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1 **Dynamics of the Baltic Sea Straits via Numerical Simulation of Exchange Flows**

2

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9

10 **Highlights:**

11 Two-layer exchange is adequately resolved with a resolution of ~100 m.

12 Horizontal resolution in the narrow channels has a large effect on the strait exchange.

13 Dynamics of strait exchange greatly differs in the individual straits.

14 Two-layer transport and blocking show non-unique dependence upon the net transport.

15 Large vertical mixing characterizes gravity currents in the Sound.

16

17

18

19 **Abstract**

20 The Semi-implicit Cross-scale Hydroscience Integrated System Model (SCHISM), which uses  
21 unstructured grids, is set up for the North and Baltic Seas. With a resolution of ~100 m in the  
22 narrow straits connecting the two basins, this model accurately resolves the inter-basin exchange.

23 Validation against observations in the straits shows the model has good skill in simulating the  
24 transport and vertical profiles of temperature, salinity and currents. The timing and magnitude of  
25 the major inflow event in 2014-2015 is also realistically simulated. The analysis is focused on  
26 the two-layer exchange, its dependence on the atmospheric forcing, and dominant physical  
27 balances. The two-layer flows in the three connecting straits show different dependencies upon  
28 the net transport. The spatial variability of this dependence is also quite pronounced. The three-  
29 strait system developed specific dynamics, with time lags and differences between currents in the  
30 individual straits during inflow and outflow conditions. Analysis on the impact of resolution

31 indicates that the performance of the model changes depending on whether the narrow parts of  
32 the straits are resolved with a resolution of 500 m or 100 m. With this ultra-fine resolution,  
33 gravity flows and variability of salinity in deep layers is generally more adequately simulated.  
34 This paper identifies the needs for more profound analysis of the coupled dynamics of Baltic and  
35 North Seas with a focus on the Danish straits.  
36

37 **1. Introduction**

38

39 European straits linking different semi-enclosed seas or connecting them with the ocean (e.g., the  
40 Bosphorus, Dardanelles, Great Belt) are from one to several kilometers wide. The net transport in  
41 those straits is largely driven by river runoff. The shallow depths (~30 m at places) keep the  
42 hydrological characteristics of adjacent basins very different. A two-layer exchange, which is  
43 similar to the transport in tidal estuaries, dominates the straits' dynamics, with upper-layer  
44 transport to basins that are more saline and bottom-layer transport in the opposite direction.

45

46 The Danish Straits between the Baltic Sea and North Sea (Figs. 1, 2) include the Little Belt,  
47 Great Belt, and Øresund (commonly known in English as the Sound). The widths of the above  
48 straits are ~1km, ~15–32km, and ~4km, respectively. The comparison of these geometrical  
49 scales with the internal (baroclinic) Rossby radius of deformation (~5km in the Kattegat, see  
50 Fennel et al., 1991) indicates that the Great Belt could be rotationally influenced.

51

52 Tides are small in the Baltic Sea and most of the mechanical energy input is provided by air  
53 pressure and wind. The balance between the pressure gradient and friction roughly dominates  
54 flow regime in the straits. The analysis of cross-channel density structure by Umlauf and  
55 Arneborg (2009a, b) reveals dynamics that are more complex; the observed transverse Ekman  
56 transport is balanced by the geostrophic transport due to the down-channel tilt of the interface. In  
57 the Baltic Sea, there also are numerous sills critical to the separation between sub-basins and  
58 water exchange (Leppäranta and Myrberg, 2009). Thus the processes over the shallows are  
59 important for the internal mixing and transport of surface and bottom waters (Reissmann et al.,  
60 2009).

61

62 Much progress has been made in recent decades in the physical oceanography of the Baltic Sea  
63 (Feistel et al., 2008, Leppäranta and Myrberg, 2009), including a growing understanding of the  
64 role of Baltic Sea's straits and sills (Omstedt et al., 2014). One of the major gaps in our regional  
65 knowledge is in the field of exchange between sub-basins, turbulent mixing (Reissmann et al.,  
66 2009) and water mass formation. These processes are crucial for the deep-water ventilation  
67 (Meier et al., 2006) and upwelling in the Baltic Sea (Lehmann and Myrberg, 2008). So far, the

68 physical oceanography of the Baltic Sea is rather incomplete because in most modelling studies  
69 the two-layer exchange is neither sufficiently resolved nor considered as fully (two-way) coupled  
70 with the general circulation of interconnected basins. Elucidating and solving some problems in  
71 this field is the basic motivation for the present study and the main difference from our previous  
72 studies (Stanev et al., 2015; Zhang et al., 2016).

73  
74 The water and salt balances, which are intimately related to their major physical drivers, such as  
75 evaporation, precipitation and river run-off, are at the heart of dynamics of estuarine basins.  
76 However, these balances are largely dependent on the dynamical control in the straits connecting  
77 the semi-enclosed basins and open ocean, and in particular on the atmospheric and tidal forcings.  
78 There are a number of process studies dealing with hydraulics in the straits, two-layer exchange  
79 and outflows, which captured the basic physics (Stigebrandt, 1983; Armi, 1986; Armi and  
80 Farmer, 1988; Farmer and Armi, 1988; Borenäs and Lundberg, 1986; Pratt and Lundberg, 1991;  
81 Laanearu and Lundberg, 2000; Gustafsson, 2004; Garrett, 2004; Arneborg, et al., 2007). There  
82 are also many 3D numerical model studies (Lehmann, 1995; Schrum, 1997; Schrum &  
83 Backhaus, 1999; Meier et al., 1999; Janssen, 2002), some of which show large bias in the water  
84 balance and a tendency towards reduced salinities. As recognized by Janssen (2001) and Omstedt  
85 et al. (2014), the ability of the models to simulate saltwater inflows through the Kattegat into the  
86 Baltic Proper, to continuously renew the Baltic deep water and keep the halocline stable is a  
87 prerequisite for multi-year simulations of the Baltic Sea.

88  
89 In earlier 3D modelling studies, the transition zone between the Baltic Sea and North Sea  
90 (hereinafter the area including the Kattegat, Danish straits and the western part of the Baltic Sea  
91 will be referred to as the North Sea–Baltic Sea Transition Zone, NBTZ) was resolved in the best  
92 case with grids of ~1 km, and even coarser in scenario studies. This resolution is not optimal for  
93 narrow straits such as the Sound or Little Belt. Cross-sectional area in the straits depends also on  
94 the position of sea level, which is not fixed; therefore climate model scenarios (Meier et al.,  
95 2017) could be affected by sea-level rise. Sensitivity to global changes is expected to be  
96 strongest in the shallow straits where the dynamic balances could change if sea-level change is  
97 comparable with the depth.

98

99 Some positive trends of the structured-grid modelling of water exchange between the North Sea  
100 and Baltic Sea with respect to model resolution requirement are documented by Gräwe et al.  
101 (2014) who used a multi-nested modeling system with horizontal resolution ranging between 8  
102 km and 600 m in the straits. Mohrholz et al. (2015) also reported model simulations with  
103 resolution of 600 m. Even with this fine resolution, models cannot fully resolve the geometry of  
104 the Little Belt, or the complex topographic structures of the other two straits. Therefore another  
105 strong motivation for this study is to investigate the model performance when using ultra-fine  
106 resolution scales, e.g., between 100 and 500 m.

107

108 Using one-way nesting techniques is also not adequate to address the dynamics of inter-  
109 connected basins (e.g. the coupled system North Sea – Baltic Sea). In this case, the possible  
110 interaction between dynamics in the straits and in the basins connected by the straits is missing.  
111 Thus insufficient model resolution and one-way nesting are considered the major sources of  
112 uncertainties and explain the limited or controversial knowledge of the straits' role in the  
113 dynamics of the European seas.

114

115 The key (and different) role of individual Baltic Sea straits and sills in water exchange and  
116 mixing still remains largely unclear. One problem revealed by the field campaigns is the  
117 intermittent regime of straits exchange and diverse appearances of inflow and associated mixing  
118 and entrainment, all of which have relatively small spatial scales. A clear 4D view based on  
119 observations on temporally variable inflows and outflows in the straits areas is still missing.  
120 Numerical modelling is considered here as an important research tool (as complementary to  
121 observations) to address the complexity of straits dynamics.

122

123 Unstructured-grid models overcome some nesting and resolution problems and allow addressing  
124 various ocean and coastal scales at the same time (Lermusiaux et al., 2013; Danilov, 2013;  
125 Scholz et al., 2013, Stanev et al., 2017). The simulation of water exchange in the NBTZ (Zhang  
126 et al., 2016a) also demonstrated promising perspectives. Earlier, Kliem et al. (2006) described  
127 simulation for the Baltic Sea using a 2D unstructured-grid model.

128

129 In the present study, we describe the improvements in the set-up used here in comparison to the  
130 model of Zhang et al. (2016a) for the same area. It is not possible in a single study to address all  
131 interesting physical aspects studied in several dozen previously published papers. Therefore we  
132 will focus our analysis on (1) model validation against observations in the NBTZ, (2) the role of  
133 resolution, (3) responses to atmospheric forcing with time scales ranging from synoptic to  
134 annual, and (4) the appearances of the two-layer strait exchange in the individual straits.  
135 Dynamics studied earlier will be presented in more general terms just to demonstrate the  
136 consistency of the present numerical simulations with the previous studies. This study is an  
137 extension of the work of Zhang et al. (2016a), but focused on the major Baltic Sea Inflow (MBI)  
138 in 2014-2015. It adds to the study of Stanev et al. (2015), which addressed simulations of earlier  
139 MBI-s and the inter-dependence between transports in the individual straits. One improvement  
140 here is that we increase the horizontal resolution in the straits by about ten times compared to the  
141 0.5 nm horizontal resolution of Stanev et al. (2015), who used a two-way nested modelling  
142 approach. Another new aspect is the more profound model validation in the NBTZ and inter-  
143 comparison of results from numerical simulations using grids with different resolutions.

144

145 One specific research challenge (not addressed in our previous studies) motivating the present  
146 study is the impact of sea level dynamics on the variability of water and salt exchange in the  
147 North Sea and Baltic Sea. This issue is relevant to the causality of inflow events. We will also  
148 address the interdependency of the exchange flows in the individual straits and the temporal and  
149 spatial variability of the two-layer exchange. In a following publication the emphasis will be on  
150 the quantification of individual processes governing the two-layer exchange and mixing in the  
151 NBTZ.

152

153 The paper is structured as follows: Section 2 presents the numerical model; its validation against  
154 observations is presented in Section 3; Sections 4 and 5 describe the circulation in the NBTZ and  
155 its temporal and spatial variability; Section 6 addresses the response of individual straits to  
156 atmospheric forcing and regional inter-dependence between straits transport and sea level;  
157 Section 7 presents the two-layer exchange in the three straits connecting the North Sea and the  
158 Baltic Sea; and, Section 8 quantifies the advantage of using ultra-fine resolution in the straits.  
159 The paper ends with a brief conclusion.

160

## 161 **2. Numerical model**

### 162 **2.1 Model description**

163 Semi-implicit Cross-scale Hydroscience Integrated System Model (SCHISM) is a derivative  
164 product of the original SELFE (semi-implicit Eulerian–Lagrangian finite-element) model (Zhang  
165 and Baptista, 2008), with many improvements described in Zhang et al. (2016b). SCHISM  
166 solves the primitive equations using a hybrid Finite Element and Finite Volume approach (an  
167 example of the grid is shown in Fig. 3a). Terms that place stringent stability constraints (e.g.  
168 CFL) are treated implicitly. Eulerian-Lagrangian method (ELM) is used for the momentum  
169 advection. The model version used in this study is hydrostatic with Boussinesq approximation.

170

171 The combination of Galerkin Finite Element Method (GFEM) with (1) the implicit time-stepping  
172 (which enables efficiency and robustness) and with (2) the ELM enables a good balance in terms  
173 of numerical diffusion and dispersion, because numerical diffusion (inherent in an implicit  
174 method and ELM) balances out by the numerical dispersion (inherent in GFEM). The model is  
175 not immune to sensitivity with respect to grid generation (see next section).

176

177

178 SCHISM has been previously used to simulate the circulation in the North Sea and Baltic Sea  
179 (Zhang et al., 2016a) and therefore its presentation here is very short. The parameterizations (see  
180 Zhang et al., 2016a, b) allow resolving the baroclinic instability, which is very important for  
181 areas dominated by eddy dynamics. Bottom roughness is set to a constant value of 0.5mm; the  
182 bi-harmonic viscosity used is described by Zhang et al. (2016b). No explicit horizontal  
183 diffusivity is used as the higher-order solver is monotone by design; the vertical viscosity and

184 diffusivity are calculated from the generic length-scale model (Umlauf and Burchard, 2003) with  
185 a k-kl configuration. The improvements in the present paper compared to the setup of Zhang et  
186 al. (2016a) are basically associated with better resolution in some critical areas and with  
187 improved forcing.

188

## 189 **2.2 Model area**

190 Bathymetry data used in the present study are the same as the ones used by Zhang et al. (2016a).  
191 However, additionally we use here the Baltic Sea Bathymetry Database version 0.9.3  
192 (<http://data.bshc.pro/>, last accessed on June 5, 2015) with 500 m resolution to improve the  
193 bathymetry in the NBTZ. Model refinements (compared to bathymetry and grid of Zhang et al.,  
194 2016a) have also been done in Skagerrak, Norwegian Trench, Wadden Sea and the area around  
195 the mouth of Oder River.

196

197 The computational grid has ~400K nodes (compared with about 300K nodes in the topography  
198 of Zhang et al., 2016a) with a minimum grid side length of ~80m in the narrow areas of the Little  
199 Belt (Fig. 3). The model grid for the other two straits is shown for example in the supplementary  
200 material (Fig. S1 and Fig. S2). Most of the change of resolution is specified on the shallow shelf  
201 where dynamics are dominated by friction. An essentially uniform resolution of ~3 km is used in  
202 the open-sea parts of two basins minimizing wave distortion because of non-uniform resolution  
203 in unstructured grid models. The vertical LSC<sup>2</sup> grid described by Zhang et al. (2015) is used here  
204 (see Fig. 3b). It allows flexible placement of vertical nodes at each horizontal position; the  
205 Vanishing Quasi Sigma (VQS, Dukhovskoy et al., 2009) ensures smoothness among neighboring  
206 nodes. Shaved cell technique (Zhang et al., 2015) eliminates staircases, shuts down the diapycnal  
207 mixing and reduces the co-ordinate slope and thus the pressure gradient errors. Tests conducted  
208 to demonstrate the performance of the LSC<sup>2</sup> grid can be found in Zhang et al. (2015). As  
209 demonstrated by Zhang et al. (2016a) on the example of Baltic proper (see their figure Fig.A.1),  
210 the use of LSC<sup>2</sup> grid contributes to simulating realistic stratification. This couldn't be achieved in  
211 *S*-grid even with the number of layers being doubled. The vertical LSC<sup>2</sup> grid used here consists  
212 of up to 59 layers in the Norwegian Trench, with an average number of 31 levels in the whole  
213 model domain.

214

### 215 **2.3 Initialization and forcing**

216 Monthly climatological salinity and temperature data (Janssen et al., 1999) are used to initialize  
217 the model, like this was the case in the paper by Zhang et al. (2016a). However, we use  
218 here finer-resolution data for atmospheric forcing, including hourly wind, atmospheric  
219 pressure, air temperature, dew point temperature and cloud cover from the 7 km-  
220 resolution COSMO-EU model of German Weather Service (DWD). From these data, the wind  
221 stress, fluxes of sensible and latent heat, as well as short wave and long wave radiation are  
222 computed. The Swedish Meteorological and Hydrological Institute (SMHI) EHYPE (pan-  
223 European HYdrological Predictions for the Environment) product is used for the  
224 freshwater fluxes from 34 rivers discharging into the Baltic Sea and North Sea.

225  
226 The model has two open boundaries (west of the English Channel and between the British Isles  
227 and Scandinavia, Fig. 1). At these boundaries hourly values of elevation, horizontal velocity,  
228 salinity, and temperature were used, which were taken from the Copernicus product  
229 (<http://marine.copernicus.eu/>; last accessed in May 2017) interpolated at each time step onto the  
230 model grid. The use of these data is considered an optimal solution because they are dynamically  
231 consistent, based on up-to-date modelling (O’Dea, 2012) and have been validated extensively.

232  
233 After an initialization period of four years the model is run for another two years, 1 March 2014  
234 to 31 March 2016, which is the period analyzed in this paper. We will refer to this reference  
235 experiment as the control run (CR). An additional experiment was carried out in which all areas  
236 in the NBTZ where the resolution in the CR was finer than 500 m were resolved with a  
237 horizontal resolution of 500 m. We will refer to this experiment as the E-500. Comparison  
238 between Fig. 3c, d and Fig. 3a, b illustrates the difference in the model resolution of two  
239 experiments for the area of Little Belt. Fig. S1 and Fig. S2 illustrate the difference between the  
240 CR and E-500 for the straits of Sound and Great Belt, respectively.

241  
242 The simulations were conducted on Mistral peta-scale supercomputer of the German Climate  
243 Computing Center (Deutsches Klimarechenzentrum GmbH (DKRZ)). On 1024 CPUs the model  
244 runs ~150 times faster than real time.

245

### 246 3. Validation against observations

#### 247 3.1 Sea level and transport in the straits

248 The overall performance of SCHISM for the area in the present study has been addressed by  
249 Zhang et al. (2016a). Therefore the validation here will focus primarily on areas and specific  
250 periods, which have not been addressed in this earlier study, and include the NBTZ and periods  
251 of recent extreme events. The studied period is chosen such that it includes the MBI in 2014-  
252 2015, for which there are already observations (Mohrholz et al., 2015) and analyses. The realism  
253 of the model with respect to the transport in the straits will be assessed. We will compare our  
254 estimates with the computations based on the method proposed by Håkansson (citation from  
255 Meier et al., 2003), which assumes a balance between along-strait pressure gradient and bottom  
256 friction term. This dominant balance is proven in those studies after estimating the correlation  
257 between sea level difference in two locations at both sides of the straits and the observed  
258 volumetric flows obtained from ADCP ship-borne transects and moored Aanderaa current meters  
259 across the Drogden Sill. The calibration proposed by those authors used the two tide gauge  
260 stations Viken and Klagshamn, located in the northern and southern entrance of the Sound,  
261 respectively (see Fig. 2 for their positions).

