ABSTRACT

Title of Dissertation:

NONLINEAR INTERNAL WAVES AND SHORT-TERM VARIABILITY OF CARBON SYSTEM DRIVEN BY LATERAL CIRCULATION IN COASTAL PLAIN ESTUARY

Renjian Li, Doctor of Philosophy, 2023

Dissertation directed by:

Professor Ming Li Marine Estuarine and Environmental Sciences Program

Recent observations in Chesapeake Bay showed that the interaction between lateral circulation and channel-shoal bathymetry generated internal lee waves which subsequently propagated onto shallow shoals and evolved into internal solitary waves, leading to overturning and enhanced turbulent mixing. However, it is unknown under what hydrodynamic conditions the lee waves could be generated and how the nonlinear internal waves evolved. Using an idealized straight channel representative of a coastal plain estuary, we conducted numerical simulations to investigate internal wave generation over a range of river flows and tidal amplitudes. The model results are summarized using the estuarine classification diagram based on the freshwater Froude number Fr_f and the mixing parameter M. Δh decreases with increasing Fr_f as stronger stratification suppresses waves, and no internal waves are generated under large Fr_f . Δh initially increases or saturates to a certain amplitude as M further increases. This regime diagram suggests that internal lee waves can be generated in a wide range of estuarine

conditions. To examine the nonlinear evolution of internal waves, a three-dimensional nonhydrostatic model with nested model domains and increasing grid resolution was configured. The lee wave steepens into a shorter elevation wave due to shoaling and soon evolves into a depression with a train of undular waves at its tail as bottom boundary mixing elevates the halocline above the mid-depth. These nonlinear internal waves enhance the turbulent dissipation rate over the deep channel and shallow shoal, suggesting an important energy source for mixing in stratified coastal plain estuaries. In addition, a pH sensor deployed at the middle reach of Chesapeake Bay recorded high-frequency variability in bottom pH driven by along-channel winds. Though wind-driven lateral circulation can advect high pH water downward, the slow airsea exchange of CO_2 limits the lateral ventilation. With DIC and TA budget analysis and comparison with cross-sections at upper- and lower-Bay where strong lateral circulation was confined in the surface layer, we found vertical mixing and replenishment of oceanic water by longitudinal advection could be more important mechanisms to ventilate bottom pH.

NONLINEAR INTERNAL WAVES AND SHORT-TERM VARIABILITY OF CARBON SYSTEM DRIVEN BY LATERAL CIRCULATION IN COASTAL PLAIN ESTUARY

by

Renjian Li

Dissertation submitted to the Faculty of the Graduate School of the University of Maryland, College Park, in partial fulfillment of the requirements for the degree of Doctor of Philosophy 2023

Advisory Committee: Professor Ming Li, Chair Professor Wei-Jun Cai Professor Patricia Glibert Associate Professor Jeremy Testa Assistant Professor Joe Jurisa © Copyright by Renjian Li 2023

Acknowledgements

First I want to express my endless gratitude to my advisor Dr. Ming Li for his guidance and support throughout my Ph.D. study. I learned a lot from him and he is very supportive for my career pursuit. I really appreciate his help with organizing my ideas and his patience for editing my manuscript. I also would like to thank my committee members, Dr. Pat Glibert, Dr. Jeremy Testa, Dr. Wei-Jun Cai, and Dr. Joe Jurisa for their guidance. Such a wonderful committee gave me opportunities to work on interdisciplinary research. Discussion with my committee members broadened my research interests and gave me inspirations. Besides, I want to thank Dr. Jian Zhao for his concern and encouragement. Former group members, Dr. Fan Zhang, Dr. Wenfei Ni, Dr. Xiaohui Xie and Yijun Guo gave me a lot of help not only on my research but also on my life at HPL. Other friends at HPL and visiting scholars also gave me a lot of help and I want to thank them for their company during my life there. I also need to thank our collaborator Dr. Chunqi Shen for helping me grasp the carbonate chemistry model.

Finally, I must thank my family and friends from high school and undergraduate. Without my family's insistence and continuous encouragement and comfort from my friends, I could not finish this Ph.D. study.

Table of Contents

Acknowledgements	ii
Table of Contents	iii
List of Tables	v
List of Figures	vi
Chapter 1: Introduction	1
1.1 Generation of internal lee wave in estuaries	2
1.2 Generation and evolution of internal solitary wave	5
1.3 Drivers of short-term variability in coastal pH	8
1.4 Dissertation objectives and layout	. 12
Chapter 2: A regime diagram for internal lee waves in coastal plain estuaries	. 14
2.1 Abstract	. 15
2.2 Introduction	. 16
2.3 Methods	. 18
2.3.1 Model descriptions and numerical experiments	. 19
2.3.2 Froude number analysis	. 22
2.4 Lateral wave generation	. 23
2.4.1 Generation and propagation of internal lee waves	. 23
2.4.2 Along-channel variations in wave generation	. 29
2.5 Internal lee wave generation under different hydrodynamic conditions	. 33
2.5.1 Effects of river flow	. 33
2.5.2 Effects of tidal amplitude	. 35
2.5.3 Different wave structures	. 39
2.5.4 Interpretation in terms of internal hydraulics	. 41
2.6 A regime diagram	. 43
2.7 Discussion and conclusion	. 46
2.8 Acknowledgements	. 49
2.9 Data availability statement	. 49
Chapter 3: Generation and evolution of internal solitary waves in a coastal plain estuary	. 50
3.1 Abstract	. 51
3.2 Significance statement	. 51
3.3 Introduction	. 52

3.4 Methods	55
3.4.1 Model configuration	55
3.4.2 Diagnostics of model results	57
3.5 Results	58
3.5.1 Lee wave generation and propagation	58
3.5.2 Wave steepening, dispersion and propagation	61
3.5.3 Emergence of ISWs	63
3.5.4 Dissipation of ISWs	67
3.6 Discussion and Conclusion	68
3.7 Acknowledgements	71
Chapter 4: Short-term variability and ventilation of bottom pH in a stratified estuary	
4.1 Abstract	73
4.2 Introduction	73
4.3 Methods	
4.3.1 High-frequency observation	78
4.3.2 ROMS-RCA-CC model configuration	79
4.3.3 Diagnostic of DIC and TA budget	83
4.4 Results	84
4.4.1 Wind-driven variability of bottom pH	84
4.4.2 Ventilation of bottom pH	
4.5 Concluding remarks	
4.6 Acknowledgements	100
Chapter 5: Conclusion	101
Bibliography	106

List of Tables

Chapter 2

Table 2.1 Summary of numerical experiments in which η_t is the tidal amplitude (m) at the open boundary, M is the estuarine mixing number, U_r is the river flow velocity (m s⁻¹), Fr_f is the freshwater Froude number, L_1 is the salt intrusion length (km), $Fr_{2\text{max}}$ is the maximum mode-2 Froude number at the left channel-shoal interface of the mid-estuary cross-section, \overline{N} is the averaged buoyancy frequency over the deep channel of at the mid-estuary cross-section, $\overline{N}H/V$ is the topographic Froude number, and Vk is the intrinsic frequency for the lee waves.

List of Figures

Chapter 1

Figure 1.1 A schematic diagram illustrating the generation of internal solitary waves by lateral circulation adapted from Xie et al. (2019). Here, Fr_2 is the Froude number with respect to mode-2 wave speed. When $Fr_2 \ge 1$, supercritical lateral flows generate a mode-2 lee wave at the edge of the deep channel (a). When $Fr_2 < 1$ as lateral flows weaken, the lee wave propagates onto the shoal, evolving into a mode-1 elevation wave (b). The elevation wave subsequently evolves into a train of internal solitary waves (c).

Chapter 2

- Figure 2.1 (a) Schematic of the numerical model domain consisting of a straight estuarine channel and a shelf. (b) Cross-channel section featuring a triangular-shaped deep channel and flat shallow shoals. The black dashed lines mark the location of site A, site B and site C (shown in Fig. 2.3) respectively.
- Figure 2.2 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 13 with $\eta_t = 0.8$ m and $U_r = 0.03$ m/s. Vertical lines indicate the timing of the six cross-channel snapshots shown below. The grey shaded region represents flood tide and the yellow shaded region represents ebb tide. (b)-(d), (h)-(j) Distributions of salinity (contours), velocity vectors (arrows), and dissipation rate (background color) at the mid-estuary cross-section at times T1-T6 marked in (a). Contour intervals are at 1 psu increments. (e)-(g), (k)-(m) Cross-channel distribution of Froude number Fr_1 and Fr_2 at T1-T6. The solid lines indicate rightward bottom flows and the dashed lines indicate leftward bottom flows. The vertical dashed lines in (b)-(m) mark the location of the channel-shoal interface.
- Figure 2.3 (a)-(c) Time-depth distributions of the salinity (contours) and vertical velocity (color) at sites A, B, and C in the mid-estuary cross-section (their locations marked in Fig. 1b). The magenta contours highlight the internal waves.
- Figure 2.4 (a)-(c) The vertical structure of the vertical velocity normalized by its maximum value (blue), mode-1 structure function $\Phi_1(z)$ (green) and mode-2 structure function $\Phi_2(z)$ (red) at times T7 and T8 (marked in Fig. 2.3) and sites A and C respectively.
- Figure 2.5 (a)-(c) Time series of sectionally averaged along-channel velocity (blue) and mode-2 Froude number Fr_2 (red) at the left channel-shoal interface in the upper-, mid- and lower-estuary cross-sections (their locations marked in Fig. 2.8). (d)-(l) Snapshots of lateral velocity (color) and salinity distribution (contours) at these sections [here timing marked as the dotted black lines in (a)-(c)]. Contour

intervals are at increments of 1.5 psu in (d), (g), and (j), 1 psu in (e), (h), and (k), 0.5 psu in (f), (i), and (l). In (d) the two dashed lines mark the depths of the lateral velocity maxima and their distance is used to calculate the wave amplitude.

- Figure 2.6 Along channel distributions of (a) internal lee wave amplitude Δh , (b) maximum bottom lateral velocity V and the depth-averaged stratification N^2 when Fr_2 reaching maximum at the left channel-shoal interface, (c) maximum mode-2 Froude number Fr_{2max} , and (d) the timing of lateral flow reaching critical condition ($T_{Fr_2} = 1$) after ebb slack at estuary mouth. The red dashed line in (d) indicates the function of $\frac{x}{\sqrt{gD}}$ +10. The black dashed lines mark the locations of upper-, mid- and lower-estuary cross-sections respectively.
- Figure 2.7 (a)-(d) Snapshots of cross-channel distributions of salinity (contours) and lateral velocity (arrows) at the mid-estuary section in model runs with different river discharges but fixed tidal forcing (runs 7–10). Contour interval is 0.5 psu in (a), and 1 psu in (b)-(d). The snapshots are taken at the time when Fr_2 at the left channel-shoal interface reaches a maximum.
- Figure 2.8 (a) The stratification at the left channel-shoal interface and (b) the internal lee wave phase speed as a function of river discharge U_r . Values are calculated at the mid-estuary sections from the model runs featuring internal waves (runs 1-15, 17-19).
- Figure 2.9 (a)-(d) Snapshots of cross-channel distributions of time-averaged viscosity K_{ν} during the ebb tide (background color), salinity (contours), and lateral velocity (arrows) at the mid-estuary section in model runs with different tidal amplitudes but fixed river discharge (runs 7, 12, 17, 22). Contour interval is 0.5 psu.
- Figure 2.10 The maximum bottom lateral velocity as a function of tidal velocity at the estuary mouth η_t . Values are calculated at the mid-estuary sections from the model runs featuring internal waves (runs 1-15, 17-19).
- Figure 2.11 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 17 with $\eta_t = 1.1$ m and $U_r = 0.01$ m/s. (b)-(d) Distributions of salinity (contours) and velocity vectors (arrows) at the midestuary cross-section at times T12-T14 marked in (a). Contour intervals are at 0.5 psu increments. Magenta contour lines mark the isohaline of 13 psu. (e)-(g) Cross-channel distribution of Froude number Fr_1 and Fr_2 at T12-T14.
- Figure 2.12 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 15 with $\eta_t = 0.8$ m and $U_r = 0.07$ m/s. (b)-(g) Distributions of salinity (contours) and velocity vectors (arrows) at the midestuary cross-section at times T1-T3 marked in (a). Contour intervals are at 1 psu increments.
- Figure 2.13 Internal lee wave amplitude Δh versus Fr_{2max} (a) and V/\overline{N} (b) from all model

runs featuring internal waves. The black dashed line in (b) is a linear fit for V/\overline{N} > 1.7. In the model runs, 10 cross-sections are selected to spread over the entire estuary, at a distance of (1 to 10)/(10 L_1) from the mouth of the estuary. Each open circle represents Δh calculated from a cross-section, along with Fr_{2max} , V and \overline{N} .

- Figure 2.14 Regime diagram of normalized wave amplitude $\Delta h/H$ as a function of Fr_f and M. Stars are the runs whose results show lateral frontogenesis. The black dashed lines denote the boundaries among four different estuary classes. The rectangle indicates the approximate influence of spring-neap tidal variation, river flow variation for the estuaries indicated.
- Chapter 3
- Figure 3.1 (a) Schematic of the numerical model domain consisting of a straight estuarine channel and a shelf. The red rectangle denotes a child domain with 10 m resolution. (b) Schematic of the nested model domains. The magenta rectangle denotes the child domain of 2.5 m resolution. (c) Cross-channel section featuring a channel-shoal bathymetry at mid-Chesapeake Bay.
- Figure 3.2 (a) Time series of the depth-averaged along-channel velocity and lateral velocity in the bottom layer at the channel-shoal interface. The dashed vertical lines indicate the timing of the cross-channel snapshots shown in (b)-(d) and in Figs. 3.3-3.6 and 3.8. The grey shaded region marks the flood tide and the yellow shaded region marks the ebb tide. (b)-(e) Distributions of salinity (contours) and the velocity vectors (arrows) at a mid-estuary cross-section. Contour intervals are at 0.5 psu increments. The magenta dashed line in (b)-(d) marks the location of the channel-shoal interface where the mode-2 Froude numbers (Fr₂) is calculated.
- Figure 3.3 Distributions of salinity (contour lines) and the vertical velocity *w* (color) at the mid-estuary cross-section at T3-T5 marked in Fig. 3.2a. Contour intervals are at 0.2 psu increments. The purple arrow line marks the phase line of the lee wave and the magenta arrow line marks the propagation of maximum *w* from T3-T5.
- Figure 3.4 Snapshots of (a-d) the lateral velocity (color) and salinity (contour), (e-h) the vertical velocity (color) and salinity (contour), (i-l) the nonlinearity coefficient α and dispersion coefficient β in the KdV equation, and (m-p) the mode-1 phase speed c_1 at T5-T8 marked in Fig. 3.2a. Contour intervals of salinity are at 0.5 psu increments.
- Figure 3.5 Snapshots of the vertical velocity (color) and salinity (contour) at T8-T12 marked in Fig. 3.2a. Contour intervals of salinity are at 0.5 psu increments. The green contour in (a) marks the isopycnal tracked in Fig. 3.6. The magenta dashed line in (d) marks the location of the time series shown in Fig. 3.7.
- Figure 3.6 Hovmöller diagram for isopycnal displacement of 9 psu marked in Fig. 3.5a. In

the vertical coordinate, time interval of each line is 10 minutes, equivalent to 2.5 m isopycnal displacement. The grey shaded region represents the bottom topography on the left shoal.

- Figure 3.7 (a) Time-depth distributions of salinity (contours) and the vertical velocity (color) at a location on the left shoal marked by the magenta line in Fig. 3.5d. (b) Time series of the lateral velocity at the depths of 2 and 6 m at the same location on the shoal.
- Figure 3.8 Distributions of salinity (contours) and dissipation rate ε (color) on the left shoal at times T12-T15 marked in Fig. 3.2a.
- Figure 3.9 Distributions of salinity (contours) and the along-channel velocity shear (a), the lateral velocity shear (b), and Richardson number (c) at T12 marked in Fig. 3.2a.

Chapter 4

- Figure 4.1 Map showing bathymetry (a) and model grids (b) for Chesapeake Bay. The red dot in (a) marks the location of the Gooses Reef. The black lines in (a) mark the cross-sections and the black line in (b) marks the along-channel section used in later analysis.
- Figure 4.2 Time series of wind speed vector (a), bottom salinity (b) and bottom pH (c) from observations at the Gooses Reef (marked as red dot in Fig. 4.1a). The blue, red, green rectangles mark the duration of selected westerly, up-estuary, and down-estuary wind events in later analysis. The blue lines are original time series including tidal fluctuations and the red lines and wind vector are low-passed with a 34-hour Butterworth filter.
- Figure 4.3 Distributions of salinity (a), DIC (b), TA (c), chlorophyll-a (CHLA; d) pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the weak westerly wind period marked in 4.2a. The black dashed line marks the location of Gooses Reef.
- Figure 4.4 Distributions of lateral circulation vector (a), salinity (b), DIC (c), TA (d), pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the upestuary wind event marked in 4.2a.
- Figure 4.5 Distributions of lateral circulation vector (a), salinity (b), DIC (c), TA (d), pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the downestuary wind event marked in 4.2a.
- Figure 4.6 Along channel distributions of subtidal along-channel current (a, f, k), salinity (b, g, l), DIC (c, h, m), pH (d, i, n), Ω_{Ar} (e, j, o) during the selected wind periods. The along-channel section is marked by the black line in Fig. 1b. The magenta

and white contour lines in b, g, l mark the isohaline of 17 and 25 psu respectively. The black dashed lines in d, i, n mark the location of upper-, mid-, and lower-Bay cross-sections respectively. The white contour lines in e, j, o mark the isoline of $\Omega_{Ar} = 1$.

- Figure 4.7 Distributions of salinity, pH, and Ω_{Ar} at an upper-bay cross-section during the westerly winds (a-c) and up-estuary winds (d-f).
- Figure 4.8 Distributions of salinity, pH, and Ω_{Ar} at a lower-bay cross-section during the westerly winds (a-c) and up-estuary winds (d-f).
- Figure 4.9 Time series of along-channel wind speed (a) and model-estimated terms in the DIC-TA budget for bottom water (below 10-m depth) at the upper-, mid-, and lower-Bay cross-sections (b-d) in August, 2016.
- Figure 4.10 Horizontal distributions of surface pCO2, DIC change induced by air-sea exchange, dissolved inorganic nitrogen (DIN), chlorophyll-a (CHLA), and DIC change induced by net ecosystem metabolism (NEM) during the westerly winds (a-e) and up-estuary winds (f-j).
- Figure 4.11 Time series of time-integrated terms in the DIC-TA budget for bottom water (below 10-m depth) at the upper-, mid-, and lower-Bay cross-sections in August, 2016.

Chapter 1: Introduction

Nonlinear internal waves are widely observed in the stratified coastal ocean and play an important role in generating turbulent mixing and transporting biochemically important materials. The conversion of barotropic tidal energy to internal waves is now generally accepted as a major source for mixing in the ocean (Munk and Wunsch 1998). However, in shallow coastal plain estuaries, turbulence has been mostly attributed to boundary layer turbulence (Geyer and MacCready 2014) and internal waves have not attracted much attention (Wang 2006). This introduction chapter reviews the basic concepts of internal waves and current research advances on internal waves in shallow estuaries as well as drivers of short-term variability of pH in coastal ocean, and proposes the motivation and objectives of this dissertation.

<u>1.1 Generation of internal lee wave in estuaries</u>

Internal lee waves are waves forced by flow over an obstacle (e.g., a mountain range in the atmosphere, sea floor topography in the ocean) in a stably stratified fluid. They are observed in the lee (i.e., downstream) of the topography, hence the name "lee waves" (Legg 2021). In the ocean, internal lee waves generated by flows over rough topography can extract energy from the mean flows and produce turbulent mixing when they break (MacKinnon et al. 2017). Therefore, lee waves play an important role in the global energy budget and mixing tracers across density interfaces in the stratified ocean interior (Nikurashin and Ferrari 2011; Melet et al. 2014).

In the atmosphere and deep ocean, forcings such as large-scale jets are slowly varying and regarded as steady flows. The generation of internal lee wave by steady flow is mainly controlled by the lee wave Froude number Nh/U, where N is buoyancy frequency (N^2 represents stratification), h is topographic height, and U is flow velocity (Legg 2021). When $Nh/U \ll 1$, lee

waves are linear with upward energy flux. When Nh/U > 1, the mean flow is not energetic enough to move fluid parcels over the topography and blocking will occur on the upstream side of the topography. The generated wave amplitude and wavelength at the lee side of the topography will be reduced due to blocking. Meanwhile, a hydraulic jump could form downstream with strong mixing (Winters 2016).

In addition to steady geostrophic flow, lee waves can also be generated by oscillating tidal flow in coastal regions and submarine ocean ridges. The tidal flow given by $U = U_0 cos(\omega t)$ can excite both internal waves at the tidal forcing frequency ω (internal tides) and transient internal lee waves at frequency of Uk where $k = 2\pi/L$ and L is the horizontal length scale of the obstacle (Bell 1975; Nakamura et al. 2000). For $U_0k/\omega \ll 1$, the generated internal waves are dominant by internal tides, whereas lee waves will dominate if $U_0k/\omega \gg 1$ (Garrett and Kunze 2007; Mohri et al. 2010). The control of lee wave Froude number Nh/U_0 is also applicable in the oscillating condition. Observations at the Knight Inlet revealed a rich variety of internal lee wave structures under different stratification and tidal conditions, including mode-1 wave, mode-2 wave, and hydraulic jump (Farmer and Smith 1980). Further observations indicate tidally driven hydraulic jumps are locations of enhanced mixing (Klymak and Gregg 2003; Klymak et al. 2008; Legg and Klymak 2008).

Despite lack of much attention, several previous observations did find internal lee waves in shallow estuaries. Early measurements in the partially mixed Rotterdam Waterway estuary observed internal lee waves trapped over undular bottom topography (Pietrzak et al. 1991). Surveys in Tamar Estuary also found an internal lee wave generated by tidal flow over a bed depression and the distortion of the thermocline by the internal lee wave was thought to enhance the local vertical mixing (Sturley and Dyer 1992). Later observations in Hudson River directly observed enhanced turbulent dissipation rates as well as internal lee waves above a trench (Peters 1999). However, Peters (1999) thought the enhancement was not large enough to significantly affect spatial averages in mixing over the larger surroundings. In contrast, using an idealized model with estuarine stratification and water depth, Wang (2006) argued tidal flow-topography interaction could be an important energy source for halocline mixing in partially mixed estuaries. Different from former along-channel observations, recent high-resolution CTD surveys across a cross-channel section in Chesapeake Bay captured an internal lee wave over the edge of the deep channel, suggesting lateral circulation interacting with channel-shoal bathymetry could also generate lee waves (Xie et al. 2017b). In the following study, Xie and Li (2019) used a realistic model of Chesapeake Bay to reproduce the internal lee waves observed during the field experiment. However, it remains unknown what river flow and tidal current conditions are conducive to the internal lee wave generation and whether the mechanism is applicable to a generic coastal plain estuary.

Former studies on lee wave generation in the ocean focused on the interaction between flow and sill, whereas valley-like topographies are also common in estuaries. Experiments suggested the behavior of flow interacting with a valley could be different from a sill. If the valley is filled with stagnant heavy fluid, as flow moves downstream, the isopycnals in the valley will tilt upward in the downstream direction, generating a baroclinic forcing to oppose the downstream movement (Baines 1995). Similar phenomena have been observed and simulated in the atmosphere that wind flows go directly across a stratified valley or crater with stagnant valleyflows decoupled from the flows aloft (Holden et al. 2000; Lehner et al. 2016; Rotunno and Lehner 2016). However, as oceanic scenario differs strongly from these atmospheric studies, how tidally driven flow interacts with valley-like deep channel is unknown.

1.2 Generation and evolution of internal solitary wave

Internal solitary waves are hump-shaped nonlinear and nonhydrostatic gravity waves that propagate horizontally along pycnocline in the stratified ocean (Bourgault et al. 2016). Despite the name "solitary", they are usually composed of several oscillations confined to a limited region of space as a wave packet (or wave train). Different from lee waves that do not propagate far away from their generation sites, internal solitary waves can even propagate hundreds of kilometers in the coastal oceans and marginal seas. They play an important role in generating turbulent mixing, modulating short-term variability of nearshore ecosystem, and transporting sediment and biochemical materials (Lamb 2014; Woodson 2018; Boegman and Stastna 2019).

