



# Cyanobacteria net community production in the Baltic Sea as inferred from profiling $p\text{CO}_2$ measurements

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## Abstract.

Organic matter production by cyanobacteria blooms is a major environmental concern for the Baltic Sea as it promotes the spread of anoxic zones. Partial pressure of carbon dioxide ( $p\text{CO}_2$ ) measurements carried out on Ships of Opportunity (SOOP) since 2003 have proven to be a powerful tool to resolve the carbon dynamics of the blooms in space and time. However, SOOP measurements lack the possibility to directly constrain the depth-integrated net community production (NCP) due to their restriction to the sea surface. This study tackles the resulting knowledge gap through (1) providing a best-guess NCP estimate for an individual cyanobacteria bloom based on repeated profiling measurements of  $p\text{CO}_2$  and (2) establishing an algorithm to accurately reconstruct depth-integrated NCP from surface  $p\text{CO}_2$  observations in combination with modelled temperature profiles.

Goal (1) was achieved by deploying state-of-the-art sensor technology from a small-scale sailing vessel. The low-cost and flexible platform enabled observations covering an entire bloom event that occurred in July and August 2018 in the Eastern Gotland Sea. For the biogeochemical interpretation, recorded  $p\text{CO}_2$  profiles were converted to  $C_T^*$ , which is the dissolved inorganic carbon concentration normalised to alkalinity. We found that the investigated *Nodularia*-dominated bloom event had many biogeochemical characteristics in common with blooms in previous years. In particular, it lasted for about three weeks, caused a  $C_T^*$  drawdown of  $80 \mu\text{mol kg}^{-1}$ , and was accompanied by a sea surface temperature increase of  $10 \text{ }^\circ\text{C}$ . The novel finding of this study is the vertical extension of the  $C_T^*$  drawdown up to 12 m water depth. Integration of the  $C_T^*$  drawdown across this depth and correction for vertical fluxes permit a best-guess NCP estimate of  $\sim 1.2 \text{ mol-C m}^{-2}$ .

Addressing goal (2), we combined modelled hydrographical profiles with surface  $p\text{CO}_2$  observations recorded by SOOP *Finnmaid* within the study area. Introducing the temperature penetration depth (TPD) as a new parameter to integrate SOOP observations across depth, we achieve a reconstructed NCP estimate that agrees to the best-guess within 10%.



Applying the TPD approach to almost two decades of surface  $p\text{CO}_2$  observations available for the Baltic Sea bears the potential to provide new insights into the control and long-term trends of cyanobacteria NCP. This understanding is key for an effective design and monitoring of conservation measures aiming at a Good Environmental Status of the Baltic Sea.

## 1 Introduction

### 25 1.1 Net community production (NCP) in marine ecosystems

Net community production (NCP) of organic matter triggers many biogeochemical processes that control the functioning and state of marine ecosystems. Globally relevant examples are the biological carbon pump (Henson et al., 2011; Sanders et al., 2014) and the establishment of oxygen minimum zones (Gilly et al., 2013; Oschlies et al., 2018). In this biogeochemical context, we define NCP as the net amount of carbon fixed in organic matter (gross production minus respiration) that is produced in a defined water volume over a defined period. The reliable quantification of NCP is a prerequisite to understand subsequent biogeochemical transformation of the organic matter and its imprint on environmental conditions.

### 1.2 Baltic Sea

On a regional scale, NCP quantification is of particular importance to study the formation of anoxic conditions in stratified water bodies caused by the mineralisation of organic matter that was exported across a permanent pycnocline. This situation is typically encountered in semi-enclosed, silled estuaries such as the Baltic Sea. The deep basins of the Baltic Sea receive substantial amounts of oxygenated, salty water from the North Sea only during occasional major inflow events. Between inflow events, those water masses can stagnate for more than a decade below the permanent halocline (Mohrholz et al., 2015), which is located at around 60 m water depth in the Central Baltic Sea. The export of organic matter into the deep waters is the ultimate cause for the expansion of anoxic areas in the Baltic Sea, which are nowadays considered “the largest anthropogenically induced hypoxic areas in the world [a state which is] primarily linked to increased inputs of nutrients from land” (Carstensen et al., 2014). A quantitative and mechanistic understanding of near-surface organic matter production is key to understand, predict, and eventually counteract the expansion of those anoxic areas. The development of measures to reduce eutrophication and deep water anoxia represents a core component of the EU Marine Strategy Framework Directive (MSFD), which is implemented as the HELCOM Baltic Sea Action Plan (BSAP) and aims at a Good Environmental Status (GES).