262

263 The index of agreement  $D$  proposed by Willmott (1981) measures the degree to which the  
264 observed data  $O$  is estimated by the predicted value  $P$ ,

$$265 \quad D = 1 - \frac{\sum_{i=1}^n (P_i - O_i)^2}{\sum_{i=1}^n (|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \quad (1)$$

266

266 Here,  $n$  is the number of observations (index  $i$ ) and the overbar is the temporal mean of the  
267 observed data. A value of 1 would indicate perfect agreement, whereas a value of 0 would  
268 indicate no agreement at all. In the third and fourth line of Table 1,  $P$  and  $O$  are the normalized  
269 transports estimated from the parametric model presented by Meier et al. (2003) and numerical  
270 model, respectively.

271

272 The observed and simulated sea levels at these two stations are in a very good agreement (Fig.  
273 4a-b and Table 1). Noteworthy is the phase difference between sea level at these stations  
274 (compare Fig. 4a and Fig. 4b). The pressure gradient between the two of them changes to  
275 strongly negative (Fig. 4e) giving the first “push” of the MBI in 2014. The timing of this event is

276 shown by the vertical green line. The model errors are small in comparison to the variances of  
 277 analyzed variables and therefore  $D$  is quite high. The index of agreement from the parametric  
 278 model of 0.97 is considered here as an “ideal” agreement because it is based on calibrated data.  
 279 Our simulations yield 0.94, which demonstrated that the agreement between the observations and  
 280 the fluxes ( $Q_m$ ) computed with SCHISM is very close to that “ideal” case.  
 281

	<b>D</b>	<b>RMSE</b>	<b>B</b>
$\xi_{obs}, \xi_m$ (Viken)	0.88	0.15 (m)	0.04 (m)
$\xi_{obs}, \xi_m$ (Klagshamn)	0.92	0.09 (m)	0.10 (m)
$\Delta\xi_{obs}, Q_{par}$ (normalized)	0.97	0.33	-0.03
$\Delta\xi_{obs}, Q_m$ (normalized)	0.94	0.42	-0.08

282  
 283 Table 1. Index of agreement, root mean square error (rmse) and bias of sea levels (first and second  
 284 lines) at the gauges Viken and Klagshamn (see Fig. 2 for their positions). The agreement between  
 285 the normalized (non-dimensional) data series of sea-level differences between the same stations  
 286 and the net transport estimated from the parametric model of Håkansson (citation from Meier et  
 287 al., 2003) are shown in the third line. The present simulations are shown in the fourth line.  
 288  
 289  
 290

291 The temporal evolution of sea level (Fig. 4a, c) up to the Baltic Sea stations Visby and Degerby,  
 292 the latter known recently as Föglö, (see Fig. 1 for their position) demonstrates a synchronous  
 293 sea-level dynamics over a larger area (the green vertical line shows that phase differences are  
 294 relatively small). These stations are representative of the volume change of the whole Baltic Sea  
 295 (e.g. Jacobsen 1980). As demonstrated by Janssen et al. (2001), Station Degerby has high skill in  
 296 describing the variability of Baltic Sea surface elevation. The accurate predictions of sea level  
 297 elevation in stations Visby and Degerby manifests the model skill with respect to the dominant  
 298 dynamics in the Baltic Sea.  
 299

300 According to Håkansson (citation from Meier et al., 2003), the agreement between the observed  
 301 and simulated sea levels at stations Viken and Klagshamn guarantees a correct prediction of the

302 volumetric transport through the Sound. This concept is based on the assumption of balance  
 303 between along-strait pressure gradient and bottom friction term. It is supported by the third and  
 304 fourth lines in Table 1, which show the agreement between non-dimensional sea-level  
 305 differences at these two stations and net transport (see also Fig. 4e). Notably, the parametric  
 306 estimations of Håkansson were calibrated to observations; SCHISM was not specifically  
 307 calibrated. These results indicate that also in SCHISM the balance between along-strait pressure  
 308 gradient and bottom friction plays the major role in the Sound. Furthermore, the correct estimate  
 309 of the straits' transport is a prerequisite for the good model skill in the entire Baltic Sea.  
 310 Obviously, the good skill in stations Visby and Degerby (Fig. 4a, c) and in the straits are  
 311 consistent with each other.

312

### 313 **3.2 Currents in the straits**

314 Data from three ADCP stations in the Danish straits operated by the DMI are used here to  
 315 validate simulated currents. Two stations, Østerrenden (55.363266N 11.022787E) and  
 316 Vengeancegrund (55.207542 N11.086632E), are in the Great Belt, and the third , Drogden Fyr  
 317 (55.536380N 12.711413E), is in the Sound (see Fig. 2 for their position). Data used here are  
 318 recorded at 3 depths at all three stations during 01 October 2014-01 June 2015. Comparison with  
 319 simulations demonstrated a good qualitative agreement at the three stations (Fig. 5). The model  
 320 overestimates slightly the velocity maxima. The quantitative validation shows that the coefficient  
 321 of agreement is above 0.82, reaching 0.94 at Vengeancegrund (Table 2). Compared to the  
 322 relatively large amplitudes of currents the rms error is not too big. The maximum bias is ~6 cm/s,  
 323 which is also reasonable, keeping in mind that model forcing is not perfect.

324

325

<b>Station, depth</b>	<b>D</b>	<b>RMSE [m/s]</b>	<b>B [m/s]</b>
Drogden, 3m	0,86	0,39	-0,010
Drogden 5m	0,93	0,29	-0,010
Drogden 10m	0,91	0,18	-0,041

Vengeancegrund, 1m	0,94	0,28	-0,028
Vengeancegrund, 3m	0,93	0,30	-0,033
Vengeancegrund, 5m	0,94	0,28	-0,048
Oesterende 5m	0,86	0,38	0,042
Oesterende 10m	0,87	0,34	0,054
Oesterende, 14 m	0,82	0,29	0,064

326  
327 Table 2. Index of agreement (D), rmse and bias (B) of observed along-channel currents and  
328 currents estimated by the model (see Fig. 2 for the positions of observations).

329

330

331 It is noteworthy that the signals in the two straits differ substantially not only by their magnitude,  
332 but also by phase.

333

### 334 **3.3 Salinity**

335 Earlier validations of SCHISM against MARNET observations

336 ([http://www.bsh.de/en/Marine\\_data/Observations/MARNET\\_monitoring\\_network/index.jsp](http://www.bsh.de/en/Marine_data/Observations/MARNET_monitoring_network/index.jsp), last  
337 accessed July, 2017) revealed a good consistency of simulations (Zhang et al., 2016a). In the  
338 following, we will present model validation against different data source, e.g., freely available  
339 CTD and bottle data from the International Council for the Exploration of the Sea (ICES)  
340 database (<http://ocean.ices.dk/HydChem/HydChem.aspx?plot=yes>, last accessed July, 2017).

341 From this dataset we selected the observations situated along the pathway of salt intrusions (BY-  
342 1, BY-5, BY-7 and BY-15; see Fig. 1 for their positions). The validation was performed for a  
343 period of one year starting 1 September 2014 and thus covering the time of the MBI during the  
344 winter 2014-2015.

345

346 The ability of model to capture the change of thermohaline characteristics of the North Sea  
347 waters penetrating into the Baltic Sea during the MBI along their way over the sills and in the

348 small regional sub-basins is illustrated in Fig. 6. Simulations and observations show clearly the  
349 delayed appearance of salt-water intrusions with increasing distance from the straits, as well as a  
350 decrease of the amplitude of salinity outbreak associated with the MBI at stations far from the  
351 NBTZ. The model skill is good (D is above 0.91 in bottom layers in all stations). In the surface  
352 layers D is also above 0.91. Only in stations BY-7 and BY-5, D drops to 0.80 which is a  
353 reasonable value taking into consideration possible errors in the model and its forcing. Namely,  
354 using hourly data with 7 km horizontal resolution is perhaps still not fine enough. Since the  
355 Baltic Sea is enclosed basin, unresolved atmospheric dynamics in its large coastal areas could  
356 bias ocean simulations. Bulk aerodynamic formulas are also not perfect. Using coupled  
357 atmosphere-ocean models with high resolution in the straits and other sensitive areas could be an  
358 adequate step toward improvement of atmospheric forcing.

359  
360 The time versus depth diagrams of salinity (Fig. 7) demonstrate that the time when the mixed  
361 North Sea water reaches the observational locations is very well forecasted by the model. In the  
362 stations Darss and Arkona simulated salinity values exceed the observed ones, while in the  
363 Gotland Basin simulated bottom salinity values are slightly underestimated (compare Fig. 7g and  
364 Fig. 7h). Although peaks in salinity associated with the MBI are slightly overestimated in the  
365 shallow NBTZ area, the mixing on their way down to the Gotland Basin reduces the magnitude  
366 of salinity signal below the observed values. The agreement between simulations and  
367 observations in the Gotland Basin is very valuable because the Gotland Basin integrates temporal  
368 development of salinity in the Kattegat, Belt Sea and the Western Baltic (Janssen et al., 2001). In  
369 conclusion, without special tuning, the model captures salinity intrusions in the straits. The  
370 deterioration of the bottom water properties in E-500 will be addressed in section 8 (see the  
371 panels on the right of Fig.7). More realistic representation of the penetration of mixed water  
372 down to the Gotland Basin and its spreading there could be achieved after a closer look at the  
373 parameterizations used, which will be addressed in future publications

374

#### 375 **4. Overall presentation of the circulation in the NBTZ.**

376 The model allows resolving sharp fronts in salinity (the panels on the left-hand side of Fig. 8)  
377 and numerous small-scale features in the relative vorticity (the panels on the right-hand side of  
378 Fig. 8). The comparison between the inflow and outflow patterns demonstrates that the position

379 of positive and negative vorticity alternates; that is demonstrated well in the Great Belt. The  
380 vorticity alternation follows the alternating direction of flow in the straits. With a much coarser  
381 resolution, as used in earlier modelling studies based on structured grids, one cannot accurately  
382 resolve the velocity gradients in the straits. The zoom-in views of the model grid in Fig. 3 (see  
383 also supplementary Fig. S1\_and Fig. S2) and the insets in the Sound and Great Belt shown in  
384 Fig. S3 support this conclusion. The complex flow structure could be important for the resistance  
385 in the straits, which depends on the velocity shear. The above reasoning is supported by the  
386 analysis on the role of horizontal resolution (CR versus E-500) presented in section 8. With  
387 increasing distance from the straits, the scales of vorticity patterns increase. Most of them show  
388 an elongated shape, which is explained by the predominant narrow jets in the area of the Arkona  
389 and Bornholm Basins.

390  
391 The inflow and outflow situations are well distinguished in the salinity patterns (Figs. 8a, 8c).  
392 During the outflow conditions low salinity surface water displaces to the north (see also the  
393 sharp front in Fig. S3e, f), resulting in a reduction of sea surface salinity (SSS) in the Kattegat by  
394 about 6. The propagation pathways of these low-salinity water masses are well seen in the  
395 plumes originating from the Great Belt and Sound (Fig. 8a). The salinity front separating the  
396 Skagerrak water mass from the Kattegat water mass is “pushed” north of the Skagen (Fig. 8a). In  
397 most inflow cases, the Skagerrak water (with higher salinity) depicts a jet-like propagation  
398 pattern in the direction of the Sound. The front separating these two water masses is extremely  
399 strong, reaching more than 10 salinity units per km (Fig. S3f) at certain times. The two straits  
400 provide two sources of high salinity water entering the Bornholm Basin (Fig. 8c).

401  
402 The vertical salinity section through the Sound shows a typical gravity-current type propagation  
403 starting from the Drogden Sill (the shallowest location in Fig. 9). This current is seen even better  
404 in the turbulent kinetic energy (TKE) patterns; maximum values are in a thin bottom layer. TKE  
405 shows another maximum zone at the northern entrance of the Sound where the jet from the  
406 Kattegat converges towards the strait (Fig. 8c). This is a zone of extreme vertical mixing; its  
407 dynamics can change vertical stratification and strongly affect the propagation properties of  
408 gravity currents.

409

410 The TKE decreases in the middle of the water column, particularly in the Baltic Sea part of the  
411 cross-section. It further increases in the surface layer, displaying a characteristic profile known  
412 from other similar strait environments (Stanev et al., 2017).

413

## 414 **5. Temporal and spatial patterns of inflows and outflows.**

### 415 **5.1 Chronology of the MBI in 2014-2015**

416 Inflows and outflows in the Danish straits have much in common with tidally driven estuarine  
417 exchange; however in the case of the Baltic Sea the role of atmospheric forcing is more  
418 important than that of tides (Stanev et al., 2015). MBIs are to a first order barotropic phenomena  
419 driven by an emptying-refilling process of the Baltic Sea (Schimanke et al., 2014). Existing  
420 concepts explaining their chronology have been mostly based on observations (Lass and  
421 Matthäus, 1996). However, observations are not available over large areas and for sufficiently  
422 long periods. Furthermore, MBIs appear rarely (about once per ten years in the recent times) and  
423 their statistical description is difficult. Numerical modelling provides an opportunity to address  
424 the timing and causality of MBI for the entire area of inter-connected basins.

425

426 The temporal-spatial evolution of MBI during 2014-2015 is presented in Fig. 10 along the  
427 section line shown in Fig. 1. In the area of the straits this line follows the section line through the  
428 Sound as shown in Fig. 2. Sea level in the Baltic Sea is higher than in the North Sea; this is  
429 typical in estuarine basins. The mean difference between the areas to the left and to the right of  
430 Drogden Sill (see the blue arrows in Fig. 10) is ~17 cm. This sill (the shallowest depth in Fig. 9)  
431 physically separates the two basins as seen by the variability pattern in Fig. 10a (we will come  
432 again to the “separation issue” in section 6.1). In the North Sea, the temporal variability is  
433 dominated by tides. For better readability of plots, model data have been filtered with a window  
434 of 1 day, so only neap-spring variability is seen in Fig. 10.

435

436 Sea level variability in the Baltic Sea is largely driven by atmospheric forcing; the event at the  
437 beginning of December 2014 is of particular importance. On 2 December 2014 (triangle symbol  
438 on the time-axis in Fig. 10a), sea level in the Baltic Sea dropped to ~52 cm below the sea level  
439 found to the north of the Sound (see also Fig 4 manifesting the precursory period). In only 2 days  
440 this slope triggered a huge transport (MBI) resulting in an increase of sea level in the Baltic Sea

441 by 82 cm during the next ~40 days (Fig. 4c, d). A similar situation was observed in November  
442 2015, this time the MBI appearing as two strong pulses in the winter of 2015-2016 (Fig. 10a).

443

444 The presentation in Fig. 10a is instructive also for some important general circulation features.  
445 One feature is the low sea level at km 800 (in the Skagerrak) that reflects the cyclonic rotation of  
446 currents there. As seen in Fig. 10e, bottom salinity in the Baltic Sea shows an increase (positive  
447 anomaly) right after the outbreak of MBI in 2014. This signal propagates to the east, which is  
448 deduced from the slope of the salinity anomaly pattern. The speed of propagation decreases with  
449 increasing distance from the strait, particularly approaching the Gotland Basin. This basin is the  
450 “final destination” of positive bottom salinity anomaly (compare with the delay of phases of  
451 salinity signal illustrated by the blue line in Fig. 6). There is not a clear response of the bottom  
452 salinity in the North Sea to the MBI, which is easily understandable. However, this does not hold  
453 for the SSS. Indeed the surface plume propagation depicts situations with alternating positive and  
454 negative anomalies, which propagate to the west (the slope of contours in the North Sea, Fig. 10c  
455 is opposite to the one in the Baltic Sea, Fig. 10e). The overall temporal variability is  
456 approximately seasonal. What seems non-trivial is that the largest positive anomalies on both  
457 sides of the Drogden Sill are generated almost simultaneously and propagate in both directions as  
458 surface plumes in the North Sea and bottom plumes in the Baltic Sea. Another interesting result  
459 of the simulations is the entrapment of saltier water at about km 1500, which is the area of  
460 Bornholm Basin (red arrows in Fig. 10). This basin accumulates saltier water and acts as a long-  
461 term reservoir, which sporadically “discharges” parcels of salty water to the east. This is seen as  
462 short-term positive-anomaly “strips” following the direction of bottom water propagation. While  
463 the presence of these strips is consistent with the dominant concept about the periodic export of  
464 saltier bottom waters from the retention basins (e.g., the Bornholm Basin, Jakobsen, 1995), an  
465 explanation of the “vertical strips” seen in the bottom salinity anomaly is needed. This is not an  
466 unphysical result. Its appearance is explained by the fact that the anomalies of bottom salinity  
467 depend on the position of the chosen thalweg, as well as on the vertical stratification; the latter is  
468 highly variable in different depth intervals.

469

## 470 **5.2 Different dynamics in the three straits**

471 Comparison of the SCHISM simulations in the three straits (Little Belt, Great Belt and Sound)  
472 are shown in Fig. 11. In order to give more detailed views on the results, time versus distance  
473 diagrams in these figures are shown only in the NBTZ, that is along the section lines in Fig. 2.  
474 While the pressure gradient forcing appears in a semi-coherent way in the three straits, the  
475 temporal-spatial response of individual straits to atmospheric forcing is rather different. The sea-  
476 level anomalies (left panels in Fig. 11a) are extremely large in the winter months of 2014 and  
477 2015 providing the major drivers for the strong inter-basin exchange. This barotropic forcing  
478 triggers a clear salinity response in the three straits, which largely differs between the surface and  
479 bottom layers. In the Sound (Fig. 11b) pulses of higher-salinity surface water are very weak (and  
480 with a very small along-strait extension). However, bottom salinity pulses appear quasi-  
481 periodically in this strait (Fig. 11c); the strongest of them extends up to the Bornholm Basin  
482 (~km 300). The low-salinity values in the Sound area between km 150 and 250 in Fig. 11c do not  
483 mean an absence of salinity intrusions there, but demonstrate that these are shallow areas with  
484 salinity values close to the surface ones.

