac{\Delta \mathbb{V}_{\text{est}}(S, x)}{\Delta T}, \quad (\text{A7})$$

where

$$\mathbb{V}_{\text{est}}(S, x) = \int_x^0 A(S, \xi) d\xi \quad (\text{A8})$$

is the volume on the estuarine side of the transect with all $s \geq S$.

Note that (A7) is a special case of the derivation by Wang et al. (2017) who carried out the integration between two transects of non-zero salinity. Combining (5), (A4) and (A7) gives

$$Q(S, x) = -\frac{1}{2} \frac{\partial}{\partial S} \int_x^0 \int_W m(S, \xi, y) dy d\xi + \frac{\Delta \mathbb{V}_{\text{est}}(S, x)}{\Delta T}. \quad (\text{A9})$$

When defining

$$\mathbb{m}_{\text{est}}(S, x) = \int_x^0 \int_W m(S, \xi, y) dy d\xi \quad (\text{A10})$$

as the mixing per salinity class on part of an isohaline with salinity S occurring inside an estuarine volume bounded by a transect fixed at position x , then we obtain

$$Q(S, x) = -\frac{1}{2} \frac{\partial \mathbb{m}_{\text{est}}(S, x)}{\partial S} + \frac{\Delta \mathbb{V}_{\text{est}}(S, x)}{\Delta T}. \quad (\text{A11})$$

Relation (A11) shows the direct interdependence of the Total Exchange Flow profile and the derivative of the mixing per salinity class in the estuarine volume bounded by the transect, corrected by the storage term. This has indirectly been shown by Wang et al. (2017) in their Figs. 3 and 4.

In an estuarine system where the time-averaged salinity is stably stratified, a single dividing salinity $s_{\text{div}}(x)$ exists with $q > 0$ for $S > s_{\text{div}}$ and $q \leq 0$ for $S \leq s_{\text{div}}$, such that we can define

$$Q_{\text{in}}(x) = \int_{s_{\text{div}}(x)}^{S_{\text{max}}} q(S, x) dS > 0, \quad Q_{\text{out}}(x) = \int_0^{s_{\text{div}}(x)} q(S, x) dS \leq 0, \quad (\text{A12})$$

see Lorenz et al. (2019) and Fig. 1. It should be noted that (A12) gives

$$Q_{\text{in}}(x) = Q(s_{\text{div}}(x), x). \quad (\text{A13})$$

In (A12), $Q_{\text{in}}(x)$ and $Q_{\text{out}}(x)$ are the inflow and outflow volume transports defined in (1) and displayed in Fig. 1b. Evaluating (A11) at $S = s_{\text{div}}(x)$, we obtain the key relation of this study,

$$Q_{\text{in}}(x) = -\frac{1}{2} \frac{\partial \mathbb{m}_{\text{est}}(s_{\text{div}}(x), x)}{\partial S} + \frac{\Delta \mathbb{V}_{\text{est}}(s_{\text{div}}(x), x)}{\Delta T}, \quad (\text{A14})$$

including the storage term. When additionally assuming sufficient long-term averaging, i.e., vanishing of the storage term $\Delta \mathbb{V}_{\text{est}}/\Delta T$, we obtain the simplified version (9).

In a similar way, storage terms can also be added to the exchange flow - mixing relation (10) for three-layer flow (see also Fig. 1d):

$$\begin{aligned} Q_{\text{in,high}} &= -\frac{1}{2} \frac{\partial \mathbb{m}_{\text{est,high}}}{\partial S} + \frac{\Delta \mathbb{V}_{\text{est,high}}}{\Delta T}, \\ Q_{\text{in,low}} + Q_r &= \frac{1}{2} \frac{\partial \mathbb{m}_{\text{est,low}}}{\partial S} + \frac{\Delta \mathbb{V}_{\text{est,low}}}{\Delta T}. \end{aligned} \quad (\text{A15})$$

Symbol	Meaning	Unit
$A(S, x)$	Cross-sectional area below isohaline	m^2
$A_{\text{est}}(S, x)$	Area of isohaline inside the estuary	m^2
ΔT	Duration of averaging period	s
$H(S, x, y)$	Isohaline height	m
$J_{\text{est}}(S, x)$	Area-integrated diahaline diffusive salt flux on the estuarine side	$\text{m}^3 \text{s}^{-1} \text{g kg}^{-1}$
$K_h(x, y, z, t)$	Horizontal eddy diffusivity	$\text{m}^2 \text{s}^{-1}$
$K_v(x, y, z, t)$	Vertical eddy diffusivity	$\text{m}^2 \text{s}^{-1}$
$m(S, x, y)$	Local salinity mixing per salinity class	$\text{m s}^{-1} \text{g kg}^{-1}$
$\mathbb{M}_{\text{est}}(s_{\text{div}}(x), x)$	Integrated salinity mixing per salinity class on the estuarine side	$\text{m}^3 \text{s}^{-1} \text{g kg}^{-1}$
$\mathbb{M}_{\text{est,high}}(s_{\text{div,high}}(x), x)$	Integrated salinity mixing per salinity class for high salinity	$\text{m}^3 \text{s}^{-1} \text{g kg}^{-1}$
$\mathbb{M}_{\text{est,low}}(s_{\text{div,low}}(x), x)$	Integrated salinity mixing per salinity class for low salinity	$\text{m}^3 \text{s}^{-1} \text{g kg}^{-1}$
$q(S, x)$	Volume transport per salinity class	$\text{m}^3 \text{s}^{-1} (\text{g kg}^{-1})^{-1}$
$Q(S, x)$	Volume transport	$\text{m}^3 \text{s}^{-1}$
$Q_{\text{in}}(x)$	Inflowing volume transport	$\text{m}^3 \text{s}^{-1}$
$Q_{\text{in,high}}(x)$	High-salinity part of inflowing volume transport	$\text{m}^3 \text{s}^{-1}$
$Q_{\text{in,low}}(x)$	Low-salinity part of inflowing volume transport	$\text{m}^3 \text{s}^{-1}$
$Q_{\text{out}}(x)$	Outflowing volume transport	$\text{m}^3 \text{s}^{-1}$
Q_r	River runoff	$\text{m}^3 \text{s}^{-1}$
$s(x, y, z, t)$	Salinity	g kg^{-1}
S	Salinity coordinate	g kg^{-1}
$s_{\text{in}}(x)$	Inflowing salinity	g kg^{-1}
$s_{\text{out}}(x)$	Outflowing salinity	g kg^{-1}
$s_{\text{div}}(x)$	Dividing salinity	g kg^{-1}
$S_{\text{max}}(x)$	Maximum salinity	g kg^{-1}
$u_{\text{dia,z}}(S, x, y)$	Diahaline volume transport per unit horizontal area	m s^{-1}
$U_x(S, x, y)$	Vertically integrated transport in x-direction	$\text{m}^2 \text{s}^{-1}$
$U_y(S, x, y)$	Vertically integrated transport in y-direction	$\text{m}^2 \text{s}^{-1}$
$U_{\text{dia}}(S, x)$	Laterally integrated diahaline velocity	$\text{m}^2 \text{s}^{-1}$
$\mathbb{V}_{\text{est}}(s_{\text{div}}(x), x)$	Volume below dividing salinity isohaline on estuarine side	m^3
$\mathbb{V}_{\text{est,high}}(s_{\text{div,high}}(x), x)$	Volume below high dividing salinity isohaline on estuarine side	m^3
$\mathbb{V}_{\text{est,low}}(s_{\text{div,low}}(x), x)$	Volume below low dividing salinity isohaline on estuarine side	m^3
W	Width of estuary	m
$\chi_s(x, y, z, t)$	Local salinity variance destruction	$(\text{g/kg})^2 \text{s}^{-1}$

TABLE A1. List of variables including their meanings and units.

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Highlights

The role of the shoal – salt mixing mechanisms in a partially mixed tidal estuary with channel-shoal geometry

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- Enhanced mixing near the shoals plays an essential role for the exchange flow
- Salt plume formation is a major mixing mechanism at the channel-shoal transition
- Salt plume formation is enhanced by saltwater storage between flood and ebb
- Under increased stratification, additional strong boundary layer mixing occurs

The role of the shoal – salt mixing mechanisms in a partially mixed tidal estuary with channel-shoal geometry

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Abstract

The estuarine exchange flow is inherently linked to salt mixing which transports water across isohaline surfaces. This has recently been quantified as an exact relation between the distribution of local mixing and the exchange flow intensity. For the partially mixed, northwest German Elbe estuary, locally enhanced mixing occurred at the channel-shoal transition. Here, we aim to identify the mechanisms leading to such near-shoal mixing which are thus of particular importance to the estuarine exchange flow. To this end, a highly resolved numerical simulation of the Elbe estuary was accounted for in a process-oriented validation and then applied for a selected spring-neap cycle, assessing elevated mixing in space and time. For the tidal cycle of most intense mixing, occurring at neap, we find two main mechanisms of near-shoal mixing despite a high spatial variability from topographical irregularities: First, differential advection during flood leads to the formation of bottom salt plumes above plateau-shaped shoals which can be reinstated during ebb. Strong shear above the plateau leads to intense mixing at the interface of the plume and surface layer during flood and ebb. Second, the intersection of sufficiently stratified layers with the turbulent channel sidewalls results in intense mixing. Under high stratification, the intensity of near-shoal mixing compared to channel mixing increases as persistent stratification stabilizes

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the channel throughout the entire tidal cycle while sidewall mixing intensifies. We conclude that the mechanisms described here can be essential for the estuarine exchange flow in partially mixed estuaries with a channel-shoal geometry.

Keywords: estuaries, salt mixing, estuarine circulation, total exchange flow

1. Introduction

Within estuaries, salt mixing, defined as the destruction of salinity variance [1], is a process that transports water masses from terrestrial freshwater discharge across isohaline surfaces toward the ocean. As such, it is closely linked to water mass transformation and a necessary requirement for the existence of an estuarine exchange flow [see 2, 3]. This exchange flow is characterized by the up-estuary transport of saltwater and the down-estuary transport of brackish water that can be quantified across a vertical, cross-channel transect as first presented by Knudsen [4] and later refined as the Total Exchange Flow (TEF) by MacCready [5]. The understanding of estuarine mixing processes can thus be a key to understanding the exchange flow.

In estuaries, the inflows into an estuary are the river run-off $Q_r > 0$ and the salt water from the ocean $Q_{in} > 0$, while the outflow into the ocean $Q_{out} < 0$ is the brackish water that has been generated as a mixing product, with these transports relative to a fixed transect across the estuary. Under long-term averaged conditions, we obtain the volume balance $Q_{in} + Q_{out} + Q_r = 0$ [neglecting freshwater transports through the sea surface, see 4]. Under this condition the estuarine exchange flow, established by these transports can be quantified by Q_{in} alone. Recently, Burchard et al. [6] derived an exact and direct relation between the local mixing and the estuarine exchange flow, combining work from Walin [7], Wang et al. [2], and Klingbeil and Henell [8]:

$$Q_{in}(x) = -\frac{1}{2} \frac{\partial \mathbb{m}_{est}(S_{div}(x), x)}{\partial S}, \quad (1)$$

with the part of the mixing per salinity class that is landward of a fixed transect located at the position x along the estuary, $\mathbb{m}_{est}(S_{div}(x), x)$ and the dividing salinity between inflow and outflow, $S_{div}(x)$. This relation shows that the intensity of the estuarine exchange flow Q_{in} at the along-estuary position x depends on the salinity-space divergence of the diahaline mixing.

28 In their study, Burchard et al. [6] point out that this relation could be a
29 useful tool to identify local mixing mechanisms that are directly related to
30 the estuarine exchange flow.

31 Previous numerical studies by Li et al. [9], Henell et al. [10], and Reese
32 et al. [11] on different estuaries have revealed that the mixing on an isoha-
33 line surface can be highly heterogeneous in space and time, varying locally
34 and with changing forcing such as the spring-neap cycle or the freshwater
35 discharge. In case of the partially to well-mixed mesotidal Elbe estuary in
36 northwest Germany, Burchard et al. [6] quantitatively linked regions of inten-
37 sified salt mixing at the channel-shoal transition of the navigational channel
38 to the estuarine exchange flow across a given cross-channel transect near
39 the river mouth. Identifying the mechanisms behind such near-shoal mixing
40 would thus allow to explain the main processes related to the exchange flow
41 within the estuary.