A few of observations also recorded internal solitary waves in shallow estuaries. Echosounding surveys across a cross-section in a partial mixed estuary, Southampton Water, showed internal isopycnal oscillations with a wave period of 4 - 8 min and wavelength of 60 – 120 m (Dyer 1982). Observations in Tees estuary also captured propagating internal solitary waves as well as intense mixing (New et al. 1986; New et al. 1987). High-frequency measurements in a salt wedge estuary, Fraser Estuary, revealed small-scale internal solitary waves and shear instabilities associated with mixing at the halocline (Geyer and Smith 1987). High-resolution echosounder-based surveys in Saint John River Estuary also found internal solitary waves with enhanced diapycnal mixing (Delpeche et al. 2010). Using moored current measurements, Groeskamp et al. (2011) observed nonlinear internal solitary waves in the highly energetic Marsdiep channel. In Chesapeake Bay, early observations using thermistor chain showed highfrequency internal waves with large isotherm displacements (Sarabun and Dubbel 1990). Later observations found high-frequency variability of dissolved oxygen and salinity, which was thought to be associated with internal solitary waves (Sanford et al. 1990). Recent observation found internal solitary waves on the shallow shoal with energy dissipation rate in the pycnocline reaching 1×10^{-4} m² s⁻³ during the passage, three orders of magnitude larger than the background value (Xie et al. 2017a; Xie et al. 2017b). In general, internal solitary waves have a wavelength of O(10) m and a period of O(1) min in shallow estuaries and are intermittent in time. They could affect mixing in the halocline and high-frequency variability of chemical tracers in estuaries, but are hard to be captured without a dedicated observational program and thus often overlooked.

Multiple mechanisms have been proposed to interpret the generation of internal solitary waves in the coastal ocean. For example, supercritical tidal flow can generate a lee-wave depression on the lee side of a ridge which then propagates upstream and evolves into a train of internal solitary waves as the tidal flow slackens, which is known as the "lee wave" mechanism (Maxworthy 1979). Another generation mechanism involves the disintegration of an upstream propagating internal hydraulic jump. For example, at an entrance to the Knight Inlet, superficial tidal flows were observed to generate an undular bore or internal hydraulic jump upstream of the sill crest. This jumplike structure subsequently propagates upstream and disperses into a packet of internal solitary waves (Cummins et al 2003; Cummins et al 2006). In addition to flow-topography interaction, internal solitary waves can also originate from a river plume that flows

as a gravity current into the coastal ocean, generating horizontal flow convergence at the plume front and vertical displacement downward of near-surface waters (Nash and Moum 2005). In coastal plain estuaries, complex hydrodynamics and topography add to the difficulties in identifying the generation sites and mechanisms of the internal solitary waves and hypotheses for different cases are circumstantial. For example, the origin of the internal solitary waves in Geyer and Smith (1987) was though to correspond to a point of channel constriction. New and Dyer (1987) argued the lateral solitary waves in Southampton Water were generated by interaction of surface seiches with estuarine topography. Groeskamp et al. (2011) speculated the lateral solitary waves in Marsdiep channel originated from the lateral intrusion of freshwater plume. In Chesapeake Bay, Xie et al. (2017a) attributed internal solitary waves on the shoal to a winddriven gravity current, whereas Xie et al. (2017b) hypothesized internal solitary waves in another case were evolved from an internal lee wave generated by lateral circulation interacting with channel-shoal bathymetry. None of these hypotheses have been confirmed by either further observation or model simulation.

Once internal solitary waves are generated, they will experience nonlinear evolution and dissipation during propagation due to the varying topography, currents, and stratification (Helfrich and Melville 2006). For example, in a two-layer system, when the density interface locates above the mid-depth, an internal solitary wave tends to exist as a depression wave (downward displacement), and contrarily as a wave of elevation (upward displacement) when the density interface is closer to the bottom (Scotti et al. 2008). The phenomenon that an internal solitary wave transforms from a depression in the deeper region to an elevation entering a shallower region has been widely observed in the coastal ocean (Klymak and Moum 2003; Scotti

and Pineda 2004; Bourgault et al. 2007). The shape of a nonlinear internal wave is affected by the balance between nonlinear steepening and dispersion (Lamb 2014). Shoaling internal solitary waves will break by strong overturning on a steep slope, whereas on a gentle slope shoaling solitary waves can fission into a train of much shorter waves or boluses propagating along the bottom (Vlasenko and Hutter 2002; Aghsaee et al. 2010; Sinnett et al. 2022). In coastal plain estuaries, stratification changes over a tidal cycle, which means wave evolution is not only subject to spatial variability but also temporal variability. How internal solitary waves evolve under such complicated estuarine environment is poorly understood.

<u>1.3 Drivers of short-term variability in coastal pH</u>

Ocean acidification (OA), a consequence of oceanic uptake of increasing anthropogenic CO₂, is an important stressor on marine ecosystem. How acidification will affect marine organisms in coastal habitats is more difficult to predict as coastal carbonate chemistry is highly variable (Waldbusser and Salisbury 2014). Monitoring of pH at coastal habitats shows diurnal pH changes are much greater than the predicted pH decline in the open ocean within the next 100 years (O'Boyle et al. 2013; Baumann and Smith 2018). Hofman et al. (2011) analyzed high-resolution time series of surface pH over a variety of systems from coastal to coral reef and found diel pH fluctuations range from 0.1-1.4, depending on the local temperature, metabolism, and total alkalinity (TA). The range of the diurnal variability also varies seasonally with larger value in summer (Wootton et al. 2008; Baumann et al. 2015). Moreover, model predictions for a seagrass habitat showed increasing anthropogenic carbon would reduce the system ability to buffer natural extremes in pH, leading to amplification of extremely low pH events in future

(Pacella et al. 2018). Those extreme events in pH have been recognized as an important stressor on marine organisms such as bivalves (Hauri et al. 2013; Harris et al. 2013).

The diurnal variability of pH is mostly attributed to the diel pattern in photosynthesis and respiration: pH increases as photosynthesis takes up CO₂ over the day, and then declines as respiration replenish CO₂ during the night (Wootton et al. 2008; Hofman et al. 2011; O'Boyle et al. 2013; Saderne et al. 2013; Baumann et al. 2015; Akhand et al. 2016; Baumann and Smith 2018; Pacella et al. 2018). Reum et al. (2014) argued diel vertical migrators whose movement can perturb stratified water could be another driver in fjord estuaries as they live in the deep water during the day and migrate to the near-surface water at night. In addition to biological drivers, physical processes can also drive the short-term variability in pH and pCO_2 . As oceanic water typically has a lower DIC/TA ratio than riverine water, tidal advection in estuaries can drive pH variability at semi-diurnal or diurnal frequency with high pH, low pCO_2 during flood tides and low pH, high pCO_2 during ebb tides (Ribas-Ribas et al. 2013; Akhand et al. 2016; McCutcheon et al. 2021; Sims et al. 2022). Baumann et al. (2015) noticed the overlapping of tidally driven variability and diel metabolism cycle can lead to extreme pH values in a tidal salt marsh. Besides, Dai et al. (2009) found temperature was the major driver of the diurnal variability in surface pCO_2 in the oligotrophic regions in the South China Sea. Another observation in the northern South China Sea argued internal waves generated by tidal currents interacting with bottom topography could be another driver, as they can transport nutrient-replete subsurface water into the euphotic zone, stimulating phytoplankton production and lowering surface pCO_2 (Tai et al. 2020). Moreover, observations at a urbanized estuary, Hudson River, found land-sea temperature gradients built up on warm days could drive sea breezes and diurnal

wind cycles, which enhanced surface turbulent mixing and pCO_2 by a factor of 10–100 in the mid-afternoon of a day (Orton et al. 2010). In a longer event time scale (days to weeks), wind-driven upwelling can transport high nutrient and low pH water from the bottom to the surface in the coastal region (DeGrandpre et al. 1998; Gago et al. 2003; Saderne et al. 2013). Whether the upwelling would elevate or lower surface pH depends on the competition between flow advection and enhanced primary production (Cheresh and Fiechter 2020). Extreme heat events or marine heatwaves could also lead to low pH events of several days to weeks at estuarine habitats (Tassone et al. 2022). In addition, observations in the turbid Hudson River suggested strong spring-neap tidal cycle could drive a fortnight variability of surface pCO_2 with high value during the spring tide and low value during the neap tide (Scully et al. 2022).

Previous studies on short-term variability of pH focused on surface pH or shallow wellmixed coastal water. In many stratified estuaries with high turbidity, primary production is confined in the surface layer and net respiration prevails in the bottom layer, so no diel metabolic cycle exists in the bottom water (Carstensen et al. 2003; Testa et al. 2012). It raises a question whether high-frequency variability of pH also exists in the bottom water and what drivers should be responsible for the variability. Chesapeake Bay, as a large partially stratified estuary with relatively low buffer capacity (Cai et al., 2017), is an ideal study site to address the question. Recent observations in Chesapeake Bay found pH and surface pCO_2 to have large spatial gradients. The pH ranges from a minimum value of 7.1 in the upper Bay and the bottom waters of the mid Bay to a maximum value as high as 8.5 at in the surface waters of in the mid and lower Bay (Brodeur et al., 2019). pCO_2 also displays a strong along-channel gradient from the estuary's head to mouth, resulting in outgassing in the upper Bay, sink of atmospheric CO_2 in the mid Bay, and near-equilibrium conditions in the lower Bay (Chen et al. 2020; Friedman et al. 2020). Due to stratification and biological processes that consume DIC in the surface euphotic layer and produce DIC in the bottom layer, strong vertical gradients in DIC and pH develops (Cai et al., 2011, 2017). These strong horizontal and vertical gradients make the carbonate system susceptible to disruptions from physical forcing. Observations from a moored sensor showed high frequency (days-weeks) fluctuations of surface pH and pCO_2 driven by a combination of physical and biological processes (Shadwick et al. 2019). However, the single sensor cannot identify which physical processes are responsible for the variability. Another measurement of pCO_2 and salinity at a cross-channel transect in the mid Bay showed wind could drive lateral variations in surface pCO_2 (Huang et al. 2019). Coupled hydrodynamicbiogeochemical-carbonate chemistry models (ROMS-RCA-CC) have been developed for Chesapeake Bay (Shen et al. 2019). A hindcast simulation suggested wind-driven lateral upwelling could transport low pH water from the deep channel to the shallow shoal, harming the oyster habitats (Li et al. 2020). These studies all focused on surface pH and pCO2 and the shortterm variability of bottom pH in the deep channel remain unclear. In addition, wind-driven lateral exchange of oxygen between well-oxygenated shallow shoals and hypoxic deep channel is thought to be an important mechanism for ventilation of bottom oxygen (Scully 2010, 2016). CO_2 dynamics often mirror O_2 dynamics, since the production and consumption of DIC and O_2 are affected by common biological processes and all chemical tracers are advected or diffused by the same physical processes. However, surface-water pCO₂ adjusts more slowly than O₂ and rarely reaches equilibrium with respect to the atmospheric pCO_2 (Cai et al. 2021). Thus, whether the wind-driven lateral ventilation mechanism is applicable to bottom pH requires further examination.

1.4 Dissertation objectives and layout

This dissertation mainly surrounds the internal wave generation mechanism proposed by Xie et al. (2017b), in which an internal lee wave is generated over the flank of the deep channel when tidally-driven lateral currents become supercritical and the lee wave subsequently propagates toward the shallow shoal, evolving into a train of solitary waves (shown as Fig. 1.1). Based on the unknowns mentioned in the sections above, the main objectives of this dissertation are to identify what river flow and tidal current conditions are conducive to the lee wave generation and how the lee wave evolves into the internal solitary waves in a generic coastal plain estuary. Another objective is to investigate the drivers of the short-term variability of bottom pH in Chesapeake Bay using observation data from a mooring sensor and coupled physical-biochemical models.



Figure 1.1 A schematic diagram illustrating the generation of internal solitary waves by lateral circulation adapted from Xie et al. (2019). Here, Fr_2 is the Froude number with respect to mode-2 wave speed. When $Fr_2 \ge 1$, supercritical lateral flows generate a mode-2 lee wave at the edge of the deep channel (a). When $Fr_2 < 1$ as lateral flows weaken, the lee wave propagates onto the shoal, evolving into a mode-1 elevation wave (b). The elevation wave subsequently evolves into a train of internal solitary waves (c).

The dissertation is organized as follows. Chapter 2 investigates under what river flow and tidal current conditions the internal lee waves could be generated by lateral circulation in a generic coastal plain estuary. Chapter 3 interprets the generation and evolution processes of internal solitary waves associated with lateral processes. In chapter 4, short-term variability and ventilation of bottom pH in Chesapeake Bay is studied by observation and model simulation.

The final chapter summarizes the overall findings and suggests the future work to improve the knowledge on nonlinear internal waves and short-term variability of pH in estuaries.

Chapter 2: A Regime Diagram for Internal Lee Waves in Coastal Plain Estuaries

Preface

This chapter is a reproduction of work published in *Journal of Physical Oceanography* with coauthor Ming Li. The right to reuse this work was retained by the authors when publication rights and nonexclusive copyright were granted to the American Meteorological Society.

Li, R., and M. Li, 2022: A regime diagram for internal lee waves in coastal plain estuaries. Journal of Physical Oceanography, 52(12), 3049-3064. doi: https://doi.org/10.1175/JPO-D-21-0261.1

2.1 Abstract

Recent observations in Chesapeake Bay showed that the interaction between lateral circulation and channel-shoal bathymetry generated internal lee waves, but it is not known under what hydrodynamic conditions the lee waves could be generated. Using an idealized straight channel representative of a coastal plain estuary, we conducted numerical simulations to investigate internal wave generation over a range of river flows and tidal amplitudes. It is shown that the lee waves can be generated across all salinity regimes in an estuary. Since the lateral currents are relatively weak and usually subcritical with respect to the lowest mode, mode-2 lee waves are most prevalent but a hydraulic jump can develop during the transition to subcritical flows in the deep channel, producing high energy dissipation rate and strong mixing. Unlike stratified flows over a sill, stratified water in the deep channel may become stagnant and uncoupled from the flows above such that a mode-1 depression wave can form higher up in the water column. With the lee wave Froude number well above 1 and the intrinsic wave frequency between the inertial and buoyancy frequency, the lee waves generated in coastal plain estuaries are nonlinear lee waves with the wave amplitude scaling approximately with V/\overline{N} where V is the maximum lateral flow velocity and \overline{N} is the averaged buoyancy frequency in the deep channel. The model results are summarized using the estuarine classification diagram based on the freshwater Froude number Fr_f and the mixing parameter M. Δh decreases with increasing Fr_f as stronger stratification suppresses waves, and no internal waves are generated under large Fr_f . Δh initially increases with increasing M as the lateral flows become stronger with stronger tidal currents, but decreases or saturates to a certain amplitude as M further increases. This modeling study suggests that internal lee waves can be generated in a wide range of estuarine conditions.

2.2 Introduction

Nonlinear internal waves are widely observed in the stratified coastal ocean and play an important role in generating turbulent mixing and transporting biochemically important materials. The conversion of barotropic tidal energy to internal waves is now generally accepted as a major source for mixing in the ocean (Munk and Wunsch 1998). In contrast, internal waves in estuaries have not attracted much attention (Wang 2006), except for flows over sills at the entrance to deep fjords (e.g. Farmer and Armi 1999; Cummins et al. 2003; Gregg and Pratt 2010) and in deep estuaries (e.g. Bourgault and Kelley 2003; Bourgault et al. 2007; Richards et al. 2013). In shallow coastal plain estuaries, turbulence has been mostly attributed to boundary layer turbulence (Geyer and MacCready 2014). Dissipation by bottom friction is assumed to be the dominant sink for the barotropic tidal energy, and most studies have focused on the bottom dissipation.

Several previous observations however did find internal waves in coastal plain estuaries. Echo-sounding surveys across a cross-section in a partial mixed estuary, Southampton Water, showed internal isopycnal oscillations with a wave period of 4 - 8 min (Dyer 1982). Using moored current measurements, Groeskamp et al. (2011) observed nonlinear internal solitary waves in the highly energetic Marsdiep channel. In Chesapeake Bay, early observations using thermistor chain showed high-frequency internal waves with large isotherm displacements (Sarabun and Dubbel 1990). Recent observation found that energy dissipation rate ε in the pycnocline reached 1×10^{-4} m² s⁻³ during the passage of internal solitary waves, three orders of magnitude larger than the background value (Xie et al. 2017a). Strong mixing has also been associated with the passage of internal waves in other estuaries (New et al. 1986, Sturley and

Dyer 1992). For example, internal waves generated by tidal flow over a trench in the Hudson River estuary produced enhanced turbulent dissipation above the trench (Peters 1999). These observations suggest that internal waves can be another pathway to turbulent mixing in the stratified estuaries, but mechanisms for internal wave generation are not yet well understood. Neither is it known how prevalent internal waves are in coastal plain estuaries.

Based on high resolution temperature and velocity measurements at a mid-bay section of Chesapeake Bay, Xie et al. (2017b) proposed a mechanism in which an internal lee wave is generated over the flank of the deep channel when tidally-driven lateral currents become supercritical and the lee wave subsequently propagates toward the shallow shoal, evolving into a train of solitary waves. To test the first part of this hypothesis, Xie and Li (2019) used a realistic model of Chesapeake Bay to simulate the internal lee waves observed during the field experiment and confirmed the mechanism of lee wave generation by the lateral currents. However, this study did not identify hydrodynamic conditions at which the stratified lateral flows are conducive to generating the internal lee waves. It remains unknown under what river flow and tidal current conditions that the internal lee waves could be generated in a generic coastal plain estuary.

Observations at the Knight Inlet revealed a rich variety of internal lee wave and hydraulic jump structures under different river flow and tidal conditions (Farmer and Smith 1980). Under typical summer conditions the tidal flow is subcritical with respect to the lowest mode but supercritical with respect to higher modes, resulting a mode-2 lee wave or jump. When tidal flows become supercritical with respect to all modes, however, the transition from subcritical

upstream flow to an accelerating supercritical downslope flow generates an internal hydraulic jump (Farmer and Armi 1999). Flow interactions with a topographic depression such as the deep channel in a coastal plain estuary could be different from flow interactions with a sill. Previous modeling studies of atmospheric flows over a valley showed flow structures such as valley-flow stagnation, lee waves, internal wave breaking, and hydraulic jumps, which are quite different from flows over a hill (Rotunno and Lehner 2016, Lehner et al. 2016). Therefore, modeling studies are needed to document possible range of internal wave and flow structures that might be produced by the interaction between the lateral flows and the valley in the deep channel. Moreover, coastal plain estuaries are much shallower than fjords and costal oceans such that bottom friction and turbulent mixing generated in the bottom boundary layer could affect the generation of the internal lee waves.

In this study an idealized straight estuarine model with channel-shoal bathymetry is used to examine the generation of internal lee waves under a range of river flows and tidal forcing conditions. The paper is structured as follows. In section 2.3, the model configuration and numerical experiments are described as well as the nondimensional parameter relevant to internal lee wave generation. Section 2.4 presents a detailed analysis of processes and features of the lateral wave generation in a coastal plain estuary. In section 2.5 we explore lee waves over a range of river flows and tidal forcing conditions and interpret the wave generation in terms of internal hydraulics. The model results are summarized in a regime diagram in section 2.6. Concluding remarks are made in section 2.7.

2.3 Methods

2.3.1 Model descriptions and numerical experiments

The Regional Ocean Modeling System (ROMS) is used to configure a model for the idealized straight estuarine channel. The model domain is an estuary-shelf system (Fig. 2.1a), following Hetland and Geyer (2004), Cheng et al. (2010, 2011) and Li et al. (2014). The estuary part of the model domain is a straight channel and does not have slope in the along-channel direction. The channel is 750 km long to damp out tides before they reach the upstream boundary and the width of the channel is set at 8 km. The cross-channel section has a channel-shoal bathymetry consisting of a triangular deep channel in the center and two flat shoals on each side (Fig. 2.1b). The shoal is 10 m deep (D = 10 m). The relative depth (H) of the deep channel is 10 m and the width (L) is 2 km. The continental shelf is 80 km wide and has a fixed cross-shelf slope of 0.05%. The total model domain has 240 grid cells in the east-west direction, 79 grid cells in the north-south direction, and 20 layers in the vertical direction. The estuarine channel has 200 grid cells in the along-channel direction and 41 grid cells in the cross-channel direction. The along-channel grid size increases exponentially from the estuary mouth (100 m) to its head (12 km), providing a highly resolved estuarine region near the mouth. In the numerical experiments conducted, the estuary length (L_1) , defined as the distance from the estuary mouth to the upstream location where the vertically averaged salinity is 1 psu, is less than 300 km. The cross-channel grid in the estuary is uniformly distributed and the vertical layers are uniformly discretized.



Figure 2.1 (a) Schematic of the numerical model domain consisting of a straight estuarine channel and a shelf. (b) Cross-channel section featuring a triangular-shaped deep channel and flat shallow shoals. The black dashed lines mark the location of site A, site B and site C (shown in Fig. 2.3) respectively.

The model is forced by tides at the offshore (eastern) open boundary and by river flow at the upstream (western) end of the estuarine channel. At the upstream boundary, a momentum boundary condition is imposed on the depth-averaged velocity. The inflowing river water is prescribed to have zero salinity. To simplify time series analysis, we impose a semidiurnal tide with the period of 12 h. The salinity of the coastal ocean is set at 35 psu. The open-ocean boundary is treated with a Chapman condition for surface elevation, a Flather condition for barotropic velocity, and an Orlanski-type radiation condition for baroclinic velocity and scalars (Marchesiello et al. 2001). A quadratic stress is exerted at the seabed, assuming that the bottom boundary layer is logarithmic with a roughness height of 0.5 mm. The Coriolis parameter is set at 1.0×10^{-4} rad s⁻¹.

The vertical eddy viscosity and diffusivity are computed using the *k-kl* turbulence closure scheme (Warner et al. 2005) with the background diffusivity and viscosity set at 1×10^{-5} m² s⁻¹. In

this closure scheme, the turbulent kinetic energy k and turbulent length scale l are calculated by solving two prognostic equations for k and kl. The eddy viscosity K_V and eddy diffusivity K_S are then given by

$$K_V = \sqrt{2k} l S_M + \gamma, \ K_S = \sqrt{2k} l S_N + \gamma_S, \tag{2.1}$$

where γ and γ_S are the background eddy viscosity and diffusivity. S_M and S_N are stability functions that describe the effects of shear and stratification (Kantha and Clayson, 1994). The energy dissipation rate is calculated using

$$\varepsilon = \left(c_{\mu}^{0}\right)^{3} k^{\frac{3}{2}} l^{-1}, \qquad (2.2)$$

where $c_{\mu}^{0} = 0.5544$. We also conducted model runs using the *k*- ε and *k*- ω turbulence closure schemes and found almost identical results.

The model was initialized with no flow, a flat sea surface, and a uniform salinity of 35 psu. To simplify, temperature is uniform everywhere and does not change with time. Using a tidal amplitude (η_i) of 1.1 m and a sectionally averaged river flow (U_r) of 0.03 ms⁻¹, the model was run for 360 days to reach a quasi-steady state. The salinity distribution from this run was then used as the initial salinity condition in each of the following numerical experiments. Results obtained at the quasi steady state, during which tidally averaged circulation and stratification did not change with time (after 120 or so more days of integration), were used for the analysis.

A total of 24 model runs were conducted over a range of river discharges and tidal amplitudes to investigate the generation of internal lee waves by lateral circulation in the idealized estuary (Table 2.1).