485  
486 Saltier mixed North Sea water shows much longer excursions in the Great Belt, both in the  
487 surface and bottom layers, than in the surface layers of Sound. Great Belt section reveals the  
488 zones of saltier bottom waters in the Arkona Basin (about km 300). Note that the position of 300  
489 km along the Sound pathway almost coincides with the position of 500 km along the Great Belt  
490 section (Fig. 2). These positions demarcate the Bornholm Basin, an area of salt-water  
491 accumulation. In the two straits, MBI is better identified by the salinity change in the bottom  
492 layers. The comparison between the sections along the Great Belt and Sound, which slightly  
493 overlap at the end of the Great Belt section, demonstrates that the high bottom salinity reflects  
494 the water originating from the Sound. This conclusion is justified by the fact that the bottom  
495 salinity maximum at about km 500 along the Great Belt section is separated from the main pulse  
496 of saltier bottom water.

497  
498 The Little Belt shows more “diffuse” patterns, which is due to the fact that the narrow opening in  
499 this strait needs more time to propagate the saltier North Sea water. While the importance of the  
500 Little Belt for the exchange between the North Sea and Baltic Sea is small under normal events,

501 it becomes more substantial during the MBI. In the southernmost part of the section line in this  
502 strait (at about km 200) a backward propagation of positive salinity anomaly occurs, which is  
503 identified by the opposite slope of the contours in the time versus distance diagram. This  
504 illustrates the fact that saltier water in the Great Belt, which tends to fill the western Baltic Sea,  
505 reaches this location faster and in bigger amounts than water originating from the Little Belt.

506

## 507 **6. Synchronous and asynchronous responses in the individual straits**

### 508 **6.1 Interdependence of straits transport and sea level**

509 It is still unclear whether the changes of sea level in the Baltic Sea and North Sea are equally  
510 important for the net transport, and what the expected dependence during inflow and outflow  
511 situations is. To answer these questions we analyze first the dependence of the volume fluxes  
512 integrated over the three straits on the difference between sea level in the Kattegat and central  
513 Baltic Sea. Unlike the analysis presented in section 3.1, which was focused on the dominant  
514 frictional control in the straits, the difference between sea levels in the Kattegat and central  
515 Baltic Sea reflects the role of general oceanographic conditions in the two basins and can  
516 potentially elucidate the leading role of one of them (see the discussion in section 3.1 about the  
517 representativeness of sea level in the central Baltic Sea).

518

519 The scatter plots in Fig. 12 are shown for two 14-days periods during which the transport was  
520 dominated by either outflow from the Baltic Sea (1-15 Nov, 2014) or inflow (6-21 Dec, 2014).  
521 As expected, there is a clear correlation between sea-level difference and net flow. The smaller  
522 correlation during the inflow situation (the period of MBI) is not so trivial and is explained with  
523 the help of Fig. 12d. The inflow period-1 was characterized by multiple pulses, which is  
524 consistent with a similar situation during the 1993 MBI (Stanev et al., 2015). This is comparable  
525 with the salinity change described by Jakobsen (1995): inflows were characterized by larger  
526 oscillations, while outflows showed smoother changes. Obviously, the 1993 case observed by  
527 Jakobsen (1995) was almost repeated in 2014-2015. The unstable dynamics during inflows thus  
528 makes it possible that large outflows occur in times of small sea-level differences between the  
529 Kattegat and Central Baltic Sea, i.e., oscillations of sea levels in the two basins and the strait  
530 flow could become asynchronous.

531

532 The correlation between the sea level differences between the two basins and the sea level in the  
533 Kattegat (Fig. 12b), from one side, and the central Baltic Sea (Fig. 12c), from the other,  
534 demonstrates that the variability of sea level in the Kattegat plays the leading role (correlation  
535  $\sim 0.91$ ). Sea level in the central Baltic Sea correlates weakly with the sea level difference during  
536 outflows (correlation  $\sim -0.38$ ). Changes of sea level in the central Baltic Sea are more important  
537 for the inflows. In this case the correlation reverses with  $-0.73$  and  $0.5$  for the Baltic Sea and the  
538 Kattegat, respectively. This result is reminiscent of similar results for the Black Sea-  
539 Mediterranean Sea system based on analysis of observations (Volkov et al., 2016) and numerical  
540 simulations (Stanev et al., 2017), i.e. the major driver is the forcing from the outside basin.  
541 However, inflows are strongly dependent on the sea level in the central Baltic Sea, which  
542 supports the existing concepts (Lass and Matthäus, 1996).

543  
544 The areal distribution of correlation between net straits transport and sea level (Fig. 12e) reveals  
545 an overall anti-symmetric pattern (positive correlation in the Kattegat and negative correlation in  
546 the Southern Baltic Sea). With increasing distance from the straits, the magnitude of correlation  
547 decreases. This reflects the delay associated with the propagation of barotropic signal to remote  
548 locations. The areas of transition from positive to negative values are very sharp and identify the  
549 natural (physical) boundaries between the North Sea and Baltic Sea. The trend of larger negative  
550 correlations along the Scandinavian Baltic Sea coast reveals the role of geostrophic control. The  
551 larger correlation along the western coast of Kattegat is explained with the larger tidal range  
552 there (see Fig. 6 of Stanev et al., 2015).

## 553 554 **6.2 Similarities and differences in the response of individual straits to atmospheric forcing.**

555 Using a numerical model with horizontal resolution of  $0.5$  nm, Stanev et al. (2015) demonstrated  
556 that the correlation between transports in the Sound and Great Belt cannot be represented with a  
557 simple linear regression line. This does not fully conform to the simple idea that the transports in  
558 the straits are linearly proportional, the coefficient being the ratio between cross-sectional areas.  
559 There are different estimates for this ratio. Mattsson (1996) claims that the narrow passages in  
560 the Belt Sea have vertical cross-sectional areas on the order of  $300\,000\text{ m}^2$ , while the narrow  
561 cross-sectional areas in the Sound are about  $60\,000\text{ m}^2$ . They found that the mean partition of the  
562 instantaneous flows through the Great Belt Sea and Sound is  $8:2$ , rather than the generally

563 accepted (at that time) estimate of 8:3. Kullenberg and Jacobsen (2000) reported a quite different  
564 ratio between cross-sectional areas of two straits. They claimed that the cross-sectional area over  
565 the sill in the Sound was 0.1 km<sup>2</sup>; in the Belt Sea the narrowest section was 0.16 km<sup>2</sup>. The ratio  
566 between the transports in the two straits estimated by Sayin and Krauss (1996) was 3:1. The  
567 estimations of Fischer and Matthäus (1996) and Jakobsen and Trebuchet (2000) for the transport  
568 ratio (TR) was 2.67. The estimation of Fu (2013) was 2.78. Besides the ratio between transports  
569 in the two strait, the response times are also subject to large uncertainties (Stanev et al., 2015).

570

571 One could expect that the differences between previous estimates of exchange flows were most  
572 probably due to the use of different cross-sectional areas (more generally topographies). The  
573 areas of narrowest cross-sections in the two straits based on the topography and model resolution  
574 used in the present study are 121100 m<sup>2</sup> and 73000 m<sup>2</sup>. The ratio between the smallest cross-  
575 sectional areas of the Great Belt (between Nakskov and Langeland) and Sound in our model is  
576 1.66. We will call this number area ratio (AR).

577

578 The barotropic transports in the Great Belt and Sound for October 2014- May 2015 indicate that  
579 the magnitudes of oscillations in the two straits largely exceed the mean values (Fig. 13a). In the  
580 Great Belt the the rms difference of barotropic transport from its mean value is  $6.64 \times 10^4$  m<sup>3</sup>/s;  
581 the corresponding number for the Sound is  $2.89 \times 10^4$  m<sup>3</sup>/s, while the net transport for the Baltic  
582 Sea is about  $1.5 \times 10^4$  m<sup>3</sup>/s (Liljebladh and Stigebrandt, 1996). The averaged TR for October  
583 2014 - May 2015 estimated here is 2.70 (see the regression curve in Fig. 13b), which compares  
584 well with the numbers 2.63-2.75 of Stanev et al. (2015) who used a model of the same area with  
585 a resolution of 1 km. This result can serve as a justification that the TR is reasonably simulated  
586 even with this “coarse” resolution of ~1km.

587

588 There is a substantial difference between the TR estimated from the regression curve (2.70) and  
589 the AR (1.66) demonstrating that the narrower and shallower strait (Sound) exerts larger  
590 resistance. The scatter plot (Fig. 13b) gives an idea about the robustness and stability of the  
591 above averaged estimates. The comparison between this averaged number (2.70) and the large  
592 variance of TR (2.30) demonstrated the complex inter-relationship between transports in the two

593 straits (see Fig. 13g) and their large variations over time. Stronger variability in the Great Belt  
594 compared to the Sound is partially due to high frequency (tidal) oscillations in the former; the  
595 Sound effectively filters out the tidal oscillations (Stanev et al., 2015).

596

597 The distribution of the TR is non-Gaussian (Fig. 13e). There is a clear inflow-tail, i.e. the  
598 transport in the Sound gets relatively stronger during inflow events. This tendency during  
599 inflows is illustrated in the comparison between Fig. 13c and Fig. 13d where the distribution of  
600 the TR is separately shown for inflow and outflow cases. Although the shapes of these  
601 histograms are not fully identical with the results of Stanev et al. (2015, compare with their Fig.  
602 8) the overall result suggests that the change in transport starts first in the Sound. The temporal  
603 evolution of the distribution of the transport ratio (Fig. 13g) clearly explains the non-Gaussian  
604 shape of histograms.

605

606 The asynchronous responses of the two straits revealed by the asymmetry of the curve in Fig. 13f  
607 against zero time lag is explained as a result of the Sound being closer to the inflowing waters,  
608 which follow the eastern Kattegat coast (see Fig. 8c). Unlike the similar analysis in Stanev et al.  
609 (2015), we did not filter out the tides, therefore the lagged-time-correlation in Fig. 13f is affected  
610 by M2 tides.

611

612 The basic difference between the correlation of barotropic transports in the Little Belt and Great  
613 Belt (not shown here) from the case addressed above (Sound and Great Belt) is that the  
614 coefficient in the regression curve is about two times smaller, because the transport in the Little  
615 Belt is about half of that in the Sound. Notably, the average TR (5.11) is much smaller than its  
616 variance of 12.96 due to a very low correlation between the flows in the Little Belt and Great  
617 Belt.

618

## 619 **7. Two-layer exchange in the straits**

620 In some straits connecting estuarine basins with the neighboring seas, the net transport in the  
621 upper and bottom layers shows opposite trends. With the increase of net outflow, i.e. the  
622 transport in the direction of the long-term mean (barotropic) transport, the upper layer flow  
623 increases and the bottom flow decreases and is sometimes blocked. During the inflow situation,

624 the upper-layer transport decreases and the bottom layer transport increases (Möller, 1928). This  
625 old concept usually assumes that there are two water masses in the upper and bottom layers  
626 moving in opposite directions separated by an interface where velocity tends to zero. This is a  
627 typical situation in estuarine circulation. One such case is the Strait of Bosphorus where the two-  
628 layer exchange is well known.

629

630 In the NBTZ the frontal area separating the Kattegat and Baltic Sea water masses is periodically  
631 displaced back and forth by the atmospheric forcing (Fig. 9a, c); the vertical structure of the two-  
632 layer flow is not always well pronounced, unlike in the Bosphorus Strait (see for more detail  
633 Stanev et al., 2017) . The latter resembles a salt wedge where the interface is almost horizontal  
634 (slope of 1-2 m per kilometer) and covers the entire strait. The simulated dynamics in the Baltic  
635 Sea straits show rather different and more diverse appearances.

636

637 The lack of profile observations over large areas in the straits makes it impossible to validate  
638 extensively the two-layer volume exchange. We can at least compare the present simulations  
639 against other similar cases and check whether concepts valid for other straits hold for the Baltic  
640 Sea straits, whether this is the case everywhere in these straits, and what the differences are.

641

642 As shown in section 3.1 the volumetric transport is simulated reasonably well (Fig. 4). This  
643 (barotropic) transport integrated over the sections shown in Fig. 14a is used as the independent  
644 variable (x-axis in Fig. 14), against which we compare the transports in the upper and bottom  
645 layers across the same sections (y-axis). Along most of these sections, the simulated upper-layer  
646 flow decreases and the bottom-layer flow increases with decreasing net transport. This supports  
647 the previous estimates based on simulations with the same model and observations in other  
648 similar straits (Stanev, 2017). It is noteworthy that the model has not been specially tuned to  
649 earlier theoretical analyses, some of which were based on simpler theoretical concepts or  
650 observations. This demonstrates that these results have general applicability. What has not been  
651 sufficiently addressed in earlier analyses in the NBTZ is the spatial variability of the dependence  
652 of transport in each layer on the total net transport. This is illustrated in Fig. 14 for three sections  
653 in the Little Belt (on the left), four sections in the Belt Sea (in the middle), and four sections in  
654 the Sound (on the right). The positions of the analyzed sections are shown in Fig. 14a. The plots

655 on the top correspond to the northernmost transect, and the plot on the bottom to the  
656 southernmost transect.

657  
658 The comparison between two-layer flows in the three straits shows similar trends, but the  
659 magnitudes are different (notice different ranges for each strait). With the exception of the  
660 northernmost section in the Sound (Fig. 14c) and the southernmost section in the Little Belt (Fig,  
661 14j), all other plots show that in most cases the flow is unidirectional for most of the transport  
662 variability ranges. This means that either the surface or bottom flow equals the net transport, i.e.  
663 we observe a blocking of transport in one of the layers (Oğuz et al., 1990). As the magnitude of  
664 net transport decreases below some critical value the transport becomes two-directional; this  
665 transition is not linear as seen by the curvature of transport dependence.

666 In an idealized case, the surface and bottom transports can be represented by two crossing curves  
667 (Oğuz et al., 1990). This would mean that for one value of net transport there is one and only one  
668 pair of values for the upper and bottom layer transports. The scatter of data suggests that the  
669 appearance of two-layer transport is quite diverse (different possible combinations of surface and  
670 bottom flows could correspond to the same net transport). Furthermore, the scatter is different in  
671 different straits and at different locations in the straits. This manifests that there are not a unique  
672 critical values of net water transport, beyond which two-layer transport transforms into one-layer  
673 transport. Several representative examples are addressed below, one for each strait.

674  
675 Extreme transports in the Little Belt are more than five times smaller than the extreme transports  
676 in the Great Belt. Two-way transport is observed for only very low net transports (below  $3 \times 10^3$   
677  $\text{m}^3 \text{s}^{-1} = 0.003 \text{ Sv}$ ). At the southernmost end of this strait the spread of data is large, which  
678 suggests that the two-layer transport there is substantially affected by other processes (e.g., the  
679 local circulation) after the flow leaves this narrow strait.

680  
681 Along the entire Great Belt, from the northernmost reaches down to the Fehmarn Belt the  
682 transport curves look very similar. The largest scatter of data at the Fehmarn Belt and at the  
683 northernmost section is due to larger-scale oceanographic conditions that is in these areas simple  
684 concept of straits transport are not applicable. Blocking events for surface and bottom flows  
685 occur at different net transports, which is most pronounced for the section across Langeland

686 Fjord (Fig. 14h). In this case, the asymmetry of curves (left and right of the zero transport value)  
687 is clearly seen. Furthermore, for all sections there is no unique magnitude of net transport beyond  
688 which blocking events occur. At the Great Belt South section (Fig. 14e) upper layer transport is  
689 blocked for net transport above  $\sim 0.3 \times 10^5 \text{ m}^3 \text{ s}^{-1}$ . For the bottom layer transport the respective  
690 value is  $\sim 0.2 \times 10^3 \text{ m}^3 \text{ s}^{-1}$ .

691  
692 North of the Sound the scatter of data demonstrates that this area is subject to oceanographic  
693 conditions originating from the Kattegat (e. g. transport appears rather stochastic and not fully  
694 constrained by the straits dynamics) and therefore for the same net transport different  
695 combinations of surface and bottom transport are possible. The upper and bottom layer transport  
696 across the southern sections in the Sound are much more constrained by the straits physics and  
697 therefore the scatter of data is smaller. Nevertheless, the scatter of data is too big to define a  
698 threshold value for blocking either surface or bottom transport in the Sound. It is interesting to  
699 see that this scatter increases in some sections (Fig. 14f), but only under the inflow situation.  
700 This is similar to the case in the Great Belt (Fig. 14h), but much more clearly pronounced in the  
701 Sound asymmetric response. This is in qualitative agreement with the results shown in Fig. 12  
702 and previous analyses of Jakobsen (1995) and Stanev (2015).

703  
704 In conclusion, the scatter of individual transports is usually larger at both ends of the strait, while  
705 in the middle of the straits the relationships are reminiscent of the “canonical” relationship  
706 known for other straits. Although the simulated two-layer transport is similar to other strait cases,  
707 there are specific asymmetries in the Baltic Sea straits. The relationships between the net  
708 transport and transport in the surface and bottom layer are not unique, thus deviating from simple  
709 theoretical estimations.

710

## 711 **8. Fine versus coarse- resolution simulations**

712 With a resolution of 500 m in the NBTZ, the cross-sectional areas in the Great Belt and Sound  
713 are  $122300 \text{ m}^2$  and  $68800 \text{ m}^2$ , respectively ( $121100 \text{ m}^2$  and  $73000 \text{ m}^2$  in CR). The TR is 1.78  
714 (1.65 in CR) thus it changed relatively little ( $\sim 8$  percent) with changing the resolution. This small  
715 change is at least partially due to the fact that the DEM used in the CR and E-500 is the same.  
716 However, as seen in Fig. 3, the straits are resolved in the CR with only a few vertical columns.

717 Therefore, although the changes of topography in the CR and E-500 were relatively small, the  
718 different horizontal resolution led to substantial effects, which will be considered below.

719

720 In the Great Belt, the mean magnitude of barotropic transport during October 2014-May 2015  
721 changed from  $9.32 \times 10^4 \text{ m}^3/\text{s}$  in the CR to  $8.49 \times 10^4 \text{ m}^3/\text{s}$  (in E-500). The respective numbers  
722 for the Sound are  $4.66 \times 10^4 \text{ m}^3/\text{s}$  and  $4.08 \times 10^4 \text{ m}^3/\text{s}$ . The averaged TR between the simulated  
723 transports in the two straits for the same period changed from 2.70 (CR) to 3.0 (E-500). The  
724 analysis of transport properties in the two straits (similar to what has been shown in Fig. 13 for  
725 CR, and in Fig. S4 for the E-500) demonstrated that the changes in the model resolutions  
726 affected the TR-distribution curves (compare the histograms in Fig. 13 and Fig. S4). The inflow  
727 histogram in E-500 tends to a Gaussian type, which can be interpreted as a trend to lower  
728 asymmetry between strait exchanges in the case of coarser resolution of straits. The temporal  
729 evolution of the distribution of the TR (compare Fig. 13 g and Fig. S4g) gives another illustration  
730 of the differences between the two experiments. Each time slice in these plots represents a  
731 normalized histogram of the TR analyzed for a period of three days. The secondary maximum in  
732 the histograms during outflow conditions (Fig. S4d) is clearly seen for small and negative values  
733 of TR (Fig. S4g). Although the transport in the straits does not change drastically in the two  
734 experiments, their relative distribution and correlation is strongly affected by the horizontal  
735 resolution.