42 Generally, the occurrence of near-shoal mixing is dependent on the impact
43 of lateral topography on the local current, e.g., in form of lateral circulation.
44 Early work by Erdogan and Chatwin [12] showed that for laminar flow in
45 a pipe, lateral circulation can enhance cross-channel tracer mixing. Later,
46 Smith [13] presented similar findings for a highly idealized estuary. Further-
47 more, differential advection of an along-channel density gradient, caused by
48 increased turbulence above flat shoals compared to the deep channel, plays
49 an important role in the dynamics of tidal estuaries and the creation of lateral
50 circulation as it turns longitudinal baroclinic pressure gradients into lateral
51 gradients [13, 14, 15, 16, and others]. Lateral circulation, in turn, can also
52 influence the along-channel estuarine exchange flow [see, e.g., 17, 18, 19].
53 Other drivers of lateral circulation have been summarized and quantified,
54 e.g., by Lerczak and Geyer [17]. In studies by Collignon and Stacey [20] and
55 Huguenard et al. [21], lateral circulation was found to promote mixing above
56 channel-adjacent shoals by destabilizing the water column through lateral
57 straining of isopycnals and vertical shear of horizontal velocities.

58 Further, Wang and Geyer [22] identified hotspots of salt mixing in along-
59 channel direction of the Hudson river which Warner et al. [23] later related
60 to lateral salt fronts occurring during ebb tide due to hydraulic effects at
61 local topographical constrictions. In the same study by Warner et al. [23], it
62 was confirmed that mixing in form of salinity variance destruction generally
63 occurs in locations with an ideal overlap of locally strong stratification and
64 sufficiently strong turbulence.

65 With respect to the temporal variability in partially mixed estuaries, mix-

ing was found to be ebb-enhanced by several studies [see, e.g., 20, 21, 23], which can be attributed to the availability of increased stratification for mixing. Within the spring-neap cycle, mixing in such estuaries tends to be most intense during the transition from neap to spring, when high levels of stratification co-occur with increasing levels of tidal energy [see, e.g., 2, 3, 9].

The previous paragraphs show that numerous studies have been performed on the timing and localization of mixing within partially mixed estuaries. Yet, these studies primarily address singular mechanisms without bringing them into the context of estuarine circulation. Within this study, we therefore build on the work by Reese et al. [11] and Burchard et al. [6] to explicitly localize enhanced mixing in space and time consistent with the estuarine circulation within a mesotidal estuary with a channel-shoal geometry. We then identify the specific processes leading to these regions of enhanced mixing. In doing so, we contribute to the understanding of how large-scale exchange flow patterns can be related to local processes and provide a guideline on how key mechanisms for estuarine mixing and the total exchange flow can be identified also in other estuaries.

2. Materials and Methods

In this study, we made use of the mixing definition by Burchard and Renau [1] as well as a vertical salinity variance decomposition by Li et al. [24] as described below. We applied these methods to the output from a realistic, high-resolution numerical hindcast simulation of the northwest German mesotidal Elbe estuary.

2.1. Theoretical framework

2.1.1. Estuarine mixing

Here, we define local salt mixing $\chi(x, y, z, t)$ as the destruction of salinity variance [1]:

$$\chi = 2K_h(\partial_x S)^2 + 2K_h(\partial_y S)^2 + \underbrace{2K_v(\partial_z S)^2}_{\chi_v}, \quad (2)$$

where $K_h(x, y)$ is the horizontal and $K_v(x, y, z, t)$ is the vertical diffusivity of salt, and $\chi_v(x, y, z, t)$ is the vertical mixing. In our simulations, K_h is a function of the horizontal grid size (see also Section 2.2.2). Further, $S(x, y, z, t)$ is the local salinity and ∂_i is the partial derivative in each spatial direction $i \in \{x, y, z\}$.

From the local mixing χ , the estuary-wide mixing can be computed using different choices for the estuarine boundary. A simple choice is to bound the estuary in seaward direction with a fixed vertical transect at a given along-channel location x . Integration over the resulting estuarine volume $V(x, t)$ yields the estuary-wide mixing $M(x, t)$ as used, e.g., by MacCready et al. [3]:

$$M(x, t) = \int_{V(x, t)} \chi(x, y, z, t) dV. \quad (3)$$

Alternatively, the estuary can be bounded by an isohaline surface of salinity S , yielding the volume $V(S, t)$. For stable stratification, the estuary-wide mixing $M(S, t)$ can then be computed as [see 25]

$$M(S, t) = \int_{V(S, t)} \chi(x, y, z, t) dV. \quad (4)$$

For a more general definition of $M(S, t)$ that is also valid for unstable stratification, we refer to Klingbeil and Henell [8]. On long-term average, such that salt and volume storages vanish, and neglecting surface fluxes, the mixing $M(S)$ is easily determined by a universal law of estuarine mixing [25]:

$$M = S^2 Q_r, \quad (5)$$

which states that the mixing within the estuarine volume $V(S, t)$ is solely determined by the freshwater discharge Q_r entering the estuary and by the choice of the bounding isohaline S . A good agreement between the LHS and RHS of (5) consequently indicates that the freshwater input and mixing within the estuary are balanced.

2.1.2. Mechanisms of stratification and destratification

Additionally, we make use of the vertical salinity variance $(S')^2(x, y, z, t)$ to quantify the vertical stratification of a water column as presented in Li et al. [24]:

$$S = \bar{S} + S', \quad (6)$$

where $\bar{S}(x, y, t)$ is the vertically averaged salinity. Consequently, $S'(x, y, z, t)$ yields the vertical anomaly of the salinity S .

To separate different mechanisms of stratification and destratification in a single water column, Li et al. [24] derived a dynamic equation for the rate

of change of the vertically integrated vertical salinity variance,

$$\underbrace{\frac{\partial}{\partial t} \int_{-H}^{\eta} (S')^2 dz}_{\text{Tendency}} + \underbrace{\nabla_h \int_{-H}^{\eta} \mathbf{u} \cdot (S')^2 dz}_{\text{(A): Advection}} = \underbrace{-2 \int_{-H}^{\eta} \mathbf{u}' S' \cdot \nabla_h \bar{S} dz}_{\text{(B): Straining}} - \underbrace{\int_{-H}^{\eta} \chi_v dz}_{\text{(C): Vertical Mixing}} \quad (7)$$

with the water depth $H(x, y)$ below $z = 0$, the surface elevation $\eta(x, y, t)$ above $z = 0$, where ∇_h is the horizontal gradient and the horizontal velocity vector $\mathbf{u}(x, y, z, t) = \bar{\mathbf{u}} + \mathbf{u}'$ is split into its depth-average $\bar{\mathbf{u}}$ and vertical velocity anomaly $\mathbf{u}'$ analogously to (6). The equation neglects horizontal mixing, which was indeed found to be considerably weaker than vertical mixing within our study (not shown), as well as the divergence of horizontal diffusive fluxes. It further neglects surface fluxes of salinity variance, such as precipitation and evaporation.

It should further be noted that (7) will also yield an increase in vertical salinity variance for the creation of unstable stratification since $(S')^2$ quantifies any deviation from the vertical average as expressed in (6). However, conditions in the Elbe estuary are almost exclusively stable. Unstable stratification only occurs locally and for a short duration preferably during flood [not shown, but for generally stable conditions cf. 26, 11], such that we are confident in using (7) as a measure for stratification changes in this study.

For the purpose of this study, we further split term (B) into its respective along-channel (x -) and cross-channel (y -) components u, v to better differentiate between impacts from lateral and longitudinal circulation.

2.2. Numerical simulations

2.2.1. Study region

A thorough description of the Elbe estuary is found in Reese et al. [11], but we note here that it is an M₂-dominated mesotidal, single-channel estuary adjacent to the German Bight, a southeastern part of the North Sea (see Fig. 1a,d). Due to past dredging activities as well as ongoing maintenance, the Elbe estuary has a well-defined navigational channel surrounded by extensive tidal flats leading to a simple channel-shoal geometry. The estuary is partially to well-mixed depending on discharge conditions and the spring-neap cycle [27, 28]. The tidal intrusion within the Elbe is limited in upstream direction by a weir in Geesthacht (see Fig. 1a).

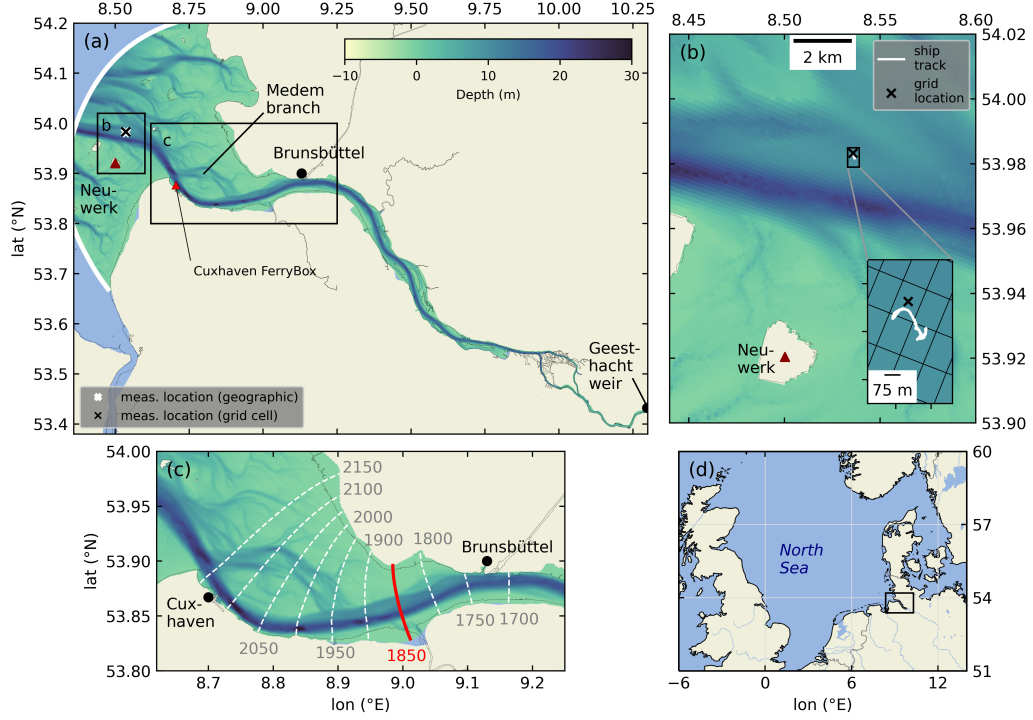


Figure 1: Overview of the tidal Elbe. (a) Model domain and topography used for the numerical simulation of the Elbe estuary as marked by the black rectangle in (d). The white cross marks the measurement location from Section 3, and the black cross shows the nearest grid location chosen for the comparison of simulation and observations in the same section. The bold white line shows the location of the open model boundary and the black rectangles mark the details shown in (b) and (c), respectively. In (b) and the inset in (b), the white line shows the ship track during the observations, the black lines show the horizontal grid lines of the numerical setup, and the remaining contents are as explained in (a). In (c), the bold red line marks the transect 1850 explicitly presented in Section 4, while dashed white lines and gray labels indicate all remaining cross-estuary transects used for the analysis of mixing processes for the present study. (d) Location of the estuary at the North Sea coast.

153 2.2.2. Numerical model and setup

154 For our numerical simulations, we used the General Estuarine Transport
155 Model [GETM; 29, 30], coupled to the General Ocean Turbulence Model
156 [GOTM; 31, 32] for a k - ε turbulence parameterization with a second-order,
157 algebraic closure [33]. The setup used here has been derived from the Elbe
158 setup presented and validated by Reese et al. [11] and further used by Bur-
159 chard et al. [6]. For the present study, the vertical grid resolution was in-
160 creased from 30 to 40 layers, now using adaptive coordinates that allow for
161 a flexible zoom in stratified regions [34]. The horizontal, curvilinear grid
162 resolution was increased to 2404×397 grid cells in along-channel and cross-
163 channel direction, respectively, while the thalweg-following grid shape itself
164 was only subject to minor changes. This specific shape yields cross-estuary
165 grid lines which can directly be used for analyses on cross-channel transects.