### 45 1.3 Cyanobacteria blooms

The annual cycle of organic matter production in the Baltic Sea can be broadly divided into two events (Schneider and Müller, 2018). After a nitrate-fueled spring bloom, which is usually followed by a so-called blue water period with close-to-zero NCP rates, mid-summer cyanobacteria blooms develop in most years and cause a next pulse of NCP. The cyanobacteria blooms are limited to the months of June to August (Kownacka et al., 2020) and represent a common feature of the Baltic Sea ecosystem at least since the 1960s (Finni et al., 2001). The blooms are a major public concern, because they produce toxins and form



thick surface scums lowering the recreational value of the Baltic Sea. From a biogeochemical perspective, the ability to fix nitrogen makes cyanobacteria independent from nitrate and aggravates the eutrophication state of the Baltic Sea. Whether their growth is limited by the availability of phosphate remains an ongoing debate (Nausch et al., 2012), although the highly variable C:P ratio of their biomass (Nausch et al., 2009) indicates phenotypic plasticity. Other ongoing debates in the field of cyanobacteria research address the fate of the produced organic matter and its transfer into the food web (Karlson et al., 2015), the intensification of cyanobacteria blooms through positive feedback loops between organic matter production, deep water anoxia and the release of phosphate from anoxic sediments (Vahtera et al., 2007), as well as their response to ongoing changes in salinity, temperature and the partial pressure of carbon dioxide ( $p\text{CO}_2$ ) (Olofsson et al., 2019, 2020). The limited understanding of the factors that control the blooms hinders the reliable prediction of the future state of the Baltic Sea and therefore the prioritisation of conservation measures (Elmgren, 2001). In particular, it remains challenging to disentangle how expected trends – including warming, reduced nutrient loads, and increasing  $p\text{CO}_2$  – might impact cyanobacteria growth (Meier et al., 2019; Saraiva et al., 2019).

#### 1.4 Quantification of NCP

Striving for a better understanding of the ecosystem impact of cyanobacteria blooms, the accurate quantification of produced organic matter is key. In this regard, NCP could in principle be quantified directly as an increase in particulate organic carbon (POC). However, POC measurements would not detect the amount of organic matter that was exported between observations (Wasmund et al., 2005) and also fail to achieve the required spatio-temporal resolution due to a low degree of automation. As an alternative, it is possible to quantify NCP through the drawdown of dissolved inorganic carbon ( $\text{C}_T$ ) from the water column (Schneider et al., 2003). From a biogeochemical perspective, the determination of NCP in terms of carbon is ideal, because carbon is the major component of organic matter and directly related the amount of oxygen ( $\text{O}_2$ ) that is consumed during mineralisation. In principle, NCP could as well be estimated from  $\text{O}_2$  time series. However, the equilibrium reactions of carbon dioxide ( $\text{CO}_2$ ) in seawater result in higher re-equilibration times of  $\text{CO}_2$  with the atmosphere compared to  $\text{O}_2$ , which results in substantially longer signal preservation and makes  $\text{C}_T$  the preferred tracer for NCP. During the Baltic Sea spring bloom, the tracing of nutrient consumption is a meaningful alternative to quantify NCP and convincingly leads to comparable results to the  $\text{C}_T$  approach (Wasmund et al., 2005). However, nutrient time series do not allow for determining cyanobacteria NCP due to the organism's ability to fix nitrogen and their highly variable C:P ratios. In conclusion, the well established  $\text{C}_T$  approach is the favorable method to determine cyanobacteria NCP. However, it should be noted that NCP estimates derived from this approach include the formation of POC and dissolved organic carbon (DOC). The produced DOC contributes ~20% to POC (Hansell and Carlson, 1998; Schneider and Kuss, 2004) and is not likely to be vertically exported.

#### 1.5 Previous studies

Among previous attempts to trace and quantify the organic matter production of cyanobacteria blooms, automated measurements of the partial pressure of carbon dioxide ( $p\text{CO}_2$ ) on the Ship of Opportunity (SOOP) *Finnmaid* played a pivotal role. Those measurements were started in 2003 and it was demonstrated that highly accurate time series of changes (not absolute



values) in  $C_T$  can be derived from  $p\text{CO}_2$  observations (Schneider et al., 2006). The conversion from  $p\text{CO}_2$  to  $C_T$  relies on a  
85 fixed alkalinity ( $A_T$ ) estimate and is applicable under the condition that internal sources of  $A_T$  can be excluded, which is the  
case in the Baltic Sea due to the absence of calcifying plankton (Tyrrell et al., 2008). The derived parameter is comparable to  
directly measured  $C_T$  normalised to  $A_T$ , and in the following referred to as  $C_T^*$ . For several years of SOOP observations, it was  
shown that the  $C_T^*$  drawdown during mid-summer cyanobacteria blooms occurs in pulses of days to weeks, primarily during  
90 calm, sunny days. Further, it was found that the  $C_T^*$  drawdown correlates well with the co-occurring increase in sea surface  
temperature (SST), rather than with absolute SST. This relationship was attributed to a common driver, which is the light dose  
received by the water mass under consideration (Schneider and Müller, 2018).