736

737 The areal distribution of correlation between the transport in the straits and sea level in E-500  
738 almost repeats the pattern shown in Fig. 12 e. The difference between the respective correlations  
739 in two experiments can be used to identify areas where changes in the dynamical balances occur.  
740 This difference does not exceed several percent (Fig. 12f), however its pattern is not trivial.  
741 Notably, far from the straits, where the horizontal resolution in the two experiments is the same,  
742 the areal distribution of this correlation is different. The coarser resolution of narrow sections in  
743 E-500 results in an overall decrease of correlation in the Kattegat. The maximum decrease is  
744 along the western coast where the tidal range is larger (Stanev et al., 2015). South of the straits  
745 the correlation increases in E-500 (in comparison to CR) and the difference pattern in Fig. 12f  
746 depicts approximately the propagation pathway of the North Sea mixed water. The correlation  
747 pattern shows strong sensitivity to horizontal resolution in narrow channels, e.g. between the

748 Langeland and the Fyn (Sio Sound) and in the area around Darss Sill. In both areas, Fig. 12f  
749 shows reversals of correlation and small-scale patterns demonstrating that dynamical changes  
750 can be locally strongly affected by the resolution. In particular, the response to changed  
751 resolution in the Sound could explain at least some of the differences in the water mass  
752 transformation and propagation towards the Gotland Basin.

753

754 Differences between the CR and E-500 originate from the areas where horizontal resolution has  
755 substantially been changed, as can be seen in the enlarged diagrams in Fig. S3 and Fig. S5.  
756 Inflow salinities are higher in the CR (compare Fig. S3b, f and S5b, f) and in the Sound the core  
757 of high salinity water is very pronounced in the CR (see the difference between Fig. S3f and  
758 S5f). In the outflow situations shown in these figures, salinity is lower in the CR. Of particular  
759 importance to illustrate the differences between the two experiments is the comparison of  
760 vorticity in the straits, which yields information about the velocity shear. In the Sound, these  
761 differences are much clearer during inflow events (compare Fig. S3h and Fig. S5h). The  
762 respective outflow situations (Fig. S3g and S5g) show much better similarity. The conclusion is  
763 that with finer resolution in the CR (compare Fig. S1b and S1d), velocity shear along straits'  
764 coasts is better resolved, which changes the patterns of velocity and salinity.

765

766 In several of the illustrations (Figs. 6, 7, 10, 11) simulations with E-500 were shown next to ones  
767 from the CR, but were not commented on because the analyses were focused on physical  
768 interpretation of results. In the following, we will present briefly the major differences between  
769 the CR and E-500. Overall, the fine resolution model overestimates bottom salinity in Arkona  
770 Basin (Fig. 6a). Before the MBI, bottom salinity in the Bornholm Basin simulated in the CR was  
771 closer to the observed one, while after the MBI observed data lay between E-500 and the CR  
772 simulations (Fig. 6c). In the Stolpe Channel and further down to the Gotland Basin, the quality of  
773 CR simulations was better (notice the different colors in Fig. 6d corresponding to individual  
774 experiments). SSS values were much closer in the two models than the bottom ones. Obviously,  
775 changing the resolution affects the properties of bottom layers.

776

777 The panels on the right hand side of Fig. 10 are based on the results from E-500. Qualitatively,  
778 both simulations look similar, but differences on both sides of the straits are also clearly seen.

779 The low sea level in the area of Skagerrak is further reduced in the E-500 simulations.  
780 Furthermore, the positive SSS anomaly is more pronounced in the North Sea in E-500. These  
781 changes are explained by larger mixing in the straits (overturning of water) during extreme  
782 situations bringing bottom water closer to the sea surface, which further propagates in the  
783 direction of the North Sea (compare also Fig. S3a, e and Fig. S5a, e). After the MBI the  
784 freshening trend in E-500 is stronger. These results prove that the resolution in the straits can  
785 affect remote areas.

786

787 The differences between two models are more obvious in the Baltic Sea where the bottom  
788 salinity anomaly is much clearer in the CR. In E-500, the signal almost does not reach the  
789 Gotland Basin. This is seen from the comparison between Fig. 7h and Fig. 7i and the data (Fig.  
790 7g) and supports the conclusions from analysis of Fig 6. With more realistic bottom topography  
791 and better resolution of the narrow flows, the penetration of saltier water in the straits simulated  
792 in the CR is larger and their accumulation in the Arkona Basin and Bornholm Deep reservoir  
793 provides enough source water to be “pushed” via the Stolpe Channel in the direction of the  
794 Gotland Basin under favorable conditions (compare Fig. 10e and Fig. 10f). This is in line with  
795 the analysis of Janssen (2002) who stated that ventilation of the Gotland Basin is only possible  
796 when water mass characteristics in the Arkona Basin are beyond a critical value enabling  
797 sufficient salty water to reach the Bornholm Basin. Obviously, the CR fulfilled these  
798 requirements.

799

800 More complete presentation of the agreement between the two models is shown in Fig. 11. SSS  
801 and bottom salinity along section lines in Fig. 2 simulated in the two experiments (Fig. 11b, c)  
802 agree with each other, as was also the case with the larger-scale analysis in Fig. 10. Although  
803 SSS patterns qualitatively agree and the bottom salinity shows similar appearances of salt  
804 intrusions, the magnitude of the variability is different in the two models, particularly in the  
805 Sound. At all analyzed stations, the CR gives larger salinity values. More detailed analysis shows  
806 larger differences, e.g., in station Viken, where E-500 shows lower amplitudes of oscillations. In  
807 this location the position of the salinity front shifts under different resolutions, which explains  
808 the relatively larger salinity differences there ( $D=0.73$ ). This changing skill of SCHISM in  
809 different areas depending upon the resolution in the straits (Fig. 6 and Fig. 7) gives a motivation

810 to further address the parameterizations used to more reasonably simulate the penetration of the  
811 mixed North Sea water along its way from the Kattegat down to the Gotland Basin. Obviously,  
812 the problem with realistic propagation of bottom water could not be resolved with the increased  
813 resolution in the straits alone.

814

## 815 **9. Conclusions**

816 One basic idea behind this research was to use results from numerical modelling to address  
817 different issues of straits physics and dynamics of interconnected basins. This approach is  
818 justified by the fact that observations are not available over large areas and for sufficiently long  
819 periods with the needed resolution. An unstructured-grid model was presented, which overcame  
820 some deficiencies in past studies caused by the coarse resolution of the two-layer exchange in the  
821 straits and/or not using two-way coupling between the general circulation of interconnected  
822 basins and straits physics. Analyses gave a closer look at the impact of ultra-fine resolution  
823 scales, e.g., between 100 and 500 m. The extensive validation against available observations  
824 demonstrated a very good model skill giving sufficient credibility to simulations as 4D  
825 representation of dominant processes. We used these synthetic data to explain the key (and  
826 different) role of individual Baltic Sea straits and the temporal and spatial variability of their  
827 dynamics.

828

829 The realism of the model was first demonstrated with respect to the transport in the straits and  
830 the variability of sea levels at two ends of the straits. The volumetric transport showed a very  
831 good skill, revealing the leading role of the balance between along-strait pressure gradient and  
832 bottom friction. Furthermore, the consistency between basin-scale and strait-scale dynamics  
833 appeared crucial for the quality of the simulated gravity flows and basin-scale baroclinic  
834 dynamics. The model appeared capable of capturing the change of thermohaline characteristics  
835 of the North Sea waters penetrating into the Baltic Sea during the MBI along their way over the  
836 sills and in the small regional sub-basins. The timing of arrival of mixed North Sea water at  
837 several observational locations was accurately forecasted. The penetration of the bottom salinity  
838 signal into the Gotland Basin matched the observed one, particularly well up to Stolpe Channel.

839

840 There are number of geophysical specificities which have been revealed from the simulations.  
841 The Sound appeared as an area where extreme vertical mixing changes vertical stratification and  
842 strongly affects the propagation properties of gravity currents (in the Baltic Sea) and surface  
843 plume (in the North Sea). While the former can be expected, the fate of the surface plume in the  
844 North Sea was not so trivial. This plume was seen as alternating positive and negative anomalies,  
845 which propagated to the west. It was demonstrated that the Drogden Sill played the role of the  
846 generator of large salinity anomalies (mixer because of shallow depths). These anomalies  
847 propagated in either direction (depending on the alteration of the straits transport) as surface  
848 plumes in the North Sea and bottom plumes in the Baltic Sea.

849

850 Substantial differences between short-term variability during inflow and outflow situations were  
851 identified. The inflows were characterized by multiple pulses and large oscillations in transport  
852 and salinity, while the outflows showed smoother changes. During periods of strong currents, the  
853 flow in the straits was unidirectional. Decreasing the magnitude of the net transport below some  
854 critical value, caused the transport to become two-directional. However, the appearance of two-  
855 layer transport was quite diverse, which was seen by the different pairs of surface and bottom  
856 flows corresponding to the same net transport. The magnitude of net flow beyond which one of  
857 the two-way currents was blocked was also not unique. This “ambiguity” was different in  
858 different straits and at different locations in the straits. In the interior of the straits, the two-layer  
859 transport tended to the “canonical” one known from theory (Oguz et al., 1990). North and south  
860 of the straits the scatter of transport pairs (surface and bottom ones) increased because these  
861 areas were exposed to oceanographic conditions. Furthermore, the two-layer exchange was not  
862 symmetric for inflow and outflow conditions (non-canonical behavior under the inflow  
863 situation).

864

865 The three individual straits revealed very different dynamics. Saltier mixed North Sea water  
866 showed much longer excursions in the Great Belt, both in the surface and bottom layers than in  
867 the surface layers of the Sound. Nevertheless, during the MBI of 2014-2015, the salinity signal in  
868 the Bornholm Basin reflected water originating from the Sound.

869

870 Although there are concepts about the *causality of inflow events* (Svansson, 1959; Jakobsen et  
871 al., 2010; Schimanke et al., 2014) the contribution of the sea level changes in the Baltic Sea and  
872 North Sea for transports in the straits have not been previously quantified. The model  
873 simulations were reminiscent of similar results for the Black Sea-Mediterranean Sea system  
874 (Volkov et al., 2016), i.e. the major driver was the forcing from the outside basin. However,  
875 inflows were strongly dependent on the sea level in the central Baltic Sea, which supported the  
876 existing concepts (Lass and Matthäus, 1996). The correlation between net straits transport and  
877 sea level revealed an overall anti-symmetric pattern; the transition from positive to negative  
878 values made it possible to identify the natural (physical) boundaries between the North Sea and  
879 Baltic Sea.

880

881 The interdependence of the exchange in the individual straits does not fully conform to the  
882 simple idea that transports in the straits are linearly proportional, the coefficient being the ratio  
883 between the smallest cross-sectional areas. In fact, the transport in the Sound is smaller, which  
884 reveals the stronger frictional control there. We demonstrated that there are very complex  
885 relationships between transports in the two straits partially manifested by the large magnitudes of  
886 oscillations (comparable to the mean values). The coefficient of linear regression between  
887 transports in the Sound and Great Belt increased during the MBI-dominated cases, demonstrating  
888 the role of the Sound as a pathway for North Sea waters associated with extreme events.  
889 Furthermore, the transport in the Great Belt lags the one in the Sound, which was explained as a  
890 result of the Sound being closer to the inflowing waters following the eastern coast of Kattegat.

891

892 The changes in the model resolutions (from fine to ultra-fine) affected the strait exchange. The  
893 almost Gaussian-type histograms in the coarser simulation (E-500) can be interpreted as a trend  
894 to lower asymmetry between strait exchanges in the case of coarser resolution of straits. In the  
895 Sound the position of the salinity front shifts under different resolutions. Overall, the fine  
896 resolution model (CR) overestimated slightly bottom salinity in the Arkona Basin. However, in  
897 the Stolpe Channel and further down to the Gotland Basin, the CR simulations were superior.  
898 Comparisons between the CR and E-500 proved that the resolution in the straits affects remote  
899 locations in both inter-connected basins. The improvements due to using ultra-fine resolution  
900 appeared fundamental in the Baltic Sea, allowing more realistic simulation of the propagation of

901 the salinity signal down to the Gotland Basin. This was due to the fact that in the CR the  
902 penetration of saltier water in the straits was larger and its accumulation in the Bornholm Deep  
903 reservoir provided enough source water for the deep-ocean ventilation. It is questionable whether  
904 the increased resolution in the straits alone could fully solve the problem with realistic  
905 propagation of bottom water. Some further improvement of model skill could be achieved after a  
906 closer look at the physical parameterizations contributing to more accurate simulation of the  
907 penetration of the mixed water down to the Gotland Basin and its spreading there.

908  
909

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1050

1051 **List of figures**

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1055 section. The black box in the NBTZ identifies the position of Fig. 2.

1056  
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1064  
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1068 Little Belt.

1069  
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1077  
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1081

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1084

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1088

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1091 inflow periods, respectively. Time is shown in the title of each plot. (b) and (d) shows relative  
1092 vorticity for the same times. Rectangles identify the position of the insets shown in Fig. S3

1093

1094 Fig. 9. Salinity and turbulent kinetic energy along the blue-colored section line (Fig. 2) in the  
1095 Sound. (a) and (c) show salinity during outflow and inflow period, respectively. Time is shown  
1096 in the title of each plot. (b) and (d) show turbulent kinetic energy for the same times. The  
1097 outflow-situation (upper plots) corresponds to the period just before the MBI, the inflow one ,  
1098 during the MBI, is shown in the bottom plots.

1099

1100 Fig. 10. Time versus distance along the section line in Fig. 1 diagrams of sea level in [m], (a, b),  
1101 SSS anomaly (c, d) and bottom salinity anomaly (e, f). Panels on the left are from the control  
1102 run, the ones on the right from the coarse-resolution one. The blue arrow shows the position of  
1103 Drogden Sill, this is the shallow most depth in Fig, 7. Bornholm Deep is indicated by the red  
1104 arrow.

1105

1106 Fig. 11 Time versus distance diagrams along the transect lines in Fig. 2. Each group of six panels  
1107 depicts CR simulations (on the left) and E-500 ones (on the right) for the individual straits: upper  
1108 two figures-Sound (So), the two figures in the middle – Great Belt (GB), the two bottom figures  
1109 – Little Belt (LB). (a) is sea level, (b) is SST, (c) is bottom salinity.

1110

1111 Fig. 12: (a) Net volume flux [ $\text{m}^3/\text{s}$ ] integrated over the three straits (positive in the direction of  
1112 BalticSea) versus sea level difference [m] between the Kattegat (area averaged) and central

1113 Baltic Sea (area averaged). A positive sea level difference means that sea level in the Kattegat is  
1114 higher. (b) sea level difference [m] between the same areas as in (a) versus sea level [m] in the  
1115 Kattegat. (c) sea level difference [m] between the same areas as in (a) versus sea level [m] in the  
1116 central Baltic Sea. Data have been detided with a running average window of 1 day. (d)  
1117 Temporal evolution of net transport in the Sound during the MBI in 2014-2015. (e) correlation  
1118 map of volume flux integrated over the three straits [ $\text{m}^3/\text{s}$ ] and sea level [m] in the NBTZ.(f)  
1119 shows the difference between (e) and similar plot from E-500.

1120

1121 Fig.13.(a)Vertically integrated water transport through the Great Belt and Sound across the  
1122 section lines 5 and 3, respectively (see Fig.2a for their positions) during October 2014 - May  
1123 2015. Negative values are towards the Baltic Sea. The ratio between the transports in the Great  
1124 Belt and Sound is also given (green line) as a running average of 7 days. (b) is a scatter plot of  
1125 the transport in the Sound versus the one in the Great Belt. The equation for the regression curve  
1126 is also given; (c) and (d) show the distribution of the ratio between the transport in the Great Belt  
1127 and Sound during the inflow and outflow conditions, respectively. The transport values in the  
1128 Sound smaller than  $9\text{e}3\text{m}^3\text{s}^{-1}$  have been excluded; (e) is the same as (c) and (d) but for all  
1129 conditions. (f) is the correlation of the water transport in the Great Belt and Sound as a function  
1130 of time lag. (g) is the distribution of the ratio between the transport between the Great Belt and  
1131 Sound, where each time slice represents a normalized histogram of this ratio analysed for a  
1132 period of three days. The white solid line illustrates the average ratio of fluxes through Great  
1133 Belt and Sound. The thick vertical lines in (a) and (g) indicates the beginning of the MBI in  
1134 2014.

1135

1136 Fig. 14. The volumetric flow rates across sections shown in (a) in the upper layer (red symbols)  
1137 and bottom layer (green symbols) as a function of the net flow. Positive flows are from the North  
1138 Sea to the Baltic Sea. The panels on the left are transports in the Little Belt, the ones in the  
1139 middle in the Great Belt and the ones on the right in the Sound.

1140

1141 **Supplementary figures**

1142

1143 Fig. S1. Horizontal grid in the Sound in the CR (a) and in the E-500 experiment (c). The  
1144 respective vertical grids are shown exemplarily in (b) and (d) along the section plotted by the  
1145 thick black lines. For the position of (a) and (c), see the respective box in Fig. 2 in the area of  
1146 Sound.

1147

1148 Fig. S2. Horizontal grid in the Sound in the CR (a) and in the E-500 experiment (c). The  
1149 respective vertical grids are shown exemplarily in (b) and (d) along the section plotted by the  
1150 thick black lines. For the position of (a) and (c), see the respective box in Fig. 2 in the area of  
1151 Great Belt.

1152

1153 Fig. S3. Dynamics in the Great Belt (upper panels) and Sound (bottom panels) represented by  
1154 the patterns of surface salinity and relative vorticity normalized by the Coriolis parameter. The  
1155 individual figures are zooms of Fig. 8 in the straits. (a), (b) show SSS in the Great Belt during  
1156 outflow and inflow periods, respectively. (c) and (d) shows relative vorticity in the Great Belt for  
1157 the same times as (a) and (b). The same as in (a-d) is shown in (e-h) for the Sound.