166 The setup version used here applies forcing for the year 2024. Boundary
167 forcing, prescribed at the open boundary in the German Bight as illustrated
168 in Fig. 1a, was taken from E.U. Copernicus Marine Service [35] and includes
169 tidal elevations as well as vertical temperature and salinity distributions.
170 Initial distributions for salinity and temperature within the model domain
171 were taken from the same dataset. Meteorological forcing consists of data
172 from the MET Nordic operational archive [36], which has a 1 km-horizontal
173 resolution. For the model topography, the most recent available tidal Elbe
174 topography dataset from the year 2022 [37] was used for the majority of
175 the estuary. Remaining sections in the outer regions of the model domain
176 were taken from topography sets from Sievers et al. [38] for the German
177 Bight and from Wasserstraßen- und Schifffahrtsamt Hamburg [39] as well as
178 Wasserstraßen- und Schifffahrtsamt Weser-Jade-Nordsee [40] for the Outer
179 Weser. The different datasets were interpolated at their respective margins.

180 The horizontal diffusivity was constant in Reese et al. [11], but is now
181 computed locally on the horizontal curvilinear model grid using a Smagorin-
182 sky eddy parameterization [41]. It is therefore a function of the local grid
183 size. For calibration of the salinity distribution within the estuary, the fresh-
184 water discharge entering the setup at the weir in Geesthacht (see Fig. 1a)
185 was multiplied by a factor of 1.3. This correction was required as the avail-
186 able discharge measurements [42] are known to have a wide error margin
187 (Bundesanstalt für Wasserbau, personal communication), such that the to-
188 tal discharge intensity is a measure of model calibration. The discharge at
189 Geesthacht was prescribed at a constant salinity of 0.5 g/kg. Since the trib-

190 utaries between Geesthacht and the German Bight where found by Reese
191 et al. [11] to be neglectable with respect to the overall salt mixing dynamics,
192 they have not been included here.

193 The model was run from the 1st of January 2024. For this study, we
194 analyze model output from 16th-30th April 2024, covering one spring-neap
195 cycle.

196 The updated model domain and topography are shown in Fig. 1a.

197 3. Process-oriented Setup Validation

198 Based on the regions of enhanced mixing described in Reese et al. [11]
199 and Burchard et al. [6], measurements were performed in the outer Elbe
200 Estuary in April 2024, near such a region of proposed elevated local mixing
201 (see Fig. 1a,b and Fig. 4a). Due to limitations proposed by maritime traffic
202 and ship specifications, it was not possible to measure directly at a location
203 of high near-shoal mixing. Yet, as will be shown in the following, a process
204 of ebb-enhanced, shoal-related mixing can still be seen in the data. Due
205 to the short and recent simulation period, a statistical model validation as
206 performed by Reese et al. [11] for the old version of the setup is not possible.
207 Instead, the above-mentioned measurements are used here for a process-
208 oriented validation of the updated numerical Elbe setup, demonstrating that
209 it is capable of reproducing the type of mixing process that is the subject of
210 the present study.

211 3.1. Measurements in the outer Elbe estuary

212 Observations were performed as continuous measurements from aboard
213 the research vessel FK Littorina, anchored by the northern Elbe channel shoal
214 in the German Bight near Neuwerk (outer estuary; see Fig. 1a,b), covering
215 almost one full tidal cycle on the 28th of April 2024. The water depth ranged
216 from 7.5 m at low tide to 10.6 m at high tide. In detail, the measurements
217 were taken with an acoustic doppler current profiler (1200 kHz Workhorse,
218 RDI, US) mounted on a metal pole at the starboard side of the ship in approx.
219 1 m water depth, measuring current velocities within the water column. The
220 ADCP sampled with 1 Hz in platform coordinates, and a bin size of 0.25 m.
221 The ADCP measurements were running continuously without interruptions
222 during the time of anchoring. Additionally vertical profiles at the stern of the
223 ship were sampled with a micro-structure shear sonde (MSS90L, Sea & Sun
224 Technology, Germany). Profiles at a free falling speed of 0.6 m/s were taken

continuously with the exception of slack tide, where breaks were required due to a risk of the sonde being carried underneath the ship. The device was equipped with two PNS06 airfoil probes, measuring the dissipation rate of turbulent kinetic energy (ε) together with CTD profiles. The distance between the MSS and ADCP was approx. 20 m. The weather conditions were relatively calm, with an average wind speed of 7 m/s from a southeasterly direction [computed for the nearest grid point of the weather model output from 36]. The spectral significant wave height at the two nearest available stations ElbeWR and Nordergründe varied between 0.2 and 0.5 m and 0.1 and 0.4 m throughout the duration of the measurements, respectively [43]. During the last two hours of measurements, the wave height started increasing steeply to the respective maximum values and continued to rise after the end of the measurements. No rain occurred during the measurements, and it was mostly cloudy, such that no influence of extreme weather conditions should be found in our data. The measured freshwater discharge into the Elbe estuary from Neu Darchau scaled at about 550 m³/s during the period 25th-29th April [44], which is only half of the average April discharge [1110 m³/s for the period 1925-2014; 45].

For processing of the ADCP data, the velocities in N and E direction were computed with a moving platform correction, using the bottom track and external heading as reference. Spikes and side lobe interferences right above the bed were removed and missing data points interpolated. Additionally, the velocities were filtered with a 5 min moving average and rotated to point in the same along-channel and cross-channel directions as the model velocities in the nearest grid location, i.e., by 292.5° from the North and East axis, respectively. The magnitude of the vertical shear $[(\partial_z u)^2 + (\partial_z v)^2]^{(1/2)}$ was computed from the processed, non-rotated horizontal velocities.

Dissipation rates and other mixing parameters were estimated from the MSS as described in detail by Holtermann and Umlauf [46]: all sensors were sampled at 1024 Hz, digitized with 16 bit resolution, and transferred online to the computer. After despiking, all data were averaged to 256 Hz resolution for noise reduction, and temperature and conductivity data were corrected for different sensor response times. A sensor protection cage allowed us to sample turbulence down to approximately 0.1 m above the sediment. Dissipation rates were obtained by integrating vertical shear spectra over half overlapping 256-point Hanning windows (corresponding to 1 s segment length in time, or 0.5–0.7 m in depth), assuming local isotropy in the dissipative subrange.

262 The upper wave number for integration was found iteratively as a function
 263 of the Kolmogorov wavenumber with a correction for lost variance due to
 264 unresolved scales [47]. Dissipation rates estimated with this method from
 265 both shear probes were averaged into nonoverlapping bins of 0.5 m thickness.
 266 The noise level of this coastal profiler is of the order of 10×10^{-9} W/kg, which is
 267 sufficient to resolve the turbulence in the highly energetic outer Elbe Estuary.
 268 For better comparison with our model data, the local vertical mixing χ_v was
 269 computed from K_v and the vertical gradient of the observed salinity, $\partial_z S$, as
 270 defined in (2). K_v was computed by

$$K_v = \Gamma \frac{\varepsilon}{N^2}, \quad (8)$$

271 with a constant mixing efficiency Γ of 0.2 [48] and the buoyancy frequency
 272 $N(x, y, z, t)$. Lastly, we computed the gradient Richardson number $Ri(x, y, z, t)$,

$$Ri = \frac{N^2}{(\partial_z u)^2 + (\partial_z v)^2}, \quad (9)$$

273 from the ADCP shear interpolated onto the MSS sampling times and the
 274 MSS buoyancy frequency. The same quantities were also computed for the
 275 model output.

276 *3.2. Comparison of measurements and simulation*

277 To ensure that our simulations are capable of correctly reproducing mix-
 278 ing processes at the channel-shoal transition, we here compare our model
 279 output to the measurements described above. The two datasets are depicted
 280 in Fig. 2.

281 Note that in the model, the tidal phase near Neuwerk lags behind the
 282 observations by about half an hour due to a lag in the boundary forcing, so
 283 the model results are shown for a time span shifted by 30 minutes relative
 284 to the time axis from the observational dataset.

285 The main process found in the observational data is an incoming salt
 286 intrusion that forms during later flood and persists throughout ebb, leading
 287 to ebb-enhanced mixing (Fig. 2g,i; 12:00-17:00h UTC). It consists of an ini-
 288 tially water column-wide increase in salinity S followed by the main intrusion,
 289 which is topped by a fresher layer with strong stratification in between. The
 290 near-bottom salt intrusion coincides with a lateral circulation pattern with a
 291 (fresher) surface flow of water from the shoal toward the navigational chan-
 292 nel ($v < 0$) and an opposed (saltier) bottom flow from the channel toward

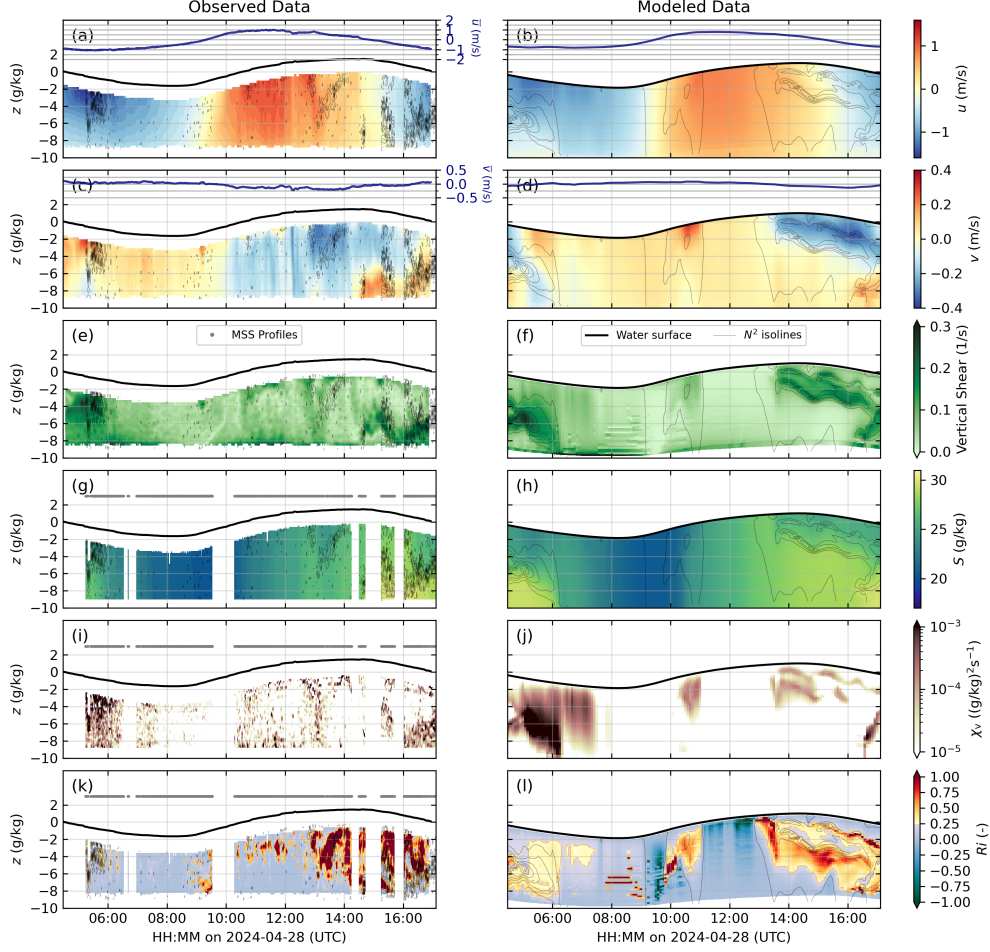


Figure 2: Comparison of observed and modeled data from a measurement location near Neuwerk as shown in Fig. 1a,b for one M_2 tidal cycle. Left-hand side: observations from the location marked in white in Fig. 1a,b, right-hand side: simulated data from the location marked with a black cross in Fig. 1a,b. (a), (b): observed and modeled along-channel velocity u , respectively, where $u > 0$ is flood-directed, $u < 0$ is ebb-directed. The blue line at the top shows the depth-averaged along-channel velocity $\bar{u}$. (c), (d): observed and modeled cross-channel velocity v , respectively, where $v > 0$ is shoal-ward, and $v < 0$ is channel-ward. The blue line at the top shows the depth-averaged cross-channel velocity $\bar{v}$. (e), (f): magnitude of the vertical shear of the horizontal velocities $[(\partial_z u)^2 + (\partial_z v)^2]^{(1/2)}$. (g), (h): salinity S . (i), (j): local vertical mixing χ_v . (k), (l): gradient Richardson Number Ri . Gray dots in the observations show the timing of each MSS profile. Note that due to a lag in the boundary forcing, the model results have been shifted by half an hour with respect to the time axis to allow for a better compatibility of the tidal phase with the observations.

the shoal ($v > 0$, Fig. 2c; 14:00-17:00h). Weak vertical mixing χ_z occurs within the shear layer between the lateral inflow and outflow during earlier ebb (Fig. 2c,i; 14:00-17:00h). At late ebb (05:00-07:00h), stronger mixing is observed throughout the entire water column, but is most intense within the stratified upper half of the water column (Fig. 2i).