Despite the successful investigation of cyanobacteria blooms through SOOP  $p\text{CO}_2$  observations, providing a depth-integrated  
estimate of NCP in units of moles carbon fixed per surface area remains challenging due to the restriction of SOOP observations  
to surface waters. Previous studies aiming at a depth-integrated NCP estimate either simply assumed that the  $C_T$  drawdown  
95 reached as far down as the water inlet of the measurement system (Schneider and Müller, 2018) or relied on a modelled mixed  
layer depth for the integration of surface observations across depth (Schneider et al., 2014). However, in the absence of any  
vertically resolved measurements, neither approach could be validated. Likewise, remote sensing approaches resolve the spa-  
tial coverage of the blooms (Hansson and Hakansson, 2007; Kahru and Elmgren, 2014), but fail to detect their vertical extent  
(Kutser et al., 2008) and quantify NCP. Finally, regular research vessel cruises allow for the determination of a full suite of bio-  
100 geochemical parameters from discrete water samples and even the experimental determination of carbon fixation rates through  
 $^{14}\text{C}$  incubations (Wasmund et al., 2001, 2005). Incubation experiments can provide valuable information about instantaneous  
rates of NCP, but – in contrast to time series observations such as obtained by SOOP measurements – do not allow to integrate  
observed changes over time and constrain budgets of biogeochemical transformations. This integration over time requires sev-  
eral weeks of repeated observations to resolve the progression of entire bloom events, ideally covering a station network to  
105 average bloom patchiness.

## 1.6 This study

This study builds upon the previous success to determine NCP based on  $p\text{CO}_2$  time series, but extends the approach to vertically  
resolved observations for the first time. The primary goals of this study are to

- 110 (1) provide a best-guess estimate for the depth-integrated NCP of an individual cyanobacteria bloom based on the full suite  
of depth-resolved in situ measurements and
- (2) establish an algorithm to reconstruct depth-integrated NCP based on surface  $p\text{CO}_2$  observations and modelled hydro-  
graphical profiles

Achieving goal (2) and applying the algorithm to almost two decades of SOOP  $p\text{CO}_2$  observations in the Baltic Sea would not  
only allow to determine long-term trends of cyanobacteria NCP, but also enable disentangling its drivers through a comparison  
115 of NCP across years characterized by different environmental conditions such as SST,  $p\text{CO}_2$  and nutrient availability.



## 2 Methods

### 2.1 Overview

Profiling in situ sensor measurements and water sampling were performed on board the 27ft sailing vessel *SV Tina V* in the framework of the field sampling campaign “BloomSail”. The study area was located in the Central Baltic Sea and extended  
120 about 25 nautical miles from the coast of Gotland into the Eastern Gotland Basin (Fig. 1). Measurements were performed during eight cruises covering the period July 6 to August 16, 2018 (Fig. 2).

A custom-made sensor package configured at IOW’s Innovative Instrumentation department was deployed to perform  $p\text{CO}_2$  and conductivity, temperature and depth (CTD) measurements. The sensor package was either towed near the water surface while cruising or lowered to at least 25 m water depth at designated profiling stations. This study focuses exclusively on the vertical profiles recorded at stations 02 – 12 (Fig. 1b), whereas profiles in coastal regions with water depths below 60 m and towed  
125 surface measurements were not taken into account. In addition to the sensor measurements, discrete samples for dissolved inorganic carbon ( $C_T$ ), total alkalinity ( $A_T$ ) and phytoplankton counts were collected. Track coordinates were continuously recorded with a tablet computer (Galaxy Tab Active, Samsung Electronics, Suwon, South Korea).

In addition to the field sampling campaign, atmospheric measurements of wind speed and  $p\text{CO}_2$  were provided by an ICOS  
130 (Integrated Carbon Observation System) station permanently operated on the island Östergarnsholm (Fig. 1B). Furthermore, sea surface  $p\text{CO}_2$  and temperature (SST) were also determined on the SOOP *Finnmaid*, regularly crossing the field study area (Fig. 1B). High-resolution hydrographical model data were obtained from the Generalized Estuarine Turbulence Model (GETM) along a vertical section following the *Finnmaid* track.