1158

1159 Fig. S4. As Fig. 13 but from E-500.

1160

1161 Fig. S5. As Fig. S3 but for E-500D.

1162

1163

# *Figures*

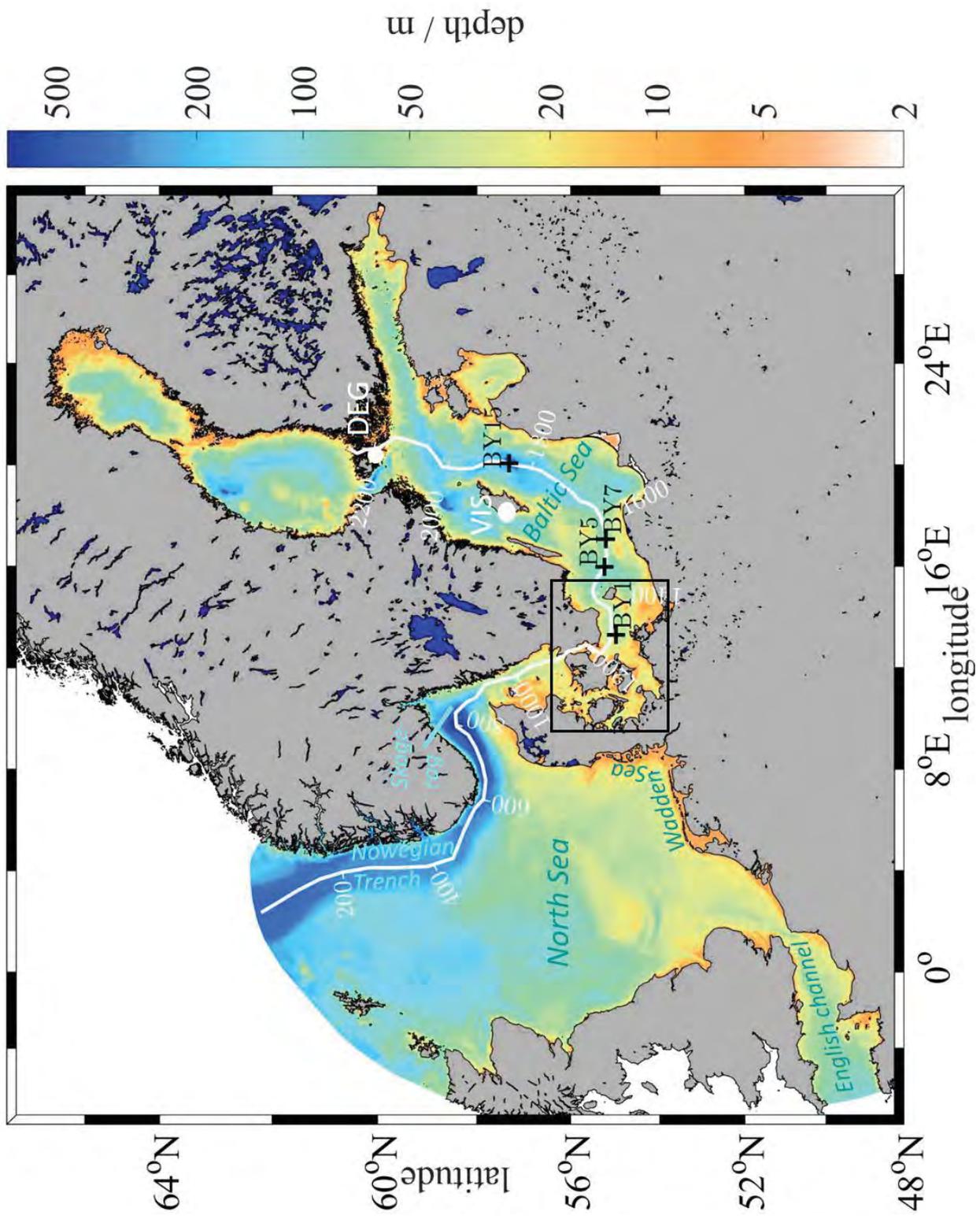


Fig. 1.

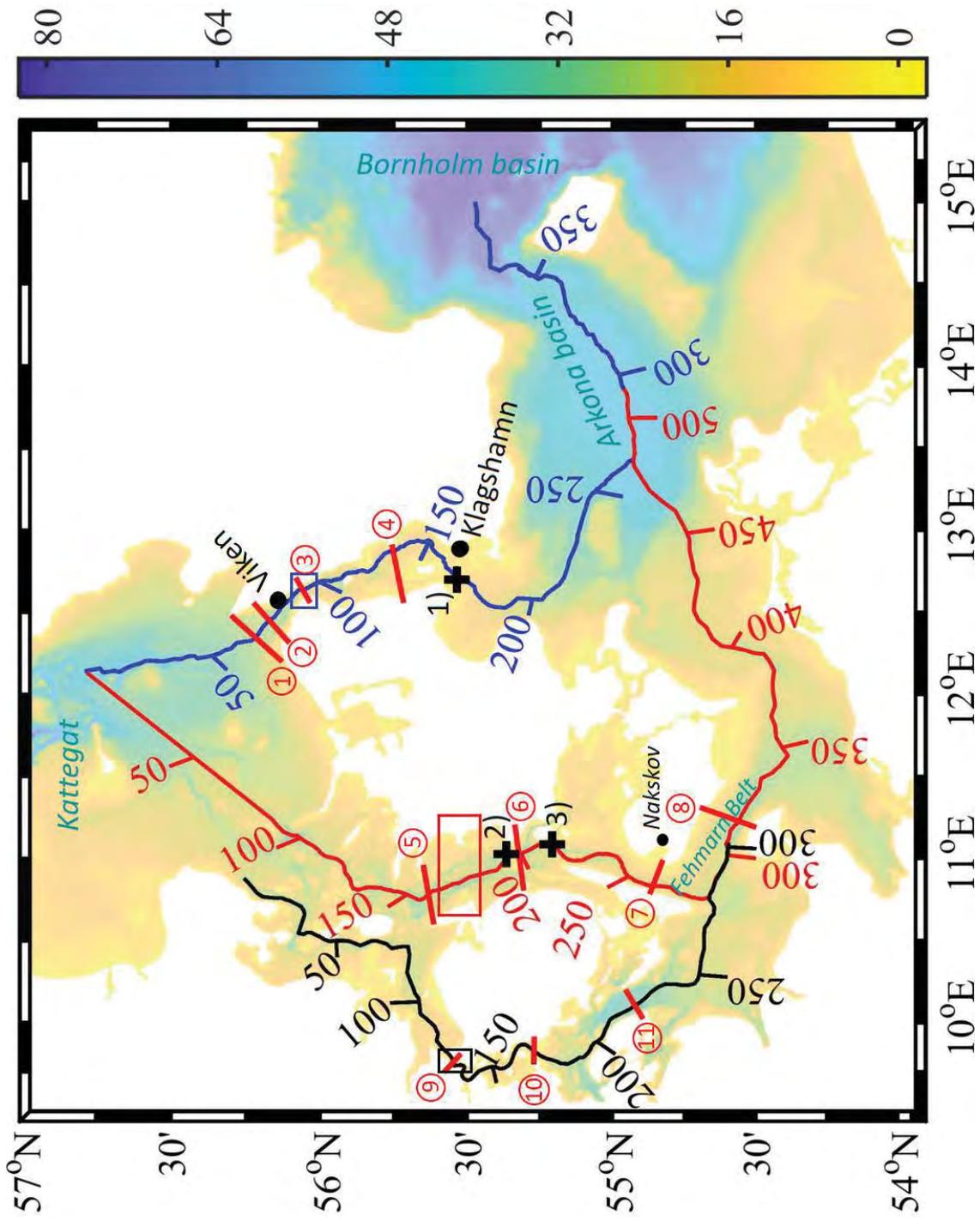


Fig. 2.

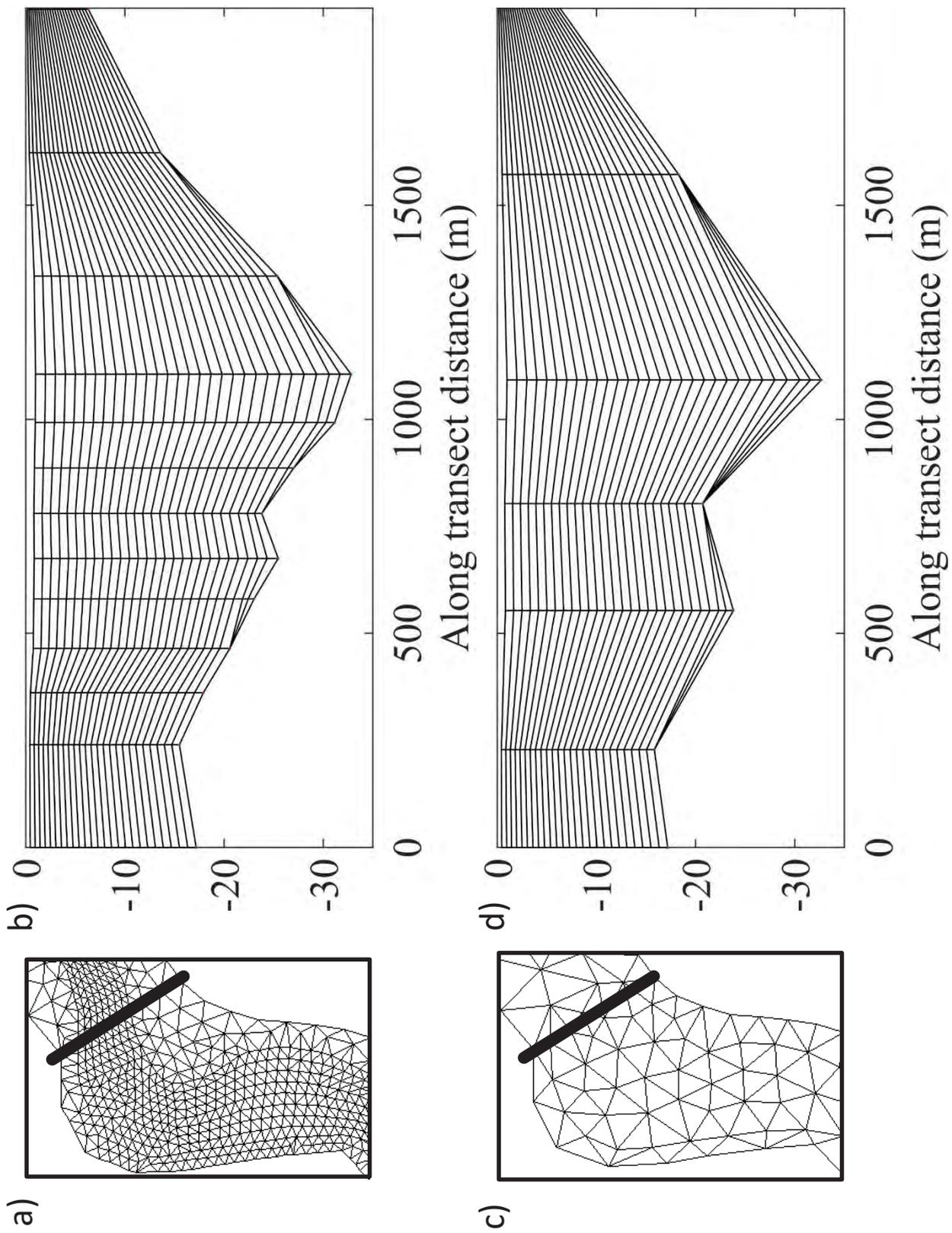
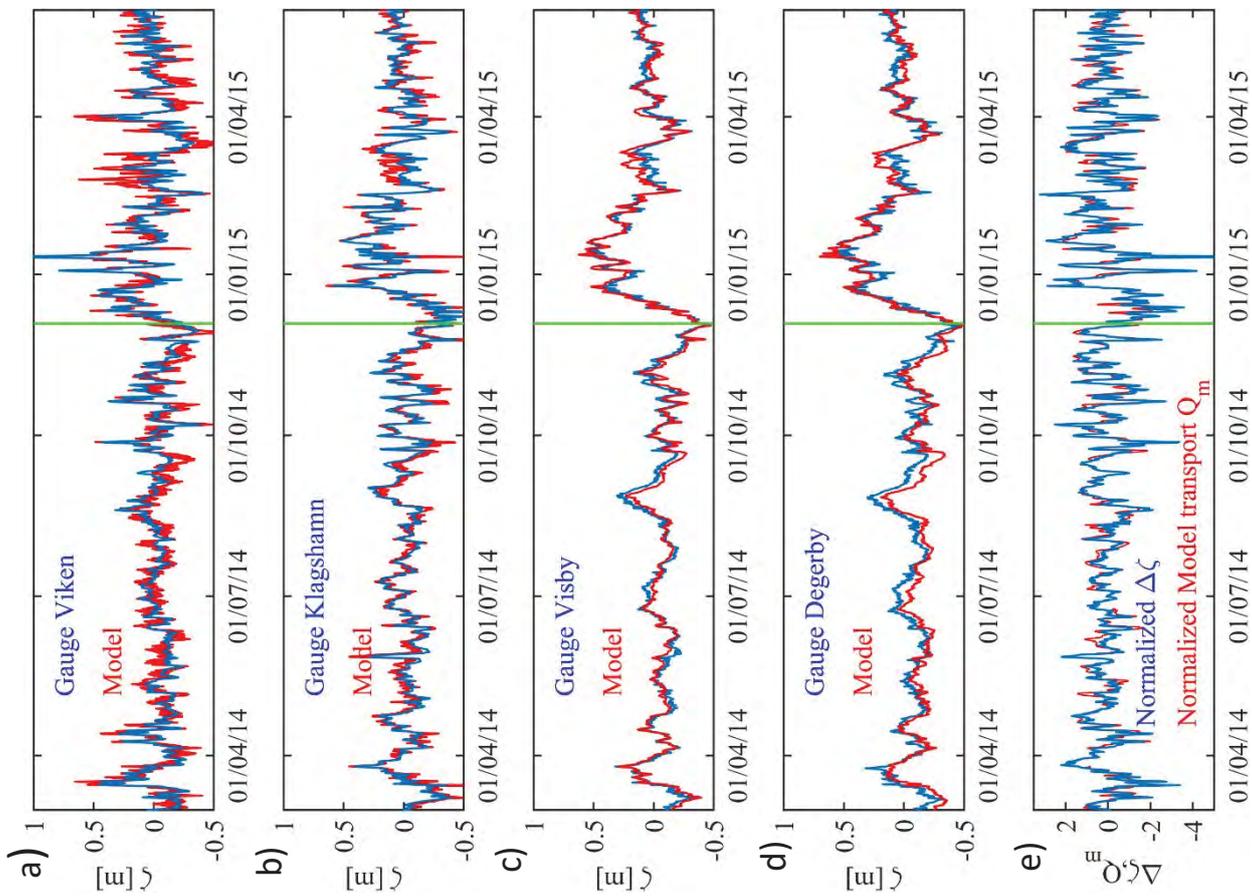