While the along-channel velocity u is well reproduced within our simulation for the entire observation period aside from a slight underestimation of the velocity amplitude (Fig. 2a,b), the salt intrusion initially reaches too high into the water column compared to the observations (Fig. 2g,h; 12:00-17:00h). Nonetheless, the general observed pattern of the intrusion is also found in the model output, including the lateral circulation pattern at early flood and the timing and vertical localization of mixing (Fig. 2d,h,j). As in the observations, our model shows an ebb tide gradient Richardson number $Ri > 0.25$ in most of the water column away from the turbulent bottom layer, and strongest mixing occurs in regions of marginal stability [$0.25 < Ri < 1$, see 49, and citations therein], see Fig. 2k,l. Marginal stability is mostly found at late ebb, where strong shear can overcome the vertical stratification in the observations as well as the simulation, such that strong mixing can occur. Meanwhile, slack after flood and early ebb display a mostly stable water column with high $Ri \gg 1$, such that mixing is weak and limited to the shear layer.

The main difference between our observations and measurements is found in the lateral velocity v during flood (10:00-14:00h), which is weakly positive in the model but weakly negative in the observations. Since the along-channel velocity u is reproduced well and of considerably higher magnitude than v , this indicates a slight difference in the angle between the observed and simulated flood currents. A reason for the slightly shifted angle, as well as the too-strong salt intrusion, may be topographical inaccuracies in the model. The ship track throughout the measurements covered a distance of roughly the size of one to two adjacent grid cells (see inset in Fig. 1b), so that small-scale topographical variations that might have influenced the observations cannot be properly resolved within the model.

Mixing during most of flood tide is weak despite the vertical shear that leads to a low gradient Richardson number $Ri < 0.25$ in the simulation and observations (Fig. 2k,l; 07:00-13:00h). Although a small Ri is generally associated with strong mixing, we here have to differentiate between strong turbulence and available stratification for mixing as defined in (2): during flood, the conditions in the measurement location are overall well-mixed,

331 so that the small Ri is here associated with low mixing due to the lack of
332 available stratification.

333 Despite the differences regarding the lateral current during flood tide
334 due to a weak shift in the angle of the local velocities, we have shown here
335 that our model is generally capable of reproducing one of the key features
336 within the focus of this study: ebb-enhanced mixing that is related to a
337 lateral salt intrusion toward the channel shoal. In our simulations, we find a
338 similar process to also occur along the shoals of the inner estuary, upstream of
339 Cuxhaven (see Fig. 1c for the location of Cuxhaven), which will be presented
340 and discussed among other processes in the following sections.

341 4. Results and Discussion

342 4.1. Elevated mixing in time

343 In a previous study of mixing dynamics in the Elbe estuary, Reese et al.
344 [11] pointed out a potential spring-neap signal of estuary-wide mixing: while
345 the magnitude of mixing throughout the seasonal cycle was dominated by
346 the incoming freshwater discharge Q_r as predicted by the universal law of
347 estuarine mixing (5) [25], the amount of this mixing on shorter time scales
348 appeared to vary with the spring-neap cycle, in particular during periods of
349 reduced and relatively constant freshwater discharge. Here, we will quantify
350 the temporal development of estuary-wide mixing in more detail for a selected
351 spring-neap cycle.

352 In Fig. 3d, the integrated mixing $M(S)$ within the estuarine volume $V(S)$
353 bounded by the isohaline surface at $S = 20$ g/kg as defined in (4) is shown
354 for one spring-neap cycle in the later half of April 2024, averaged by M_2
355 tidal cycles and scaled with the universal law (5). The freshwater discharge,
356 shown as a black line in the same panel, varied only by about $60 \text{ m}^3\text{s}^{-1}$ during
357 this period, which corresponds to about 8 % of the average magnitude of Q_r
358 within the same period. No correlation between the mixing intensity and
359 freshwater discharge can be seen. Instead, mixing of the highest intensity
360 occurs on the 17th and 18th of April, during a period of low tidal energy as
361 evident by the reduced tidal amplitude at Cuxhaven FerryBox (Fig. 3b, see
362 also Fig. 1a for the location of the station), i.e., at neap tide. This coincides
363 with generally increased levels of vertical salt stratification inside the estuary,
364 see Fig. 3c.

365 Throughout the remaining analysis period, including spring tide at the
366 26th of April, the mixing is of constant, reduced intensity and follows the uni-

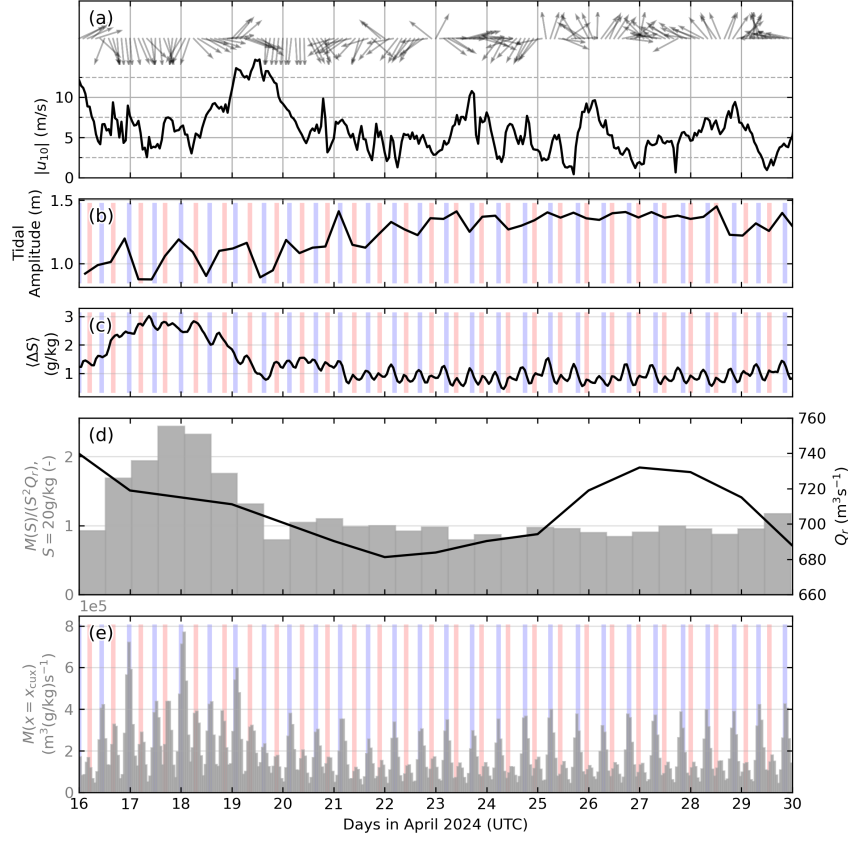


Figure 3: Simulated time series of salt mixing and related properties from the Elbe estuary throughout a full spring-neap cycle on 16th-30th April 2024. (a) Direction (arrows pointing in the direction in which the wind is blowing) and magnitude $|u_{10}|$ (black line) of the wind 10m above the surface; (b) tidal amplitude at Cuxhaven (station FerryBox in Fig. 1a), computed as the difference between adjacent high and low tide water levels and vice versa; (c) area-averaged stratification $\langle \Delta S \rangle$ within the estuarine area $A(x)$ where the vertically averaged salinity $\bar{S}(x, y, t)$ is within the bounds $0.6 \text{ g/kg} \leq \bar{S} \leq 15 \text{ g/kg}$. ΔS is the difference between the salinity in the bottom and surface sigma layers of each horizontal model grid cell; (d) volume-integrated mixing $M(S)$ as in (4) within an estuarine volume bounded by the isohaline surface at $S = 20 \text{ g/kg}$, averaged over time intervals of one M_2 tidal cycle each (gray bars). Additionally, the freshwater discharge prescribed to the model at Geesthacht is shown as a black line; (e) hourly averaged, volume-integrated mixing $M(x, t)$ as in (3) within the estuarine volume $V(x, t)$ bounded by a transect at the along-channel position x_{cux} of the station Cuxhaven FerryBox. In (b), (c), and (e), the vertical blue lines correspond to the timing of peak ebb and vertical red lines correspond to the timing of peak flood, defined as the timing of the highest ebb and flood current within a tidal cycle at Cuxhaven FerryBox, respectively.

versal law, i.e., $M(S)/S^2Q_r \approx 1$ which implies balanced conditions between mixing and freshwater discharge. We find a similar tendency for the volume-integrated mixing $M(x)$ (eq. 3) within an estuarine volume bounded by a vertical transect at Cuxhaven, at the along-channel position of the station CuxhavenFerryBox, as shown in Fig. 3e.

Within the period of balanced mixing (i.e., outside of neap tide), stratification also maintains a steady level superimposed by periodic variations throughout the M_2 tidal cycle (see Fig. 3c): stratification tends to be lowest at the transition from ebb to flood, then increases until peak flood. At late flood, stratification is reduced again until a local minimum occurs around slack after flood. At early ebb, stratification increases once more until it reaches its peak around peak ebb. For the remaining ebb tide, it is strongly reduced again. The overall highest stratification from the 21st of April on occurs at peak ebb, while the flood peak is of secondary nature. The mixing $M(x)$ follows this pattern, such that the highest mixing rates occur shortly after peak ebb (see Fig. 3e). A secondary, less pronounced mixing maximum occurs shortly after peak flood.

At neap tide, the M_2 variability of stratification and mixing is superimposed by a diurnal pattern: in particular, the mixing $M(x)$ here displays a different type of variability that coincides with a pronounced diurnal pattern of the tidal amplitude on 17th-19th April. In this period, distinct maxima of mixing occur at the beginning of the 17th, 18th, and 19th of April around peak ebb tides that coincide with semidiurnal peaks of the tidal amplitude. In between, flood and ebb display comparable levels of salt mixing. From the 19th to 21st of April, the diurnal variability of the tidal amplitude weakens and a transitional stratification and mixing pattern are found.

While the freshwater discharge is steady enough to allow for the predominance of a spring-neap related mixing signal, this signal seemingly stands in contrast to the general finding that salt mixing in partially mixed tidal estuaries peaks at the transition from neap to spring, as reported, e.g., by Wang et al. [2] for the Hudson river and Li et al. [24] for the Changjiang river. Even for the Elbe estuary itself, Reese et al. [11] pointed out increased mixing rates at the transition from neap to spring, although this signal was often obscured by a strong variability of the freshwater discharge.

To explain this disparity, the wind magnitude and direction at the Elbe river mouth are displayed in Fig. 3a. It appears that a strong wind from a westerly direction on the 19th of April hampered the re-establishment of stratification after each tidal cycle on that day. Westerly winds in the Elbe

405 estuary are upstream-directed such that they have the potential to destratify
 406 the estuary [50, 51]. Since the storm does not coincide with a clear mixing
 407 signal, it is possible that it predominantly reduced stratification via wind-
 408 driven straining. After the passing of the storm event, the tidal amplitude
 409 has already increased to such a degree that no more excess stratification can
 410 be created. Indeed, a re-evaluation of data from Reese et al. [11] during
 411 the period of mostly constant discharge in the Elbe from August 2012 to
 412 the end of December 2012 (see Fig. S1, Supplemental Material) showed that
 413 mixing can increase strongly from the beginning of neap tide, particularly at
 414 times of a strongly diurnally varying tidal amplitude under the condition that
 415 sufficient stratification is available. Depending on the continued availability
 416 of stratification, mixing may continue to increase throughout the transition
 417 from neap to spring, leading to either neap-pronounced mixing or the well-
 418 known mixing peak at the neap-spring transition. The timing of available
 419 stratification around neap tide shows a high variability which is likely driven
 420 by weather and discharge conditions. Adding to this, the time series of tidal
 421 velocity and mixing in the Hudson river shown in Warner et al. [23] seem to
 422 display a similar variability of the exact timing of mixing despite the overall
 423 tendency of highest mixing rates at the transition from neap to spring.

424 The semidiurnal pattern of mixing peaks after peak ebb and secondary
 425 peaks after peak flood is known from Warner et al. [23]. It corresponds to
 426 the timing of the tidal cycle where increased stratification is available and
 427 the tidal energy is highest. Warner et al. [23] further point out the shifted
 428 mixing pattern during periods of strong diurnal inequality of the tidal energy,
 429 where flood mixing can become comparable to ebb mixing. To that remark,
 430 we here add a more thorough explanation: the coincidence of such diurnal
 431 inequality with neap tides allows for an early onset of increased salt mixing
 432 already during neap tide, where the tidal energy would otherwise tend to
 433 be relatively low. Then, diurnal “flood” peaks coinciding with M_2 ebbs can
 434 provide sufficient tidal energy for a premature increase of mixing. Under
 435 these conditions, it is the availability of salt stratification that determines
 436 the intensity of mixing throughout the spring-neap cycle rather than the
 437 availability of tidal energy.