Run	η_t	М	U_r	Fr_{f}	L_1	Fr _{2max}	\overline{N}	$\overline{N}H/V$	Vk
1	0.5	0.30	0.005	0.0029	371	1.10	0.033	3.12	2.9×10 ⁻⁴
2	0.5	0.30	0.01	0.0058	310	0.68	0.048	5.68	2.0×10^{-4}
3	0.5	0.29	0.03	0.017	211	0.57	0.080	10.88	1.9×10^{-4}
4	0.5	0.26	0.05	0.029	184	0.46	0.092	15.10	1.6×10^{-4}
5	0.5	0.25	0.07	0.041	171	0.42	0.11	18.40	1.6×10^{-4}
6	0.6	0.39	0.005	0.0029	334	1.29	0.036	2.61	3.5×10^{-4}
7	0.6	0.41	0.01	0.0058	280	1.15	0.039	3.22	3.3×10^{-4}
8	0.6	0.38	0.03	0.017	191	1.00	0.071	5.48	3.6×10^{-4}
9	0.6	0.36	0.05	0.029	157	0.82	0.093	7.96	3.0×10^{-4}
10	0.6	0.37	0.07	0.041	144	0.79	0.10	8.78	3.1×10 ⁻⁴
11	0.8	0.62	0.005	0.0029	307	1.60	0.022	1.88	4.1×10 ⁻⁴
12	0.8	0.61	0.01	0.0058	249	1.50	0.032	2.21	4.6×10 ⁻⁴
13	0.8	0.61	0.03	0.017	147	1.38	0.051	2.75	5.6×10 ⁻⁴
14	0.8	0.67	0.05	0.029	119	1.37	0.067	3.26	5.8×10^{-4}
15	0.8	0.72	0.07	0.041	106	1.31	0.086	4.01	5.7×10 ⁻⁴
16	1.1	0.92	0.005	0.0029	188	1.32	0.035	3.41	2.4×10 ⁻⁴
17	1.1	0.93	0.01	0.0058	163	1.46	0.033	2.06	4.4×10^{-4}
18	1.1	0.98	0.03	0.017	116	1.41	0.037	2.33	5.3×10 ⁻⁴
19	1.1	1.27	0.05	0.029	81	1.60	0.072	3.09	6.1×10 ⁻⁴
20	1.1	1.31	0.07	0.041	72	0.63	0.11	9.97	2.2×10 ⁻⁴
21	1.3	1.27	0.01	0.0058	114	1.97	0.080	5.55	3.4×10 ⁻⁴
22	1.3	1.54	0.03	0.017	80	2.24	0.10	9.83	3.0×10 ⁻⁴
23	1.3	1.45	0.05	0.029	76	1.30	0.086	4.84	3.4×10 ⁻⁴
24	1.3	1.69	0.07	0.041	60	2.30	0.12	10.80	4.9×10 ⁻⁴

Table 2.1 Summary of numerical experiments in which η_t is the tidal amplitude (m) at the open boundary, M is the estuarine mixing number, U_r is the river flow velocity (m s⁻¹), Fr_f is the freshwater Froude number, L_1 is the salt intrusion length (km), $Fr_{2\text{max}}$ is the maximum mode-2 Froude number at the left channel-shoal interface of the mid-estuary cross-section, \overline{N} is the averaged buoyancy frequency over the deep channel of at the mid-estuary cross-section, $\overline{NH/V}$ is the topographic Froude number, and Vk is the intrinsic frequency for the lee waves.

2.3.2 Froude number analysis

To interpret the internal lee wave generation process, we calculated the Froude number

$$Fr_i = \frac{v}{c_i} \tag{2.3}$$

where v is the depth-averaged lateral flow velocity in the lower layer (Xie et al., 2017) and c_i is

the phase speed of the *i*th mode of internal waves. The phase speed c_i is found by solving the following eigenvalue problem (Gill, 1982):

$$\frac{d^2 \Phi(z)}{dz^2} + \frac{N^2(z)}{c_i^2} \Phi(z) = 0, \qquad (2.4)$$

with the boundary conditions $\Phi(0) = \Phi(-h) = 0$ where $\Phi(z)$ is the modal function of the vertical velocity, *h* is the water depth and *N*(*z*) is the buoyancy frequency. The Froude number has been widely used in previous studies of internal lee waves by flow-topography interaction (e.g. Vlasenko et al. 2013; da Silva et al. 2015).

A mode-1 lee wave can develop when $Fr_1 > 1$ and typically features a depression or elevation in isopycnals. A mode-2 lee wave can develop when $Fr_2 > 1$ and typically features a bulge in isopycnals. An internal hydraulic jump involves an abrupt isopycnal lift during a transition from supercritical to subcritical flows.

2.4 Lateral wave generation

2.4.1 Generation and propagation of internal lee waves

We first present a detailed case study of wave generation by lateral circulation in the estuarine channel, with the tidal amplitude $\eta_t = 0.8$ m and river flow $U_r = 0.03$ m s⁻¹ (run 13 in Table 2.1). The estuary length (L_1), as defined by the location of vertically averaged 1 psu isohaline in the along channel section, is 147 km. The mid-estuary cross-section at $L_1/2$ is chosen to investigate the wave generation process. Figure 2.2a shows the time series of sectionally averaged along-channel tidal velocity and depth-averaged lateral flow velocity in the bottom layer. There is a phase lag of 2-3 hours between the lateral velocity and along-channel velocity.
The lateral flows at the left channel-shoal interface reach a peak speed of 0.18 m s^{-1} during the ebb tide.

Snapshots of lateral circulation and salinity distribution at the mid-estuary cross-section are shown in Fig. 2.2. A counter-clockwise lateral circulation (looking into the estuary) develops during the ebb tide (Figs. 2.2b-d). At the maximum ebb tide T1, no isohaline displacements appear over the deep channel and $Fr_2 < 1$ (Figs. 2.2b & 2.2e). At T2, wave perturbation of small amplitude starts to be generated over the left edge of the deep channel as the lateral flows (v)become critical at the left channel-shoal interface (Figs. 2.2c & 2.2f). When the bottom lateral flows become supercritical at T3, a large-amplitude internal wave with a characteristic mode-2 bulge structure appears at this location and is arrested (Figs. 2.2d & 2.2g). Subsequently, the ebb tide subsides and the lateral currents weaken. At T4 when the lateral flows become subcritical (Fig. 2.2k), the lee wave propagates upward and onto the left shoal while its amplitude decreases (Fig. 2.2h). Meanwhile, the trailing edge of the wave steepens and an internal wave reminiscent of a mode-1 elevation wave is formed at the rear of the wave, possibly due to second-order nonlinear processes which become important as the depression enters shallower water (Lamb 1994). At T5, the tidal flow switches to the flood phase and strong mixing on over the left shoal destroys the wave depression (Fig. 2.2i). At the late flood tide T6, the wave completely disappears (Fig. 2.2j).



Figure 2.2 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 13 with $\eta_t = 0.8$ m and $U_r = 0.03$ m/s. Vertical lines indicate the timing of the six cross-channel snapshots shown below. The grey shaded region represents flood tide and the yellow shaded region represents ebb tide. (b)-(d), (h)-(j) Distributions of salinity (contours), velocity vectors (arrows), and dissipation rate (background color) at the midestuary cross-section at times T1-T6 marked in (a). Contour intervals are at 1 psu increments. (e)-(g), (k)-(m) Cross-channel distribution of Froude number Fr_1 and Fr_2 at T1-T6. The solid lines indicate rightward bottom flows and the dashed lines indicate leftward bottom flows. The vertical dashed lines in (b)-(m) mark the location of the channel-shoal interface.

The time-depth distributions of the vertical velocity (w) and salinity at three locations in the mid-estuary cross-section further illustrate the propagation and evolution of the internal lee wave (Fig. 2.3). Site A is on the left flank of the deep channel; site B is located at the left channel-shoal interface; and site C is farther left on the left flat shoal. The magenta isohaline contours in Fig. 2.3a show a mode-2 wave at site A. The wave speed is ~ 0.13 m s⁻¹ relative to the background flow, while the lateral flow velocity is up to 0.17 m s⁻¹. Hence the wave is trapped at site A for about 1.5 hours due to opposing lateral currents. The trailing edge of the wave arrives at site A. From T7 to T8, the lateral velocity drops from 0.10 m s⁻¹ to 0 and then switches its direction to -0.04 m s⁻¹, such that the background flow changes from resisting the leftward wave propagation to assisting it. It takes about 1 hour for the mode-2 wave to travel from site A to site B (400 m distance), at a mean speed of 0.11 m s⁻¹ (Fig. 2.3b). The maximum w decreases from 1.3 mm s⁻¹ at site A to 0.8 mm s⁻¹ at site B. It takes another hour for the wave to travel to site C further left on the shoal (Fig. 2.3c). The wave also propagates upward during this transit (compare Figs. 2.3b and 2.3c). The maximum value of w decreases to 0.3 mm s⁻¹ at site C, which is almost one order of magnitude smaller than that at site A, signaling a significant loss of the wave energy.



Figure 2.3 (a)-(c) Time-depth distributions of the salinity (contours) and vertical velocity (color) at sites A, B, and C in the mid-estuary cross-section (their locations marked in Fig. 1b). The magenta contours highlight the internal waves.

Figures 2.2 and 2.3 show isohaline patterns reminiscent of mode-1 and mode-2 waves. To quantify the wave modal structure, a modal decomposition was performed for the vertical velocity at sites A and C. Contribution of each mode can be determined by solving a weighted least squares problem (Nash et al. 2005),

$$w(z) = \sum_{i=1}^{m} W_i \Phi_i(z),$$
(2.5)

where W_i is the *i*th modal amplitude of vertical velocity *w*, $\Phi_i(z)$ is the *i*th mode structure function and m is the number of modes attained from equation (4). At site A and T7, mode-2 explains 45% of the total vertical velocity variance and mode-1 explains 12% (Fig. 2.4a), indicating a dominant mode-2 wave consistent with the bulge structure seen in the isohaline pattern (Fig 2.3a). At site C, the mode-1 structure explains 60% while mode-2 structure explains 24% (Fig. 2.4b), indicating a predominant mode-1 wave consistent with the elevation wave pattern seen in the isohaline (Fig 2.3c). Hence the lee waves shown in Fig. 2.3 are strictly a mixture of mode-1 and mode-2 waves but with one mode dominating.



Figure 2.4 (a)-(c) The vertical structure of the vertical velocity normalized by its maximum value (blue), mode-1 structure function $\Phi_1(z)$ (green) and mode-2 structure function $\Phi_2(z)$ (red) at times T7 and T8 (marked in Fig. 2.3) and sites A and C respectively.

In contrast to the ebb tide, no internal lee waves are generated during the flood tide. The strong bottom boundary mixing over the right shoal extends from the bottom almost to the surface (Figs. 2.2i & 2.2j). Despite the strong leftward bottom lateral flows across the right channel-shoal interface, stratification in the bottom water (below 5 m depth) over the right shoal is too weak (Fig. 2.2j) such that no stratified water is advected from the shoal to the deep channel. Consequently, the flood tide is not conducive to internal lee wave generation. Only one lee wave is generated over a flood-ebb tidal cycle.

It is interesting to note that the internal lee wave leads to localized high energy dissipation rate in the stratified water over the deep channel (Figs. 2.2d-2.2h). At the slack tide T3, a pocket of relatively high ε is found under the upper crest of the mode-2 wave while the bottom boundary

layers on the two shallow shoals nearly disappear (Figs. 2.2d). Similarly, a region of high energy dissipation with $\varepsilon \sim 3.2 \times 10^{-5} \text{ m}^2 \text{ s}^{-3}$ coincides with the steepening of isohalines at the left edge of the deep channel at T4 (Fig. 2.2h). Although these regions are considerably smaller the bottom boundary layers generated by tidal currents moving over the shallow shoals, the wave-induced turbulent dissipation enhances mixing in the stratified region in the estuary and could play an important role in the circulation dynamics.

2.4.2 Along-channel variations in wave generation

The analysis above focuses on the mid-estuary cross-section. To investigate the wave generation across different salinity regimes in the estuary, we first selected three cross-sections: a lower-estuary section $(L_1/4)$, mid-estuary section $(L_1/2)$ and upper-estuary section $(3/4L_1)$, respectively, and followed the evolutions of the lateral velocity and salinity fields over time (Fig. 2.5). Internal waves appear at all the three sections, but the wave amplitude and timing of wave generation are different. At T9 when $Fr_2 = 1.2$ at the lower-estuary section (Fig. 2.5a), an internal lee wave with an amplitude of 2.7 m is generated over the left edge of the deep channel at the lower-estuary (Fig. 2.5d), while the lateral flows at the mid-estuary and upper-estuary remain subcritical (Figs. 2.5b & 2.5c). Since the salinity field in the estuary changes over a tidal cycle, it is difficult to measure the internal wave amplitude by tracking the vertical isopycnal displacements (Martin et al. 2005). Instead we calculated the wave amplitude Δh using the maximum depth difference of the lateral velocity maxima (see Fig. 2.5d for an illustration of this method), following the approach by Legg and Klymak (2008). When Fr_2 at the mid-estuary becomes supercritical at T10 (Fig. 2.5b), an internal lee wave of 4.6 m is generated at the midestuary (Fig. 2.5h). In the meantime, the internal lee wave generated at the lower-estuary section propagates toward the shoal (Fig. 2.5g) and the lateral flows at the upper-estuary section approaches critical (Fig. 2.5c). At T11, an internal lee wave of 8.4 m is generated by the supercritical lateral flows at the upper-estuary section (Fig. 2.5l), while the internal lee waves at the lower-estuary and mid-estuary sections are propagating onto the shallow shoal (Figs. 2.5j & 2.5k).



Figure 2.5 (a)-(c) Time series of sectionally averaged along-channel velocity (blue) and mode-2 Froude number Fr_2 (red) at the left channel-shoal interface in the upper-, mid- and lower-estuary cross-sections (their locations marked in Fig. 2.8). (d)-(l) Snapshots of lateral velocity (color) and salinity distribution (contours) at these sections [here timing marked as the dotted black lines in (a)-(c)]. Contour intervals are at increments of 1.5 psu in (d), (g), and (j), 1 psu in (e), (h), and (k), 0.5 psu in (f), (i), and (l). In (d) the two dashed lines mark the depths of the lateral velocity maxima and their distance is used to calculate the wave amplitude.

Figure 2.5 shows that internal lee waves can be generated at different regions of the estuary across a range of salinity regimes (5 - 20 psu). To illustrate how the lee waves vary from the

mouth to the head of the estuary, we plot the along-channel distribution of the wave amplitude Δh in Fig. 2.6. Δh is about 3 m in the lower estuary (within ~ 45 km from the estuary's mouth), increases linearly to 6 m in the mid-estuary (45 - 90 km), and peaks around 8 m at 110 km before rolling off to 4 m in the upper estuary (Fig. 2.6a). This along-channel variation in the wave amplitude is consistent with an interpretation based on the maximum Froude number at the left channel-shoal interface during a tidal cycle (Fr_{2max}). V decreases from the lower-estuary to the upper-estuary, which goes in an opposite direction to Δh (Fig. 2.6b). However, the depthaveraged stratification (N^2) at the left channel-shoal interface decreases faster in the alongchannel direction, indicating that the wave amplitude depends on the competition between the lateral velocity and stratification. Fr_{2max} increases gradually from the lower-estuary to the upperestuary before rolling off (Fig. 2.6c). Moreover, Fr_{2max} exceeds 1 in most parts of the estuary, affirming that supercritical lateral flows are a pre-condition for the internal lee wave generation. In the most upstream region of the estuary (130-150 km), stratification is too weak to support the internal wave generation. In addition, the time when the lateral flows become critical $(T_{Fr_2=1})$, corresponding to the timing of the lee wave generation at different parts of the estuary (Fig. 2.6d), can be fit as

$$T_{Fr_2=1} \approx \frac{x}{\sqrt{gD}} + 10,$$
 (2.6)

where x is the distance from the estuary mouth, g is the gravity acceleration and D is the shoal depth, as the tidal wave propagates upstream and produces lateral flows that interact with stratified water over topography to generate the internal lee wave.



Figure 2.6 Along channel distributions of (a) internal lee wave amplitude Δh , (b) maximum bottom lateral velocity V and the depth-averaged stratification N^2 when Fr_2 reaching maximum at the left channel-shoal interface, (c) maximum mode-2 Froude number $Fr_{2\text{max}}$, and (d) the timing of lateral flow reaching critical condition ($T_{Fr_2} = 1$) after ebb slack at estuary mouth. The red dashed line in (d) indicates the function of $\frac{x}{\sqrt{gD}}$ +10. The black dashed lines mark the locations of upper-, mid- and lower-estuary cross-sections respectively.

2.5 Internal lee wave generation under different hydrodynamic conditions

Since the internal lee wave generation depends on the stratification and lateral current speed, we ran the model over a range of tidal amplitudes and river flows and identify the hydrodynamic conditions that might be conducive to the lee wave generation.

2.5.1 Effects of river flow

Figure 2.7 shows the results from 4 model runs with a fixed offshore tidal amplitude $\eta_t = 0.6$

m but at different values of the river flow: $U_r = 0.01$, 0.03, 0.05 and 0.07 m s⁻¹ (runs 7 - 10 in Table 1). These snapshots are taken at the time when Fr at the left channel-shoal interface reaches the maximum during the ebb tide and the isohaline displacement is nearly largest. At $U_r = 0.01$ m s⁻¹, $Fr_{2\text{max}}=1.15$ and Δh is 4.4 m while the depth-averaged stratification (N^2) is 3.2×10^{-3} s⁻² (Figs. 2.7a and 2.8a). At $U_r = 0.03$ m s⁻¹, N^2 increases to 5.3×10^{-3} s⁻², $Fr_{2\text{max}} = 1.0$ and Δh decreases to 1.3 m (Fig. 2.7b). At higher river flows ($U_r = 0.05$, 0.07 m s⁻¹), the estuary becomes highly stratified ($N^2 = 5.9 \times 10^{-3}$, 6.3×10^{-3} s⁻²) and the lateral flow remains subcritical such that no significant perturbations of isohalines are seen over the left channel-shoal interface (Figs. 2.7c-d). At a fixed tidal amplitude, both $Fr_{2\text{max}}$ and Δh decrease as the river discharge increases.



Figure 2.7 (a)-(d) Snapshots of cross-channel distributions of salinity (contours) and lateral

velocity (arrows) at the mid-estuary section in model runs with different river discharges but fixed tidal forcing (runs 7–10). Contour interval is 0.5 psu in (a), and 1 psu in (b)-(d). The snapshots are taken at the time when Fr_2 at the left channel-shoal interface reaches a maximum.

The river flow affects the generation of internal lee wave mainly through its effects on stratification (Fig. 2.8). At a fixed tidal amplitude, the stratification increases with U_r : N^2 at the channel-shoal interface in the mid-estuary section increases from 2.5 - 3 s⁻² at $U_r = 0.005$ m s⁻¹ to 5.5 - 7 s⁻² at $U_r = 0.07$ m s⁻¹ (Fig. 2.8a). The internal wave phase speed c_i depends on the stratification and also increases with U_r (Fig. 2.8b). The mode 2 wave phase speed, c_2 , increases from 0.08 m s⁻¹ at low river discharge to 0.12 - 0.14 m s⁻¹ at high river discharge. Therefore, it is harder for the lateral flow to reach a critical speed and the internal lee wave to develop as the river discharge increases.



Figure 2.8 (a) The stratification at the left channel-shoal interface and (b) the internal lee wave phase speed as a function of river discharge U_r . Values are calculated at the mid-estuary sections from the model runs featuring internal waves (runs 1-15, 17-19).

2.5.2 Effects of tidal amplitude

The internal lee wave shows a nonlinear response to increasing tidal amplitude η_t at a fixed river flow ($U_r = 0.01 \text{ m s}^{-1}$) (Fig. 2.9). $Fr_{2\text{max}}$ does not increase monotonically as η_t increases. As η_t increases from 0.6 to 0.8 m, $Fr_{2\text{max}}$ increases from 1.15 to 1.5 and the internal wave amplitude Δh increases from 4.4 to 5.7 m (Figs. 2.9a & 2.9b). The maximum lateral flow velocity increases from 0.106 to 0.143 m s⁻¹ while the stratification is relatively unchanged. However, when η_t is 1.1 m, the maximum lateral flow velocity decreases slightly to 0.140 m s⁻¹, Fr_{2max} decreases slightly to 1.46, and wave amplitude Δh decreases to 4.9 m (Fig. 2.9c). In these three model runs stratification persists on the shallow left shoal and deep channel, creating a favorable condition for the lee generation when the lateral currents advect the stratified water from the left shoal to the deep channel. One also notices pockets of high vertical diffusivity K_v in Figs. 2.9b and 2.9c where the lee wave steepens to produce localized strong mixing, in addition to high K_v in the bottom boundary layer on the shoals. When η_t reaches 1.3 m, however, water on both left shallow shoals becomes well-mixed and stratification is confined to the deep channel (Fig. 2.9d). The maximum lateral flow velocity decreases dramatically to 0.094 m s⁻¹. No internal waves are generated but salinity fronts are developed over the channel-shoal interfaces.



Figure 2.9 (a)-(d) Snapshots of cross-channel distributions of time-averaged viscosity K_v during the ebb tide (background color), salinity (contours), and lateral velocity (arrows) at the mid-estuary section in model runs with different tidal amplitudes but fixed river discharge (runs 7, 12, 17, 22). Contour interval is 0.5 psu.

This nonlinear relationship between the internal wave amplitude and tidal amplitude η_l can be attributed to the nonlinear response of the lateral circulation to changes in the magnitude of tidal currents. As η_l increases, the maximum lateral flow velocity increases first but then saturates or even decreases slightly (Fig. 2.10). The lateral circulation strength depends on the balance among three terms: the generation of streamwise vorticity by lateral Ekman forcing, the lateral baroclinic forcing and the vertical diffusion (Li et al., 2014). Although a stronger tidal flow produces stronger vorticity generation, it also leads to stronger vorticity diffusion that tends to spin down the lateral circulation (see the region of high K_{ν} expanding from Fig. 2.10a to Fig. 2.10d). As a result, the lateral velocity initially increases as η_t increases from 0.6 to 0.8 m but then decreases as η_t increases to 1.1 and 1.3 m. Since the lee wave is generated by the lateral currents, Δh also shows a parabolic response to the tidal amplitude.



Figure 2.10 The maximum bottom lateral velocity as a function of tidal velocity at the estuary mouth η_t . Values are calculated at the mid-estuary sections from the model runs featuring internal waves (runs 1-15, 17-19).

At $U_r = 0.01 \text{ m s}^{-1}$, strong turbulent mixing destroys stratification over the shallow shoals when the tidal amplitude η_t reaches 1.3 m, thereby inhibiting the generation of the internal lee wave (Fig. 2.9d). This remains true at all the river flows: no internal waves could be generated when tidal currents are strong enough to erase stratification on the shoals. Due to the effects of the Coriolis force, brackish water typically hugs along the southern (left) boundary as it moves seaward, setting up stratification over the left shoal. During the ebb tide, the lateral currents advect this stratified water to the deep channel and generate the internal lee wave. When the tidal currents are very strong, however, K_v reaches O(10⁻²) m²s⁻¹ on the shallow shoals such that turbulence completely mix the water column there (Fig. 2.9d). The vertical stratification is confined to the deep channel and salinity fronts separate the stratified water over the deep channel from the well-mixed water on the two shoals.

2.5.3 Different wave structures

In addition to changes in the wave amplitude, wave structure also changes under different river flow and tidal conditions. The isohalines in Fig. 2.9c plunge into the deep channel and then rebound abruptly as an internal hydraulic jump, with the eddy diffusivity reaching $O(10^{-2})$ m² s⁻¹). A time sequence of snapshots in Fig. 2.11 illustrates the generation process of this hydraulic jump. The downslope flow causes the isohaline marked as the magenta contour line to depress (Fig. 2.11b) when the bottom lateral flows just become supercritical (Fig. 2.11e). As the lateral flow strengthens, the depression wave grows in amplitude over the left edge of the deep channel (Fig. 2.11c). On the other hand, the lateral flows in the deeper center channel are subcritical (Fig. 2.11f). The transition from the supercritical to subcritical flows is accomplished via a hydraulic jump with the isohalines at the trailing edge lifted sharply upward (Fig. 2.11c). As the lateral flows at the channel-shoal interface get weaker and become subcritical during the flood tide (Fig. 2.11g), the hydraulic jump propagates onto the left shoal (Fig. 2.11d). This sequence of events is similar to the internal hydraulic jump generated by tidal flow over a tall steep ridge in the deep ocean (Legg and Klymak 2008, Klymak et al. 2008), with the accompanied strong local mixing.



Figure 2.11 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 17 with $\eta_t = 1.1$ m and $U_r = 0.01$ m/s. (b)-(d) Distributions of salinity (contours) and velocity vectors (arrows) at the mid-estuary cross-section at times T12-T14 marked in (a). Contour intervals are at 0.5 psu increments. Magenta contour lines mark the isohaline of 13 psu. (e)-(g) Cross-channel distribution of Froude number Fr_1 and Fr_2 at T12-T14.