Fig. 3



**Fig. 4.**

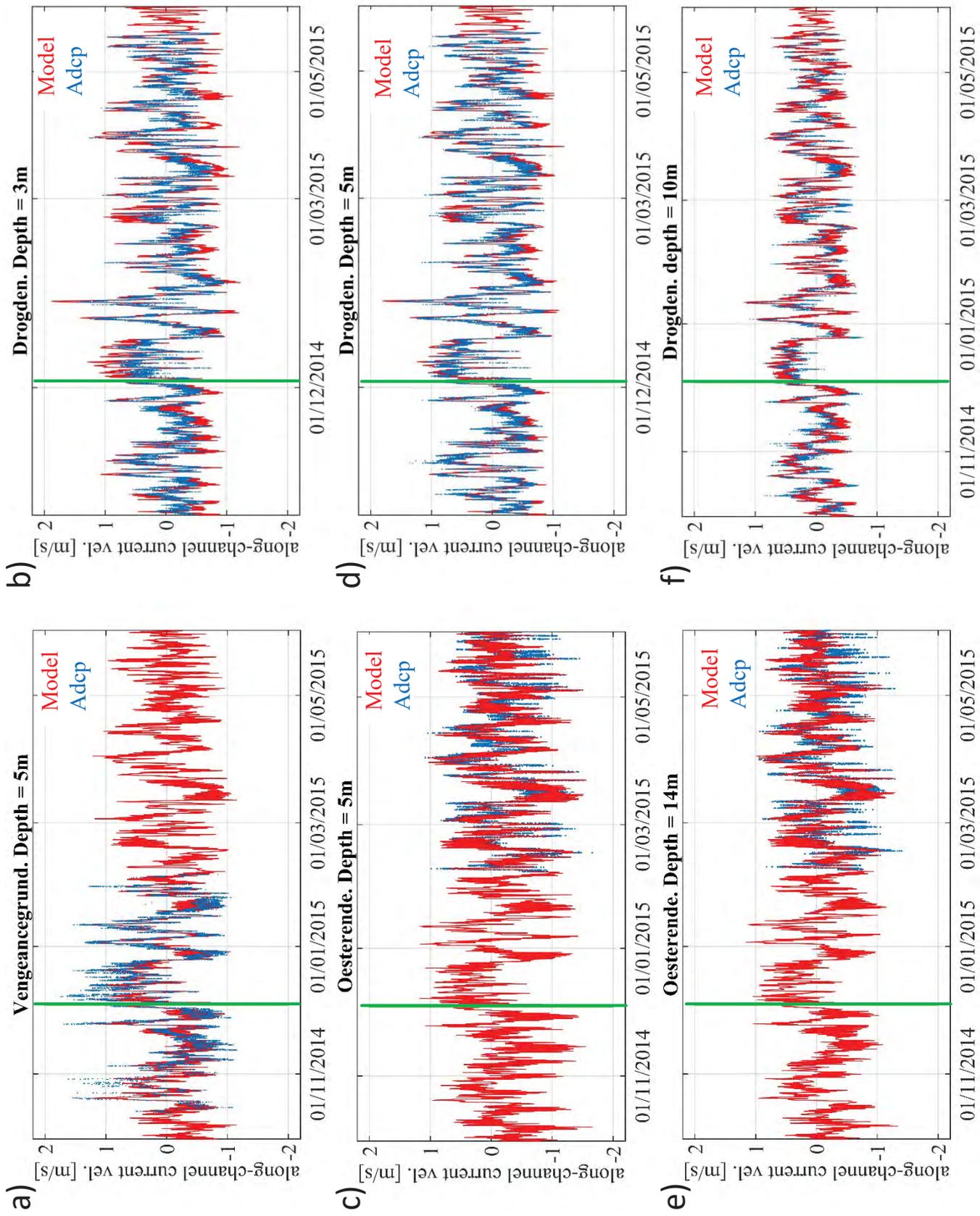


Fig. 5

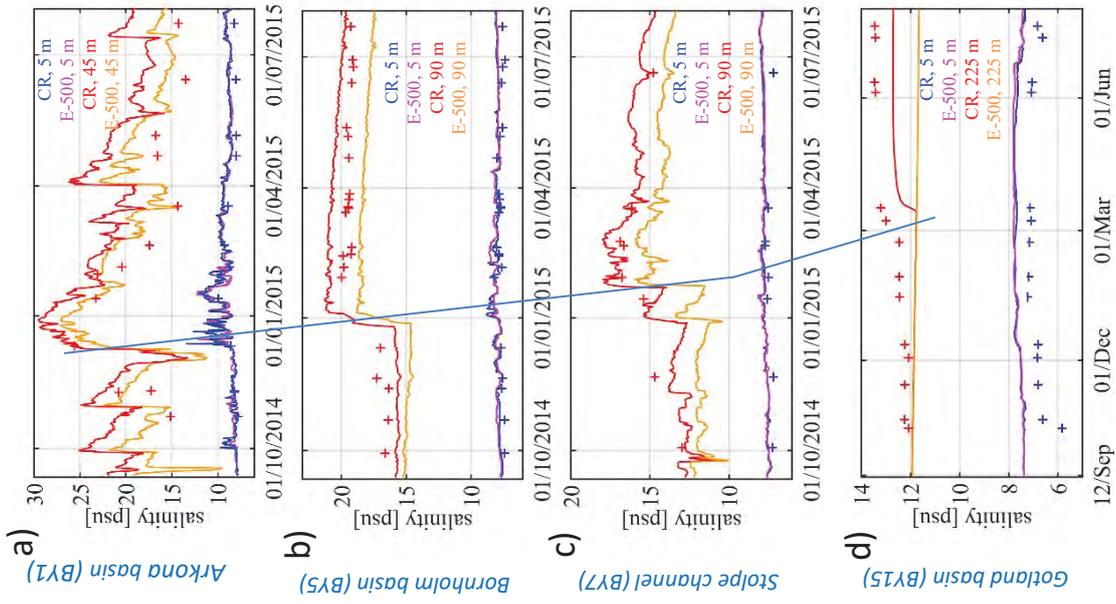


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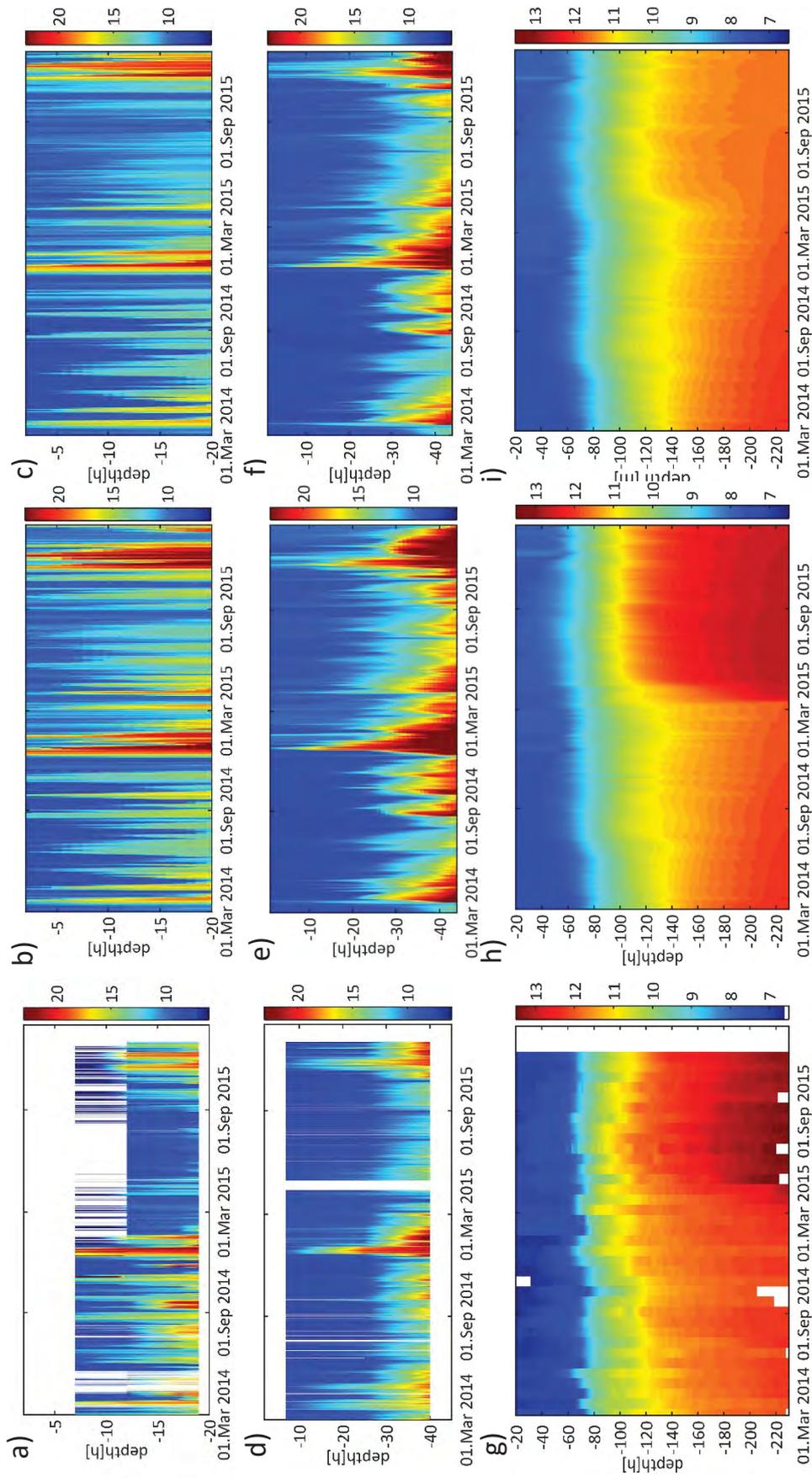


Fig. 7.

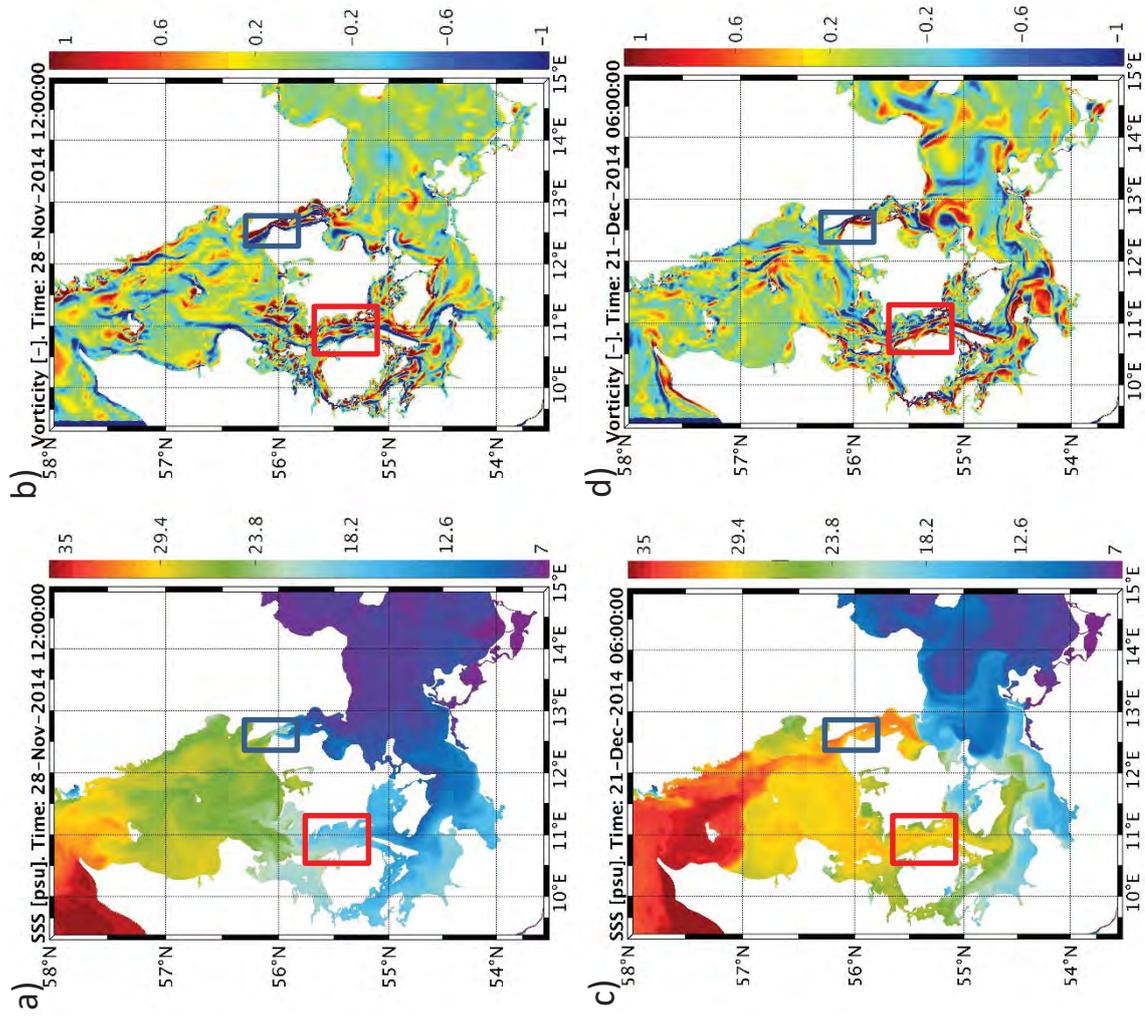


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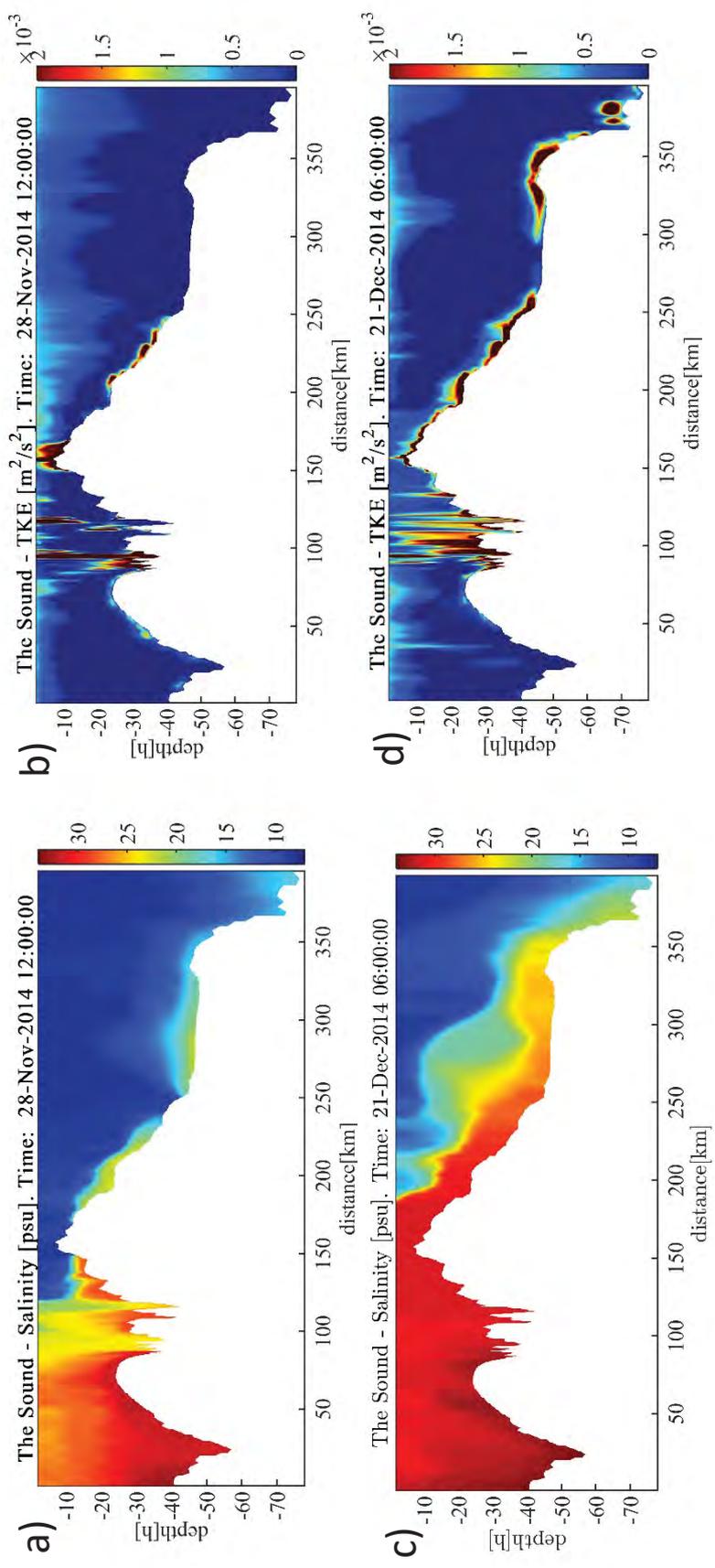


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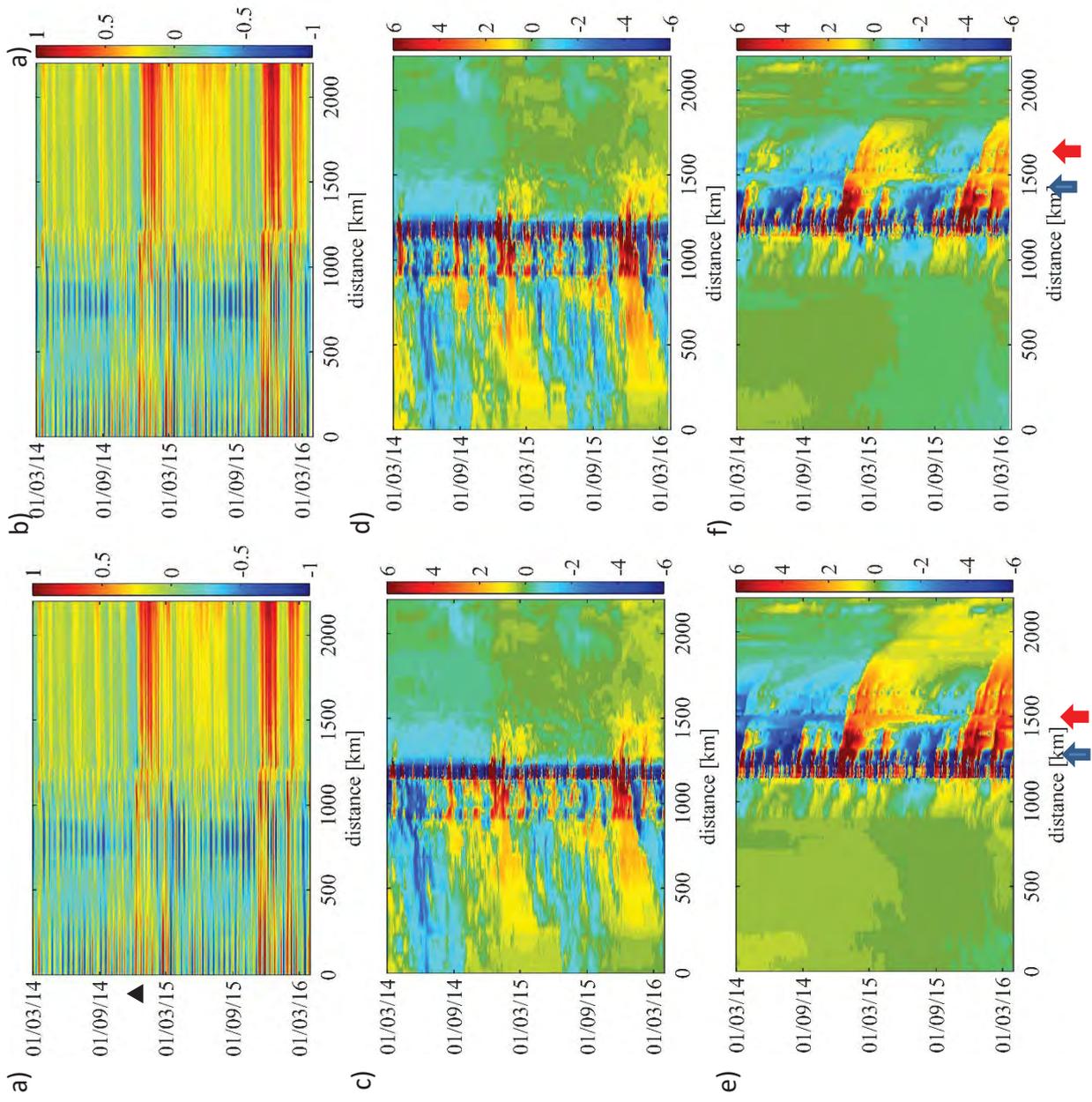


Fig. 10.