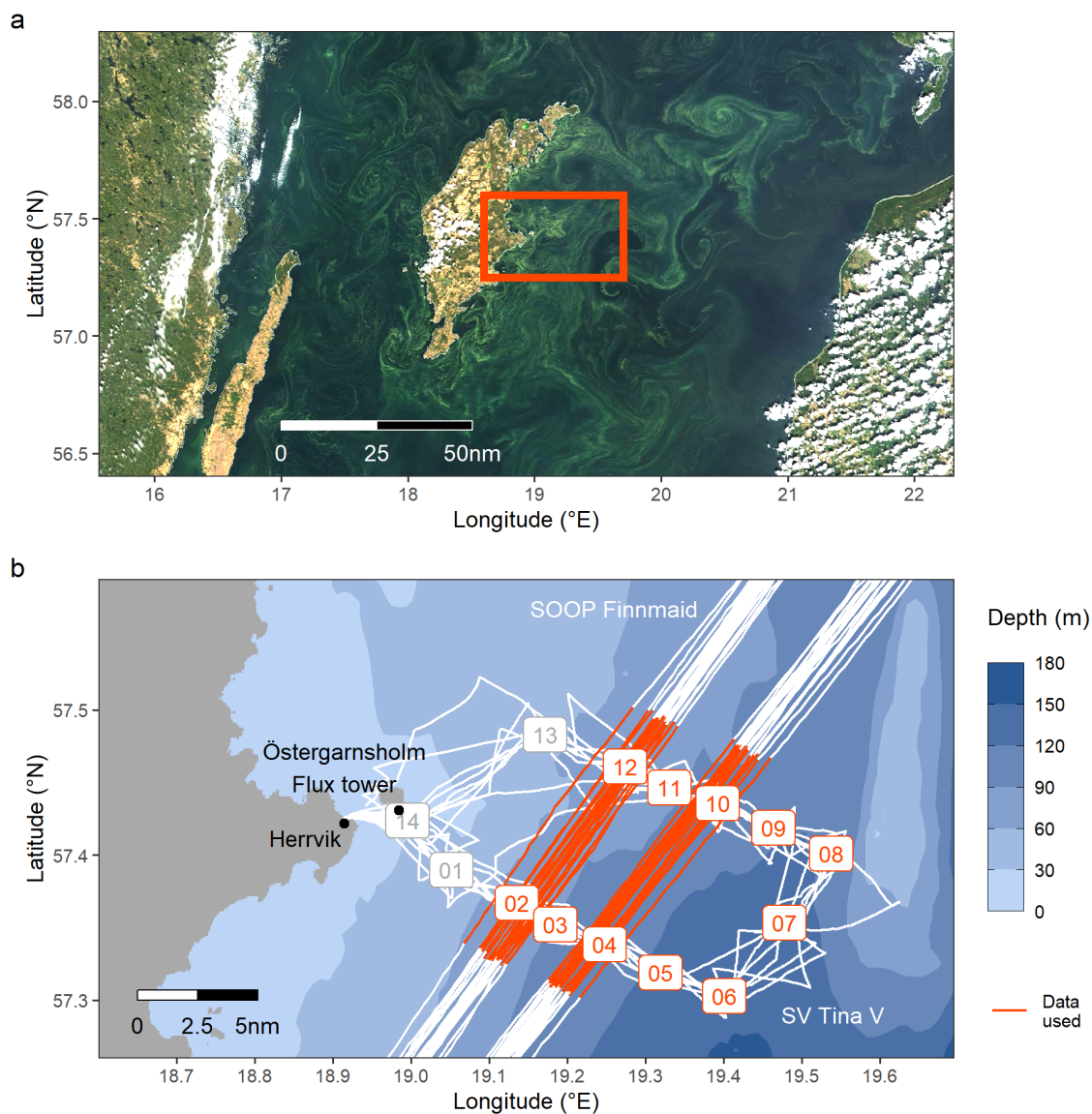
### 2.2 Field sampling campaign

#### 135 2.2.1 CTD measurements

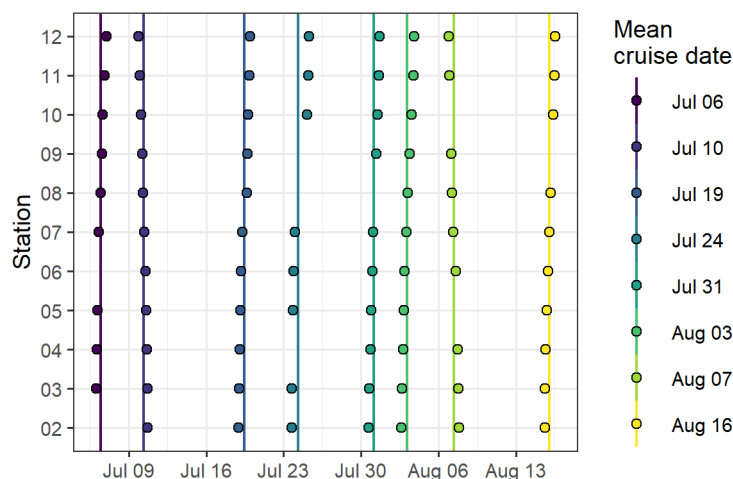
CTD measurements were performed with a SBE 16 SEACAT instrument (serial number 2557; Sea-Bird Electronics, Bellevue, USA). Temperature and salinity sensors were pre-calibrated at IOW’s sensor calibration laboratory. The manual operation of the sensor package was guided by real-time display of data submitted through a strain-relieved cable. Data stored on an internal memory were used for analysis. The CTD logging frequency was 15 seconds and observations were linearly interpolated to  
140 match the higher measurement frequency of the  $p\text{CO}_2$  sensor (for additional details see Appendix A2). The CTD instrument supplied auxiliary sensors with power and served as a central unit to record and transmit analogue output signals.

#### 2.2.2 $p\text{CO}_2$ sensor measurements

The submersible  $\text{CO}_2$  sensor used in this study, a CONTROS HydroC®  $\text{CO}_2$  (formerly Kongsberg Maritime Contros, Kiel, Germany; now -4H-JENA engineering, Jena, Germany), uses membrane equilibration of a headspace and subsequent optical  
145 Non-Dispersive Infra-Red (NDIR) absorption to determine the  $p\text{CO}_2$  in water (Fietzek et al., 2014).



**Figure 1.** (a) Extent of the cyanobacteria bloom on July 26, detectable as greenish patterns in a true color satellite image (MODIS Aqua/Terra, Nasa Worldview) showing the Central Baltic Sea around the island of Gotland. The box indicates the study area as shown in (b), a bathymetric map with the cruise tracks of *SV Tina V* (BloomSail campaign) and *SOOP Finnmaid*. BloomSail stations and the SOOP sub-transects used in this study are highlighted in red. The ICOS flux tower for atmospheric measurements is located on the island of Östergarnsholm.



**Figure 2.** Overview on profiling sensor measurements performed at stations 02 – 12 (Fig. 1). Individual sampling events are displayed as points, whereas vertical lines indicate the mean date of each cruise event.

A pre- and post-deployment calibration of the sensor was performed by the manufacturer.  $p\text{CO}_2$  data were post-processed taking into account the pre- and post-deployment calibration polynomials, as well as zeroing signals regularly recorded during each deployment. The post-processing resulted in an accuracy of 1% of reading (Fietzek et al., 2014). For details concerning sensor calibration, configuration, and signal post-processing, see Appendices A1 – A3.