In addition to mode-2 lee wave and hydraulic jump, a wave in the form of a mode-1 depression is found when both tidal amplitude and river discharge are large. An example is found in run 15 with $U_r = 0.07$ m s⁻¹ and $\eta_t = 0.8$ m. At T15 a small-amplitude mode-2 wave is generated well above the left edge of the deep channel as Fr_2 reaches 1 (Fig. 2.12b). No wave perturbations can be seen in the isohalines in the deep channel due to the establishment of strong stratification there. As the lateral flows strengthen and Fr_1 approaches 1, a mode-1 depression wave appears near the left edge of the deep channel (Fig. 2.12c). This mode-1 wave subsequently propagates onto the shallow shoal as the lateral currents weaken (Fig. 2.12d). It is interesting to

note that the heavier stratified flow in the deep channel becomes stagnant, with the lateral velocity dropping to near zero. The rightward lateral currents on the left shoal run across the top of the deep channel, causing the isohalines near the right edge of the deep channel to tilt up (Figs. 2.12b-e). In the meantime, the downward tilt of the isohalines on the left edge of the deep channel leads to the generation of a mode-1 depression wave in the stratified water above (Figs. 2.12d-e). The heavy stratified water in the deep channel is essentially decoupled from the flows above. This flow pattern is very different from stratified flows over a sill in the ocean but is similar to stratified flows over a valley in the atmosphere (Baines 1995, Lehner et al, 2016a, b, Rotunno and Lehner 2016).



Figure 2.12 (a) Time series of sectionally averaged tidal velocity and depth-averaged lateral velocity in the bottom layer for run 15 with $\eta_t = 0.8$ m and $U_r = 0.07$ m/s. (b)-(g) Distributions of salinity (contours) and velocity vectors (arrows) at the mid-estuary cross-section at times T1-T3 marked in (a). Contour intervals are at 1 psu increments.

2.5.4 Interpretation in terms of internal hydraulics

We calculated the wave amplitude Δh at 10 cross-sections of the estuary from all the model

runs featuring the internal lee waves (runs 1-15, 17-19) and plot it against $Fr_{2\text{max}}$. Figure 2.13a shows that Δh ranges between 1 and 8 m when $Fr_{2\text{max}} > 1$. Waves of smaller amplitude are also found when $0.5 < Fr_{2\text{max}} < 1$. In the laboratory experiments Maxworthy (1979) observed internal lee waves at those values of the Froude number. For a tidal flow over a sill, Fr can be calculated using the vertically averaged tidal velocity and the wave phase speed estimated from the background stratification (Farmer and Smith 1980). Here the calculation of Fr is more complicated due to the two-layer lateral flows and varying stratification (see Eq. 2.6). Nevertheless, the generation of internal lee waves as shown in Figs. 2.2, 2.5, 2.7 and 2.9 is highly consistent with an interpretation base on the internal hydraulics, although the Fr threshold is not necessarily identical to 1 due to the uncertainty in estimating $Fr_{2\text{max}}$ and the previous observation indicating that small amplitude lee waves can still be generated when Fr falls below 1. Nevertheless, the wave amplitude does not show a simple relationship with $Fr_{2\text{max}}$: e.g., Δh varies from 1 to 8.5 m at $Fr_{2\text{max}} = 1.5$.

On the other hand, V/\overline{N} provides a reasonable scaling for the wave amplitude, where V is the maximum lateral flow velocity and \overline{N} is the averaged buoyancy frequency in the deep channel. It sets a limit on the maximum possible isopycnal displacement since the conversion of the potential energy of a displaced isopycnal in the lee wave to the kinetic energy takes place within V/\overline{N} , based on the energetics argument (Mayer and Fringer 2017). In Fig. 2.13b Δh varies approximately linearly with V/\overline{N} when $V/\overline{N} > 1.7$. Here \overline{N} is the sectionally averaged buoyancy frequency over the deep channel at the time of Fr_{2max} . We calculated the lee wave Froude number $\overline{N}H/V$ for all the model runs (Legg 2021) where H is the height of the deep channel (see Fig. 2.1b). Table 1 shows that $\overline{N}H/V$ varies between ~2 and ~18, indicating that the generated

lee waves are highly nonlinear. In this regime, Legg and Klymak (2008) also found that Δh scales with V/\overline{N} in their simulations of tidal flows over a tall ridge in the deep ocean.



Figure 2.13 Internal lee wave amplitude Δh versus $Fr_{2\max}$ (a) and V/\overline{N} (b) from all model runs featuring internal waves. The black dashed line in (b) is a linear fit for $V/\overline{N} > 1.7$. In the model runs, 10 cross-sections are selected to spread over the entire estuary, at a distance of (1 to 10)/(10 L_1) from the mouth of the estuary. Each open circle represents Δh calculated from a cross-section, along with $Fr_{2\max}$, V and \overline{N} .

2.6 A regime diagram

To put in a broader context, the model results are organized in terms of the freshwater Froude number Fr_f and the estuarine mixing parameter M that are used to classify different types of estuaries (Geyer and MacCready 2014). The freshwater Froude number Fr_f is defined as

$$Fr_f = \frac{U_r}{\sqrt{g\beta S_{ocean}h}},$$
(2.7)

where U_r is the river flow velocity, β is the saline contraction coefficient, S_{ocean} is the oceanic salinity, and h is the mean water depth. Fr_f measures the strength of the river flow against the maximum possible frontal propagation speed in an estuary. The mixing parameter M is defined as

$$M^2 = \frac{C_d U_t^2}{\omega N_0 h^2},$$
(2.8)

where C_d is bottom drag coefficient, U_t is the amplitude of depth-averaged tidal current velocity, and $N_0 = (g\beta S_{ocean}/h)^{1/2}$ is the buoyancy frequency for maximum top-to-bottom salinity variation in an estuary. *M* quantifies the effectiveness of tidal mixing.

Mapping the internal wave amplitude in the Fr_f - M parameter space helps identify which types of estuaries might be conducive to internal lee wave generation (Fig. 2.14). At a fixed value of M, the normalized wave amplitude $\Delta h/H$ decreases with increasing Fr_f as stronger river flow leads to stronger stratification that tends to suppress waves. No internal waves are generated when $Fr_f > \sim 0.03$. At a fixed value of Fr_f , $\Delta h/H$ initially increases with increasing M but decreases or saturates to a certain amplitude as M further increases. This results from the nonlinear dependence of the lateral circulation strength on the tidal amplitude. Gever and MacCready (2014) classified different types of estuaries in the Fr_f - M parameter space. In the regime of strongly stratified estuaries on the left (shaded in dark green color), $\Delta h/H$ decreases from 0.7 to 0 as Fr_f increases from 0.003 to 0.03. When $Fr_f > 0.03$, river flows produce strong stratification such that the lateral flows remain to be subcritical throughout the tidal cycle and no lee waves can be generated (e.g. Fig. 2.14a). On the other hand, $\Delta h/H$ increases with increasing M because stronger tides lead to stronger lateral flows in this regime. In partially mixed estuaries in the middle (shaded in light green color), internal lee waves can be generated over a larger part of the parameter space. Most of the lee waves generated in the strongly stratified and partially mixed estuaries are mode-2 waves (e.g. Fig. 2.14d). With increasing Fr_f , $\Delta h/H$ still decreases, as the strong stratification in the deep channel suppresses the wave growth. Under medium M and large Fr_{f} , wave structure also changes into mode-1 wave due to the strongly stratified deepchannel water (e.g. Fig. 2.14b). At lower values of Fr_{f} , $\Delta h/H$ first increases with M, reaches a maximum around $M \approx 0.6$ and then decreases when M increases further. The wave structure changes into hydraulic jump when M > 0.6 as the flow transitions from a supercritical flow on the shoal to a subcritical flow in the deep channel (e.g. Fig. 2.14e). However, $\Delta h/H$ becomes nearly independent of M when $Fr_{f} > \sim 0.02$. No internal waves are found under the regime for periodically stratified estuaries. Water on the shoals becomes well mixed and salinity fronts are developed to separate the well-mixed shallow shoals from the stratified deep channel (e.g. Fig. 2.14f).



Figure 2.14 Regime diagram of normalized wave amplitude $\Delta h/H$ as a function of Fr_f and M. Stars are the runs whose results show lateral frontogenesis. The black dashed lines denote the boundaries among four different estuary classes. The rectangle indicates the approximate influence of spring-neap tidal variation, river flow variation for the estuaries indicated.

2.7 Discussion and conclusion

Using a numerical model for an idealized straight estuary with channel-shoal bathymetry, we investigated the generation of internal lee waves. Our study confirms that tidally-driven lateral flows can generate internal lee waves across all the salinity regimes in coastal plain estuaries

featuring channel-shoal bathymetry. The wave amplitude decreases with increasing river flow as stronger stratification suppresses the lee waves. The wave amplitude however shows a nonlinear dependence on the tidal amplitude: it initially increases with the tidal amplitude but saturates or decreases as the tide amplitude further increases. When the tidal currents become strong enough to erase stratification on the shallow shoals, no internal lee waves could be generated but fronts are developed at the channel-shoal interface.

With the lee wave Froude number $\overline{N}H/V > 1$ and the intrinsic frequency *Vk* between *f* and \overline{N} (Table 2.1), the lee waves generated in coastal plain estuaries fall into Regime 3 in the regime diagram of lee waves (Legg 2021). It is featured by the generation of nonlinear lee waves of vertical length scale V/\overline{N} , which agrees with the scaling shown in Fig. 2.13b. For stratified flows over a sill, this flow regime is also characterized by blocking, hydraulic control of the jet above the topographic crest, and the possibility of a stagnant wedge downstream of the crest, with mixing occurring primarily in the hydraulic jump downstream if present (Klymak et al. 2010, Winters 2016). Obviously no blocking occurs for the stratified flow over a valley (deep channel) but the lateral flows are hydraulically controlled at the edge of the deep channel. If the flows in the deep channel are subcritical, a hydraulic jump forms with the isohalines at the trailing edge of the lee wave lifted sharply upward, producing high dissipation rate and strong mixing there (Figs. 2.2h, 2.9c). Similar to the tidal flows over a tall steep topography in the deep ocean (Legg and Klymak 2008), these hydraulic jumps may be an important mechanism for generating strong local mixing in the stratified estuary.

Most studies of lee waves in the ocean focused on stratified flows over a sill. The stratified

flows over a valley (the deep channel) have received much less attention. While they share some characteristics as the flows over a sill such as the hydraulic control, they also differ in important aspects. For example, the heavier stratified water in the deep channel may become stagnant and uncoupled from the lateral flows above (Fig. 2.12). This flow deceleration and stagnation have been found in stratified flows over the valley when $\overline{N}H/V$ is large (Baines 1995), such as katabatic flows over a valley in the atmosphere. For example, the stratified flows over the Arizona's Meteor Crater often lead the formation of waves and hydraulic jumps in the lee of the upwind rim (Holden et al. 2000, Leher et al. 2016a). Numerical simulations of different valley depths and shapes revealed a rich variety of wave and flow structures, ranging from complete flows through the valley to valley-flow stagnation to situations involving internal wave breaking, lee waves, and quasi-stationary waves in the valley (Leher et al. 2016b, Rotunno and Leher 2016). Further research is needed to explore tidal flows over a valley in the ocean. In this study we modeled the deep channel as a triangle as a simplification. Future modeling studies need to consider different geometric shapes of the deep channel.

To place the model results in a broad context, we plot the lee wave amplitude in the $Fr_f - M$ parameter space. Strongly stratified and partially mixed estuaries cover a wide range of estuaries such as Hudson River and San Francisco Bay and may be conducive to the lee wave generations. According to the estuarine classification diagram by Geyer and MacCready (2014), Chesapeake Bay is a strongly stratified estuary. Indeed mode-2 internal lee waves were observed in the middle part of the estuary (Xie et al. 2017b) and the numerical simulation reproduced the mode-2 lee wave (Xie and Li 2019). Xie et al. (2017b) also observed that the lee wave subsequently propagated onto the shallow shoal and evolved into a group of internal solitary waves of

elevation. A non-hydrostatic model would be required to simulate the transformation of the lee wave into solitary waves, a topic for the future research.

2.8 Acknowledgements

We thank two reviewers for their helpful comments. We are grateful to NSF (OCE-1756155) for the financial support. This is UMCES contribution number 6201.

2.9 Data availability statement

All model results analyzed in this study have been uploaded and openly available at https://zenodo.org/record/5652345#.YYqN37pOk2w.

Chapter 3: Generation and Evolution of Internal Solitary Waves in

a Coastal Plain Estuary

Preface

This chapter is a reproduction of work which is submitted to Journal of Physical Oceanography with coauthor Ming Li. The right to reuse this work was retained by the authors when publication rights and nonexclusive copyright were granted to the American Meteorological Society.

Li, R., and M. Li, 2023 (submitted.): Generation and evolution of internal solitary waves in a coastal plain estuary. Journal of Physical Oceanography.

<u>3.1 Abstract</u>

Large-amplitude internal solitary waves were recently observed in a coastal plain estuary and were hypothesized to evolve from an internal lee wave generated at the channel-shoal interface. To test this mechanism, a 3D nonhydrostatic model with nested domains and adaptive grids was used to investigate the generation of the internal solitary waves and their subsequent nonlinear evolution. A complex sequence of wave propagation and transformation was documented and interpreted using the nonlinear wave theory based on the Korteweg-de Vries equation. During the ebb tide a mode-2 internal lee wave is generated by the interaction between lateral flows and channel-shoal topography. This mode-2 lee wave subsequently propagates onto the shallow shoal and transforms into a mode-1 wave of elevation as strong mixing on the flood tide erases stratification in the bottom boundary layer and the lower branch of the mode-2 wave. The mode-1 wave of elevation evolves into an internal solitary wave due to nonlinear steepening and spatial changes in the wave phase speed. As the solitary wave of elevation continues to propagate over the shoaling bottom, the leading edge moves ahead as a rarefaction wave while the trailing edge steepens and disintegrates into a train of rank-ordered internal solitary waves, due to the combined effects of shoaling and dispersion. Strong turbulent mixing in the bottom boundary layer dissipates wave energy and causes the eventual destruction of the solitary waves. In the meantime, the internal solitary waves can generate elevated shear and dissipation rate in local regions.

3.2 Significance statement

In the coastal ocean nonlinear internal solitary waves are widely recognized to play an important role in generating turbulent mixing, modulating short-term variability of nearshore ecosystem, and transporting sediment and biochemical materials. However, their effects on shallow and stratified estuaries are poorly known and have been rarely studied. The nonhydrostatic model simulations presented in this paper shed new lights into the generation, propagation and transformation of the internal solitary waves in a coastal plain estuary.

3.3 Introduction

In the coastal ocean nonlinear internal solitary waves (ISWs) are widely recognized to play an important role in generating turbulent mixing, modulating short-term variability of nearshore ecosystem, and transporting sediment and biochemical materials (Lamb 2014; Woodson 2018; Boegman and Stastna 2019). Their effects on shallow and stratified estuaries are poorly known and have been rarely studied, however. Since the buoyancy frequency in estuaries is typically 1-2 orders of magnitude larger than that in the coastal ocean, the ISWs in estuaries have a short wavelength of O(10) m and a short period of O(1) min. They are also highly intermittent in time and only emerge during certain periods in a tidal cycle (Dyer 1982; New et al. 1986; Sarabun and Dubbel 1990; Xie et al. 2017a, b). These ISWs are hard to be captured in field surveys and thus often overlooked. In addition, tidal advection of background fields makes the ISWs difficult to trace (Martin et al. 2005). Nevertheless, recent mooring observations in Chesapeake Bay showed that the ISWs had a large vertical displacement (4-5 m or about 1/3 of the water depth), leading to overturning and a dissipation rate of ~ $1 \times 10^{-4} \text{ m}^2 \text{ s}^{-3}$, that is 3 orders of magnitude larger than the background value (Xie et al. 2017).

Several mechanisms have been shown to be responsible for the ISWs generation in the coastal ocean. In the classic "lee wave" mechanism (Maxworthy 1979), a supercritical tidal flow generates a lee-wave depression on the lee side of a sill which subsequently propagates upstream

and evolves into a train of ISWs as the tidal flow slackens. The disintegration of an upstream propagating internal bore can also lead to ISWs. For example, at an entrance to the Knight Inlet, an undular bore or internal hydraulic jump is generated upstream of the sill crest when the tidal flow becomes supercritical, and this bore subsequently propagates upstream and disperses into a packet of ISWs (Farmer and Armi 1995; Cummins et al. 2003; Cummins et al. 2006). ISWs can also be generated by a river plume that spreads over the coastal ocean as a gravity current: the horizontal flow convergence at the plume front and downward vertical displacement of the underlying water can develop into ISWs (Nash and Moum 2005).

Once ISWs are generated, they experience nonlinear evolution and eventually dissipate. The shape of an ISW is preserved due to the balance between nonlinear steepening and dispersion. Both processes are sensitive to changes in the stratification and vertical shear as well as variations in the bottom topography (Helfrich and Melville 2006). When the pycnocline is located close to the sea surface, an ISW usually propagates as a wave of depression. In contrast, it propagates as a wave of elevation when the pycnocline sits near the bottom (Scotti et al. 2008). Observations in the coastal ocean found ISWs tend to transform from a depression wave to an elevation wave as they enter the shallower region and experience shoaling as the pycnocline approaches the bottom (Klymak and Moum 2003; Scotti and Pineda 2004; Bourgault et al. 2007).

The breaking and dissipation of shoaling ISWs can take different pathways, depending on the initial wave amplitude, stratification, and the slope of the bottom topography (Lamb 2014). A large-amplitude ISW of depression on a steep slope usually breaks by overturning with energy

loss to turbulent dissipation as the trailing edge overtakes the wave trough (Vlasenko and Hutter 2002; Aghsaee et al. 2010; Masunaga et al. 2016). On the other hand, an ISW on a gentle slope tends to fission into a train of shorter waves or boluses, which propagate along the slope with elevated dissipation levels (Bai et al. 2019; Davis et al. 2020; Sinnett et al. 2022).

Little is understood about the generation, propagation and transformation, and dissipation of ISWs in coastal plain estuaries. Recent observations in Chesapeake Bay found an internal lee wave over the flank of the deep channel that preceded the appearance of the ISWs at mooring sites over the shallow shoal (Xie et al. 2017b). Later modeling studies confirmed the hypothesis that the lee wave can be generated by lateral flows interacting with channel-shoal topography (Xie and Li 2019; Li and Li 2022), but the connection between the ISWs and the internal lee waves has not been ascertained. A major obstacle to a mechanistic modeling investigation is the enormous computer resource required to run a 3D nonhydrostatic model of an estuary at a scale of O(100) km and a resolution of O(1) m. Most of the previous nonhydrostatic modeling studies of flow-topography interactions and ISWs are based on the 2D models (Scott et al. 2008; Chen et al. 2017; Davis et al. 2020; Urbancic et al. 2022).

The Coastal and Regional Ocean Community Model (CROCO) is a new ocean modeling system built upon the Regional Ocean Modeling System (ROMS) and the non-hydrostatic kernel for free surface ocean modeling (Auclair et al. 2018). The combination of domain nesting (Penven et al. 2006; Mason et al. 2010), adaptive grid refinement in Fortran (AGRIF, Debreu et al. 2008, 2012), and nonhydrostatic algorithm makes it feasible to resolve fine scale processes and their interactions with larger-scale flows while keeping the computational cost reasonable.

Recently the 3D CROCO model has been used to simulate surf eddies in Grand Popo Beach off Benin in the Gulf of Guinea (Marchesiello et al. 2021). In this modeling study we use the 3D CROCO model to investigate the generation, propagation and transformation of ISWs in a coastal plain estuary featuring the channel-shoal bathymetry.

3.4 Methods

3.4.1 Model configuration

To resolve large-scale estuarine circulation as well as small-scale ISWs, we used CROCO to configure triply nested model domains with increasing grid resolution but decreasing domain size (Fig. 3.1). Such an approach is widely used in the mesoscale atmosphere models such as the Weather Forecasting Model (WRF) Zhang et al. 2017). (e.g. Depth [m] Depth [m] 0 (c) (a) 25 40 NA -5 Land 8 20 30 <u></u> -10 y [km] 6 15 Shelf Depth Depth Riv Estuan 20 4 10 -20 Land 2 5 -25 Ъ°

Figure 3.1 (a) Schematic of the numerical model domain consisting of a straight estuarine channel and a shelf. The red rectangle denotes a child domain with 10 m resolution. (b) Schematic of the nested model domains. The magenta rectangle denotes the child domain of 2.5 m resolution. (c) Cross-channel section featuring a channel-shoal bathymetry at mid-Chesapeake Bay.

1.5

0

5

Distance from the southern coastline [km]

10

0.5

x [km]

The outer domain covers an estuary and its adjacent shelf, with a coarse resolution of 250 m inside the estuary (Fig. 3.1a). This model configuration follows from previous estuarine modeling studies (e.g. Li et al. 2014; Li and Li 2022). The continental shelf is 80 km wide and has a fixed cross-shelf slope of 0.05%. The estuarine channel is straight and does not have slope in the along-channel direction. The cross-channel section features a channel-shoal bathymetry representative of a coastal plain estuary such as Chesapeake Bay (Fig. 3.1c). There are 2100 grid cells in the east–west direction, 79 grids in the south-north direction and 20 layers in the vertical direction. The middle domain covers a short section (length of 1.6 km and width of 10 km) in the middle of the estuary at a resolution of 10 m (Fig. 3.1a). Based on the results from the middle domain model, we refined the resolution on the shallow part of the estuarine cross-section using the adaptive grid refinement approach, such that the inner domain has a grid size of 2.5 m (Fig. 3.1b). Results from the parent model domain are automatically used as the boundary forcing to drive the child model domain through one-way nesting (Penven et al. 2006) such that the outer, the middle and inner domain models are run simultaneously.

The estuarine model is forced by semidiurnal tides at the offshore (eastern) open boundary and by river flow at the upstream (western) end of the estuarine channel. In this study, the tidal amplitude η_t was set to be 1.0 m and the river flow U_r was set to be 0.01 m s⁻¹ (equivalent to a river discharge of 1400 m³ s⁻¹ over a cross sectional area of 1.4×10^5 m²). The inflowing river water is prescribed to have zero salinity while the salinity of the coastal ocean is set at 35 psu. To simplify, temperature is uniform everywhere and does not change with time. A quadratic stress is exerted at the seabed, assuming that the bottom boundary layer is logarithmic with a roughness height of 0.5 mm. The Coriolis parameter *f* is set at 1.0×10^{-4} rad s⁻¹. The vertical eddy viscosity and diffusivity are computed using the k- ε turbulence closure scheme (Warner et al. 2005) with the background diffusivity and viscosity set at 1×10^{-5} m² s⁻¹. The model was initialized with no flow, a flat sea surface, and salinity distribution from 0 to 35 psu along the estuarine channel. The outer domain model was first run for 360 days to reach a quasi-steady state. The salinity distribution from this model run was then used as the initial salinity condition for the nested domain model simulations. Results obtained after 10 tidal cycles were used for analysis.

3.4.2 Diagnostics of model results

To better understand how the ISWs evolve over time, we used the model outputs to analyze the nonlinearity and dispersion parameters in the Korteweg-de Vries (KdV) equation:

$$\frac{\partial \eta}{\partial t} + (c_1 + \alpha \eta) \frac{\partial \eta}{\partial x} + \beta \frac{\partial^3 \eta}{\partial x^3} = 0, \qquad (3.1)$$

where η is the vertical displacement of isopycnals, c_1 is the mode-1 phase speed, α is the quadratic nonlinear coefficient, and β is the dispersion coefficient (Grimshaw et al. 2004). The nonlinear and dispersion coefficients are calculated as follows:

$$\alpha = \frac{3\int_{-h}^{0} c_1^2 \left(\frac{\partial\Phi}{\partial z}\right)^3 dz}{2\int_{-h}^{0} c_1 \left(\frac{\partial\Phi}{\partial z}\right)^2 dz},$$
(3.2)

$$\beta = \frac{\int_{-h}^{0} c_1^2 \Phi^2 dz}{2 \int_{-h}^{0} c_1 (\frac{\partial \Phi}{\partial z})^2 dz},$$
(3.3)

where *h* is the water depth. The wave phase speed c_1 and vertical structure function $\Phi(z)$ are obtained by solving the following eigenvalue problem (Gill 1982):

$$\frac{d^2 \Phi(z)}{dz^2} + \frac{N^2(z)}{c_i^2} \Phi(z) = 0, \qquad (3.4)$$

with the boundary conditions $\Phi(0) = \Phi(-h) = 0$ where N(z) is the background buoyancy frequency and c_i is the phase speed of the *i*th mode internal wave.

The variability of the coefficients α and β has been studied to understand the nonlinear transformation of ISWs in the coastal ocean (Holloway et al. 1999; Small 2001a, b). The sign of the quadratic nonlinear coefficient α determines the polarity (elevation or depression) of an ISW and mostly depends on the location of pycnocline (maximum N^2), according to the solution of the KdV equation for a two-layer fluid (Grimshaw et al. 1997). If the pycnocline lies closer to the sea bed, $\alpha > 0$, favoring an elevation wave. If the pycnocline lies closer to the sea surface, $\alpha < 0$, favoring a depression wave. The dispersion parameter β quantifies the strength of wave dispersion such that a large value of β usually signals the dispersion of an ISW into a train of waves. When analyzed in combination with wave amplitude and wavelength, α and β yield insights into the nonlinear transformation processes of ISWs.