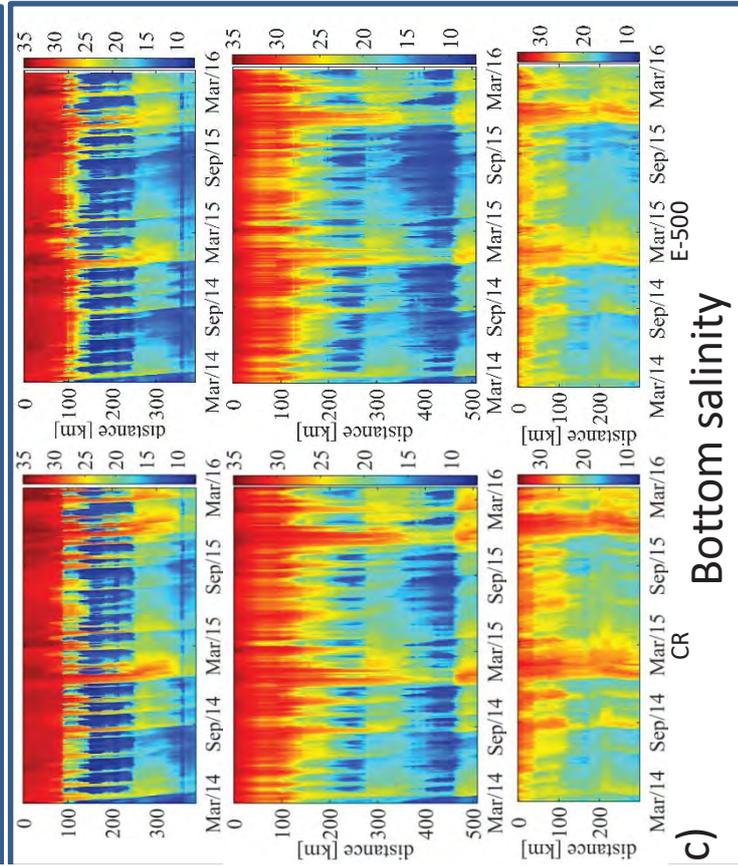
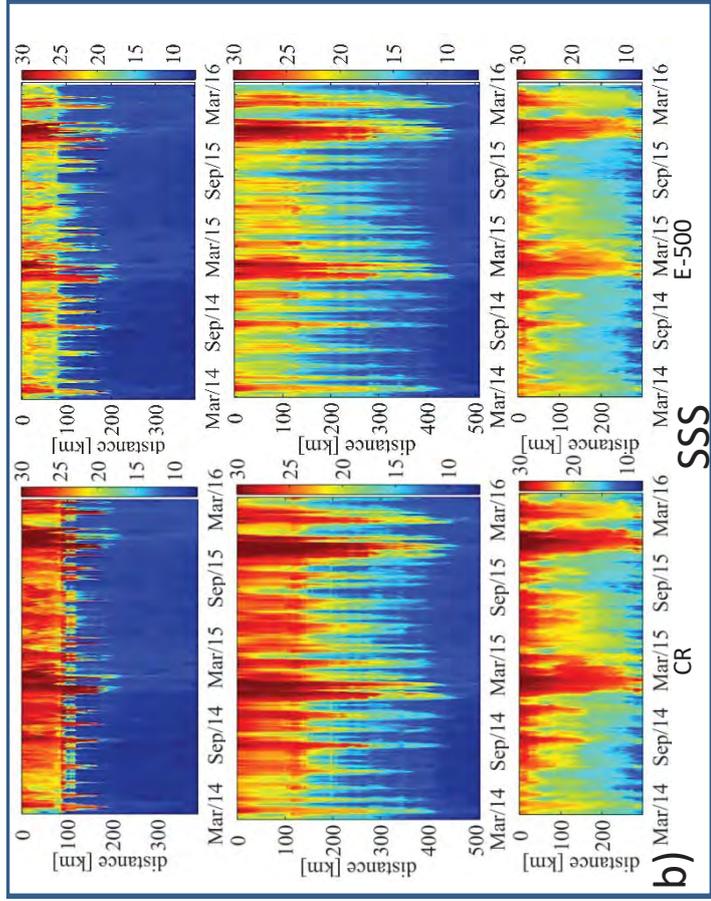
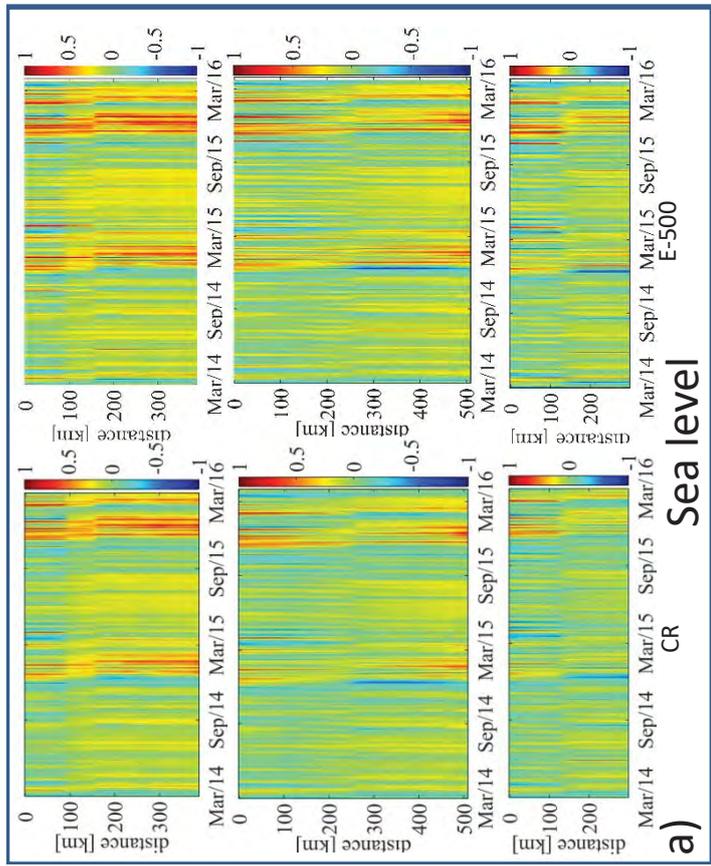


Fig. 11

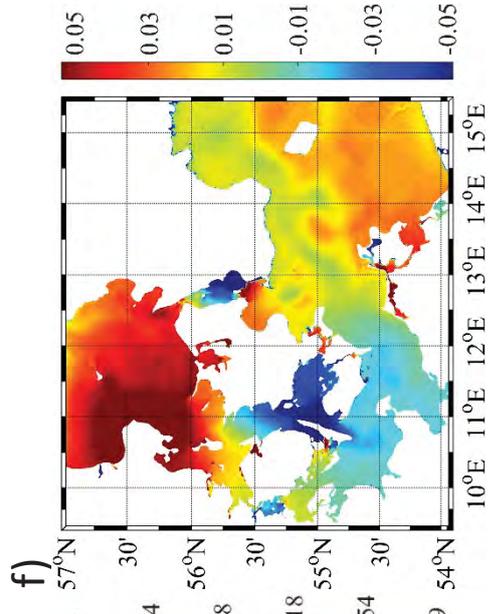
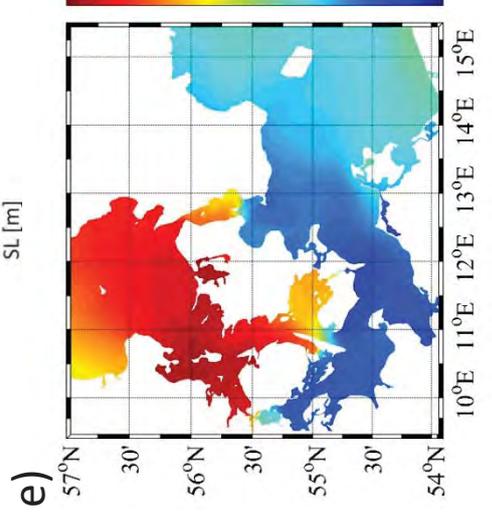
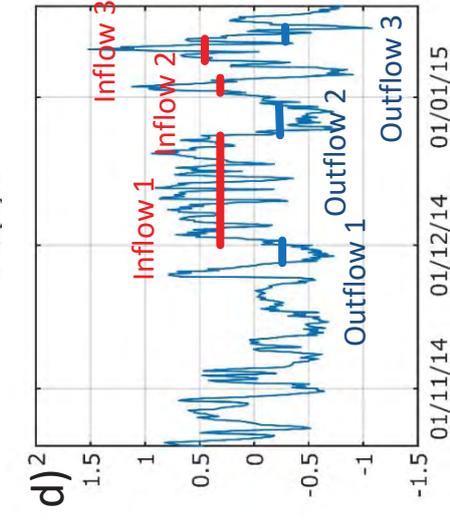
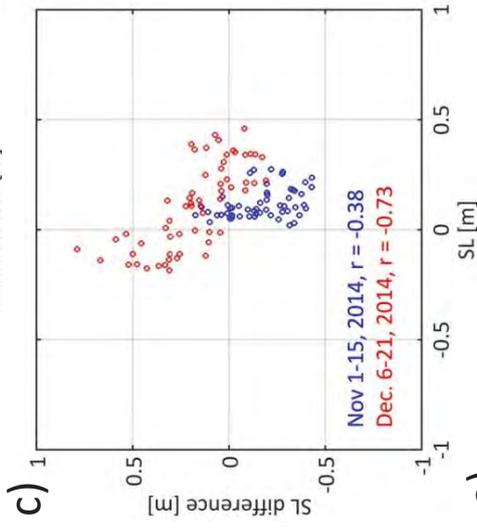
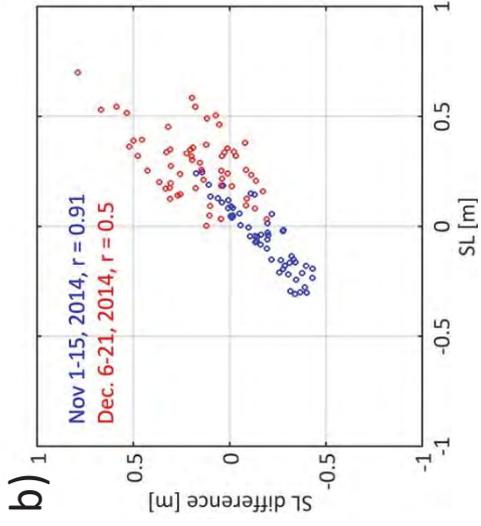
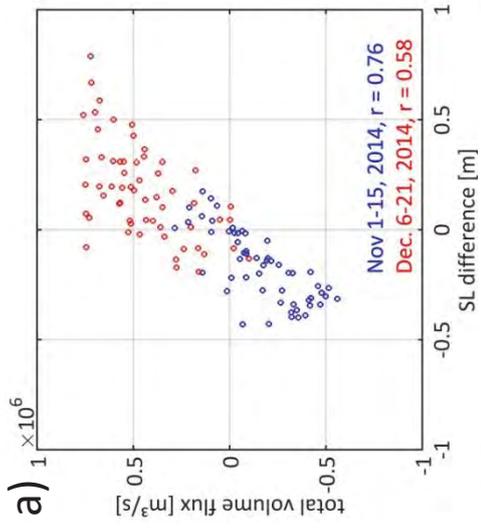


Fig. 12.

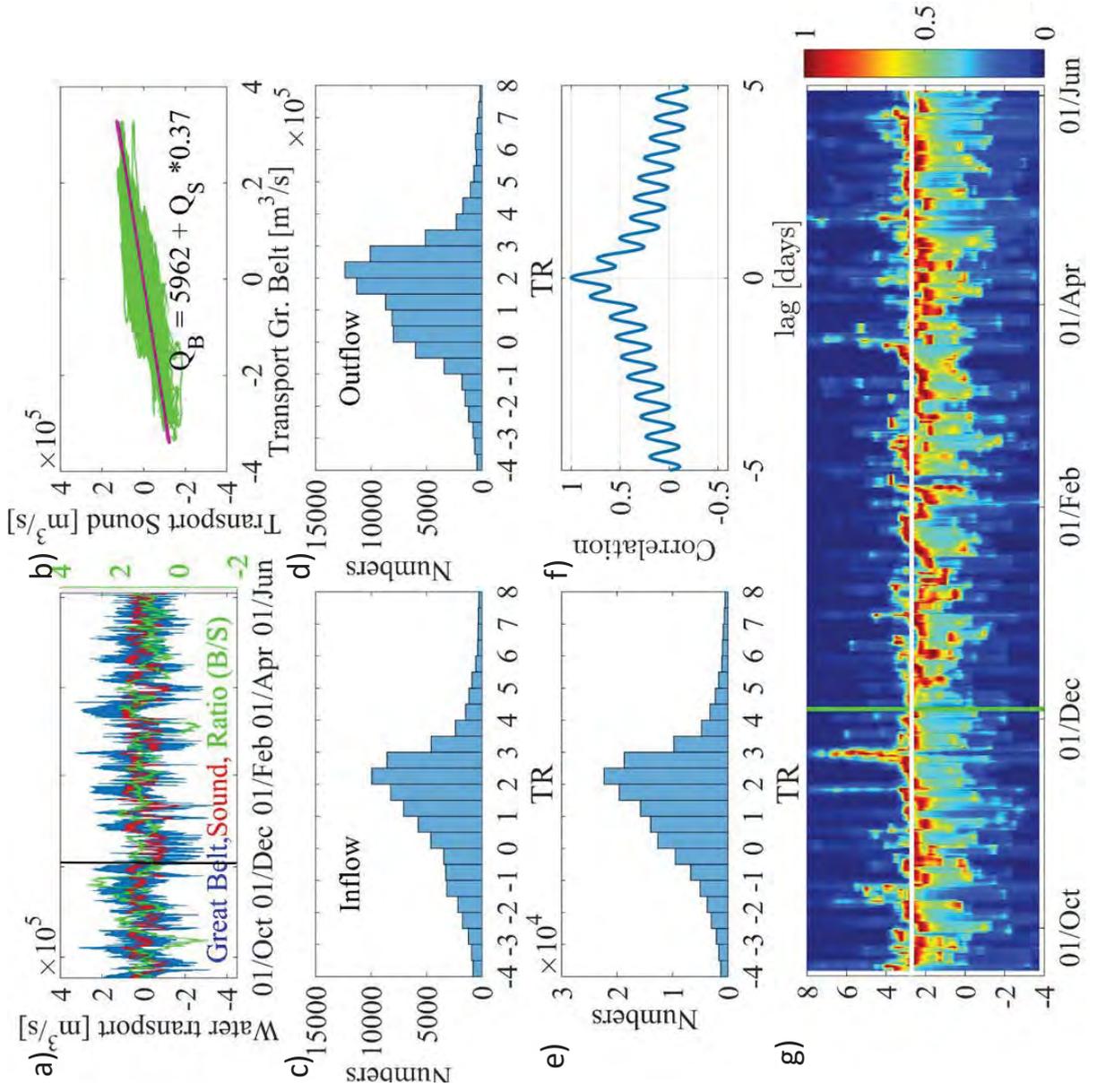


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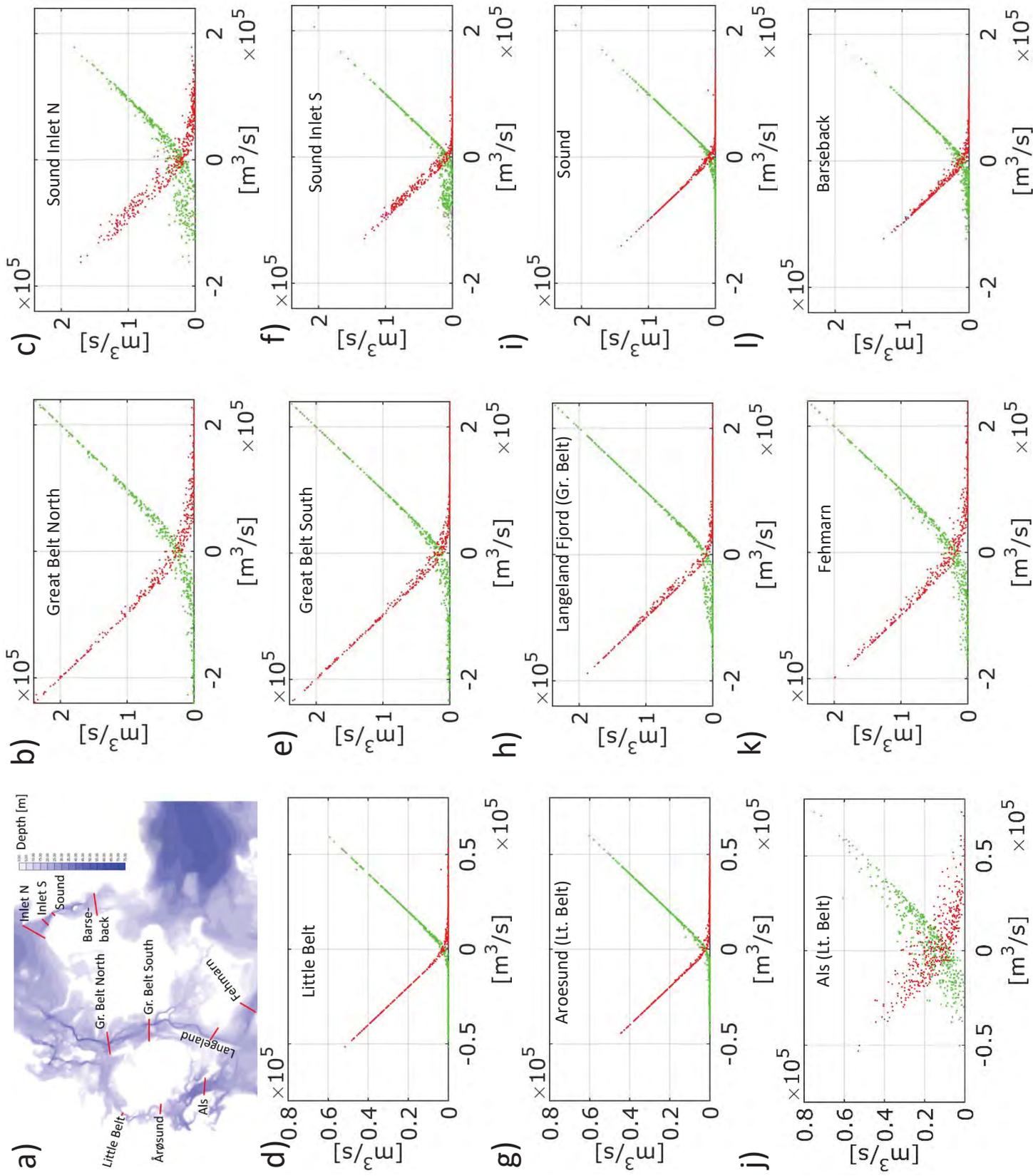


Fig. 14.