438 *4.2. Elevated mixing in space*

439 To localize mixing not only in time, but also in space, we consider the
 440 vertically integrated local mixing $\int \chi_z dz$ for each horizontal grid cell of our
 441 numerical setup. The vertically integrated mixing, averaged over the full

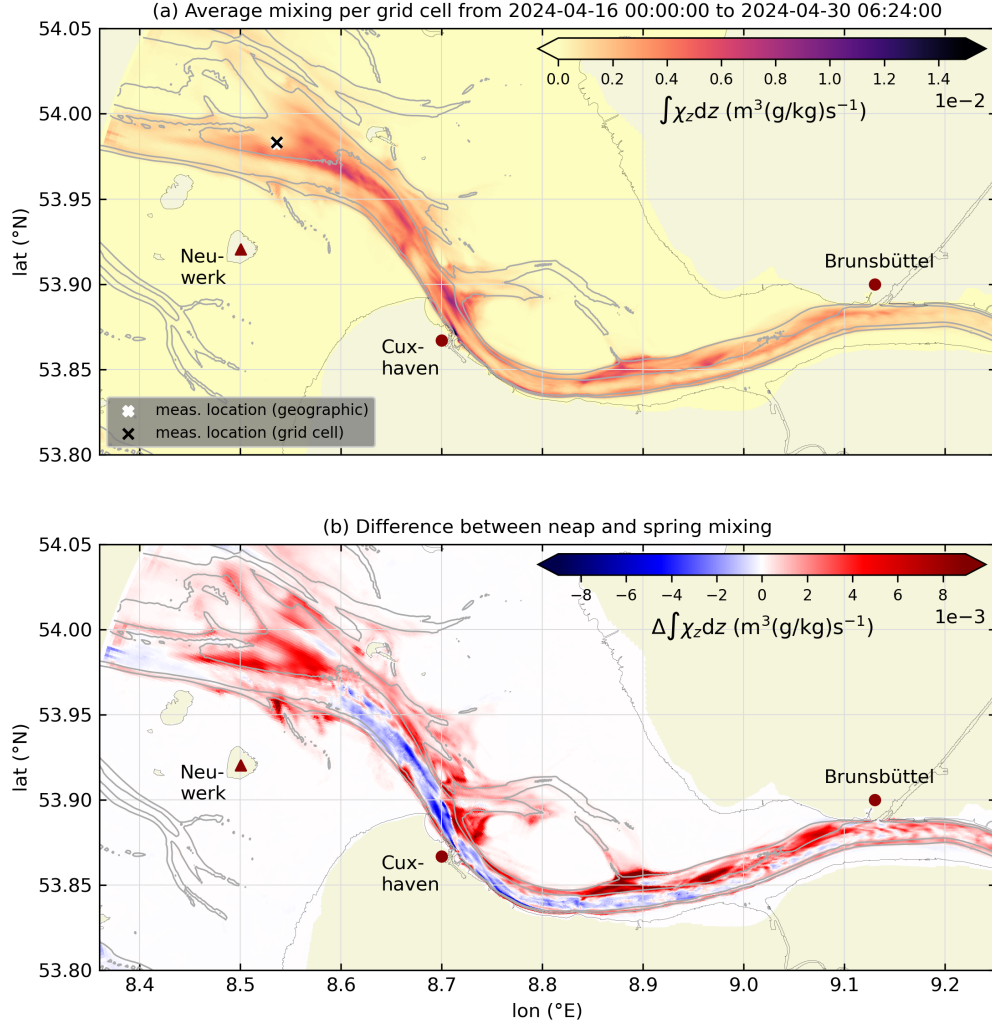


Figure 4: Salt mixing distribution within the Elbe estuary. (a) Vertically integrated local mixing $\int \chi_z dz$, averaged over a full spring-neap cycle from 16th to 30th April 2024. The white cross marks the measurement location from Section 3, and the black cross shows the nearest grid location chosen for the comparison of simulation and observations in the same section. (b) Difference between $\int \chi_z dz$ at the timing of maximum mixing as identified in Section 4.1 (neap tide; averaged from 17th April 12:00h UTC to 18th April 12:00h UTC) and $\int \chi_z dz$ at spring tide (averaged from 26th April 00:00h UTC to 27th April 00:00h UTC). Bold gray lines indicate the 12 m- and 6 m-isobaths.

spring-neap cycle from 16th to 30th April 2024, is shown in Fig. 4a. Similar to Reese et al. [11] and Burchard et al. [6], who showed the mixing intensity on a single isohaline surface, we also find regions of increased integrated mixing along the channel-shoal transition of the navigational channel, while mixing in the deeper sections of the channel is reduced.

This pattern becomes more obvious when considering the difference between the integrated mixing at neap tide and at spring tide (Fig. 4b): at neap, where mixing and stratification are strongest as shown in the previous section, mixing along the channel-shoal transition gains importance, while mixing within the channel becomes even weaker.

4.3. *Mixing mechanisms throughout an M_2 tidal cycle*

To explain the processes of the near-shoal mixing identified in Section 4.2, we will now in detail consider the estuarine dynamics throughout the M_2 tidal cycle of maximum mixing within our analysis period as identified in Section 4.1, i.e., at the transition from 17th to 18th April 2024. To this end, we first assess the horizontal distribution of the different terms from the dynamic equation for the vertical salinity variance (6) from Li et al. [24] within the estuary for flood tide and ebb tide, respectively. Additionally, data from a number of cross-channel transects from the inner estuary (Cuxhaven to upstream end of salt intrusion, see transects in Fig. 1c) is analyzed using snapshots of velocities, mixing, shear, and the gradient Richardson number Ri .

We note that in the outer Elbe estuary (downstream of Cuxhaven), the channel geometry becomes more complex and the dynamics of the river plume and of the German Bight gain importance, resulting in a higher variability of processes. In this study, we therefore restrict our analysis to the inner estuary only. However, a similar strategy could also be applied to the outer estuary.

4.3.1. *Estuary-wide processes of stratification and destratification*

Considering the different terms from the dynamic equation for the vertical salinity variance (6), a high spatial variability in magnitude and even sign of each term becomes apparent (see Fig. 5 and 6). Yet, a number of more general patterns can be found.

At flood tide, advection A and lateral straining B_y are the terms of highest intensity. Advection tends to mostly carry in less stratified water within the channel ($A < 0$, Fig. 5a) while it increases stratification above

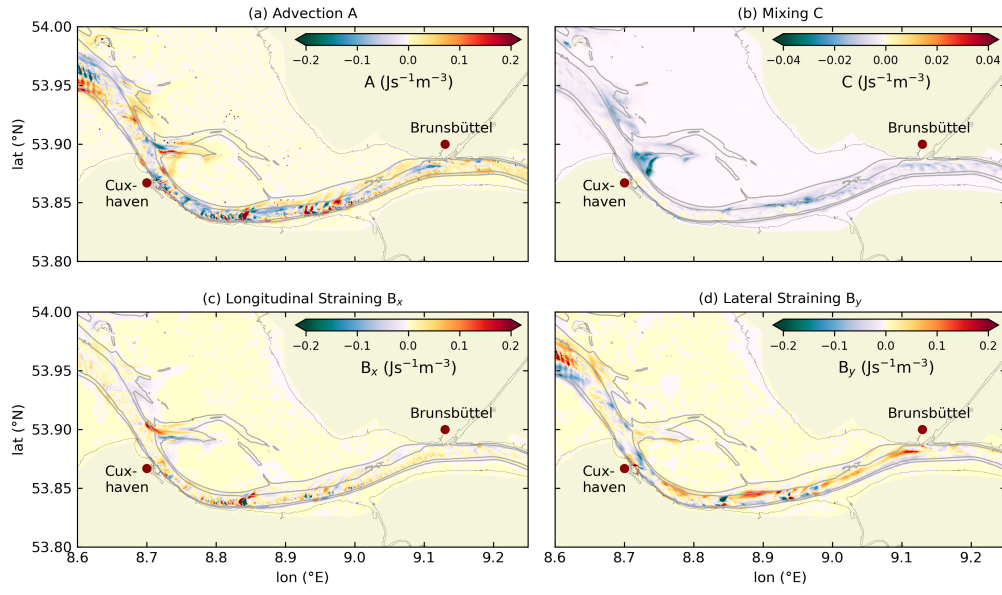


Figure 5: Different terms from (7), averaged over two hours around peak flood on 17th April 2024 (16:30h to 18:30h UTC), computed from numerical simulation output. (a): Advection term A from (7), (b): vertical mixing C, (c): along-channel straining B_x, and (d): cross-channel straining B_y from the RHS of (7). Bold gray lines indicate the 12 m- and 6 m-isobaths. Note the different colorbar scale for the mixing term in (c) compared to the remaining panels.

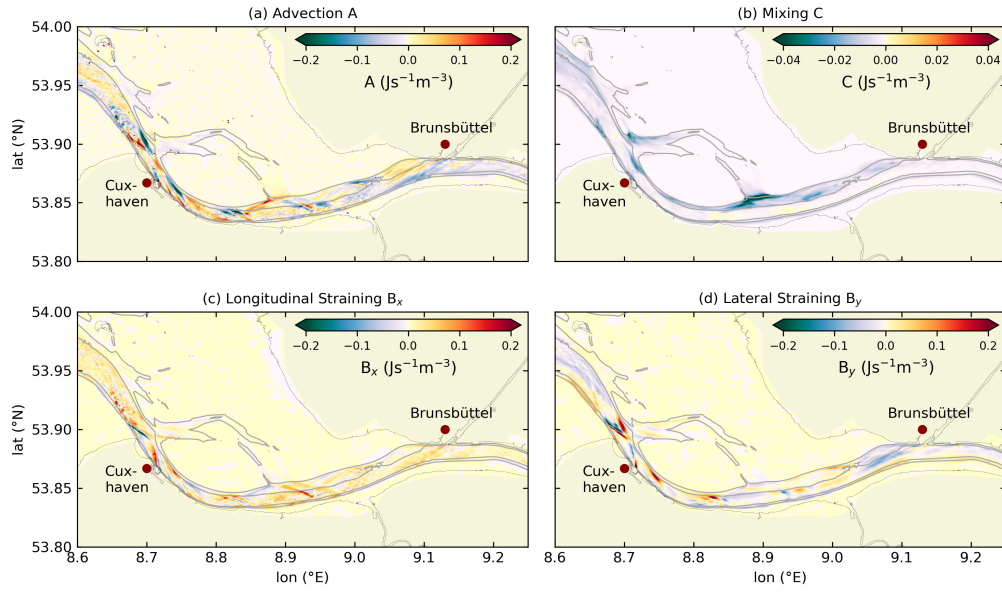


Figure 6: Different terms from (7), averaged over two hours around peak ebb on 17th to 18th April 2024 (22:30h to 00:30h UTC), computed from numerical simulation output. (a): Advection term A from (7), (b): vertical mixing C , (c): along-channel straining B_x , and (d): cross-channel straining B_y from the RHS of (7). Bold gray lines indicate the 12 m- and 6 m-isobaths. Note the different colorbar scale for the mixing term in (c) compared to the remaining panels.

the N shoal plateaus ($A > 0$). Additionally, advection carries in saltwater and thus stronger stratification at the upstream end of salt intrusion near Brunsbüttel, where the water column is mostly fresh and thus unstratified during ebb. Lateral straining is of importance only along the steep margins of the navigational channel and tends, although variable in magnitude, to be stratifying along the flat N shoal and destratifying along the steep S channel boundary (Fig. 5d). The overall flood signal of vertical salt mixing throughout the estuary is only weakly enhanced along the channel-shoal transition, and increased channel-center mixing occurs in the upstream-most region of the estuary (Fig. 5b). Lastly, longitudinal straining tends to be considerably weaker than lateral straining and advection, and does not display any distinct pattern (Fig. 5c).