3.5 Results

We present a detailed case study of the generation, evolution and dissipation of the nonlinear internal wave field generated by the interaction between the lateral circulation and the channel-shoal bathymetry in a coastal plain estuary.

3.5.1 Lee wave generation and propagation

During the ebb tide, a counter-clockwise lateral circulation (looking into the estuary) develops in the cross-channel section and the rightward currents in the bottom layer advect the

stratified water from the shallow shoal to the deep channel (Figs. 3.2a-b). To characterize the flow-topography interaction, the Froude number (*Fr*), defined as $Fr_i = v/c_i$ where v is the depth-averaged lateral flow velocity in the lower layer, is calculated. When the lateral flows become supercritical ($Fr_2 = 1.3$) at the channel-shoal interface, a large-amplitude internal lee wave with a characteristic mode-2 bulge structure appears at the left flank of the deep channel (Fig. 3.2c).



Figure 3.2 (a) Time series of the depth-averaged along-channel velocity and lateral velocity in the bottom layer at the channel-shoal interface. The dashed vertical lines indicate the timing of the cross-channel snapshots shown in (b)-(d) and in Figs. 3.3-3.6 and 3.8. The grey shaded region marks the flood tide and the yellow shaded region marks the ebb tide. (b)-(e) Distributions of salinity (contours) and the velocity vectors (arrows) at a mid-estuary cross-section. Contour intervals are at 0.5 psu increments. The magenta dashed line in (b)-(d) marks the location of the channel-shoal interface where the mode-2 Froude numbers (Fr_2) is calculated.

This lee wave subsequently propagates towards the shallow shoal and upwards as the tide
switches from the ebb to flood phase (Fig. 3.2a) and the rightward lateral currents weaken (Figs. 3.2d, 3.3a-c). The angle of the phase line to the vertical direction can be calculated from

$$\theta = \arctan(\frac{m}{k}) = \arctan(\frac{\sqrt{\frac{N^2}{V^2} - k^2}}{k}), \qquad (3.5)$$

where θ is the angle between the wave phase line and the vertical direction, k is the horizontal wavenumber, and m is the vertical wavenumber. A flow with velocity V past a topography with the vertically-averaged buoyant frequency \overline{N} can generate a lee wave with wavenumber $\frac{\overline{N}}{V}$, which can be decomposed into the horizontal and vertical directions. The horizontal wavenumber k is comparable to the length scale of the topography and then the vertical wavenumber m can be calculated from Eq. (3.5) (Mayer and Fringer 2021). At T3, with V = 0.13 m s⁻¹, $\overline{N} = 0.045$ s⁻¹, and $k \approx 0.003$ m⁻¹, m is 0.34 m⁻¹ and θ is estimated to be ~ 89.5°. An example of phase line connecting the jumplike wave trailing edge at each isopycnal is shown in Fig. 3.3a. As the water depth is two orders of magnitude smaller than the width of the deep channel, the lee wave phase lines are nearly horizontal.



Figure 3.3 Distributions of salinity (contour lines) and the vertical velocity w (color) at the mid-estuary cross-section at T3-T5 marked in Fig. 3.2a. Contour intervals are at 0.2 psu increments. The purple arrow line marks the phase line of the lee wave and the magenta arrow

line marks the propagation of maximum w from T3-T5.

In the long-wave limit ($kh \ll 1$), the horizontal group velocity $c_{g,x} \approx c_2 = 0.11 \text{ m s}^{-1}$ and the vertical group velocity $c_{g,z} = c_{g,x} \tan(90^\circ - \theta) = 0.001 \text{ m s}^{-1}$. The shoreward translation of the maximum vertical velocity w along the channel slope illustrates the wave propagation (Fig. 3.3). The maximum w is transported ~ 800 m horizontally and ~ 7 m vertically over 2 hours from T3 to T5, matching the direction of the lee wave phase line and the estimated group speeds.

3.5.2 Wave steepening, dispersion and propagation

The wave modal structure also changes as the internal lee wave propagates. The lee wave evolves from a mode-2 wave at T3 to mode-1 waves at T5 (Figs. 3.2d-3.2e). On flood tide strong mixing in the bottom boundary layer erases stratification in the deep channel and the lower branch of the mode-2 wave. On the other hand, the upper branch of the mode-2 lee wave, in the form of an elevation wave, propagates into the stratified water in the top 10 m. The upward propagation of the elevation wave perturbs the initially flat isopycnals there, such that the elevated isopycnals are followed by the depressed isopycnals to the right, indicating the formation of a trailing depression wave.

The subsequent evolution of the elevation and depression wave is shown in a sequence of snapshots of isopycnals and lateral and vertical velocity distributions (Figs. 3.4a-h). Both the elevation and depression waves flatten and disperse between T5 and T6 (Figs. 3.4e-f). Subsequently the depression wave disintegrates into a train of small amplitude waves (Figs. 3.4g-h). On the other hand, the leading edge of the elevation wave steepens, accompanied by an intensification of the upward velocity (Figs. 3.4f-h). These wave transformation processes can be

understood by studying the spatial variation of the nonlinear term $c_1 + \alpha \eta$ and dispersion parameter β in the KdV equation. The term $\alpha \eta$ determines how nonlinearity changes the wave phase speed at the wave crest/trough and may cause the steepening and flattening of the wave. The dispersion parameter β quantifies the magnitude of wave dispersion which disperses the wave energy and may cause wave fission. β increases by a factor of 2 (from 3 to 5 m³ s⁻¹) in the deeper water region where the depression wave propagates to the right. Strong dispersion causes the depression wave to flatten and disintegrate into a train of small-amplitude waves. β is considerably smaller on the left shallow shoal (in the range of 1 - 2 $\text{m}^3 \text{s}^{-1}$) where the elevation wave propagates. In the meantime, the nonlinear term becomes more important in driving the transformation of the elevation wave there. Both c_1 and α affect the wave transformation. The nonlinear parameter α is negative everywhere and would lead to the flattening of the elevation wave. However, the magnitude of α decreases as the left shore is approached (Figs. 3.4i-k), implying this flattening effect decreases as the elevation wave propagates to the left. Moreover, the spatial variation in the wave phase speed c_1 due to changes in the stratification can lead to either steepening or flattening of a wave. A decrease in the phase speed c_1 toward the left shoal will cause the steepening of the elevation wave since the wave crest moves faster than the leading edge. Indeed c_1 decreases from 0.25 - 0.3 m s⁻¹ at the channel shoal interface to under 0.2 m s⁻¹ at the left shallow region. Such a large reduction in c_1 overwhelms $\alpha\eta$, causing the elevation wave to steepen (compare Figs. 3.4g-h).



Figure 3.4 Snapshots of (a-d) the lateral velocity (color) and salinity (contour), (e-h) the vertical velocity (color) and salinity (contour), (i-l) the nonlinearity coefficient α and dispersion coefficient β in the KdV equation, and (m-p) the mode-1 phase speed c_1 at T5-T8 marked in Fig. 3.2a. Contour intervals of salinity are at 0.5 psu increments.

The steepening between T5 and T8 changes the characteristics of the elevation wave. The wave length decreases from ~ 1000 m to ~ 300 m. Moreover, this short wave is accompanied by large vertical velocities (Fig. 3.4h), with the upward velocity on the leading edge of the elevation wave reaching 3.0 mm s⁻¹ and the downward velocity on the trailing edge reaching 1.2 mm s⁻¹.

3.5.3 Emergence of ISWs

The steepening of the elevation wave leads to the formation of a soliton of elevation which can be fit into a solution to the KdV equation

$$\eta = a \operatorname{sech}^{2}(x/L) \tag{3.6}$$

where a = 0.5 m and L = 83 m (Fig. 3.5a). As the soliton propagates on the shoaling bottom, the crest of the elevation wave flattens and the leading edge moves ahead as a rarefaction wave. On the other hand, the trailing edge of the elevation soliton continues to steepen during the shoaling process, with the downward velocity reaching 5 mm s⁻¹, double of the upward velocity at the leading edge (Fig. 3.5b). In addition, the soliton of elevation cannot remain to be in a steady shape in the environment with negative α . A depression wave is formed at its tail (Fig. 3.5c). Subsequently, the effect of dispersion generates a series of high-frequency oscillations trailing the leading depression wave, forming a train of ISWs (Fig. 3.5d).



Figure 3.5 Snapshots of the vertical velocity (color) and salinity (contour) at T8-T12 marked in Fig. 3.2a. Contour intervals of salinity are at 0.5 psu increments. The green contour in (a) marks the isopycnal tracked in Fig. 3.6. The magenta dashed line in (d) marks the location of the time series shown in Fig. 3.7.

Figure 3.6 provides a detailed view of the solitary wave evolution by tracking the isopycnal

of 9 psu marked in Fig. 3.5a. The soliton of elevation has a symmetric shape at T8 but becomes asymmetric as it moves up the shoaling bottom. Its leading edge is rarefied whereas its training edge steepens. From T8 to T10, the isopycnal displacement between the wave crest and the trailing edge increases from 0.4 m to 0.8 m. At T11 the isopycnal drops down 1.2 m from the crest to the trailing edge, overshooting its equilibrium position. A small-amplitude depression wave is then formed at the tail of the elevation wave. The amplitude of the depression wave continues to grow and reaches 2 m at T12 while the trailing edge disintegrates into a train of ISWs due to dispersion, such that a large-amplitude leading depression wave is followed by a train of small-amplitude undular waves.



Figure 3.6 Hovmöller diagram for isopycnal displacement of 9 psu marked in Fig. 3.5a. In the vertical coordinate, time interval of each line is 10 minutes, equivalent to 2.5 m isopycnal displacement. The grey shaded region represents the bottom topography on the left shoal.

Time series at a site on the shoal (~ 2.5 km away from the coastline, marked in Fig. 3.5d) further illustrate the features of the wave packet (Fig. 3.7). The wave train contains 4 solitons in rank order, lasting ~ 20 min. The period of one solitary wave is only ~ 5 min on average. The leading wave in the wave packet has the largest amplitude of 2 m, accompanied by vertical velocity as strong as 0.03 m s⁻¹. The rest of the waves have much smaller amplitudes. The signal of ISWs is also shown in the time series of the horizontal velocities (Fig. 3.7b). To sustain the conservation of water mass, the internal waves generate additional surface and bottom lateral flows in opposite directions between the upward and downward vertical velocity. Unlike the elevation wave that strengthens the two-layer lateral flows in both the surface and bottom layers, the depression wave weakens and even reverses the lateral flows, leading to flow convergence in the upper layer and divergence in the lower layer. At the leading depression wave, the lateral velocity in the upper layer dramatically drops from 0.13 to -0.02 m s⁻¹ (positive is rightward) while the lateral velocity in the lower layer changes from -0.02 to 0.03 m s⁻¹.



Figure 3.7 (a) Time-depth distributions of salinity (contours) and the vertical velocity (color) at a location on the left shoal marked by the magenta line in Fig. 3.5d. (b) Time series of the lateral velocity at the depths of 2 and 6 m at the same location on the shoal.

3.5.4 Dissipation of ISWs

The subsequent destruction of the ISWs is shown in a group of snapshots in Fig. 3.8. At the beginning, the wave packet contains 4 solitary waves (Fig. 3.8a). As it propagates further shoreward, the number of solitons in the packet decreases while the amplitudes are dampened (Fig. 3.8b). When the ISWs arrive at 1.8 km away from the coastline, only the leading depression wave remains (Fig. 3.8c). The wave trailing edge rarefies, shaping the wave form into a bore front. The wave is finally merged into the salinity front adjacent to the coastline before it runs into the coast (Fig. 3.8d).



Figure 3.8 Distributions of salinity (contours) and dissipation rate ε (color) on the left shoal at times T12-T15 marked in Fig. 3.2a.

Dissipation rate ε on the shallow shoals is high due to strong turbulence in the tidal bottom boundary layer. ε below the wave is about O(10⁻⁶) m² s⁻³, which dissipates the small-amplitude ISWs. ε at the nearshore salinity front reaches O(10⁻⁵) m² s⁻³, leading to the final wave destruction. It is interesting to note that there exists a pocket of high ε anomaly at 5 m - 7 m depth below the wave (Figs. 3.8a-c). ε reaches 4×10⁻⁶ m² s⁻³ at T12 after the passage of the ISWs (Fig. 3.8b). The leading large-amplitude depression wave enhances velocity shear below the wave, lowering the local Richardson number (Fig. 3.9). The correspondence between the enhanced ε and large velocity shear suggests internal solitary wave can also contribute to local turbulent mixing in the stratified pycnocline region.



Figure 3.9 Distributions of salinity (contours) and the along-channel velocity shear (a), the lateral velocity shear (b), and Richardson number (c) at T12 marked in Fig. 3.2a.

3.6 Discussion and Conclusion

Using a 3D nonhydrostatic model with nested domains and adaptative grids, we investigated the generation, propagation, transformation and dissipation of nonlinear internal waves in a coastal plain estuary. The model results showed that the internal lee wave generated by flowtopography interaction at the channel-shoal interface can evolve into a train of ISWs when propagating over the shoaling bottom. Although the observations in Chesapeake Bay suggested a potential link between the lee wave and ISWs (Xie et al. 2017b), this modeling study provides a mechanistic explanation for the ISWs captured in the bottom-mounted ADCPs at the mooring stations on the western shore.

The first step in the wave transformation process involves a change from a mode-2 lee wave into a mode-1 elevation wave. Changes in the wave modal structure have been widely reported and are often triggered by changes in stratification and/or bottom bathymetry. Previous observational and modeling studies of lee waves in Chesapeake Bay showed that the mode-2 wave content decreases and the mode-1 wave content increases as the lee wave propagates from the deep channel to the western shoal (Xie and Li 2019; Li and Li 2022). In the South China Sea the energy of a mode-2 wave approaching a shallow plateau was scattered into mode-1 waves owing to steep bathymetric changes and wave reflection (Klymak et al. 2011). Similarly, observations on the New Jersey shelf showed the decay time scale of mode-2 wave energy is much shorter than mode-1, leading to a transformation from mode-2 to mode-1 during the wave propagation towards the coast (Shroyer et al. 2010). In this study the modal change appears to be mainly driven by changes in the stratification. With a magnitude of O(0.1) m s⁻¹, the lateral currents in estuaries are usually subcritical with respect to mode-1 but may become supercritical with respect to model-2. The lee waves generated by the interaction between the lateral flows and the channel-shoal bathymetry are typically of a mode-2 structure (Li and Li 2022). However, turbulent mixing in the bottom boundary layer can undergo large temporal changes over a floodebb tidal cycle, destroying stratification and precipitating a wave modal shift as documented in Figs. 3.2d and 3.2e.

According to the solution of the KdV equation for a two-layer fluid, nonlinear parameter α is negative if the pycnocline lies closer to the sea surface and a depression wave is favored. The presence of an elevation wave in the upper part of the water column (as shown in Fig. 3.5a) is thus surprising, despite that a negative value of α is consistent with the KdV theory (Figs. 3.4i-l). Obviously, the stratification does not fit into a two-layer system since water is nearly uniformly stratified in the top 5 m but has homogeneous salinity (density) below that depth (Fig. 3.5). It is hard to locate the pycnocline, but the isopycnal displacement is largest just above the top of the bottom boundary layer, which is near the mid-depth. Another difficulty is the separation of the wave-induced shear from the "background" shear (associated with the lateral circulation), as explained in Sweeney et al. (2020). The α values shown in Figs. 3.4i-l did not consider the background shear. We recalculated α using the instantaneous velocity shear and still obtained negative values. Nevertheless, the formation of an elevation wave makes sense given its history evolving from the upper branch of the mode-2 lee wave.

The subsequent transformation of the elevation wave into a train of rank-ordered ISWs on the shallowing shoal shares common characteristics as the transformation of a solitary wave that propagates toward the coast on the continental shelf. A solitary wave of depression usually develops in the deeper ocean where the pycnocline is located close to the ocean surface. As this wave propagates onto the shoaling continental shelf, its leading edge rarefies while its trailing edge steepens and evolves into a solitary wave of elevation followed by ranked-ordered ISWs near the sea bed (Klymak and Moum 2003, Shroyer et al. 2009). The transition from the depression to elevation wave sometimes occurs at a location where the wave's polarity changes (Grimshaw et al. 2004, Shroyer et al. 2009). In other situations, sign change in α is not necessary. In the Massachusetts Bay, the transition from the depression to elevation wave occurred at a location offshore of where the KdV theory predicts polarity switching should occur (Scotti et al. 2008). Our result is similar since α remains to be negative over the entire left shoal (Figs. 3.4i-l). The shoaling on the sloping bottom causes the rarefaction of the leading wave edge and the

steepening of the trailing wave edge. The effect of dispersion then leads to the disintegration into a train of rank-ordered ISWs (Fig. 3.6).

Our model results also highlight the role of the background turbulence (turbulence generated in the tidal boundary layer) in dissipating ISWs as well as the generation of elevated energy dissipation by large-amplitude ISWs themselves. Previous idealized numerical studies found bottom friction may significantly dampen the amplitude of ISWs (Holloway et al. 1997; Liu et al. 1998). Observations of near-bottom elevation waves also showed energy dissipated by bottom friction could be comparable to the loss to internal turbulence production (Scotti and Pineda 2004). In the coastal ocean pycnocline often locates well above the bottom, whereas in shallow coastal plain estuaries bottom friction is expected to be more important in the wave dampening. Furthermore, the ISWs in the coastal plain estuary may enhance vertical shear and generate strong energy dissipation locally, similar to the observations of enhanced local turbulent mixing via shear instability in the ISWs propagating on the continental shelf (Moum et al. 2003; Moum et al. 2007; Jones et al. 2020).

3.7 Acknowledgements

We are grateful to NSF (OCE-1756155) for the financial support.

Chapter 4: Short-Term Variability and Ventilation of Bottom pH in a Stratified Estuary

Preface

This chapter is a reproduction of work which will be submitted to *Journal of Geophysical Research: Oceans* with coauthors Ming Li, Jeremy Testa, Wei-Jun Cai, Jianzhong Su, and Chunqi Shen. The right to reuse this work was retained by the authors when publication rights and nonexclusive copyright were granted to the American Geophysical Union.

Li, R., M. Li, J. Testa, W.-J. Cai, J. Su and C. Shen, 2023 (In prep): Short-term variability and ventilation of bottom pH in a stratified estuary. Journal of Geophysical Research: Oceans.

<u>4.1 Abstract</u>

A pH sensor deployed at the middle reach of Chesapeake Bay recorded high-frequency variability in bottom pH, with fluctuation range reaching 0.5 in summer. The peaks of pH fluctuation corresponding to the trough of salinity perturbation were usually found during upestuary wind events. Using a hindcast model simulation, we confirmed wind-driven downwelling drove the short-term variability in bottom pH. Though the downwelling can advect high pH water downward, the upwelled low pH, high pCO_2 water on the other side cannot get saturated with the atmospheric pCO_2 due to the slow air-sea exchange of CO_2 . In the next wind event in the opposite direction, the low pH water on the shoal was advected back into the deep channel. Therefore, this wind-driven lateral ventilation can only temporarily relieve bottom acidity. With DIC and TA budget analysis and comparison with cross-sections at upper- and lower-Bay where strong lateral circulation was confined in the surface layer, we found vertical mixing and replenishment of oceanic water by longitudinal advection could be more important mechanisms to ventilate bottom pH.

4.2 Introduction

The large temporal pH variability and extreme pH values have been recognized in many estuarine and coastal environments (Hofman et al. 2011; Baumann et al. 2015; Baumann and Smith 2018; Cartensen and Duarte 2019). The range of pH fluctuation even over a 24-h period often exceeds projections of end-of-century acidification resulting from increasing atmospheric CO₂ (Waldbusser and Salisbury 2014). The extreme events in pH have been regarded as an important stressor on marine organisms (Hauri et al. 2013; Harris et al. 2013). However, most research focused on surface pH or well-mixed shallow water and attributed the pH fluctuations to

diel metabolism cycle (e.g. O'Boyle et al. 2013; Saderne et al. 2013; Pacella et al. 2018; Baumann and Smith 2018). In many estuaries with high turbidity, photosynthesis in the bottom water is limited by light availability (Testa et al. 2012). Whether there also exists high-frequency variability of pH in the bottom water and what drivers should be responsible for the variability remain unclear

Riverine water typically has lower dissolved inorganic carbon (DIC) and total alkalinity (TA) values and a higher DIC/TA ratio than seawater (Salisbury et al. 2008; Huang et al. 2015; Cai et al. 2021). Because of this difference between the river and ocean end members, distributions of TA, DIC, pCO_2 (partial pressure of carbon dioxide), and pH in estuaries feature strong gradients in the along-channel direction (Borges and Gypens 2010; Cai and Wang 1998; Cai et al. 2011). In stratified estuaries, strong vertical gradients in DIC and pH also develop where phytoplankton photosynthesis in the surface euphotic layer consumes DIC and respiration of organic material in the bottom layer produces DIC (Feely et al. 2010; Cai et al. 2011 and 2017). These strong horizontal and vertical gradients make estuarine carbonate chemistry susceptible to disruptions from physical forcing, but relatively few studies have addressed how physical processes affect high-frequency carbonate chemistry in estuaries. Some studies have considered tidal advection across the horizontal gradient can cause large pH fluctuations at semidiurnal or diurnal frequency (e.g. Ribas-Ribas et al. 2013; Akhand et al. 2016). Some studies also noted wind-driven upwelling and strong turbulent mixing induced by cyclones can bring acidic bottom water upwards, leading to large changes in the air-sea CO₂ flux (e.g. Saderne et al. 2013; Paerl et al. 2018; Li et al. 2020).

In stratified estuaries, stratification limits the exchange of chemical tracers between bottom layer and surface layer. This vertical decoupling leads to an upper productive layer separated from a lower layer where respiratory processes prevail (Carstensen et al. 2003). Hence, bottom pH can be extremely low especially in summer when high temperature results in more ionization of hydrogen ions (H⁺) and high microbial respiration rate. On the other hand, sea bed in estuaries is habitat for marine bivalves. Low pH and aragonite saturation state may do harm to the growth of bivalves, especially their initial shell formation (Waldbusser and Salisbury 2014). Therefore, understanding the ventilation mechanism of bottom pH is meaningful for estuarine benthic ecosystem and aquaculture.

Recent measurements in surface waters at a cross-channel transect in the middle reach of Chesapeake Bay observed large spatial variations in pCO_2 during a northerly wind event, with pCO_2 over the eastern shore was 30-40% higher than the western shore (Huang et al. 2019). Further modelling study suggests wind-driven upwelling advected high pCO_2 , low pH water from the deep channel to the shallow shoal, which could influence the oyster bed on the shoal (Li et al. 2020). At the same time with the wind-driven upwelling, a downwelling was generated on the other side of the cross-channel transect, advecting surface low pH water downward. A question is raised whether the coupled wind-driven upwelling and downwelling can ventilate the acidic water in the deep channel. In an idealized modeling study of Chesapeake Bay, Scully (2010) showed that wind-driven lateral exchange of oxygen between well-oxygenated shallow shoals and hypoxic deep channel may be more important than direct turbulent mixing in supplying oxygen to the hypoxic deep channel. CO₂ dynamics often mirror O₂ dynamics, since the production and consumption of DIC and O₂ are affected by common biological processes

such as phytoplankton photosynthesis and organic matter respiration, and all chemical tracers are advected or diffused by the same physical processes. However, surface-water O_2 equilibrates fast with the atmospheric partial pressure, while surface-water pCO_2 adjusts slowly and rarely reaches equilibrium with respect to the atmospheric pCO_2 due to the buffering effect of a much greater DIC pool on aqueous CO_2 (Cai et al. 2021). Thus, the effectiveness of wind-driven ventilation for bottom pH requires further examination.

Chesapeake Bay is a large eutrophic estuary suffering from acidification (Cai et al. 2017). Despite a mean water depth of 6.5 m, a deep paleochannel whose depth ranges from 15-30 m running in the north-south direction dominates the bathymetry in the middle reaches of the main stem. The estuarine channel is partially stratified with vertical salinity differences of 2-8 psu (Carter and Pritchard 1988). Compared with other estuaries, tidal forcing in the Bay is relatively modest with tidal range rarely exceeding 1 m (Browne and Fisher 1988). Wind forcing with dominant periods of 2-7 days is comparable to tidal forcing (Zhong and Li 2006). Therefore, Chesapeake Bay is an ideal system to study the shot-term variability and ventilation of bottom pH.