150 Although the  $p\text{CO}_2$  sensor achieves low and reproducible response times through active pumping of water onto the membrane, a correction of the response time ( $\tau$ ) was applied following Bittig et al. (2018). After the response time correction, the mean absolute  $p\text{CO}_2$  difference between the up- and downcast profile was  $<2.5 \mu\text{atm}$  in the upper 5 m of the water column and  $<7.5 \mu\text{atm}$  across the upper 20 m (Fig. A2). For details concerning the response time correction, see Appendix A4.

The biogeochemical interpretation of the  $p\text{CO}_2$  data was based on downcast profiles only. Since downcasts were started  
155 after complete equilibration of the  $p\text{CO}_2$  sensor in near-surface waters, the applied response time correction has only a minor impact on the derived NCP estimate.

### 2.2.3 Discrete $C_T$ , $A_T$ and phytoplankton sampling

Discrete samples were collected at stations 07 and 10 (Fig. 1B) with a manually released Niskin bottle. The sampling depth was estimated based on the released line.  $C_T$  and  $A_T$  samples were filled into 250 ml SCHOTT-DURAN bottles and poisoned  
160 with 200  $\mu\text{L}$  saturated  $\text{HgCl}$  solution within 24 hours after sampling. Samples were stored dark and cool, transported to IOW, and analysed in the laboratory within no more than 21 days after sampling.  $C_T$  was determined with an Automated Infra Red Inorganic Carbon Analyzer (AIRICA, MARIANDA, Kiel, Germany) and  $A_T$  was analysed by open cell titration (Dickson et al., 2007).  $C_T$  and  $A_T$  measurements were referenced to certified reference materials from batch 173 (Dickson et al., 2003). Phytoplankton samples were fixed with Lugol solution, and community composition and biomass were determined by



165 microscopic counts according to the Utermöhl method (HELCOM, 2017). For details on the analysis of discrete samples, see Appendix B.