# *Supplementary figures*

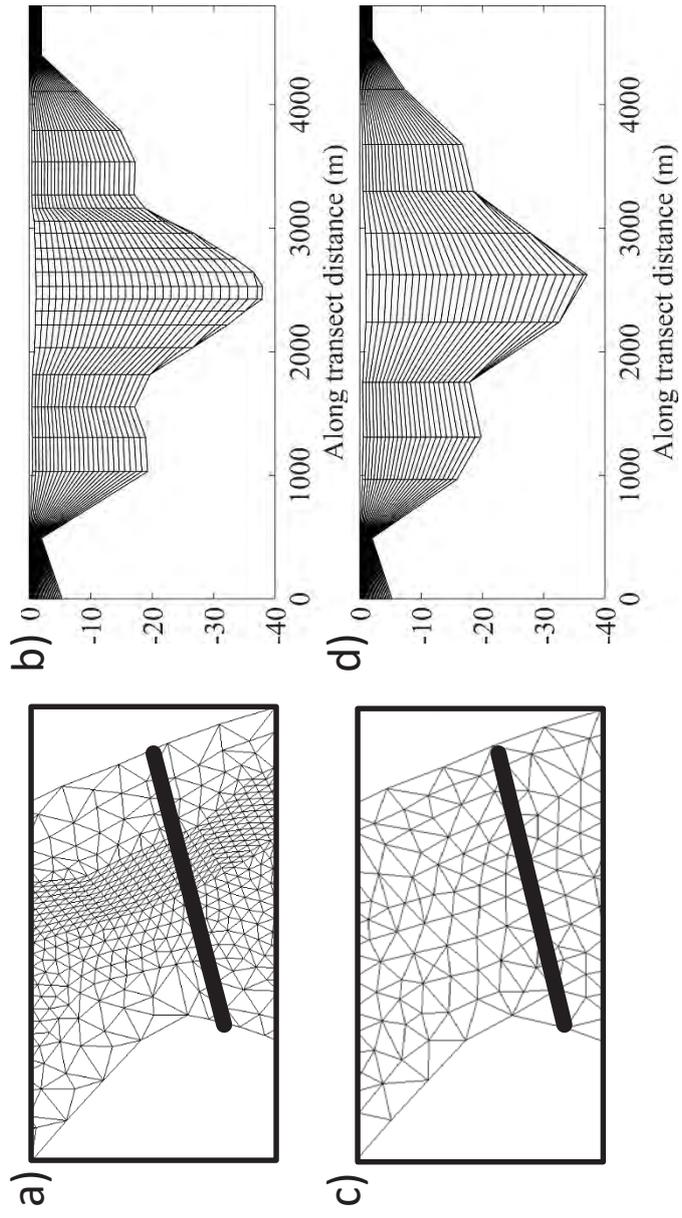


Fig. S1.

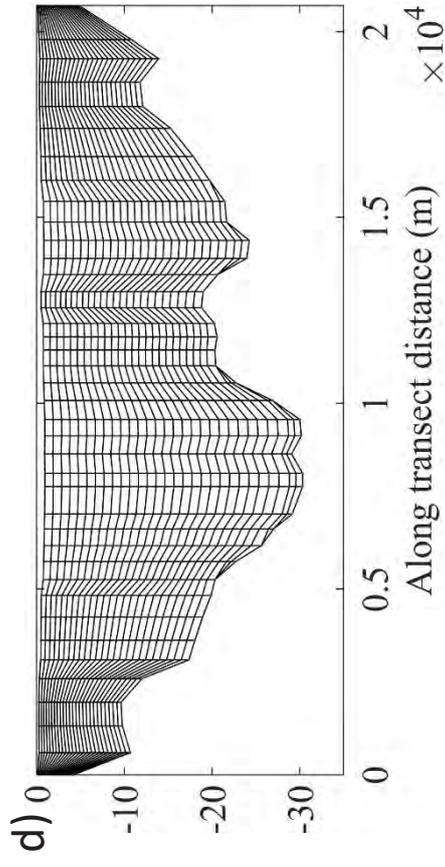
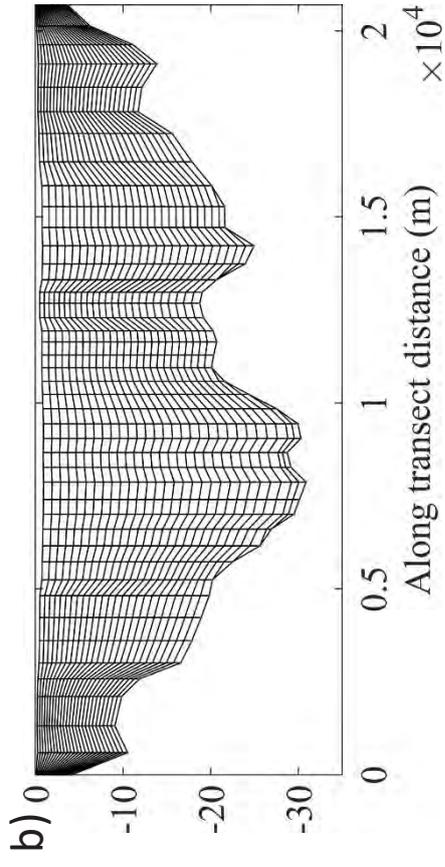
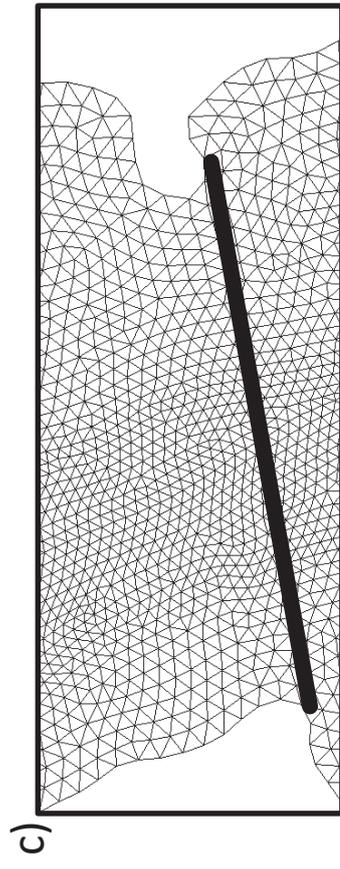
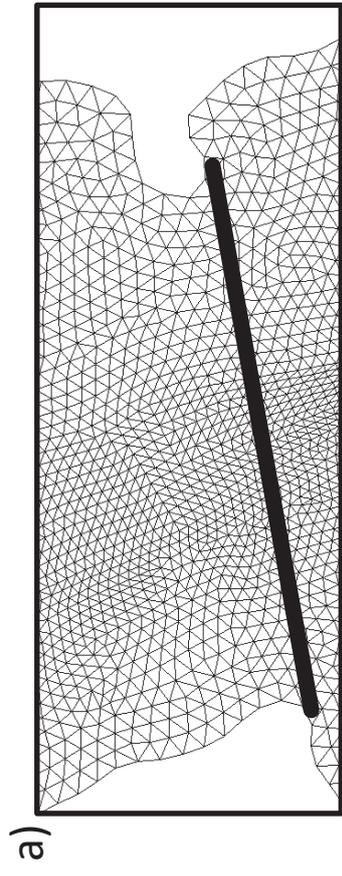


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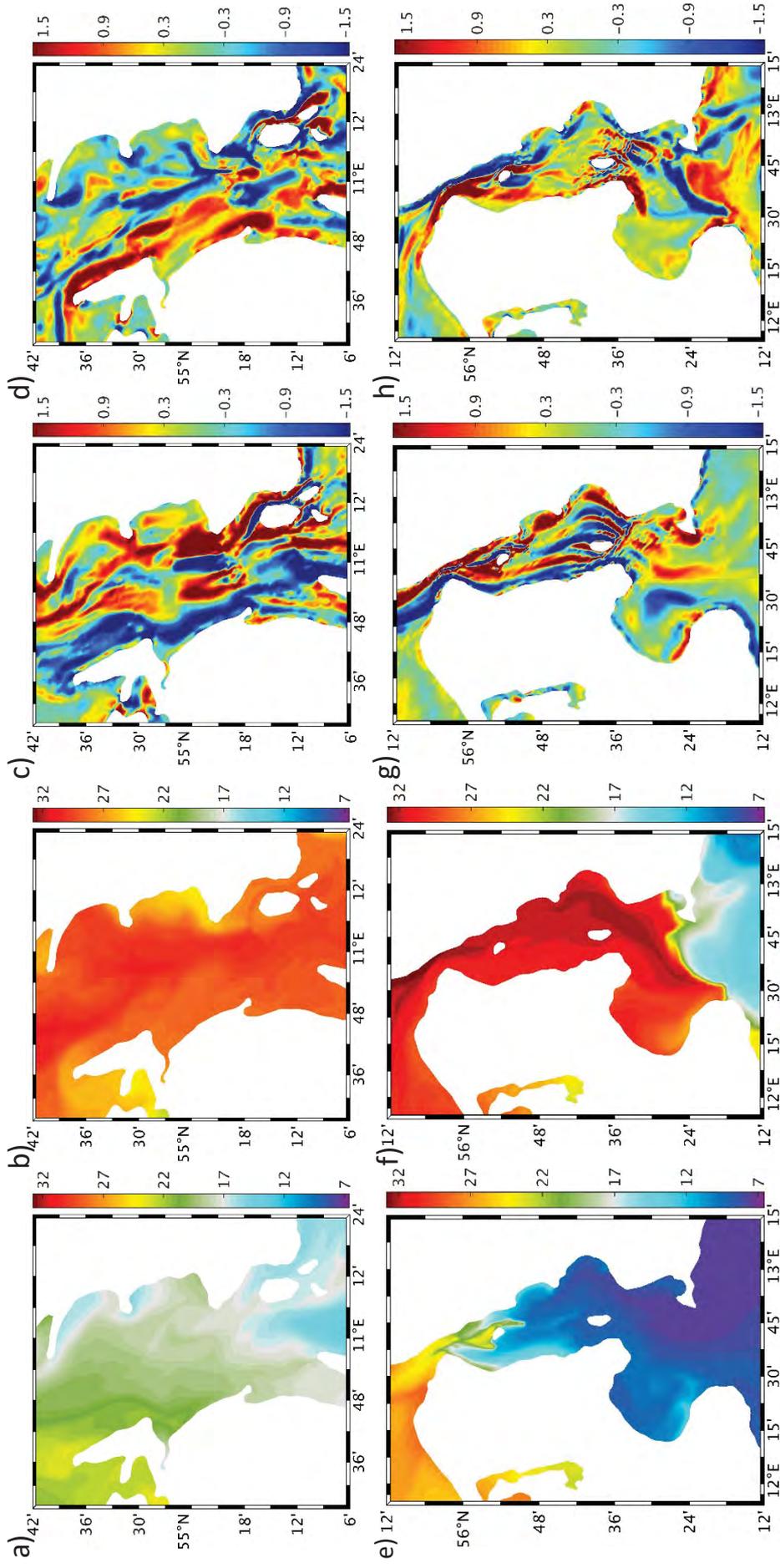


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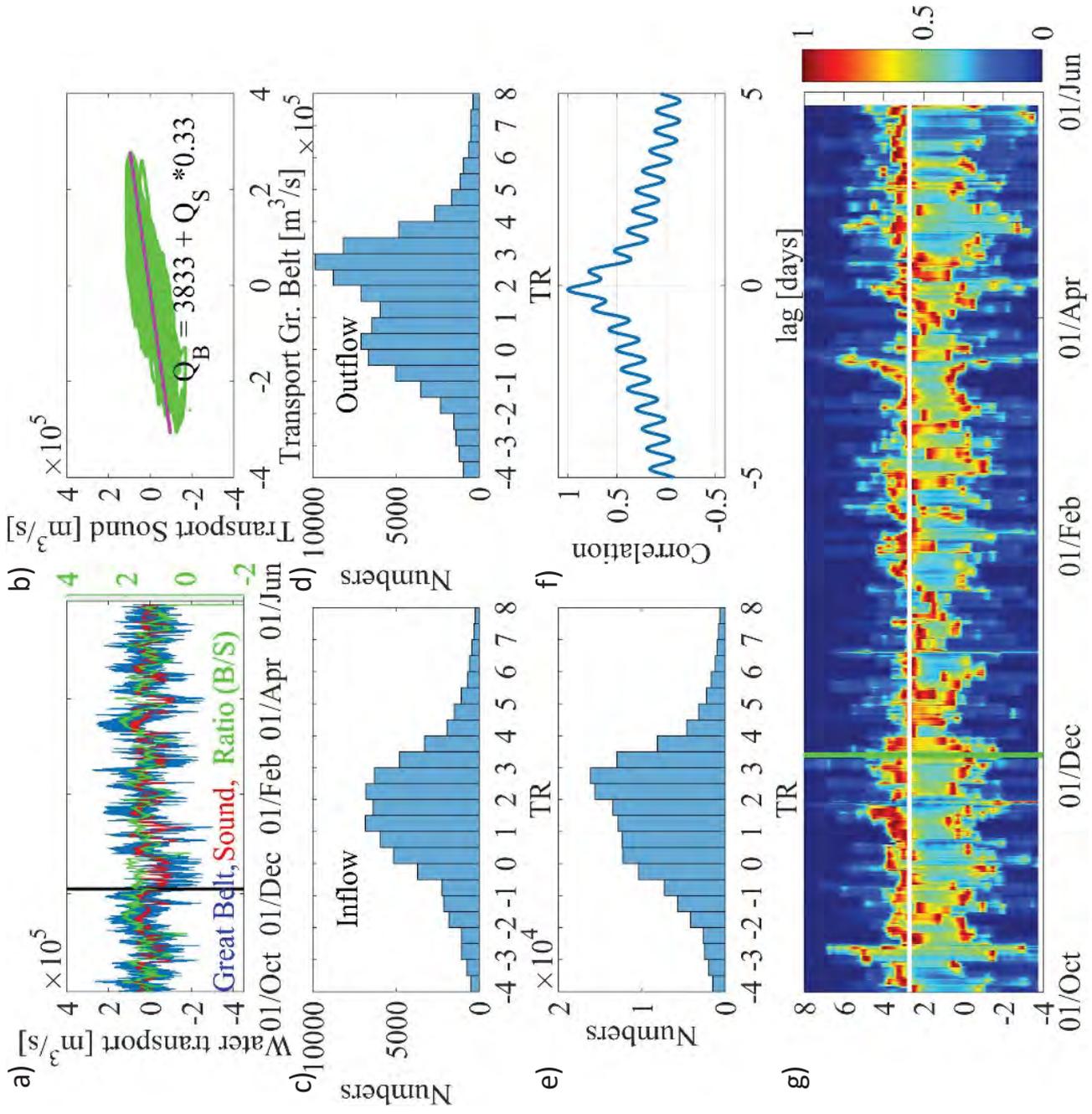


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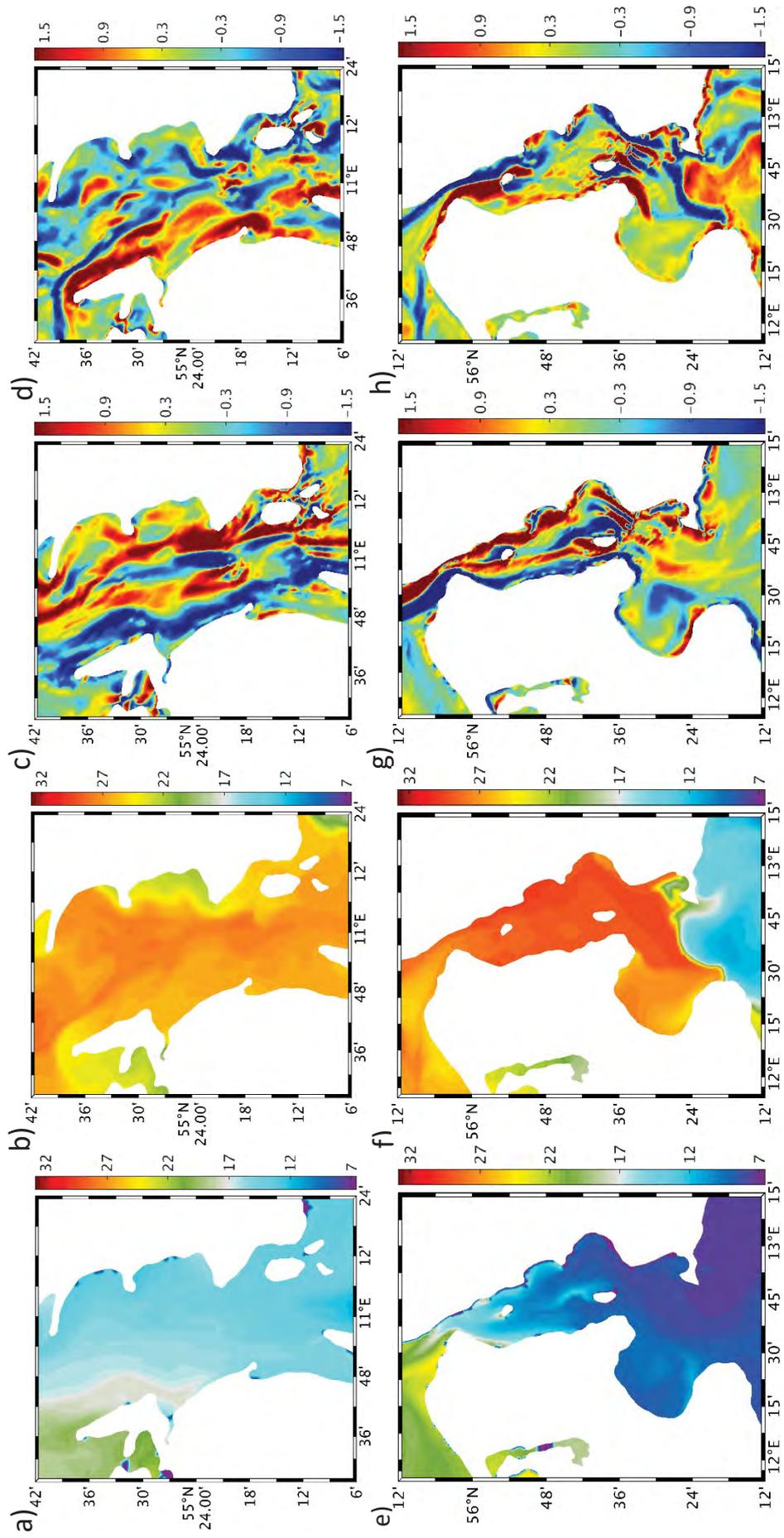


Fig. S5.