Recent observations have mapped out the distributions of DIC, TA, pCO_2 and pH in the main stem of Chesapeake Bay (Brodeur et al. 2019; Friedman et al. 2020; Chen et al. 2020). DIC and TA increased from surface to bottom and from north to south. The pH range is large, with a minimum value of 7.1 in the upper-Bay and the bottom waters of the mid-Bay and a maximum value as high as 8.5 at the surface waters of the mid- and lower-Bay (Brodeur et al. 2019). pCO_2 also displays a strong along-channel gradient from the estuary's head to mouth, resulting in outgassing in the upper Bay, uptake of atmospheric CO_2 in the mid Bay, and near-equilibrium conditions in the lower Bay (Chen et al. 2020; Herrmann et al. 2020). Seasonally, pH is high in winter and reaches minimum in summer (Friedman et al., 2020). The decomposition of autochthonous organic matter (i.e. eutrophication-stimulated primary production) is the dominant process consuming oxygen and lowering pH in summer (Su et al. 2020b). Nevertheless, calcium carbonate (CaCO₃) dissolution as an important buffering mechanism in the mid-bay, leads to higher pH values in August than in June, despite persistent hypoxic conditions during the whole summer (Su et al. 2020a, 2021). Whether there also exists a physical ventilation mechanism for bottom acidic water remains unclear. In addition, Chesapeake Bay water has relatively weak buffering capacity (Cai et al. 2017), where small changes in DIC could generate a large fluctuation of pH. High-frequency pH data from a moored sensor has showed short-term fluctuations of DIC, pH and pCO_2 associated with salinity and dissolved oxygen, hinting the influences from physical and biological processes (Shadwick et al. 2019). However, this sensor only recorded surface pH and how bottom pH fluctuates is still unknown.

Coupled hydrodynamic-biogeochemical-carbonate chemistry models (ROMS-RCA-CC) have been developed for Chesapeake Bay (Shen et al. 2019a). Shen et al. (2019a) focused their modeling analysis on the large-scale carbonate chemistry dynamics and validation against field observations. Furthermore, Shen et al. (2019b) and Shen et al. (2020) conducted 30-year hindcast simulations to examine ecosystem metabolism and carbon balance and investigate the anthropogenic impacts on pH and aragonite saturation state. Using a hindcast simulation of year 2013, Li et al. (2020) studied how wind-driven upwelling affects the carbonate chemistry on the shallow shoal. With the models, Li et al. (2023) did climate downscaling projections for

Chesapeake Bay in the mid-21st century and showed a near-doubling of CO_2 uptake, a pH decline of 0.1–0.3, and >90% expansion of the acidic volume. This study combines the observation data and model results to examine the short-term variability and ventilation mechanism of bottom pH.

4.3 Methods

4.3.1 High-frequency observation

A SeapHOx sensor was deployed at the National Oceanic and Atmospheric Administration Chesapeake Bay Interpretive Buoy System (CBIBS; https://buoybay.noaa.gov/) Gooses Reef Buoy (latitude: 38.56°N, longitude 76.41°W; red dot in Fig. 4.1a) from June to October in 2016. The SeapHOx uses an integrated sensor package consisting of a Sea-Bird SBE-37 temperature and conductivity sensor, an Aanderaa oxygen optode, and a modified Honeywell Durafet pH electrode (Bresnahan et al. 2014; Martz et al. 2010). It was placed in a custom-built stainless steel frame and suspended from the surface buoy with an intake depth of roughly 0.2 m above the bottom. Depth of the observation site is ~ 11.5 m. Raw data were acquired from a pumped flow stream at a temporal resolution of 15 minutes and then averaged hourly for analysis. The analysis focuses on the period from summer to early fall when Chesapeake Bay suffers from low pH water.



Figure 4.1 Map showing bathymetry (a) and model grids (b) for Chesapeake Bay. The red dot in (a) marks the location of the Gooses Reef. The black lines in (a) mark the cross-sections and the black line in (b) marks the along-channel section used in later analysis.

4.3.2 ROMS-RCA-CC model configuration

To further examine how winds drive short-term variability and ventilation of bottom pH in Chesapeake Bay, we used coupled hydrodynamic-biogeochemical-carbonate chemistry models to conduct hindcast simulation for year 2016. The models were configured for Chesapeake Bay and its adjacent shelf (Fig. 4.1b), consisting of 80×120 grid points in the horizontal direction and 20 evenly distributed vertical sigma levels in the vertical direction (Li et al. 2005).

The hydrodynamic model ROMS simulates water level, currents, temperature and salinity. The model is forced by freshwater discharge at river heads, water levels at the open boundary,

and heat and momentum flux across the sea surface. The freshwater input was prescribed for the eight major tributaries of Chesapeake Bay, based on measurements at US Geological Survey gaging stations. The offshore boundary water level consists of tidal and non-tidal components. The tidal component was provided by global tidal model TPXO7 (TOPEX/POSEIDON) (Egbert and Erofeeva 2002), and the non-tidal component was extracted from daily sea level measured at Duck, North Carolina, by the National Oceanic and Atmospheric Administration (NOAA). The air-sea heat fluxes were computed by using the North America Regional Reanalysis (NARR) products except for the wind speeds. As NARR products underestimate surface wind speeds over Chesapeake Bay (Scully 2013), instead the model is forced by surface wind data obtained from a variety of measurements including buoys from CBIBS and weather stations from National Data Buoy Center (NDBC; https://www.ndbc.noaa.gov/), Integrated Surface Database (ISD; Smith et al. 2011). National Estuarine Research Reserve System (NERRS; and https://coast.noaa.gov/nerrs/). These wind measurements were adjusted to 10-m wind speeds and then interpolated over the Bay's surface using a universal Kriging scheme (Fisher et al. 2015). The vertical eddy viscosity and diffusivity were parameterized using the k-kl turbulence closure scheme with the background value of 1.0×10^{-6} m² s⁻¹, and the horizontal eddy viscosity and diffusivity were set to be constant (1.0 m² s⁻¹). The ROMS model was initialized using climatological temperature and salinity conditions and run for a spin-up period of 3 years to get the initial condition for year 2016. A detailed description of the model configuration can be found in Li et al. (2005). This hydrodynamic model was previously validated against water level measurements at tidal gauge stations (Zhong and Li 2006; Zhong et al., 2008), salinity and temperature time series at monitoring stations (Li et al. 2005; Ni et al. 2020), salinity distributions collected during hydrographic surveys, and current measurements (Li et al. 2005;

Xie and Li 2018; Xie and Li 2019; Ni et al. 2020).

The biogeochemical model RCA includes a water-column component (Isleib et al. 2007) and a sediment diagenesis component (Di Toro 2001), coupled to the ROMS hydrodynamic model in an offline mode. RCA simulates pools of organic and inorganic nutrients, two phytoplankton groups (one representing winter-spring diatoms and one representing summer dinoflagellates), and dissolved oxygen concentrations (Testa et al. 2014). The RCA biogeochemical model is forced by loads of dissolved and particulate materials from the eight major rivers. Riverine constituent concentrations for phytoplankton, silica, particulate and dissolved organic carbon (C), phosphorus (P), and nitrogen (N), and inorganic nutrients $[NH_4^+, NO_2^- + NO_3^-]$ (hereafter NO_3^-), PO43-] were obtained or derived from Chesapeake Bay Program biweekly monitoring data as described in Testa et al. (2014). The ocean boundary concentrations were acquired from the World Ocean Atlas 2013 and Filippino et al. (2011). Atmospheric deposition of nutrients was much smaller than the riverine nutrient loading and thus not considered, following the previous studies (Ni et al. 2020; Li et al. 2020a; Zhang et al. 2021). The initial conditions of RCA were based on Chesapeake Bay Program monitoring data in December 2015. The RCA model has been validated against biogeochemical data at a number of stations in Chesapeake Bay (including NO₃⁻, PO₄³⁻, NH₄⁺, chlorophyll-a, dissolved oxygen, and organic C, N and P), integrated metrics of hypoxic volume, rates of water-column primary production and respiration, and nutrient fluxes across the sediment-water surface (Brady et al. 2013; Testa et al. 2013, 2014, 2017; Li et al. 2016; Ni et al. 2020).

The CC model simulating DIC, TA, and aragonite CaCO₃ has been coupled to ROMS-RCA

for Chesapeake Bay (Shen et al. 2019a, b, 2020). DIC is consumed by phytoplankton growth/photosynthesis and calcium carbonate precipitation. The sources of DIC include air-sea CO₂ flux, phytoplankton respiration, oxidation of organic matter, calcium carbonate dissolution, sulfate reduction, and sediment water fluxes. Calcium carbonate dissolution and precipitation are the primary source/sinks for TA, but the contributions of several other biogeochemical processes (e.g., nitrification and sulfate reduction) to TA are also modeled (Shen et al. 2019a). Other carbonate chemistry parameters such as pH and pCO2 are calculated from the CC model outputs using the CO2SYS program (Lewis and Wallace 1998). A detailed description of the CC model and its coupling to RCA is described in Shen et al. (2019a). The CC carbonate model is forced by the atmospheric CO₂, the riverine loads and offshore concentration of TA and DIC. Time series of TA measurements in riverine inputs were obtained from the USGS stations in the Susquehanna and Potomac Rivers (Raymond et al. 2000). The riverine DIC concentrations were calculated through CO2SYS with the available TA and pH (Shen et al. 2020). Carbonate chemistry data for the other smaller tributaries were estimated using empirical relationships as functions of freshwater discharge (Shen et al. 2019a). TA at the ocean boundary was directly estimated with the empirical equation based upon salinity at the ocean boundary (Cai et al. 2010). DIC at the offshore boundary was calculated with the available TA, fCO₂ from SOCAT (Bakker et al. 2016), salinity and temperature using CO2SYS. The atmosphere pCO_2 was set to be 403 ppm in 2016 according to the observation from NOAA-ESRL (https://www.esrl.noaa.gov/gmd/ccgg /trends). Initial conditions for DIC and TA were calculated from the two-end member mixing model. The CC model has been validated against extensive surveys of DIC, TA and pH collected during ten cruises in 2016 (Shen et al. 2019a) and long term (1985-2015) measurements of pH at a number of monitoring stations (Shen et al. 2019b,

2020).

4.3.3 Diagnostic of DIC and TA budget

To determine what caused temporal changes in bottom pH, we used the model results to investigate the DIC and TA changes in a fixed control volume V of the bottom water. As pH depends on the ratio of DIC to TA, we analyzed the change rate in DIC-TA (i.e. $\frac{\partial (DIC-TA)}{\partial t}$). The equation is given by

$$\frac{\partial (\text{DIC-TA})}{\partial t} = \frac{1}{V} (\iint_{\underbrace{A1}} -u(\text{DIC-TA})dydz + \iint_{\underbrace{A2}} -v(\text{DIC-TA})dxdz + \iint_{\underbrace{A3}} -w(\text{DIC-TA})dxdy$$
$$+ \iint_{\underbrace{A3}} K_{v} \left(\frac{\partial \text{DIC}}{\partial z} - \frac{\partial \text{TA}}{\partial z}\right)dxdy + \iint_{V} \text{BIO}dxdydz)$$
(4.1)

The first term on the right-hand side of equation (1) is the lateral advective flux across a longitudinal transect (whose area labeled as A1). The second term is the influx of DIC-TA into a cross-channel section (labeled as A2) and is called longitudinal advective flux. The third term is the vertical advective flux across the upper boundary (labeled as A3) of V. The fourth term represents the vertical diffusive flux across A3 (K_v is the vertical diffusivity). The fourth term (BIO) is biogeochemical uptake or production of DIC and TA in V, including algal and microbial respiration, CaCO₃ formation and dissolution, and benthic flux. $\frac{\partial(DIC-TA)}{\partial t} > 0$ means more DIC are produced than TA or less DIC are removed than TA, which lowers pH. In contrast, $\frac{\partial(DIC-TA)}{\partial t} < 0$ means larger DIC production than TA or smaller DIC consumption than TA, elevating pH.

4.4 Results

4.4.1 Wind-driven variability of bottom pH

The time series of salinity and pH from the observation at the bottom of the Gooses Reef showed high-frequency variabilites (Fig. 4.2). The frequency domain covers from half day to several days. Here we focus on the wind-driven variability whose period is longer than 1.5 days. Though the observed long-term pH in August was between 7.4 and 7.5, the short-term variability could elevate pH up to 7.9 (Fig. 4.2c), transiently relieving the bottom acidity. The peaks of pH corresponded to the troughs of salinity in the time series (Figs. 4.2b & 4.2c), suggesting a modulation by vertical processes as surface water in Chesapeake Bay usually has lower salinity and higher pH than bottom. In addition, the peaks of pH always occurred during the set-down or at the end of up-estuary wind events (Figs. 4.2a & 4.2c).



Figure 4.2 Time series of wind speed vector (a), bottom salinity (b) and bottom pH (c) from observations at the Gooses Reef (marked as red dot in Fig. 4.1a). The blue, red, green rectangles mark the duration of selected westerly, up-estuary, and down-estuary wind events in later analysis. The blue lines are original time series including tidal fluctuations and the red lines and

wind vector are low-passed with a 34-hour Butterworth filter.

To further check how wind modulated the bottom pH at the Gooses Reef, we chose an example sequence of a southerly wind event followed by a weak northerly wind event (highlighted in Fig. 4.2a) and used numerical simulations to illustrate the wind-driven processes. Southerly (up-estuary) winds blew over the Bay between 9 and 15 August 2016, with a maximum wind speed of $\sim 5 \text{ m s}^{-1}$. This was followed by weak northerly (down-estuary) winds lasting 1 day with a maximum wind speed of $\sim 2.5 \text{ m s}^{-1}$.

As a baseline for comparison, we first present the distributions of physical and carbonate chemistry fields at the cross-section where the Gooses Reef locates during weak westerly winds with wind speed below 2 m s⁻¹ from 8-9 August (Fig. 4.3). Before the up-estuary wind event, the cross-channel transect was vertically stratified with the top-bottom salinity difference of ~ 6 psu (Fig. 4.3a). The isohalines tilted slightly upwards on the eastern shore as the Coriolis force confined the outflowing fresher water to the west. Similarly, DIC and TA were also vertically stratified corresponding to salinity (Figs. 4.3b & 4.3c). However, the isolines of DIC and TA were almost even. The uniform cross-channel distributions of DIC and TA corresponded to the distribution of chlorophyll-a (Figs. 4.3b-d), suggesting a biological control. Chlorophyll-a did not have a strong lateral gradient but showed strong vertical gradient due to light attenuation (Fig. 4.3d). Since phytoplankton production consumed DIC in the surface euphotic layer and respiration of organic material produced DIC in the bottom layer, DIC had a larger vertical gradient than TA (Figs. 4.3b & 4.3c). The relative impacts of primary production and respiration on TA are small (Cai et al. 2021). Corresponding to DIC and TA, pH also had a strong vertical gradient, with the top-to-bottom difference reaching 0.7 (Fig. 4.3e). The homogenized low pH

water occupied the bottom layer below 9-m depth. The bottom pH at the Gooses Reef was 7.3, as low as the water in the deep channel. The aragonite saturation state Ω_{Ar} showed a similar distribution as pH (Fig. 4.3f).



Figure 4.3 Distributions of salinity (a), DIC (b), TA (c), chlorophyll-a (CHLA; d) pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the weak westerly wind period marked in 4.2a. The black dashed line marks the location of Gooses Reef.

The up-estuary wind drove a strong clockwise lateral circulation in the cross-channel section, with the eastward velocity in the near-surface layer reaching 0.05 m s⁻¹ (Fig. 4.4a). This led to upwelling on the western shore and downwelling at the eastern part of the cross-section, with the vertical velocity up to 0.1 mm s⁻¹. Consequently, eastward lateral currents in the surface layer pushed the fresher water onto the eastern shoal. Upwelling and dowelling drove the isohalines to tilt downward on the eastern slope of the deep channel (Fig. 4.4b). Besides, wind-driven turbulent mixing generated a well-mixed surface layer of 7-m depth. Due to the combination of strong surface mixing and downwelling, brackish water of 17.5 psu even penetrated from the

surface to 9-m depth over the Gooses Reef. DIC and TA showed a stronger tilt than salinity, with the downwelling of low DIC and low TA water toward the bottom at the eastern part of the crosssection (Figs. 4.4c & 4.4d). The downwelling relieved the acidity at the Gooses Reef, where bottom pH was elevated from 7.3 to 7.6 (Fig. 4.4e). Bottom Ω_{Ar} was also elevated from 1.1 to 1.7 (Fig. 4.4f). On the other hand, upwelling on the western shore brought low pH water from bottom to surface, where surface pH largely dropped from 8.0 to 7.6.



Figure 4.4 Distributions of lateral circulation vector (a), salinity (b), DIC (c), TA (d), pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the up-estuary wind event marked in 4.2a.

The following down-estuary wind after the up-estuary wind event drove a counter-clockwise lateral circulation, with upwelling on the eastern shore and downwelling on the western shore (Fig. 4.5a). Isohalines were tilted upwards, with water in the intermediate depths (~11 m) uplifted towards the eastern shoal to 7-m depth (Fig. 4.5b). Both DIC and TA were tilted back to the conditions before the up-estuary wind (Figs. 4.5c & 4.5d). Upwelling at the eastern part of

the cross-section drove the low pH water from the deep channel back to the Gooses Reef, where bottom pH dropped to 7.4 and Ω_{Ar} was decreased to 1.3 (Figs. 4.5e & 4.5f).



Figure 4.5 Distributions of lateral circulation vector (a), salinity (b), DIC (c), TA (d), pH (e), and Ω_{Ar} (f) at the mid-bay cross-section across the Gooses Reef during the down-estuary wind event marked in 4.2a.

In addition to lateral circulation, wind can also affect along-channel processes. The distributions of physical and carbonate chemistry fields along the thalweg of Chesapeake Bay are presented in Fig. 4.6 to contrast the along-channel processes under different wind conditions. Before the up-estuary wind event, the tidally averaged along-channel currents displayed a typical two-layer gravitational circulation, with seaward flow in the surface layer down to ~ 8 m and landward flow in the underlying bottom layer (Fig. 4.6a). The along-channel salinity distribution showed sloping isohalines typical of a partially mixed estuary (Fig. 4.6b). DIC also showed an along-channel gradient, but the slope of the DIC isolines was gentler than isohalines (Fig. 4.6c). Despite the delivery of lower DIC water from the river end, pH showed an increasing

longitudinal gradient from the upper-Bay to the lower-Bay as riverine water is poorly-buffered with higher DIC/TA ratio than the oceanic water (Fig. 4.6d). However, the surface along-channel gradient of pH in the mid-Bay was small due to the control from primary production. From $38.2^{\circ}N$ to $38.8^{\circ}N$, surface pH were nearly homogeneous of 8.0. Ω_{Ar} showed a similar distribution as pH (Fig. 4.6e). The highly acidic water of $\Omega_{Ar} < 1$ accumulated only in the upper-Bay.



Figure 4.6 Along channel distributions of subtidal along-channel current (a, f, k), salinity (b, g, l), DIC (c, h, m), pH (d, i, n), Ω_{Ar} (e, j, o) during the selected wind periods. The along-channel section is marked by the black line in Fig. 1b. The magenta and white contour lines in b, g, l mark the isohaline of 17 and 25 psu respectively. The black dashed lines in d, i, n mark the location of upper-, mid-, and lower-Bay cross-sections respectively. The white contour lines in e, j, o mark the isoline of $\Omega_{Ar} = 1$.

The up-estuary wind stress forced water in the surface layer to move landward whereas the pressure gradient due to sea level pileup at the head of the estuary drove the bottom water

seaward, hence reversing the gravitational circulation in the mid-Bay (Fig. 4.6f). This reversed circulation strained the salinity field towards the vertical direction, further decreasing stratification and enhancing vertical mixing (Fig. 4.6g). As the along-channel gradients in surface DIC, pH and Ω_{Ar} in the mid-Bay were small, wind-induced straining did not directly modify the surface carbonate chemistry field, but the enhanced turbulent mixing diffused surface low DIC, high pH, high Ω_{Ar} water downward (Figs. 4.6h-j). However, though the isoline of Ω_{Ar} =1 became closer to the bottom, the reversed seaward currents in the bottom layer advected the undersaturated riverine water further seaward to the mid-Bay, increasing the influenced area (Fig. 4.6j). After the up-estuary winds, the along-channel circulation recovered to the typical gravitational circulation with seaward flow in the surface layer and landward flow in the bottom layer (Fig. 4.6k). This two-layer current strained the salinity field to flatten the isohalines (Fig. 4.61). The surface mixed layer became shallower and the distribution of DIC, pH and Ω_{Ar} in the upper layer recovered to the conditions before the up-estuary wind event (Figs. 4.6m-o). However, as the duration of the down-estuary winds was much shorter than the up-estuary winds, low pH, low Ω_{Ar} water was not pushed back to its original location in the upper-Bay by landward currents in the bottom layer.

4.4.2 Ventilation of bottom pH

The observed short-term variability of bottom pH as well as model simulations suggests wind-driven downwelling can relieve bottom acidity in the mid-Bay in a short period. However, it also suggests seaward along-channel currents in the bottom layer under up-estuary wind can counteract the effects of downwelling to a certain degree. It is unknown whether wind-driven downwelling can also overwhelm along-channel process and modulate bottom pH at other cross-

sections. To answer this question, we examined two typical cross-sections in the upper-Bay and lower-Bay respectively during the same wind event with model results.

Before the up-estuary wind event, the distribution of salinity at the upper-Bay cross-section was similar to the mid-Bay cross-section (Fig. 4.7a). Nevertheless, pH and Ω_{Ar} showed lateral gradients with low pH, low Ω_{Ar} water confined to the western boundary, as primary production limited by turbidity could not homogenize the surface pH in the upper-Bay (Figs. 4.7b & 4.7c). Different from the mid-Bay, the up-estuary wind drove a three-layer lateral circulation consisting of clockwise circulation in the upper layer and counter-clockwise circulation in the lower layer (Fig. 4.7d), as lateral Ekman forcing from bottom stress becomes more significant in the shallower region (Xie et al. 2017). The clockwise lateral circulation only extended from the surface to 7-m depth, which could not advect surface water of low salinity, high pH, and high Ω_{Ar} to the bottom. Though the counter-clockwise lateral circulation in the bottom boundary layer could exchange bottom water with the mid-depth, its strength was much weaker than the clockwise lateral circulation in the surface layer. On the other hand, the landward currents in the surface layer advected high pH, high Ω_{Ar} water from the mid-Bay to the upper-Bay whereas the seaward currents in the bottom layer advected riverine water with low pH and low Ω_{Ar} , thereby enhancing the vertical gradients of pH and Ω_{Ar} (Figs 4.6i-j & 4.7e-f). Simultaneously, winddriven turbulent mixing drove a surface mixed layer of 5-m thickness, generally separating pH into two parts in the vertical direction (7.8-8.0 in the surface layer and 7.1-7.2 in the bottom layer) with a sharp vertical gradient at the mid-depth (Fig. 4.7e). Though bottom pH in the deep channel even dropped, the volume of water with Ω_{Ar} <1 at the cross-section was squeezed by the surface turbulent mixing (Fig. 4.7f).



Figure 4.7 Distributions of salinity, pH, and Ω_{Ar} at an upper-bay cross-section during the westerly winds (a-c) and up-estuary winds (d-f).

The cross-channel section in the lower-Bay is ~ 20 km wide with stratification trapped over the central deep channel (Fig. 4.8a). Due to relatively weak biological activities, the vertical gradients of pH and Ω_{Ar} were weaker than the upper- and mid-Bay (Figs. 4.8b & 4.8c). Upestuary winds also drove a complex pattern of lateral circulation at the lower-Bay cross-section (Fig. 4.8d). The relatively strong clockwise circulation was trapped at the surface layer. Though fresher water was advected from the western shoal to the eastern shoal by lateral flows, it could not be advected from the shoal into the deep channel. Besides, the weak vertical gradient of pH and Ω_{Ar} also limited the effects of vertical mixing (Figs. 4.8e & 4.8f). On the other hand, alongchannel flows in the bottom layer kept landward under up-estuary winds though their velocity was weakened (Fig. 4.6f). Thus, well-buffered oceanic water was continuously advected into the deep channel in the lower Bay, relieving the acidity in the deep channel (Figs. 4.6i-j & 4.8e-f).



Figure 4.8 Distributions of salinity, pH, and Ω_{Ar} at a lower-bay cross-section during the westerly winds (a-c) and up-estuary winds (d-f).