### 2.3 Atmospheric measurements

Meteorological observations were provided by the ICOS flux tower (Fig. 1b) located on the southernmost tip of the Island of Östergarnsholm (57.43010 °N, 18.98415 °E; Rutgersson et al., 2020). Atmospheric  $p\text{CO}_2$  was recorded with an atmospheric profile system (AP200, Campbell Scientific, Logan, USA) mounted with a  $\text{CO}_2/\text{H}_2\text{O}$  gas analyzer (LI-840A, LI-COR Bio-  
170 sciences, Lincoln, USA). Wind speed was measured with a wind monitor (Young, Michigan, USA) at 12 m above mean sea level. Wind speed and  $p\text{CO}_2$  data were averaged over 30 min intervals for further analysis. Measured wind speed was converted to  $U_{10}$ , the wind speed at 10 m above sea level (Winslow et al., 2016), to be consistent with the gas exchange parameterisation (see Sect. 2.4.3).

### 175 2.4 NCP best-guess estimate

The determination of NCP in this study relies on the interpretation of observed temporal changes in the dissolved inorganic carbon concentration ( $C_T^*$ ) across the water column. We refer to this estimate as our best-guess, as it is well-constrained by high-quality measurements and therefore as close to the truth as currently possible. Conceptually, our calculations follow the idea of a one-dimensional box model approach, which does not resolve regional variability within the research area, i.e. it  
180 neglects lateral water mass transport. With this approach it is possible to calculate NCP from the observed changes in  $C_T^*$  (Sect. 2.4.1) after vertical gridding and regional averaging of the profiles (Sect. 2.4.2) and applying corrections for  $\text{CO}_2$  fluxes caused by air-sea gas exchange (Sect. 2.4.3) and vertical mixing (Sect. 2.4.4).

#### 2.4.1 $C_T^*$ calculation

$C_T^*$  was calculated from the measured profiles of temperature and response time corrected  $p\text{CO}_2$  (Schneider et al., 2014), as  
185 well as the mean  $A_T$  ( $1720 \mu\text{mol kg}^{-1}$ ) and mean salinity (6.9) determined from discrete samples collected across the upper 20 m of the water column and the entire observation period (Fig. B1). Calculations were performed with the R package seacarb (Gattuso et al., 2020), using the  $\text{CO}_2$  dissociation constants for estuarine waters from Millero (2010).

The calculated  $C_T^*$  represents an alkalinity- and salinity-normalised estimate of the dissolved inorganic carbon concentration.  $C_T^*$  is suitable to accurately determine changes rather than absolute values of the dissolved inorganic carbon concentration and therefore the preferred variable to quantify NCP. The uncertainty in the determination of changes of  $C_T^*$  is below  
190  $2 \mu\text{mol kg}^{-1}$  when the mean  $A_T$  is constrained within  $\pm 30 \mu\text{mol kg}^{-1}$  (see Appendix C1 for a detailed assessment).

#### 2.4.2 Vertical gridding and regional averaging

The regional averaging of observations across the study area and the calculation of temporal changes at individual depth levels required a vertical gridding of the profiling sensor measurements. The vertical gridding of individual profiles was achieved





195 by calculating mean values within 1 m depth intervals. Downcast profiles with missing observations from two or more depth  
intervals caused by zeroing measurements of the  $p\text{CO}_2$  sensor were discarded, which affected 8 out of 86 recorded profiles.  
For each of eight cruise events (Fig. 2), regionally averaged profiles were further calculated as mean values within each depth  
interval across all stations. Based on those mean, vertically gridded cruise profiles, incremental and cumulative changes over  
time were calculated for each depth interval. Throughout the manuscript, observations averaged across the upper 0 – 6 m of  
200 the water column are referred to as surface observations.

### 2.4.3 Air–sea $\text{CO}_2$ flux

The air–sea gas exchange of  $\text{CO}_2$  ( $F$ ) was calculated from sea surface  $p\text{CO}_2$ , salinity and temperature, in combination with  
atmospheric  $p\text{CO}_2$  and wind speed ( $U_{10}$ ) according to Wanninkhof (2014). For the calculation, sea surface observations were  
linearly interpolated to match the temporal resolution of atmospheric measurements.