In contrast to flood, the longitudinal straining signal at ebb tide is of comparable magnitude to lateral straining and advection and shows a more consistent pattern of mainly positive (stratifying) values, in particular within the channel (Fig. 6c) because fresher water is driven on top of saltier water as in estuaries with strain-induced periodic stratification [SIPS; 52]. Lateral straining (Fig. 6d) has a weaker signal than during flood, but except for the upstream region where salt is mostly removed by the ebb current (Advection $A < 0$, Fig. 6a), it tends to be more positive along the flat N shoal and more negative along the steep S channel boundary. Ebb mixing is clearly focused on the channel-shoal transition and N shoal plateaus, with hardly any channel mixing (Fig. 6b). Depending on the exact location, increased stratification above the N shoal plateaus can be either attributed to a combination of lateral and longitudinal straining countered by advection, or vice versa.

Local, intense extrema of salt mixing occur near the western Medem branch intersect directly upstream from Cuxhaven during flood (Fig. 5b) and at the eastern Medem branch intersect during ebb (Fig. 6b) where advection carries in stratified water toward these topographical irregularities (Fig. 5a and Fig. 6a).

4.3.2. *Dynamics on transect 1850*

Although the natural variability of mixing patterns within the estuary and thus also across transects is high, a number of key mechanisms can be identified that occur to varying degrees on most transects. The features related to these mechanisms will, in the following, be presented using snapshots from transect 1850 (see Fig. 1c, red transect). It is of a characteristic, asymmetric shape with a flat, plateau-shaped shoal at its northern margin

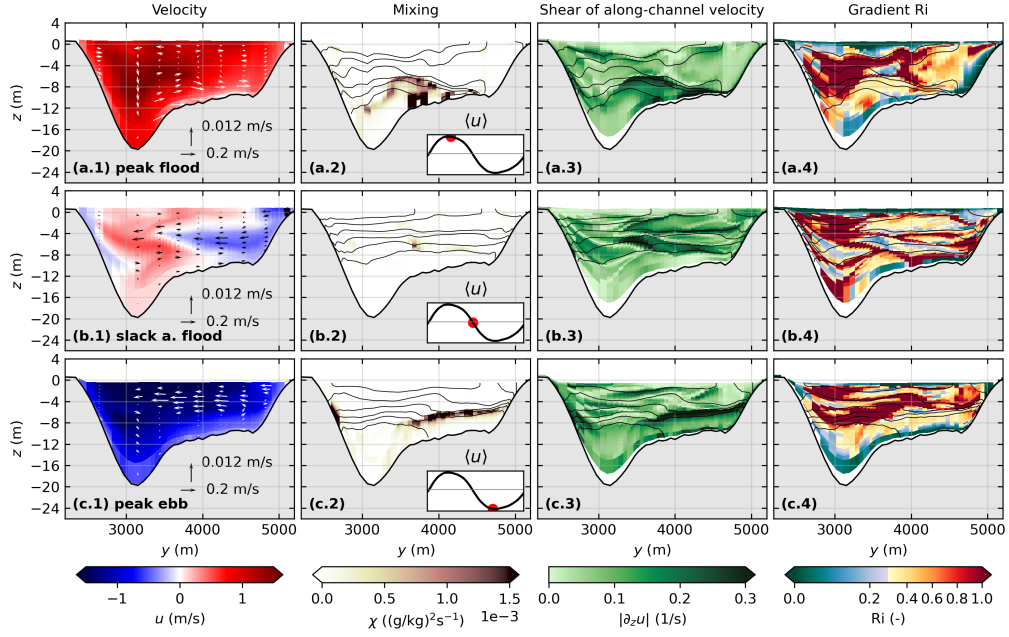


Figure 7: Snapshots of the simulated parameter distribution within cross-section 1850 (see Fig. 1c) at different times throughout the M_2 tidal cycle at the transition from 17th to 18th April 2024. (a): peak flood; (b): slack after flood; (c): peak ebb. Column 1 shows the along-channel velocity u (colormap) and cross-channel circulation v, w (arrows). Column 2 side shows the local mixing χ (colormap) and isohaline structure (contour lines). The inset axis shows the cross-section averaged along-channel velocity $\langle u \rangle$ vs. time, with the red circle marking the timing of each snapshot and the gray line indicating $\langle u \rangle = 0$. In column 3, the magnitude of the vertical shear of the along-channel velocity u , $|\partial_z u|$ is shown and column 4 shows the gradient Richardson number Ri .

515 and a steep slope at its southern margin. This geometry is typical for the
 516 inner Elbe estuary and most pronounced upstream of the eastern end of the
 517 Medem Branch (see Fig. 1a), where transect 1850 is located. Results from the
 518 remaining transects are featured in the Appendix (Section Appendix A) and
 519 Section 2 of the Supplemental Material.

520 Starting at flood, maximum current velocities occur near the center of
 521 the water column for most of the cross-section, rather than near the surface
 522 (Fig. 7a.1). Thus, salty water is transported upstream mainly along the bot-
 523 tom of the navigational channel. Nearing peak flood, this water mass spreads
 524 northward onto the plateau of the northern shoal (Fig. 7a.2). In detail, this
 525 process is accompanied by an up-shoal directed lateral current (Fig. 7a.1).
 526 From the snapshots (Fig. 7a.2-4), it can further be seen that local mixing oc-
 527 curs on top of the forming salt front at the location where the channel slope
 528 flattens toward the plateau and where the vertical shear of the along-channel
 529 velocity is sufficiently strong to partly overcome the stratification (marginally
 530 stable Ri). Additional high mixing rates are found along the bottom of the
 531 plume where the stratified layer intersects with the topography, i.e., where
 532 strong stratification is confronted with high turbulence ($Ri < 0.25$).

533 At late flood/slack after flood, the along-channel tidal current within
 534 transect 1850 slows down fastest above the northern shoal plateau because
 535 higher friction-induced turbulence allows for an earlier change of tidal direc-
 536 tion (Fig. 7b.1). This coincides with a lateral exchange flow which evens out
 537 the isohaline profile to a horizontally well-mixed and vertically uniformly
 538 stratified surface layer (Fig. 7b.2). Above the plateau, some salty bottom
 539 water is retained from peak flood to peak ebb. Within the deep naviga-
 540 tional channel, a well-mixed bottom layer persists. A relatively low shear
 541 and high $Ri \gg 0.25$ occur along the entire cross-section, such that mixing is
 542 low (Fig. 7b.2-4).

543 During ebb, fresher water preferably comes in near the surface, where
 544 the ebb current is strongest, and above the N shoal plateau. This leads
 545 to the reinstatement of a fresher region above the plateau and within the
 546 surface layer and a saltier bottom layer, comparable to the isohaline structure
 547 at peak flood (Fig. 7c.1-2). At peak ebb, elevated levels of the vertical
 548 shear of the along-channel velocity lead to a reduced gradient Richardson
 549 number Ri within the plume above the N shoal plateau. The channel is
 550 stably stratified except for the bottom and a region of similarly strong shear
 551 at the steep S slope (Fig. 7c.3-4). Regions of elevated mixing occur where high
 552 stratification is overcome by high shear: along the interface of the N shoal

553 bottom plume and the surface layer as well as in locations where the stratified
554 layer intersects with the topography, i.e., the sidewalls of the navigational
555 channel. Additionally, although of similar magnitude to the flood mixing,
556 the ebb mixing tends to be more persistent in time, often pertaining until
557 late ebb (not shown).

558 Transects 1750, 1800, and 1900 are of very similar geometry to transect
559 1850. Their respective snapshots can be found in Section 2 of the Supple-
560 mental Material (Fig. S2, S3, S4).

561 4.3.3. *Deviations on other transects*

562 In the channel region between both ends of the Medem Branch, the N
563 shoal is of intermediate geometry with a gentle slope rather than a distinct
564 plateau. As an example for the resulting dynamics, snapshots from transect
565 2050 are shown in the appendix (see Fig. A.9), but the following also applies
566 to transect 2000 (see Fig. S6, Supplemental Material). Here, a bottom salt
567 plume still forms on the slope during flood, but tends to be less pronounced
568 compared to the previously described transects with large plateaus. Less salt
569 remains above the slope at the transition from flood to ebb. The plume is
570 partly re-established toward peak ebb. The plume mixing, shear, and water
571 column stability are similar to those described for transect 1850, but can be
572 less pronounced depending on the development of the plume (see Fig. A.9).

573 As a special case, transect 1700 (see Fig. A.10) is located at the upstream
574 end of salt intrusion. Here, the dynamics are dominated by the incoming,
575 near-bottom end of the salt intrusion during flood that provides stratification
576 (see upstream section of the channel where $A > 0$ in Fig. 5a) and that leads
577 to mixing at the channel center rather than along the sidewalls. During ebb,
578 most salt is removed from the location of the transect, resulting in reduced
579 stratification (see upstream end of channel where $A < 0$ in Fig. 6a). Mixing
580 takes place mostly at peak flood and at ebb within the shear layer between
581 the salty bottom layer and the fresher surface layer.

582 Lastly, some locations within the inner Elbe estuary display topograph-
583 ical peculiarities, such as transects 1950 and 2150 which are located by the
584 intersections of the Medem branch with the main channel (not shown; see
585 Fig. S5, S7, Supplemental Material), and transect 2100 which does not dis-
586 play a gentle slope on either channel. Due to the lack of such a gentle slope,
587 no proper salt plume formation can be found (see Fig. A.11). However, at
588 late ebb, intense mixing along the S channel sidewall occurs (Fig. A.11d.2).

589 4.3.4. Discussion

590 Our findings show that regions of elevated mixing such as those reported
591 by Reese et al. [11] and Burchard et al. [6] for the Elbe estuary can occur
592 due to a multitude of mechanisms related to a high spatial variability of the
593 topography. Local topographical irregularities can disturb the lateral circu-
594 lation or lead to turbulence that results in intense mixing when stratification
595 is advected from other locations. Additionally, the locally varying aspect
596 ratios of the different transects considered in this study could also influence
597 the shape of the lateral circulation [53], which in turn strains the isohaline
598 structure and thus influences the location of elevated mixing. Nonetheless,
599 underneath this high topographical variability, we can make out two key
600 mechanisms associated with the strong near-shoal mixing that Reese et al.
601 [11] and Burchard et al. [6] linked to the total exchange flow in the Elbe.
602 These mechanisms will be explained in the following and are further summa-
603 rized in Fig. 8.

604 **(a) Mechanism 1 – salt plume formation above plateau-shaped**
605 **shoals:** For the first mechanism, the geometry of the northern shoal of
606 the navigational channel with its distinct plateau is of key importance: the
607 plateau allows for a salty bottom layer that forms throughout flood and can
608 be re-established after slack tide until peak ebb. It experiences interface
609 mixing during both its initial formation throughout flood and its final de-
610 generation beginning at peak ebb. This process is described in detail below.

611 The flood tide formation of such a salt plume can be attributed to the
612 effect of differential advection of along-channel salinity gradients [see 14,
613 15]: this causes a baroclinic pressure gradient between the initially fresher
614 (slower) shoal current and saltier (faster) channel current which drives a
615 bottom-enhanced, shoal-directed lateral current. Due to lateral straining
616 and advection from this current, a shoal-ward moving bottom salt plume is
617 formed (see Fig. 8a). Such a “lock-exchange” flow has also been described
618 by Geyer et al. [19] for the Delaware Bay estuary, which has a channel-shoal
619 geometry similar to the flat northern Elbe shoals [see also 54]. Flood mixing
620 is caused by shear of the along-channel velocity within the halocline between
621 the slow bottom plume and center-enhanced surface layer [attributed to the
622 impact of the flood-oriented lateral circulation by 18]. This shear layer can
623 extend into the navigational channel, where it leads to mixing at the interface
624 between the turbulent bottom layer and stratified surface layer as described
625 by Warner et al. [23].