To further quantify the relative contributions of physical and biochemical processes in regulating bottom pH, we analyzed a DIC-TA budget for the bottom water volume below 10-m depth at the upper-, mid- and lower-Bay cross-sections in August. As the modeled horizontal advective flux is hard to be decomposed into along-channel and lateral components accurately due to the mismatch of grid orientation with estuarine channel and along-channel variations in bathymetry could also generate vertical flows, we combined the advective fluxes in three directions (F_{xadv} , F_{yadv} , F_{vadv}) into one term (F_{adv}). At all the three cross-sections, biochemical processes worsened the acidity (Figs 4.9b-d). At the upper-Bay cross-section, contributions to relieving the bottom acidity from advection and vertical mixing were comparable (Fig 4.9b). The short-term variability in the advective flux can be interpreted by the along-channel winds to a certain degree. The advective flux sometimes worsened the acidity under up-estuary winds (Figs

4.9a & 4.9b), as reversed along-channel circulation advected riverine low-pH water to the upper-Bay. At the mid-Bay cross-section, advective flux showed large short-term variability and its amplitude was much larger than vertical diffusive flux (Fig 4.9c). During the selected up-estuary wind event, wind-driven upwelling brought the acidic water from the deep channel to the western shoal, sharply elevating the surface pCO_2 from 360~450 to 500~1000 ppm (Fig 4.10a & 4.10f). The western part of the mid-Bay transitioned from a carbon sink to a strong carbon source. The time-averaged surface DIC change from the air-sea exchange of CO₂ was negligible during the weak westerly winds before the up-estuary wind event (Fig. 4.10b). The timeaveraged reduction rate in surface DIC was elevated up to 10 µmol kg⁻¹h⁻¹ at the western boundary but sharply decreased toward the eastern shore (Fig. 4.10g). Besides, though the upwelling brought more nutrients to the surface, it did not induce a bloom over the western shoal (Figs. 4.10c-d & 4.10h-i). In contrast, the upwelling brought low-phytoplankton water from the bottom to the surface and the original phytoplankton above the western shoal was advected to the center by lateral currents. The surface DIC reduction rate induced by net ecosystem metabolism (NEM) even dropped a little as more phytoplankton was mixed downward (Figs. 4.10e & 4.10j). Compared with the consumption rate of DIC by NEM, release rate of DIC by air-sea exchange was much smaller at most of area, though their maximum values are comparable. As a result, neither fast air-sea exchange nor enhanced primary production drove the supersaturated surface pCO_2 down. After the up-estuary wind event, the acidic water on the western shoal was advected back into the deep channel by the following lateral circulation in the opposite direction. At the lower-Bay cross-section, contribution from the vertical mixing was tiny (Fig 4.9d). Longitudinal advection of well-buffered oceanic water was the dominant process to relive the bottom acidity. The advective flux also showed short-term variability, enhanced by down-estuary winds and



weakened by up-estuary winds (Figs 4.9a & 4.9d).

Figure 4.9 Time series of along-channel wind speed (a) and model-estimated terms in the DIC-TA budget for bottom water (below 10-m depth) at the upper-, mid-, and lower-Bay cross-sections (b-d) in August, 2016.


Figure 4.10 Horizontal distributions of surface pCO2, DIC change induced by air-sea exchange, dissolved inorganic nitrogen (DIN), chlorophyll-a (CHLA), and DIC change induced by net ecosystem metabolism (NEM) during the westerly winds (a-e) and up-estuary winds (f-j).

The above analysis raised a question that whether the back-and-forth advective flux in the mid-Bay helps the ventilation of bottom pH in the deep channel in a longer time-scale. To answer this question, we integrated equation (1) over time. The cumulative advective flux was smaller than the cumulative vertical diffusive flux at the upper-Bay cross-section (Fig 4.11a). Though the amplitude of advective flux at the mid-Bay cross-section was larger, the cumulative advection contribution was comparable with vertical mixing (Fig 4.11b). From 1-17 August, the cumulative advection divective flux as almost the same as vertical mixing, since the duration of up-estuary winds was long, giving more time for ventilation. After that, the cumulative advective gradually became smaller than the cumulative vertical diffusive flux. Thus, despite strong dowelling in the mid-Bay, slow air-sea CO_2 exchange limits the effectiveness of the lateral ventilation. At the

lower-Bay section, advection is the dominant mechanism to counteract the production of DIC by biochemical processes (Fig 4.11c).



Figure 4.11 Time series of time-integrated terms in the DIC-TA budget for bottom water (below 10-m depth) at the upper-, mid-, and lower-Bay cross-sections in August, 2016.

4.5 Concluding remarks

Observation in this study showed that winds can drive pH fluctuations of up to 0.5 over a period of a few days at bottom water where metabolism is limited by light in Chesapeake Bay. This adds to a growing body of evidence for large short-term pH variability in coastal and estuarine systems (Hofman et al. 2011; Baumann and Smith 2018). Previous studies focused on metabolism-driven surface pH. Hofman et al. (2011) analyzed high-resolution time series of surface pH over a variety of systems and found pH ranges at kelp forest sites are larger than coral reef ecosystems, suggesting pH ranges depend on ecosystem metabolic rates. Measurements in a salt tidal marsh found diel pH range varies seasonally due to the seasonal variations in

photosynthesis and respiration rate (Baumann et al. 2015). This study confirmed without diel metabolism cycle, physical processes such as wind-driven lateral circulation can also drive a large pH fluctuation. Nevertheless, metabolism still influences the fluctuation indirectly. Without the metabolic separation in which excess primary production is stimulated in the surface layer and net respiration prevails in the bottom layer (Testa et al. 2012), no sharp vertical gradient of pH could be interacted with by the lateral downwelling. Despite lack of observation data, we can expect during winter when photosynthesis and respiration are both weak, the vertical gradient of pH is small and the amplitude of bottom pH fluctuation also becomes small.

Different from previous studies which focus on the pH decline in a short period, this study found temporary pH elevation. As oysters typically spawn between June and August when bottom pH reaches minimum in a year, the pH elevation driven by wind can relive the harm of acidic water to oyster growth. As southerly winds over Chesapeake Bay prevail in summer, eastern part of the estuarine channel has more opportunity to experience elevated pH. Theoretically, counter-clockwise lateral circulation driven by down-estuary wind can also bring high pH water downward and relieve acidity on the western part of the channel. However, downestuary winds in summer are usually weak and short. Using an idealized numerical model of Chesapeake Bay, Li and Li (2012) found that the clockwise circulation generated under upestuary winds is much stronger than the counterclockwise circulation generated under downestuary winds. Xie et al. (2017) analyzed long-term mooring data at a cross-channel section in Chesapeake Bay and found that the lateral circulation strength increased linearly with wind speeds under up-estuary winds but was a parabolic and weaker function of wind speeds under down-estuary winds. These results suggest with the same wind speed and duration, up-estuary winds could still be more conducive to bottom pH elevation than down-estuary winds.

Model predictions for a seagrass habitat showed increasing anthropogenic carbon reduces the ability of the system to buffer natural extremes in pH, leading to amplification of extremely low pH events in future (Pacella et al. 2018). In contrast, model projections for carbonate chemistry in Chesapeake Bay showed an increase in buffer factor (Li et al. 2023). It is because the response of pH to DIC change in seawater is nonlinear with its most sensitive point at roughly 7.5 (Cai et al. 2021). The predicted pH decline in Pacella et al. (2018) is from 8.1 in 2015 to 7.8 in 2100, whereas summer bottom pH in the middle reach of Chesapeake Bay was as low as 7.4 in 2016. The increasing buffer factor means a more stable bottom pH, as more DIC will be required to remove to elevate the pH. On the other hand, global warming may enhance the vertical metabolic separation, thereby increasing the vertical gradient of pH. Thus, pH fluctuation in future Chesapeake Bay is hard to be anticipated.

Though wind-driven lateral downwelling can advect high pH water to the bottom, the upwelled high pCO_2 water on the other side cannot get saturated with the atmospheric pCO_2 due to slow air-sea exchange of CO₂. In the following wind event in the opposite direction, the low pH will be advected back to the deep channel. Therefore, the ventilation driven by lateral circulation is noneffective. The budget analysis for bottom water volume shows vertical mixing and longitudinal advection of oceanic water could be more important. It should be noted 2016 is a dry year, thereby with larger vertical diffusive flux. With a stronger stratification in a wet year, ventilation of bottom pH may be more difficult.

4.6 Acknowledgements

We are grateful to the NOAA Ocean Acidification Program (NOAA-OAP; Awards NA15NOS4780184 and NA18NOS4780179) for the financial support.

Chapter 5: Conclusion

In this dissertation, firstly an idealized estuarine model with generic channel-shoal bathymetry was used to investigate internal lee wave generation under different river flow and tidal conditions. Then a straight estuarine channel of ultrahigh resolution was configured with a state-of-art nonhydrostatic model to study the evolution from an internal lee wave to internal solitary waves over a typical channel-shoal bathymetry. Finally, with the combination of observation data and hindcast simulation by coupled hydrodynamic-biogeochemical models, the short-term variability of bottom pH in Chesapeake Bay was studied and the ventilation by wind-driven lateral circulation was examined. Despite focusing on Chesapeake Bay, the findings can be applicable to other stratified estuaries with net respiration in the bottom layer. This chapter provides a summary of major findings from the research.

Using a numerical model for an idealized straight estuary, the study confirms that tidallydriven lateral flows can generate internal lee waves across all the salinity regimes in a generic coastal plain estuary featuring channel-shoal bathymetry. The lee wave amplitude decreases with increasing river flow as stronger stratification suppresses the wave growth, whereas the wave amplitude initially increases with the tidal amplitude but saturates or decreases as the tide amplitude further increases. When the tidal currents become strong enough to erase stratification on the shallow shoals, no internal lee waves could be generated and instead fronts are developed at the channel-shoal interface. The model results are mapped into a regime diagram with estuarine parameter space to show the potential wave form in estuaries of different types. In strongly stratified estuaries, model-2 lee waves can be generated when river flows are weak. If the river flows are very strong, stratification will prevent the lateral flows from reaching critical. Partially mixed estuaries are most conducive to the generation of large-amplitude internal lee waves. A variety of wave forms including mode-2 wave, mode-1 wave and hydraulic jump can be found in this regime. No internal waves are found under the regime for periodically stratified estuaries where water on the shoals are well mixed and salinity fronts are developed to separate the well-mixed shallow shoals from the stratified deep channel.

A nonhydrostatic model further shows the evolution of an internal lee wave into internal solitary waves over the channel-shoal bathymetry. After the lee wave propagates upward and onto the shoal, it evolves into a mode-1 wave of elevation. The initial steepening of the elevation wave is due to the shallowing of water depth. After the steepening constrains the wave energy into a smaller length scale, the elevation wave evolves into a shorter wave. As bottom boundary mixing drives the halocline above the mid-depth which does not favor the polarity of elevation, the elevation wave is soon deformed into a depression wave and simultaneously releases a train of undular waves at its tail under the combined effects of nonlinearity and nonhydrostatic dispersion. The small-amplitude undular waves are dissipated by the background viscosity later. The leading depression wave propagates further and finally gets merged into a salinity front close to the lateral coastline.

Enhanced local turbulent dissipation rate is found at the steepening edge of the nonlinear internal lee waves over the deep channel. In addition, enhanced mixing is also found on the shoal after the passage of internal solitary waves. Therefore, nonlinear internal waves from interaction of lateral flows with channel-shoal topography can contribute to mixing at both channel and shoal, suggesting an important mechanism for mixing in stratified coastal plain estuaries.

Wind-driven lateral circulation drives a high-frequency pH fluctuation ranging from 0.1 - 0.5in the bottom water where diel metabolic cycle does not exist at the middle reach of a stratified estuary. The wind-driven downwelling advects high pH water downward, whereas the upwelled low pH, high pCO_2 water on the other side cannot get saturated with the atmospheric pCO_2 due to the slow air-sea exchange of CO_2 . The following wind in the opposite direction drives the low pH water on the shoal back into the deep channel. Therefore, this wind-driven lateral ventilation can only temporarily relive bottom acidity in the deep channel. At an upper-Bay cross-section, strong wind-driven lateral circulation is confined in the surface layer. Turbulent mixing plays a more important role to ventilate bottom pH. The reversed along-channel currents under upestuary winds may weaken the effects of the ventilation. Similar lateral circulation pattern is also found at a lower-Bay cross-section. However, strong stratification over the deep channel limits the turbulent ventilation. Instead replenishment of oceanic water with relatively high pH is the dominant process to modulate bottom pH in the lower-Bay. DIC and TA budget analysis shows vertical mixing and longitudinal advection could be more important mechanisms to ventilate bottom pH.

In future studies, more dedicated filed surveys need to be conducted to capture internal waves in shallow estuaries. It would be worthwhile to quantify the turbulent dissipation rate associated with internal waves in stratified estuaries. The enhanced turbulent mixing by internal lee waves over the deep channel has never been captured in filed surveys. It is deserved to confirm the mechanism in real systems and study how changes in river and tidal flows will affect the turbulent mixing over the channel-shoal topography. In addition, previous studies focused on flows interacting with a sill. Interaction between tidal flow and valley in the oceanic scenario is

also deserved to study.

Short-term variability of pH and pCO_2 should be paid more attention to as it can influence the estimate of carbon budget in a longer time scale. This dissertation only investigated changes in pH under normal winds. However, extremely wind events could have larger impacts on estuarine carbonate system though their occurrences are episodic. In future, a better hydrodynamic-biochemical model is deserved to be configured to study the response of estuarine carbonate system to hurricane and flooding.

Bibliography

- Aghsaee, P., L. Boegman, and K. G. Lamb, 2010: Breaking of shoaling internal solitary waves. *J. Fluid Mech.*, **659**, 289-317.
- Akhand, A., and Coauthors, 2016: A comparison of CO2 dynamics and air-water fluxes in a river-dominated estuary and a mangrove-dominated marine estuary. *Geophys. Res. Lett.*, **43**, 11,726-711,735.
- Auclair, F., L. Bordois, Y. Dossmann, T. Duhaut, A. Paci, C. Ulses, and C. Nguyen, 2018: A non-hydrostatic non-Boussinesq algorithm for free-surface ocean modelling. *Ocean Modell.*, 132, 12-29.
- Bai, X., Z. Liu, Q. Zheng, J. Hu, K. G. Lamb, and S. Cai, 2019: Fission of shoaling internal waves on the northeastern shelf of the South China Sea. J. Geophys. Res. Oceans, 124, 4529-4545.
- Baines, P.G., 1995: Topographic Effects in Stratified Flows. Cambridge Univ. Press. 482 pp.
- Baumann, H., and E. M. Smith, 2018: Quantifying metabolically driven pH and oxygen fluctuations in US nearshore habitats at diel to interannual time scales. *Estuar. Coast.*, **41**, 1102-1117.
- Baumann, H., R. B. Wallace, T. Tagliaferri, and C. J. Gobler, 2015: Large natural pH, CO2 and O2 fluctuations in a temperate tidal salt marsh on diel, seasonal, and interannual time scales. *Estuar. Coast.*, 38, 220-231.
- Boegman, L., G. Ivey, and J. Imberger, 2005: The energetics of large-scale internal wave degeneration in lakes. *J. Fluid Mech.*, **531**, 159-180.
- Borgesa, A. V., and N. Gypensb, 2010: Carbonate chemistry in the coastal zone responds more strongly to eutrophication than ocean acidification. *Limnol. Oceanogr.*, **55**, 346-353.
- Bourgault, D., M. Blokhina, R. Mirshak, and D. Kelley, 2007: Evolution of a shoaling internal solitary wavetrain. *Geophys. Res. Lett.*, **34**.
- Bourgault, D., and D. E. Kelley, 2003: Wave-induced boundary mixing in a partially mixed estuary. J. Mar. Res., 61(5), 553-576.
- Brady, D. C., J. M. Testa, D. M. Di Toro, W. R. Boynton, and W. M. Kemp, 2013: Sediment flux modeling: Calibration and application for coastal systems. *Estuarine Coastal Shelf Sci.*, **117**, 107-124.
- Bresnahan Jr, P. J., T. R. Martz, Y. Takeshita, K. S. Johnson, and M. LaShomb, 2014: Best practices for autonomous measurement of seawater pH with the Honeywell Durafet. *Methods in Oceanography*, **9**, 44-60.

- Brodeur, J. R., and Coauthors, 2019: Chesapeake Bay inorganic carbon: Spatial distribution and seasonal variability. *Front. Mar. Sci.*, **6**, 99.
- Browne, D. R., and C.W. Fisher, 1988: Tide and tidal currents in the Chesapeake Bay. NOAA Technical Report NOS OMA 3, 84 pp.
- Buijsman, M. C., Y. Kanarska, and J. C. McWilliams, 2010: On the generation and evolution of nonlinear internal waves in the South China Sea. J. Geophys. Res. Oceans, 115.
- Cai, W.-J., and Coauthors, 2011: Acidification of subsurface coastal waters enhanced by eutrophication. *Nat. Geosci.*, **4**, 766-770.
- Cai, W.-J., and Coauthors, 2017: Redox reactions and weak buffering capacity lead to acidification in the Chesapeake Bay. *Nat. Commun.*, **8**, 1-12.
- Cai, W.-J., and Coauthors, 2021: Natural and anthropogenic drivers of acidification in large estuaries. *Annu. Rev. Mar. Sci.*, **13**.
- Cai, W. J., and Y. Wang, 1998: The chemistry, fluxes, and sources of carbon dioxide in the estuarine waters of the Satilla and Altamaha Rivers, Georgia. *Limnol. Oceanogr.*, **43**, 657-668.
- Carstensen, J., D. Conley, and B. Müller-Karulis, 2003: Spatial and temporal resolution of carbon fluxes in a shallow coastal ecosystem, the Kattegat. *Marine Ecology Progress Series*, **252**, 35-50.
- Carstensen, J., and C. M. Duarte, 2019: Drivers of pH variability in coastal ecosystems. *Environ. Sci. Technol.*, **53**, 4020-4029.
- Carter, H. H., and D. W. Pritchard, 1988: Oceanography of Chesapeake Bay. In *Hydrodynamics* of estuaries: dynamics of partially-mixed estuaries, edited by B. Kjerfe. Vol. 1. CRC Press, 1-16.
- Chen, B., W. J. Cai, J. R. Brodeur, N. Hussain, J. M. Testa, W. Ni, and Q. Li, 2020: Seasonal and spatial variability in surface p CO2 and air-water CO2 flux in the Chesapeake Bay. *Limnol. Oceanogr.*, **65**, 3046-3065.
- Chen, Z., Y. Nie, J. Xie, J. Xu, Y. He, and S. Cai, 2017: Generation of internal solitary waves over a large sill: From Knight Inlet to Luzon Strait. *J. Geophys. Res. Oceans*, **122**, 1555-1573.
- Cheng, P., A. Valle-Levinson, and H. E. de Swart, 2010: Residual currents induced by asymmetric tidal mixing in weakly stratified narrow estuaries. *J. Phys. Oceanogr.*, **40**(9), 2135-2147.
- Cheng, P., A. Valle-Levinson, and H. E. de Swart, 2011: A numerical study of residual estuarine circulation induced by asymmetric tidal mixing in tidally dominated estuaries. J. Geophys. Res., 116, C01017, doi:10.1029/2010JC006137.

- Cheresh, J., and J. Fiechter, 2020: Physical and biogeochemical drivers of alongshore pH and oxygen variability in the California Current System. *Geophys. Res. Lett.*, **47**, e2020GL089553.
- Cummins, P. F., L. Armi, and S. Vagle, 2006: Upstream internal hydraulic jumps. J. Phys. Oceanogr., 36, 753-769.
- Cummins, P. F., S. Vagle, L. Armi, and D. M. Farmer, 2003: Stratified flow over topography: Upstream influence and generation of nonlinear internal waves. *Proc. Roy. Soc. London.*, 459A, 1467–1487.
- Dai, M., and Coauthors, 2009: Diurnal variations of surface seawater pCO2 in contrasting coastal environments. *Limnol. Oceanogr.*, **54**, 735-745.
- da Silva, J. C. B., M. C. Buijsman, and J. M. Magalhaes, 2015: Internal waves on the upstream side of a large sill of the Mascarene Ridge: A comprehensive view of their generation mechanisms and evolution. *Deep-Sea Res. I*, **99**, 87–104, doi:10.1016/j.dsr.2015.01.002.
- Davis, K. A., R. S. Arthur, E. C. Reid, J. S. Rogers, O. B. Fringer, T. M. DeCarlo, and A. L. Cohen, 2020: Fate of internal waves on a shallow shelf. J. Geophys. Res. Oceans, 125, e2019JC015377.
- DeGrandpre, M., T. Hammar, and C. Wirick, 1998: Short-term pCO2 and O2 dynamics in California coastal waters. *Deep-Sea Res. II*, **45**, 1557-1575.
- Delpeche, N. C., T. Soomere, and M.-J. Lilover, 2010: Diapycnal mixing and internal waves in the Saint John River Estuary, New Brunswick, Canada with a discussion relative to the Baltic Sea. *Estonian Journal of Engineering*, **16**.
- Debreu, L., P. Marchesiello, P. Penven, and G. Cambon, 2012: Two-way nesting in split-explicit ocean models: Algorithms, implementation and validation. *Ocean Modell.*, **49**, 1-21.
- Debreu, L., C. Vouland, and E. Blayo, 2008: AGRIF: Adaptive grid refinement in Fortran. *Computers & Geosciences*, **34**, 8-13.
- Di Toro, D. M., 2001: Sediment flux modeling, 624 pp., Wiley-Interscience, New York.
- Dyer, K., 1982: Mixing caused by lateral internal seiching within a partially mixed estuary. *Estuarine Coastal Shelf Sci.*, **15**, 443-457.
- Egbert, G. D., and S. Y. Erofeeva, 2002: Efficient inverse modeling of barotropic ocean tides. J. *Atmos. Ocean Tech.*, **19(2)**, 183-204.
- Farmer, D. M., and L. Armi, 1999: The generation and trapping of solitary waves over topography. *Science*, 283, 188–190.
- Farmer, D. M., and J. D. Smith, 1980: Tidal interaction of stratified flow with a sill in Knight Inlet. *Deep-Sea Res.*, **27A**, 239–246.

- Feely, R. A., and Coauthors, 2010: The combined effects of ocean acidification, mixing, and respiration on pH and carbonate saturation in an urbanized estuary. *Estuarine Coastal Shelf Sci.*, **88**, 442-449.
- Fisher, A. W., L. P. Sanford, and S. E. Suttles, 2015: Wind stress dynamics in Chesapeake Bay: Spatiotemporal variability and wave dependence in a fetch-limited environment. J. Phys. Oceanogr., 45, 2679-2696.
- Frieder, C. A., S. H. Nam, T. R. Martz, and L. A. Levin, 2012: High temporal and spatial variability of dissolved oxygen and pH in a nearshore California kelp forest. *Biogeosciences*, 9, 3917-3930.
- Gago, J., M. Gilcoto, F. F. Pérez, and A. R10s, 2003: Short-term variability of fCO2 in seawater and air-sea CO2 fluxes in a coastal upwelling system (R1a de Vigo, NW Spain). *Marine Chemistry*, **80**, 247-264.
- Garrett, C., and E. Kunze, 2007: Internal tide generation in the deep ocean. Annu. Rev. Fluid Mech., **39**, 57-87.
- Geyer, W. R., and P. MacCready, 2014: The estuarine circulation. Annu. Rev. Fluid Mech., 46, 175-197.
- Geyer, W. R., and J. D. Smith, 1987: Shear instability in a highly stratified estuary. J. Phys. Oceanogr., 17, 1668-1679.
- Gill, A. E., 1982: Atmosphere–Ocean Dynamics. Academic Press, 662 pp.
- Gregg, M., and L. Pratt, 2010: Flow and hydraulics near the sill of Hood Canal, a strongly sheared, continuously stratified fjord. *J. Phys. Oceanogr.*, **40**, 1087–1105.
- Grimshaw, R., E. Pelinovsky, and T. Talipova, 1997: The modified Korteweg-de Vries equation in the theory of large-amplitude internal waves. *Nonlinear Processes in Geophysics*, **4**, 237-250.
- Grimshaw, R., E. Pelinovsky, T. Talipova, and A. Kurkin, 2004: Simulation of the transformation of internal solitary waves on oceanic shelves. *J. Phys. Oceanogr.*, **34**, 2774-2791.
- Groeskamp, S., J. J. Nauw, and L. R. Maas, 2011: Observations of estuarine circulation and solitary internal waves in a highly energetic tidal channel. *Ocean Dyn.*, **61**, 1767-1782.
- Harris, K. E., M. D. DeGrandpre, and B. Hales, 2013: Aragonite saturation state dynamics in a coastal upwelling zone. *Geophys. Res. Lett.*, **40**, 2720-2725.
- Hauri, C., N. Gruber, A. McDonnell, and M. Vogt, 2013: The intensity, duration, and severity of low aragonite saturation state events on the California continental shelf. *Geophys. Res. Lett.*, 40, 3424-3428.