### 205 2.4.4 Vertical entrainment flux of $\text{CO}_2$ through mixing

Due to the stable thermocline present between June 6 and August 7, vertical mixing of  $C_T^*$  across the 12 m integration depth  
layer was neglected during this period. However, clear signals for significant vertical entrainment of  $C_T^*$  across this layer were  
recorded between August 7 and 16. This entrainment was quantified assuming an instantaneous complete vertical mixing to  
17 m water depth after August 7. For this simplified scenario, the  $C_T^*$  flux across the 12 m depth layer was estimated based on  
210 a mass–balance of  $C_T^*$ , which behaves conservatively with respect to mixing (see Appendix C2 for details).

## 2.5 NCP reconstruction from surface $p\text{CO}_2$ observations and hydrographical profiles

Calculating depth–integrated NCP from a time series of surface  $p\text{CO}_2$  observations, such as provided by SOOP lines, also  
relies on the conversion of  $p\text{CO}_2$  to  $C_T^*$ . Furthermore, the change of  $C_T^*$  over time in the surface water needs to be multiplied  
with an integration depth estimate to derive an inventory change. Here, we tested two approximations of this integration depth,  
215 which are:

- Mixed layer depth (MLD)
- Temperature penetration depth (TPD)

MLD and TPD are described in detail in Sect. 2.5.3. The two parameterisations were further applied to following two test data  
sets, both of which contain the required surface  $p\text{CO}_2$  and vertically resolved temperature and salinity data:

- 220
- In situ data from the BloomSail campaign without  $p\text{CO}_2$  data at depth (SV Tina V (surface only))
  - Combined SOOP surface  $p\text{CO}_2$  observations and modelled salinity and temperature profiles (SOOP Finnmaid + GETM  
model)

The derived four reconstructed NCP time series were compared to the best–guess estimate (i.e. the estimate based on the  
vertically resolved  $p\text{CO}_2$  observations from this study).



### 225 2.5.1 SOOP *Finnmaid* surface $p\text{CO}_2$

SOOP *Finnmaid* regularly commutes between Helsinki in Finland and Travemünde in Germany thereby crossing the entire Central Baltic Sea and our study area on the east coast of Gotland every 1 – 2 days. On board SOOP *Finnmaid*,  $p\text{CO}_2$  is measured with a bubble-type equilibrator system supplied with water from an inlet at around 3 m water depth. Details of the measurement set-up are described in Schneider et al. (2014) and data are submitted on a regular basis to the Surface Ocean  $\text{CO}_2$  Atlas SOCAT (Bakker et al., 2016). The primary measurement system used to determine  $p\text{CO}_2$  in this study is a NDIR sensor (LI-6262, LI-COR Biosciences, Lincoln, USA). The ferrybox unit is also equipped with an additional methane/carbon dioxide analyzer (Greenhouse Gas Analyzer DLT 100, type 908-0011, Los Gatos Research, San Jose, USA), providing independent  $p\text{CO}_2$  observations (Gülzow et al., 2011). Intercomparison of both systems is routinely used to ensure the correct functioning of the instrumentation. In this study, a data gap caused by malfunctioning of the primary LI-COR system was filled by including data recorded with the Los Gatos system on six cruises between July 8 and 16 (see Appendix D for details). The mean regional  $p\text{CO}_2$ , sea surface temperature (SST) and salinity (SSS) were calculated for each crossing of the study area (Fig. 1B). Based on those mean values,  $C_T^*$  was calculated following the procedure outlined in Sect. 2.4.1. A remaining gap in the SOOP time series was filled with two in situ  $C_T^*$  observations from the BloomSail campaign (July 19 and 24).

### 2.5.2 GETM model temperature and salinity

Surface SOOP measurements were complemented with the vertical distribution of salinity and temperature from the output of a numerical ocean model of the Baltic Sea. The deployed General Estuarine Turbulence Model (GETM) has a horizontal resolution of 1 nautical mile and 50 vertical terrain-following levels. The uppermost level has a thickness of maximum 50 cm to properly represent SST and ocean-atmosphere fluxes. The computation of the atmospheric fluxes is based on the parameterisation of Kara et al. (2005). The model run covers the period 1961 – 2019. A detailed analysis of the ocean model performance is given in Placke et al. (2018) and Gräwe et al. (2019). For the present study, we used a model run restarted in 2003 with the atmospheric forcing from the operational reanalysis data set of the German weather service (Zängl et al., 2015). Additionally, we implemented the Langmuir-circulation parameterisation of Axell (2002), to account for wind-wave induced variation in the mixed layer depth. Model results were averaged over 24 h and interpolated to a standardised section with 2 km horizontal and 1 m vertical resolution, which follows the mean *Finnmaid* cruise track. Based on this standard section, daily mean profiles within the study area were computed and linearly interpolated to match the exact times of *Finnmaid* crossings.