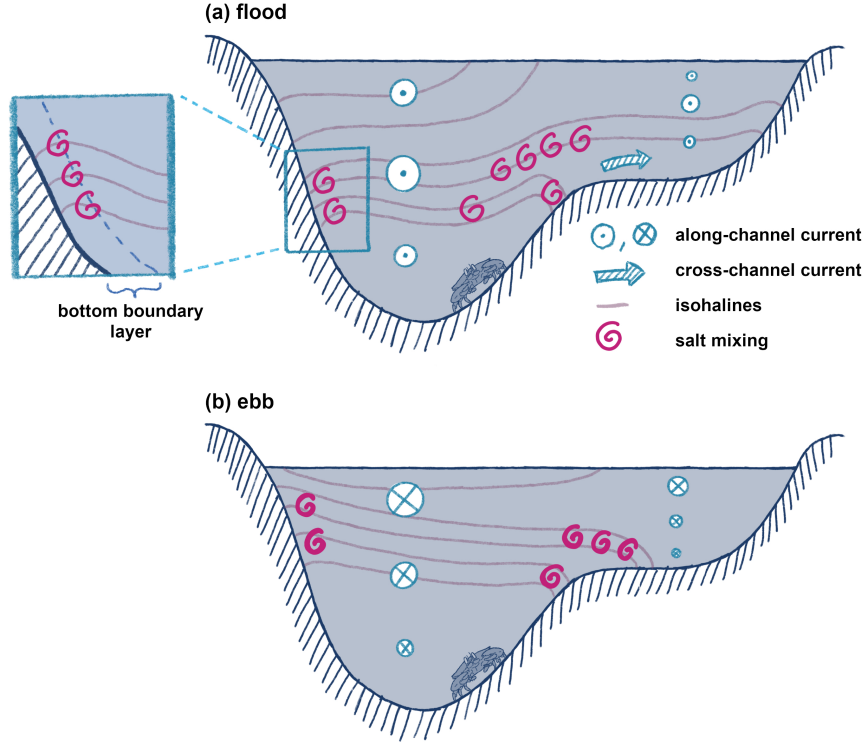


Figure 8: Schematic cross-section of an estuary with a plateau-shaped shoal on one side and a steep slope on the other side, explaining the basic mechanisms of mixing at the channel-shoal transition. (a) Flood: The effect of differential advection results in a baroclinic pressure gradient that drives a lateral current up the shoal plateau (mechanism 1). As a result, a bottom salt plume is formed on the plateau. Mixing occurs at the interface between the bottom plume and fresher surface water, where the shear is high due to the center-enhanced flood current. It may also occur at the same interface further within the channel. Additional mixing occurs where isohalines intersect with the turbulent bottom boundary layer (mechanism 2), as shown in detail in the zoom panel [adapted from Fig. 14 in 10, and references therein] (b) Ebb: After a vertically uniform stratification at slack after flood, the salt plume shape above the shoal plateau is re-established due to incoming freshwater of the surface-enhanced ebb current (mechanism 1). The vertical shear is elevated within the plume, and high mixing rates occur where high shear and high stratification overlap. Turbulent boundary layer mixing (mechanism 2) as explained in the zoom panel from (a) also occurs at ebb. The overall more persistent mixing at ebb is indicated by the bold magenta swirls.

626 An ebb tide salt plume is re-established from the uniform vertical strat-
 627 ification after slack tide. This process is a result of the faster turning of
 628 the tides above the shoal plateau, such that fresher water first occurs in
 629 the North, and the surface-enhanced ebb currents. As a consequence, the
 630 bottom layer above the plateau remains saltier and forms a channel-ward re-
 631 treating front. Even though the effect is a seemingly lateral movement, it is
 632 primarily caused by longitudinal rather than lateral currents which carry in
 633 water of laterally varying salinity and stratification. This process is further
 634 strongly aided by the plateau shape of the N shoal which enables the storage
 635 of relatively salty bottom water above the plateau throughout slack after
 636 flood (see Fig. 8b). Ebb mixing is associated with shear of the along-channel
 637 velocity within the bottom plume above the shoal plateau. Consequently,
 638 mixing is localized above the plateau, while the navigational channel itself
 639 is too stably stratified for the establishment of any significant turbulence. A
 640 spatially broader distribution and temporally longer occurrence result in the
 641 ebb-enhancement of the mixing. Collignon and Stacey [20] and Huguenard
 642 et al. [21] attribute increased ebb mixing above the shoals of comparable
 643 partially mixed estuaries to the destratifying effect of lateral circulation that
 644 reduces the water column stability and thus enables mixing. Here, we do not
 645 find a consistent signal of ebb-tide lateral straining or lateral velocity shear
 646 that directly reduces stratification above the shoal plateau. Instead, the low
 647 $Ri \lesssim 0.25$ is predominantly associated with a high shear of the along-channel
 648 velocity that is sufficiently strong to overcome the existing stratification and
 649 to lead to turbulent mixing.

650 At intermediate channel-shoal transitions such as those described in Sec-
 651 tion 4.3.3 that have no distinct plateau, the effect of differential advection
 652 as well as the N shoal salt storage capacity between flood and ebb are re-
 653 duced, thus weakening the salt plume formation at flood and ebb. At steep
 654 slopes without a plateau, this process consequently occurs to no significant
 655 extent as both the differential advection and salt storage are missing – just
 656 as the fronts described in Huguenard et al. [21] and Warner et al. [23] were
 657 restricted to the flat shoals of similarly asymmetric channels, although this
 658 is not further evaluated in those publications.

659 **(b) Mechanism 2 – intersection of isohalines with the topog-**
 660 **raphy:** In addition to mechanism 1, bottom-generated boundary layer
 661 turbulence results in high mixing rates wherever a stratified layer intersects
 662 with the local topography as shown in the zoom panel in Fig. 8 [55, 56, 10].
 663 To satisfy a net-zero salt flux condition at the channel boundary, the iso-

halines need to intersect orthogonally with the topography. The resulting structure introduces a baroclinic pressure gradient that can drive an upward directed boundary current [57, 58, 50], additionally leading to shear at the interface between the boundary layer and surrounding water that can facilitate mixing even along steeper sidewalls in contrast to the plume shear from mechanism 1, which is bound to flat shoals with plateaus.

Boundary layer mixing occurs along the head of the salt plume from mechanism 1 as well as in places where the stratified water from the deep channel intersects, preferably, with steep sections of the channel sidewalls. In the latter case, it is the deep-channel processes of stratification and destratification that determine the intensity of available stratification for the boundary layer mixing. Particularly during ebb, the channel stratification is mainly established as a result of longitudinal straining, since the surface-enhanced ebb current drives fresher water on top of saltier water as described by Simpson et al. [52] for estuaries of the SIPS-regime. Interestingly, in contrast to SIPS estuaries, the flood current does not display a clearly destratifying longitudinal straining signal, likely due to the more bottom-enhanced along-channel current structure that partly prevents the transport of (denser) saltier water on top of (less dense) fresher water and thus the creation of unstable stratification. Therefore, mechanism 2 is of similar importance in the Elbe during flood as during ebb.

At neap tide, boundary layer mixing (mechanism 2) is the main mechanism leading to mixing at the steep southern slope. Despite being very intense, it is mostly restricted to a very thin boundary layer adjacent to the channel sidewall, whereas mechanism 1 is active over an often horizontally broad region above a plateau. Resulting from the more intense stratification, both mixing mechanisms lead to more intense mixing at neap compared to spring. However, while the salt plume formation (mechanism 1) is dominant also at times of the reduced spring stratification (not shown), the intersection of the halocline with the topography (mechanism 2) naturally depends on the availability of high stratification within the channel. At the same time, such high stratification additionally stabilizes the water column within the deep channel, as evident by the consistently high $Ri \gg 1$ independent of the M_2 tidal phase, such that mixing within the channel itself is more efficiently suppressed than during weaker stratification. These facts account for the increased importance of near-shoal mixing processes in the presence of increased stratification, as found in Section 4.2.

701 5. Summary and Conclusions

702 Here, we have thoroughly analyzed which processes lead to salt mixing
703 and estuarine exchange flow inside the partially-mixed Elbe estuary. Based
704 on results from Reese et al. [11] and Burchard et al. [6], who identified mixing
705 at the channel-shoal transition as a major player for the exchange flow within
706 the Elbe estuary, we here assessed the exact timing and location of most
707 intense mixing. As a next step, this was then traced to single mechanisms of
708 near-shoal mixing and thus the exchange flow.

709 Starting with an analysis of estuary-wide mixing throughout a selected
710 spring-neap cycle, we identified the timing of maximum mixing to coincide
711 with the peak of total salt stratification at neap tide. A further increase
712 of mixing toward the transition from neap to spring, as known for partially
713 mixed estuaries from literature such as Wang and Geyer [22] and Warner
714 et al. [23], was likely hampered by a storm that prematurely reduced the
715 stratification to its typical spring tide extent. Throughout the semidiurnal
716 M_2 tidal cycle, highest mixing rates were found at peak ebb (see Fig. 3e).

717 As shown by Reese et al. [11] and Burchard et al. [6], the locations where
718 mixing and water transport across isohaline surfaces are most pronounced
719 are strongly topography dependent, with the channel-shoal transition as a
720 region of consistently enhanced mixing. We could here confirm these mixing
721 regions and further report that their relative and absolute intensity compared
722 to deep-channel mixing increases during the highly-stratified neap period of
723 maximum mixing (see Fig. 4) since persistent stratification stabilizes the
724 water column within the channel throughout the entire semidiurnal tidal
725 cycle. Despite a high local variability related to topographical differences, we
726 identified two general mechanisms of mixing at the channel-shoal transition
727 (see also summary in Fig. 8):

- 728 1. Formation of a bottom salt plume above a plateau-shaped shoal during
729 flood as a result of differential advection that is re-established at early
730 ebb due to the retainment of near-bottom saltwater and incoming near-
731 surface freshwater [see also 20, 21, 19]. Mixing of high intensity occurs
732 due to shear of the along-channel velocity around peak flood and ebb,
733 but is more abundant and more persistent during ebb.
- 734 2. Intersection of a stratified layer with the topography, which results
735 in boundary layer mixing due to high bottom-generated turbulence
736 [55, 56, 10]. This mechanism occurs along the head of the salt plume

737 from mechanism 1 as well as at the sidewalls of the navigational channel
738 during both flood and ebb. Its relative importance depends on the
739 amount of available stratification created within the channel.

740 We find here that we can differentiate between channel-adjacent shoals,
741 where both mechanisms occur, and steep channel boundaries without active
742 shoals, where only mechanism 2 is found because the steep slopes of the chan-
743 nel sidewalls neither allow for a pronounced impact of differential advection
744 nor for the retention of salt at the transition from flood to ebb. In addition to
745 these mechanisms, topographical irregularities where stratified water is car-
746 ried in from the channel were found to lead to considerable, albeit strongly
747 localized, mixing.

748 With the present study, we have thus demonstrated how the theory pre-
749 sented in Klingbeil and Henell [8] and Burchard et al. [6] can be applied to
750 conclude not only when and where, but also in connection to which mecha-
751 nisms, the exchange flow predominantly occurs in a given estuary. We have
752 successfully provided dominant underlying mechanisms of mixing and thus
753 the total exchange flow for the Elbe estuary. For estuaries with a channel-
754 shoal geometry, our findings underline the essential role that lateral processes
755 as well as shoals and their interaction with the main current play for both
756 estuarine mixing and the exchange flow. With our detailed analysis, we fur-
757 ther added to the knowledge of estuarine mixing mechanisms from earlier
758 studies such as Collignon and Stacey [20], Huguenard et al. [21] and Warner
759 et al. [23] and assessed their importance within a given estuary in space and
760 time. We have confirmed the basic finding that mixing is largest during ebb
761 flow [23], but we demonstrated that the underlying processes are much more
762 complex than the common picture of a solely longitudinally oscillating tide
763 suggests [59].

764 Declaration of competing interest

765 The authors declare that they have no known competing financial inter-
766 ests or personal relationships that could have appeared to influence the work
767 reported in this paper.

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784 **Research Data Availability Statement**

785 All Python scripts used to create the Figures shown in the present study
786 as well as the processed setup topography and freshwater discharge as used for
787 the numerical Elbe setup are preliminarily accessible via [https://git.io-](https://git.io-warnemuende.de/reese/Reese-et-al-2025)
788 [warnemuende.de/reese/Reese-et-al-2025](https://git.io-warnemuende.de/reese/Reese-et-al-2025). Together with the numerical
789 model output used for this study, they will be uploaded to a permanent
790 data repository once this manuscript has been accepted for publication. The
791 same applies to the observational data presented in Section 3. Seastate
792 data (significant spectral wave height) was collected and made freely avail-
793 able by the BSH marine environmental monitoring network (MARNET),
794 the RAVE project (www.rave-offshore.de), the FINO project ([www.fino-](http://www.fino-offshore.de)
795 [offshore.de](http://www.fino-offshore.de)) and cooperation partners of the BSH. The data was taken from
796 <https://seastate.bsh.de/rave/index.jsf>. For the modeling presented
797 in this work, the GETM source code has been archived on Zenodo ([https:](https://doi.org/10.5281/zenodo.7741730)
798 [//doi.org/10.5281/zenodo.7741730](https://doi.org/10.5281/zenodo.7741730)). The horizontal numerical grid was
799 created using the Delft3D rgfgrid GUI [60], which can be downloaded as part
800 of a software set from <https://oss.deltares.nl/web/delft3d/home> with
801 a freely available license from the same website. All forcing data used for
802 the model is freely available, including boundary forcing and initial salt and
803 temperature distributions from E.U. Copernicus Marine Service [35], mete-
804 orological forcing from the MET Nordic operational archive [36], and the
805 daily-averaged freshwater discharge at Neu Darchau from Wasserstraßen-
806 und Schiffahrtsamt Magdeburg [42]. The topography datasets used for

807 the creation of the numerical setup were taken from Wasserstraßen- und
808 Schifffahrtsamt Hamburg [37], Sievers et al. [38], Wasserstraßen- und Schiff-
809 fahrtsamt Hamburg [39], and Wasserstraßen- und Schifffahrtsamt Weser-
810 Jade-Nordsee [40]. All figures except Fig. 8 were created with Matplotlib
811 version 3.2.2 [61, 62], see also <https://matplotlib.org/>. In Fig. 1, the
812 maps were created fully (d) or partly (a-c) with cartopy v0.17.0 [63, 64],
813 see <http://scitools.org.uk/cartopy>, including the NaturalEarthFeature
814 function (made with Natural Earth. Free vector and raster map data at
815 naturalearthdata.com).