- Helfrich, K. R., and W. K. Melville, 2006: Long nonlinear internal waves. Annu. Rev. Fluid Mech., 38, 395-425.
- Herrmann, M., and Coauthors, 2020: Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay. J. Geophys. Res. Oceans, 125, e2019JC015610.
- Hetland, R. D., and W. R. Geyer, 2004: An idealized study of the structure of long, partially mixed estuaries. J. Phys. Oceanogr., 34, 2677–2691.
- Hofmann, G. E., and Coauthors, 2011: High-frequency dynamics of ocean pH: a multiecosystem comparison. *PLoS One*, **6**, e28983.
- Holden, J. J., S. H. Derbyshire, and S. E. Belcher, 2000: Tethered balloon observations of the nocturnal stable boundary layer in a valley. *Bound.-Layer Meteor.*, **97**, 1–24, doi:10.1023/A:1002628924673.
- Holloway, P. E., E. Pelinovsky, and T. Talipova, 1999: A generalized Korteweg-de Vries model of internal tide transformation in the coastal zone. J. Geophys. Res. Oceans, 104, 18333-18350.
- Holloway, P. E., E. Pelinovsky, T. Talipova, and B. Barnes, 1997: A nonlinear model of internal tide transformation on the Australian North West Shelf. *J. Phys. Oceanogr.*, **27**, 871-896.
- Huang, W. J., W. J. Cai, Y. Wang, S. E. Lohrenz, and M. C. Murrell, 2015: The carbon dioxide system on the M ississippi R iver-dominated continental shelf in the northern G ulf of M exico: 1. Distribution and air-sea CO2 flux. J. Geophys. Res. Oceans, 120, 1429-1445.
- Huang, W.-J., W.-J. Cai, X. Xie, and M. Li, 2019: Wind-driven lateral variations of partial pressure of carbon dioxide in a large estuary. *J. Mar. Syst.*, **195**, 67-73.
- Isleib, R. P. E., J. J. Fitzpatrick, and J. Mueller, 2007: The development of a nitrogen control plan for a highly urbanized tidal embayment, *Proc. Water Environ. Feder.*, **5**, 296–320.
- Jones, N., G. Ivey, M. Rayson, and S. Kelly, 2020: Mixing driven by breaking nonlinear internal waves. *Geophys. Res. Lett.*, **47**, e2020GL089591.
- Kantha, L.H., and C.A. Clayson, 1994: An improved mixed layer model for geophysical applications. J. Geophys. Res., 99, 25235–25266.
- Klymak, J. M., M. H. Alford, R. Pinkel, R.-C. Lien, Y. J. Yang, and T.-Y. Tang, 2011: The breaking and scattering of the internal tide on a continental slope. *J. Phys. Oceanogr.*, **41**, 926-945.
- Klymak, J.M., and M. Gregg, 2004: Tidally generated turbulence over the Knight Inlet Sill. J. *Phys. Oceanogr.*, **34**, 1135–1151.

- Klymak, J. M., S. M. Legg, and R. Pinkel, 2010: High-mode stationary waves in stratified flow over large obstacles. J. Fluid Mech., 644, 321-336.
- Klymak, J. M., and J. N. Moum, 2003: Internal solitary waves of elevation advancing on a shoaling shelf. *Geophys. Res. Lett.*, **30**.
- Klymak, J.M., R. Pinkel, and L. Rainville, 2008: Direct breaking of the internal tide near topography: Kaena Ridge, Hawaii. J. Phys. Oceanogr., 38(2), 380-399.
- Lamb, K. 1994. Numerical experiments of internal wave generation by strong tidal flow across a finite-amplitude bank edge. *J. Geophys. Res.*, **99**, 843–864.
- Lamb, K. G., 2014: Internal wave breaking and dissipation mechanisms on the continental slope/shelf. *Annu. Rev. Fluid Mech.*, **46**, 231-254.
- Legg, S., 2021: Mixing by oceanic lee waves. Annu. Rev. Fluid Mech., 53, 173-201.
- Legg, S., and J. Klymak, 2008: Internal hydraulic jumps and overturning generated by tidal flow over a tall steep ridge. *J. Phys. Oceanogr.*, **38**(9), 1949-1964.
- Lehner, M., and Coauthors, 2016a: The METCRAX II field experiment: A study of downslope windstorm-type flows in Arizona's Meteor Crater. Bull. Amer. Meteor. Soc., 97, 215–235,
- Lehner, M., R. Rotunno, and C. D. Whiteman, 2016b: Flow regimes over a basin induced by upstream katabatic flows—An idealized modeling study. *J. Atmos. Sci.*, **73**, 3821–3842,
- Lewis, E.R., and D.W.R. Wallace, 1998: CO2SYS-Program developed for CO2 system calculations. Carbon Dioxide Inf. Anal. Centre.
- Li, M., P. Cheng, R. Chant, A. Valle-Levinson, and K. Arnott, 2014: Analysis of vortex dynamics of lateral circulation in a straight tidal estuary. *J. Phys. Oceanogr.*, 44, 2779-2795.
- Li, M., Y. Guo, W.-J. Cai, J. M. Testa, C. Shen, R. Li, and J. Su, 2023: Projected increase in carbon dioxide drawdown and acidification in large estuaries under climate change. *Communications Earth & Environment*, **4**, 68.
- Li, M., Y. J. Lee, J. M. Testa, Y. Li, W. Ni, W. M. Kemp, and D. M. Di Toro, 2016: What drives interannual variability of hypoxia in Chesapeake Bay: Climate forcing versus nutrient loading? *Geophys. Res. Lett.*, 43, 2127-2134.
- Li, M., R. Li, W.-J. Cai, J. M. Testa, and C. Shen, 2020: Effects of wind-driven lateral upwelling on estuarine carbonate chemistry. *Front. Mar. Sci.*, **7**, 588465.
- Li, M., L. Zhong, W. C. Boicourt, 2005: Simulations of Chesapeake Bay estuary: Sensitivity to turbulence mixing parameterizations and comparison with observations. J. Geophys. Res.-Oceans, 110, C12004.

- Li, M., L. Zhong, W. C. Boicourt, S. Zhang, and D. L. Zhang, 2006: Hurricane-induced storm surges, currents and destratification in a semi-enclosed bay. *Geophys. Res. Lett.*, **33**.
- Li, R., and M. Li, 2022: A Regime Diagram for Internal Lee Waves in Coastal Plain Estuaries. J. *Phys. Oceanogr.*, **52**, 3049-3064.
- Li, Y., and M. Li, 2012: Wind-driven lateral circulation in a stratified estuary and its effects on the along-channel flow. *J. Geophys. Res. Oceans*, **117**.
- Liu, A. K., Y. S. Chang, M. K. Hsu, and N. K. Liang, 1998: Evolution of nonlinear internal waves in the East and South China Seas. *J. Geophys. Res. Oceans*, **103**, 7995-8008.
- MacKinnon, J. A., and Coauthors, 2017: Climate process team on internal wave–driven ocean mixing. *Bulletin of the American Meteorological Society*, **98**, 2429-2454.
- Marchesiello, P., F. Auclair, L. Debreu, J. McWilliams, R. Almar, R. Benshila, and F. Dumas, 2021: Tridimensional nonhydrostatic transient rip currents in a wave-resolving model. *Ocean Modell.*, **163**, 101816.
- Marchesiello, P., J. McWilliams, and A. Shchepetkin, 2001: Open boundary conditions for longterm integration of regional oceanic models. *Ocean Modell.*, 3(1), 20, doi: 10.1016/S1463-5003(00)00013-5.
- Martin, W., P. MacCready, and R. Dewey, 2005: Boundary layer forcing of a semidiurnal, crosschannel seiche. *J. Phys. Oceanogr.*, **35**, 1518-1537.
- Martz, T. R., J. G. Connery, and K. S. Johnson, 2010: Testing the Honeywell Durafet® for seawater pH applications. *Limnology and Oceanography: Methods*, **8**, 172-184.
- Mason, E., J. Molemaker, A. F. Shchepetkin, F. Colas, J. C. McWilliams, and P. Sangrà 2010: Procedures for offline grid nesting in regional ocean models. *Ocean Modell.*, **35**, 1-15.
- Masunaga, E., O. B. Fringer, H. Yamazaki, and K. Amakasu, 2016: Strong turbulent mixing induced by internal bores interacting with internal tide-driven vertically sheared flow. *Geophys. Res. Lett.*, **43**, 2094-2101.
- Maxworthy, T., 1979: A note on the internal solitary waves produced by tidal flow over a threedimensional ridge. J. Geophys. Res. Oceans, 84, 338-346.
- Mayer, F. T., and O. B. Fringer, 2017: An unambiguous definition of the Froude number for lee waves in the deep ocean. J. Fluid Mech., 831.
- Mayer, F., and O. Fringer, 2021: Resolving nonhydrostatic effects in oceanic lee waves. *Ocean Modell.*, **159**, 101763.
- McCutcheon, M. R., H. Yao, C. J. Staryk, and X. Hu, 2021: Temporal variability and driving factors of the carbonate system in the Aransas Ship Channel, TX, USA: a time series study. *Biogeosciences*, **18**, 4571-4586.

- McSweeney, J. M., and Coauthors, 2020: Observations of shoaling nonlinear internal bores across the central California inner shelf. J. Phys. Oceanogr., 50, 111-132.
- Melet, A., R. Hallberg, S. Legg, and M. Nikurashin, 2014: Sensitivity of the ocean state to lee wave-driven mixing. *J. Phys. Oceanogr.*, **44**, 900-921.
- Mohri, K., T. Hibiya, and N. Iwamae, 2010: Revisiting internal wave generation by tidetopography interaction. J. Geophys. Res. Oceans, 115.
- Moum, J., D. Farmer, E. Shroyer, W. Smyth, and L. Armi, 2007: Dissipative losses in nonlinear internal waves propagating across the continental shelf. *J. Phys. Oceanogr.*, **37**, 1989-1995.
- Moum, J., D. Farmer, W. Smyth, L. Armi, and S. Vagle, 2003: Structure and generation of turbulence at interfaces strained by internal solitary waves propagating shoreward over the continental shelf. *J. Phys. Oceanogr.*, **33**, 2093-2112.
- Munk, W., and C. Wunsch, 1998: Abyssal recipes. II: Energetics of tidal and wind mixing. *Deep Sea Res. Part I*, **45**, 1977–2010.
- Nash, J. D., and J. N. Moum, 2005: River plumes as a source of large-amplitude internal waves in the coastal ocean. *Nature*, **437**, 400-403.
- New, A., and R. Pingree, 1992: Local generation of internal soliton packets in the central Bay of Biscay. *Deep Sea Research Part A*, **39**, 1521-1534.
- New, A. L., K. R. Dyer, and R. E. Lewis, 1986: Predictions of the generation and propagation of internal waves and mixing in a partially stratified estuary. Estuarine Coastal Shelf Sci., 22, 199-214.
- Ni, W., M. Li, and J. M. Testa, 2020: Discerning effects of warming, sea level rise and nutrient management on long-term hypoxia trends in Chesapeake Bay. *Science of The Total Environment*, **737**, 139717.
- Nikurashin, M., and R. Ferrari, 2011: Global energy conversion rate from geostrophic flows into internal lee waves in the deep ocean. *Geophys. Res. Lett.*, **38**.
- O'Boyle, S., G. McDermott, T. Noklegaard, and R. Wilkes, 2013: A simple index of trophic status in estuaries and coastal bays based on measurements of pH and dissolved oxygen. *Estuar. Coast.*, **36**, 158-173.
- Orton, P. M., W. R. McGillis, and C. J. Zappa, 2010: Sea breeze forcing of estuary turbulence and air-water CO2 exchange. *Geophys. Res. Lett.*, **37**.
- Pacella, S. R., C. A. Brown, G. G. Waldbusser, R. G. Labiosa, and B. Hales, 2018: Seagrass habitat metabolism increases short-term extremes and long-term offset of CO2 under future ocean acidification. *PNAS*, **115**, 3870-3875.

- Paerl, H. W., and Coauthors, 2018: Two decades of tropical cyclone impacts on North Carolina's estuarine carbon, nutrient and phytoplankton dynamics: implications for biogeochemical cycling and water quality in a stormier world. *Biogeochemistry*, **141**, 307-332.
- Penven, P., L. Debreu, P. Marchesiello, and J. C. McWilliams, 2006: Evaluation and application of the ROMS 1-way embedding procedure to the central California upwelling system. *Ocean Modell.*, **12**, 157-187.
- Peters, H., 1999: Spatial and temporal variability of turbulent mixing in an estuary. *J. Mar. Res.*, **57**, 805–45.
- Pietrzak, J. D., C. Kranenburg, G. Abraham, B. Kranenborg, and A. van der Wekken, 1991: Internal wave activity in Rotterdam waterway. *J. Hydr. Eng.*, **117**, 738-757.
- Reum, J. C., S. R. Alin, R. A. Feely, J. Newton, M. Warner, and P. McElhany, 2014: Seasonal carbonate chemistry covariation with temperature, oxygen, and salinity in a fjord estuary: implications for the design of ocean acidification experiments. *PLoS One*, **9**, e89619.
- Ribas-Ribas, M., E. Anfuso, A. Gómez-Parra, and J. Forja, 2013: Tidal and seasonal carbon and nutrient dynamics of the Guadalquivir estuary and the Bay of Cádiz (SW Iberian Peninsula). *Biogeosciences*, **10**, 4481-4491.
- Richards, C., D. Bourgault, P. S. Galbraith, A. Hay, and D. E. Kelley, 2013: Measurements of shoaling internal waves and turbulence in an estuary. J. Geophys. Res., 118, 273–286, doi:10.1029/2012JC008154.
- Rotunno, R., and M. Lehner, 2016: Two-layer stratified flow past a valley. J. Atmos. Sci., 73, 4065-4076.
- Saderne, V., P. Fietzek, and P. M. J. Herman, 2013: Extreme variations of pCO2 and pH in a macrophyte meadow of the Baltic Sea in summer: evidence of the effect of photosynthesis and local upwelling. *PLoS One*, **8**, e62689.
- Salisbury, J., M. Green, C. Hunt, and J. Campbell, 2008: Coastal acidification by rivers: a threat to shellfish? *Eos Trans. AGU*, **89**, 513-513.
- Sanford, L. P., K. G. Sellner, and D. L. Breitburg, 1990: Covariability of dissolved oxygen with physical processes in the summertime Chesapeake Bay. *J. Mar. Res.*, **48**, 567-590.
- Sarabun C. C., and D. C. Dubbel, 1990: High-resolution thermistor chain observations in the upper Chesapeake Bay. *Johns Hopkins APL Technical Digest*, **11**, 48-53.
- Scotti, A., R. C. Beardsley, and B. Butman, 2007: Generation and propagation of nonlinear internal waves in Massachusetts Bay. J. Geophys. Res. Oceans, **112**.
- Scotti, A., R. C. Beardsley, B. Butman, and J. Pineda, 2008: Shoaling of nonlinear internal waves in Massachusetts Bay. J. Geophys. Res. Oceans, 113.

- Scotti, A., and J. Pineda, 2004: Observation of very large and steep internal waves of elevation near the Massachusetts coast. *Geophys. Res. Lett.*, **31**.
- Scully, M. E., 2010: Wind modulation of dissolved oxygen in Chesapeake Bay. *Estuar. Coast.*, **33**, 1164-1175.
- Scully, M. E., 2013: Physical controls on hypoxia in Chesapeake Bay: A numerical modeling study. J. Geophys. Res. Oceans, **118**, 1239-1256.
- Scully, M. E., A. P. Michel, D. P. Nicholson, and S. Traylor, 2022: Spatial and temporal variations in atmospheric gas flux from the Hudson River: the estuarine gas exchange maximum. *Limnol. Oceanogr.*, 67, 1590-1603.
- Shadwick, E. H., M. A. Friedrichs, R. G. Najjar, O. A. De Meo, J. R. Friedman, F. Da, and W. G. Reay, 2019: High-frequency CO2 system variability over the winter-to-spring transition in a coastal plain estuary. J. Geophys. Res. Oceans, 124, 7626-7642.
- Shen, C., and Coauthors, 2019a: Controls on carbonate system dynamics in a coastal plain estuary: A modeling study. *Journal of Geophysical Research: Biogeosciences*, **124**, 61-78.
- Shen, C., J. M. Testa, M. Li, and W. J. Cai, 2020: Understanding anthropogenic impacts on pH and aragonite saturation state in Chesapeake Bay: Insights from a 30-year model study. *Journal of Geophysical Research: Biogeosciences*, **125**, e2019JG005620.
- Shen, C., J. M. Testa, W. Ni, W. J. Cai, M. Li, and W. M. Kemp, 2019b: Ecosystem metabolism and carbon balance in Chesapeake Bay: A 30-year analysis using a coupled hydrodynamicbiogeochemical model. J. Geophys. Res. Oceans, 124, 6141-6153.
- Shroyer, E., J. Moum, and J. Nash, 2009: Observations of polarity reversal in shoaling nonlinear internal waves. *J. Phys. Oceanogr.*, **39**, 691-701.
- Shroyer, E. L., J. N. Moum, and J. D. Nash, 2010: Mode 2 waves on the continental shelf: Ephemeral components of the nonlinear internal wavefield. *J. Geophys. Res. Oceans*, **115**.
- Sims, R. P., and Coauthors, 2022: Tidal mixing of estuarine and coastal waters in the western English Channel is a control on spatial and temporal variability in seawater CO 2. *Biogeosciences*, **19**, 1657-1674.
- Sinnett, G., S. R. Ramp, Y. J. Yang, M.-H. Chang, S. Jan, and K. A. Davis, 2022: Large-Amplitude Internal Wave Transformation into Shallow Water. J. Phys. Oceanogr., 52, 2539-2554.
- Small, J., 2001: A nonlinear model of the shoaling and refraction of interfacial solitary waves in the ocean. Part I: Development of the model and investigations of the shoaling effect. J. Phys. Oceanogr., **31**, 3163-3183.

- Small, J., 2001b: A nonlinear model of the shoaling and refraction of interfacial solitary waves in the ocean. Part II: Oblique refraction across a continental slope and propagation over a seamount. J. Phys. Oceanogr., 31, 3184-3199.
- Smith, A., N. Lott, and R. Vose, 2011: The integrated surface database: Recent developments and partnerships. *Bulletin of the American Meteorological Society*, **92**, 704-708.
- Sturley, D.R. and K.R., Dyer, 1992: A topographically induced internal wave and mixing in the Tamar Estuary. *Dynamics and Exchanges in Estuaries and the Coastal Zone*, D. Prandle, Eds., Vol. 40, *Coastal and Estuarine Studies*, AGU, Washington, D.C., 57-74.
- Su, J., and Coauthors, 2020a: Chesapeake Bay acidification buffered by spatially decoupled carbonate mineral cycling. *Nat. Geosci.*, **13**, 441-447.
- Su, J., and Coauthors, 2020b: Source partitioning of oxygen-consuming organic matter in the hypoxic zone of the Chesapeake Bay. *Limnol. Oceanogr.*, **65**, 1801-1817.
- Su, J., and Coauthors, 2021: Supply-controlled calcium carbonate dissolution decouples the seasonal dissolved oxygen and pH minima in Chesapeake Bay. *Limnol. Oceanogr.*, 66, 3796-3810.
- Tai, J.-H., and Coauthors, 2020: Short-Term Variability of Biological Production and CO2 System Around Dongsha Atoll of the Northern South China Sea: Impact of Topography-Flow Interaction. *Front. Mar. Sci.*, **7**, 511.
- Tassone, S. J., A. F. Besterman, C. D. Buelo, J. A. Walter, and M. L. Pace, 2022: Co-occurrence of aquatic heatwaves with atmospheric heatwaves, low dissolved oxygen, and low PH events in estuarine ecosystems. *Estuar. Coast.*, **45**, 707-720.
- Testa, J. M., D. C. Brady, D. M. Di Toro, W. R. Boynton, J. C. Cornwell, and W. M. Kemp, 2013: Sediment flux modeling: Simulating nitrogen, phosphorus, and silica cycles. *Estuarine Coastal Shelf Sci.*, **131**, 245-263.
- Testa, J. M., and Coauthors, 2014: Quantifying the effects of nutrient loading on dissolved O2 cycling and hypoxia in Chesapeake Bay using a coupled hydrodynamic–biogeochemical model. *J. Mar. Syst.*, **139**, 139-158.
- Testa, J. M., W. M. Kemp, C. S. Hopkinson Jr, and S. V. Smith, 2012: Ecosystem metabolism. *Estuarine ecology*, 381-416.
- Testa, J. M., Y. Li, Y. J. Lee, M. Li, D. C. Brady, D. M. Di Toro, and W. M. Kemp, 2017: Modeling physical and biogeochemical controls on dissolved oxygen in Chesapeake Bay: lessons learned from simple and complex approaches. *Modeling Coastal Hypoxia: Numerical Simulations of Patterns, Controls and Effects of Dissolved Oxygen Dynamics*, 95-118.

- Urbancic, G. H., K. G. Lamb, I. Fer, and L. Padman, 2022: The generation of linear and nonlinear internal waves forced by subinertial tides over the Yermak Plateau, Arctic Ocean. *J. Phys. Oceanogr.*, **52**, 2183-2203.
- Vlasenko, V., and K. Hutter, 2002: Numerical experiments on the breaking of solitary internal wavesover a slope–shelf topography. *J. Phys. Oceanogr.*, **32**, 1779-1793.
- Vlasenko, V., N. Stashchuk, M. R. Palmer, and M. E. Inall, 2013: Generation of baroclinic tides over an isolated underwater bank. J. Geophys. Res. Oceans, 118, 4395–4408, doi:10.1002/jgrc.20304.
- Waldbusser, G. G., and J. E. Salisbury, 2014: Ocean acidification in the coastal zone from an organism's perspective: multiple system parameters, frequency domains, and habitats. *Annu. Rev. Mar. Sci.*, 6, 221-247.
- Wang, D., 2006: Tidally generated internal waves in partially mixed estuaries. *Cont. Shelf Res.*, **26**, 1469–1480, doi:10.1016/j.csr.2006.02.015.
- Warner, J. C., C. R. Sherwood, H. G. Arango, and R. P. Signell, 2005: Performance of four turbulence closure models implemented using a generic length scale method. *Ocean Modell.*, 8, 81-113.
- Winters, K.B., 2016: The turbulent transition of a supercritical downslope flow: sensitivity to downstream conditions. *J. Fluid Mech.*, **792**, 997–1012
- Woodson, C. B., 2018: The fate and impact of internal waves in nearshore ecosystems. *Annu. Rev. Mar. Sci.*, **10**.
- Wootton, J. T., C. A. Pfister, and J. D. Forester, 2008: Dynamic patterns and ecological impacts of declining ocean pH in a high-resolution multi-year dataset. *PNAS*, **105**, 18848-18853.
- Xie, X., and M. Li, 2018: Effects of wind straining on estuarine stratification: A combined observational and modeling study. J. Geophys. Res. Oceans, **123**, 2363-2380.
- Xie, X., and M. Li, 2019: Generation of internal lee waves by lateral circulation in a coastal plain estuary. *J. Phys. Oceanogr.*, **49**, 1687-1697.
- Xie, X., M. Li, and W. C. Boicourt, 2017a: Breaking of internal solitary waves generated by an estuarine gravity current. *Geophys. Res. Lett.*, **44**, 7366-7373.
- Xie, X., M. Li, M. Scully, and W. C. Boicourt, 2017b: Generation of internal solitary waves by lateral circulation in a stratified estuary. *J. Phys. Oceanogr.*, **47**, 1789-1797.
- Zhang, F., M. Li, A. C. Ross, S. B. Lee, and D.-L. Zhang, 2017: Sensitivity analysis of Hurricane Arthur (2014) storm surge forecasts to WRF physics parameterizations and model configurations. *Weather and Forecasting*, **32**, 1745-1764.

Zhong, L., and M. Li, 2006: Tidal energy fluxes and dissipation in the Chesapeake Bay. *Cont. Shelf Res.*, **26**, 752-770.

Zhong, L., M. Li, and M. Foreman, 2008: Resonance and sea level variability in Chesapeake Bay. *Continental Shelf Research*, **28**, 2565-2573.