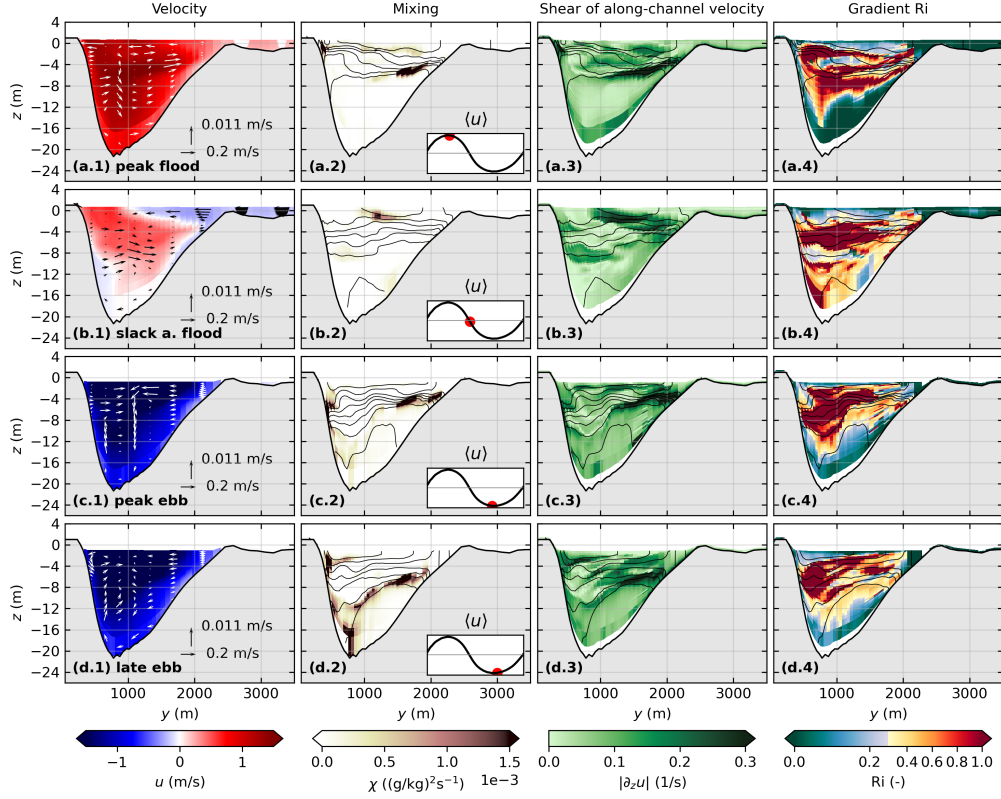


Figure A.9: Snapshots of the simulated parameter distribution within cross-section 2050 (see Fig. 1c) at different times throughout the M_2 tidal cycle at the transition from 17th to 18th April 2024. (a): peak flood; (b): slack after flood; (c): peak ebb, (d): late ebb. Column 1 shows the along-channel velocity u (colormap) and cross-channel circulation v, w (arrows). Column 2 side shows the local mixing χ (colormap) and isohaline structure (contour lines). The inset axis shows the cross-section averaged along-channel velocity $\langle u \rangle$ vs. time, with the red circle marking the timing of each snapshot and the gray line indicating $\langle u \rangle = 0$. In column 3, the magnitude of the vertical shear of the along-channel velocity u , $|\partial_z u|$ is shown and column 4 shows the gradient Richardson number Ri .

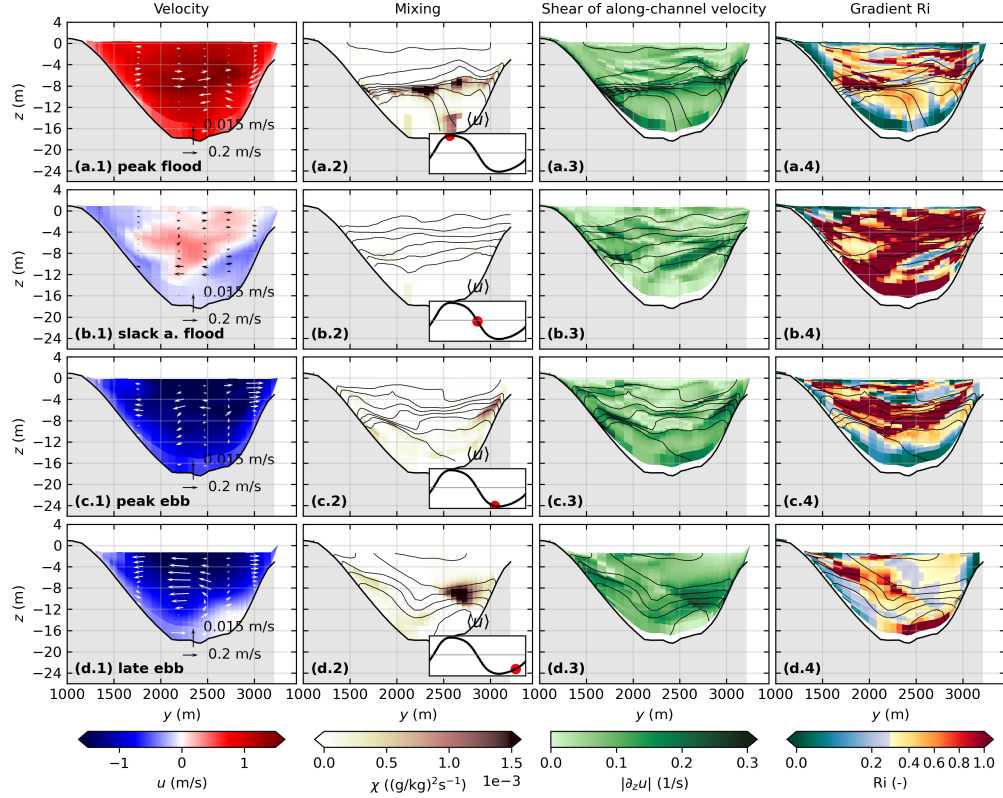


Figure A.10: Snapshots of the simulated parameter distribution within cross-section 1700 (see Fig. 1c) at different times throughout the M_2 tidal cycle at the transition from 17th to 18th April 2024. (a): peak flood; (b): slack after flood; (c): peak ebb, (d): late ebb. Column 1 shows the along-channel velocity u (colormap) and cross-channel circulation v, w (arrows). Column 2 side shows the local mixing χ (colormap) and isohaline structure (contour lines). The inset axis shows the cross-section averaged along-channel velocity $\langle u \rangle$ vs. time, with the red circle marking the timing of each snapshot and the gray line indicating $\langle u \rangle = 0$. In column 3, the magnitude of the vertical shear of the along-channel velocity u , $|\partial_z u|$ is shown and column 4 shows the gradient Richardson number Ri .

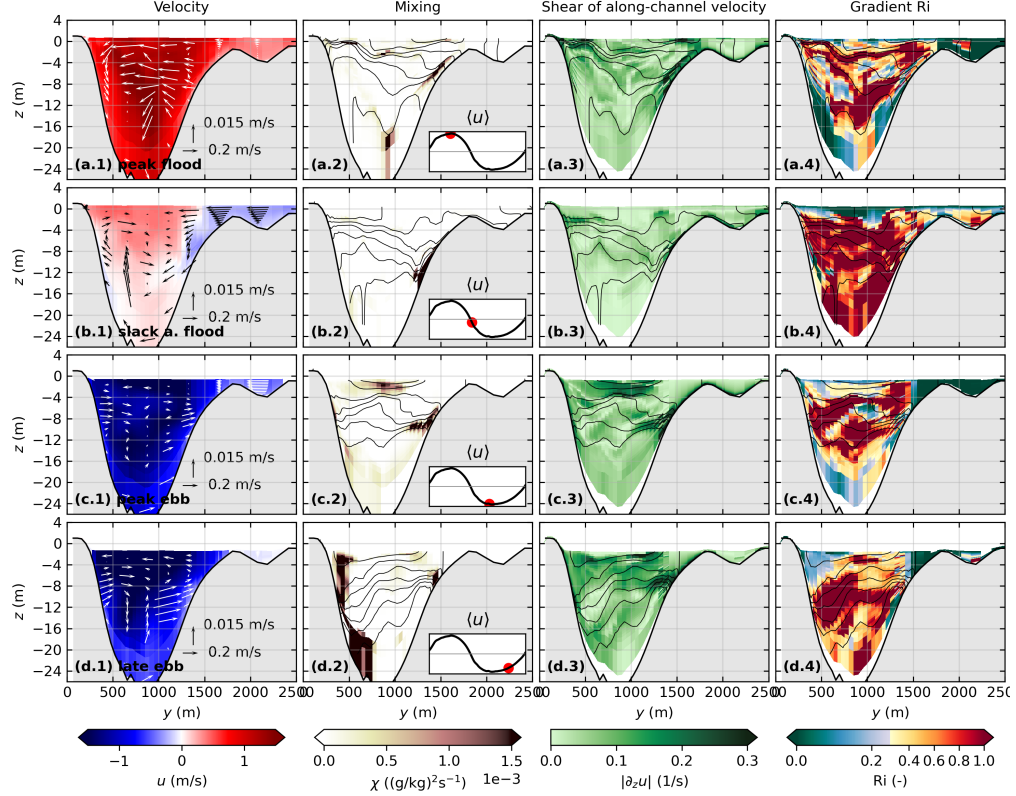


Figure A.11: Snapshots of the simulated parameter distribution within cross-section 2100 (see Fig. 1c) at different times throughout the M_2 tidal cycle at the transition from 17th to 18th April 2024. (a): peak flood; (b): slack after flood; (c): peak ebb, (d): late ebb. Column 1 shows the along-channel velocity u (colormap) and cross-channel circulation v, w (arrows). Column 2 side shows the local mixing χ (colormap) and isohaline structure (contour lines). The inset axis shows the cross-section averaged along-channel velocity $\langle u \rangle$ vs. time, with the red circle marking the timing of each snapshot and the gray line indicating $\langle u \rangle = 0$. In column 3, the magnitude of the vertical shear of the along-channel velocity u , $|\partial_z u|$ is shown and column 4 shows the gradient Richardson number Ri .

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Publications

- **Reese, L.**, Becker, M., Holtermann, P., Li, X., and Burchard, H. (2025): *Water Mass Transformation in Partially Mixed, Tidal Estuaries With Shallow Shoals Is Related to Lateral Salt Front Formation*, under review. Pre-print at: https://papers.ssrn.com/sol3/papers.cfm?abstract_id=5133686
- Rummel, K., Gräwe, U., Klingbeil, K., Kolb, P., Li, X., **Reese, L.**, and Burchard, H. (2025): *Spatially resolved salt intrusion mechanisms in a tidal estuary and the impact of channel deepening*. Journal of Geophysical Research: Oceans, 130, e2024JC022073, <https://doi.org/10.1029/2024JC022073>.
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- **Reese, L.**, Gräwe, U., Klingbeil, K., Li, X., Lorenz, M., and Burchard, H. (2024): *Local mixing determines spatial structure of diahaline exchange flow in a mesotidal estuary – A study of extreme runoff conditions*. Journal of Physical Oceanography, 54, 3–27, <https://doi.org/10.1175/JPO-D-23-0052.1>.