### 2.5.3 Parameterisation of the integration depth

In this study, two parameters were used to integrate surface observations across depth, namely the classical mixed layer depth (MLD) and the newly introduced temperature penetration depth (TPD).

MLD was defined as the shallowest depth at which seawater density exceeds the density at the surface by more than  $0.1 \text{ kg m}^{-3}$  (Roquet et al., 2015). According to this definition, MLD characterises the thermohaline structure of the water column and often (but not necessarily) approximates the depth to which surfaces water masses are actively mixed. The defini-



tion through a fixed density threshold further implies that gradual changes of temperature with depth are not reflected by this parameter.

260 TPD was defined as the SST increase divided by the integrated warming signal across the water column (i.e. the sum of all positive temperature changes within 1m depth intervals) that occurred between two sampling events (for illustration see Fig. C4A). TPD is only applicable when SST increases and has units of metres. According to its definition, TPD characterises the mean penetration depth of a warming signal and takes gradual changes of temperature across depth into account. To illustrate the TPD concept, it should be noted that a homogeneous warming signal that ceases abruptly at 10 m water depth would result in the same TPD as a warming signal that decreases linearly from the surface to 20 m water depth (TPD is 10 m in both cases). The TPD approach is motivated by the assumption that primary production and temperature increase are both primarily controlled by the light dose that a water parcel received (Schneider et al., 2014) and therefore show similar patterns.

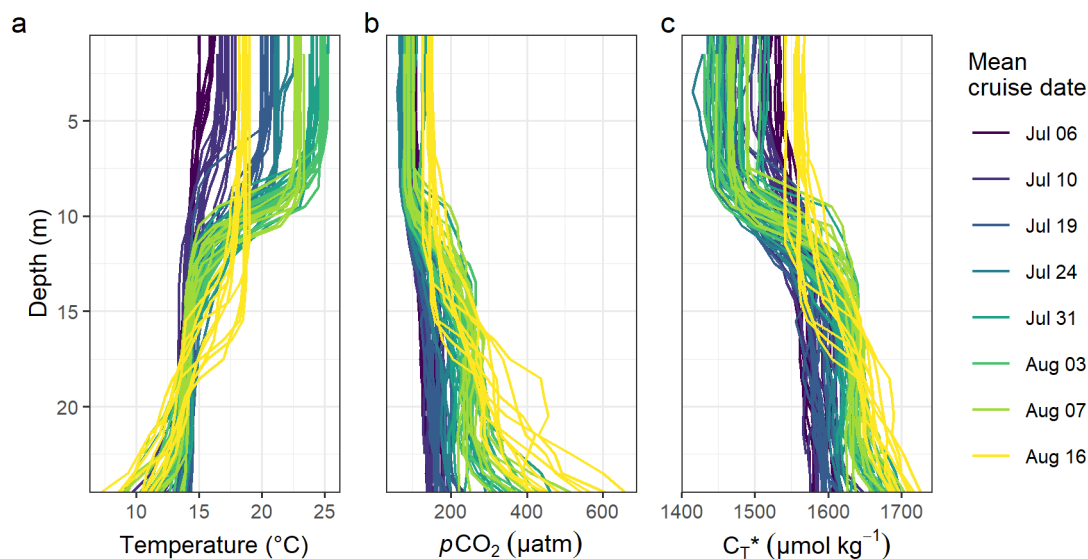
265 Based on MLD or TPD, vertically integrated changes of  $C_T^*$  were reconstructed as the product of incremental changes of surface  $C_T^*$  between cruise days and one of the two integration depth estimates. The reconstructed integrated changes of  $C_T^*$  were further corrected for air–sea fluxes of  $CO_2$  according to section 2.4.3. Please note that neither the MLD nor the TPD approach allows to resolve vertical entrainment fluxes, because profiles of  $C_T^*$  are not reconstructed (compare section 2.4.4). In analogy to TPD, the penetration depth of  $C_T^*$  drawdown (CPD) was defined as the decrease of  $C_T^*$  at the surface divided by the integrated loss of  $C_T^*$  across the water column (Fig. C4B).

### 3 Results

#### 3.1 Dynamics of temperature, $pCO_2$ , $C_T^*$ and phytoplankton biomass

275 Between July 6 and August 16, a total number of 78 complete vertical CTD and  $pCO_2$  downcast profiles were recorded (Fig. 2 and 3).  $C_T^*$  was calculated and profiles were regionally averaged for each of the eight cruise events (Fig. 4). Since the first cruise of the BloomSail expedition on July 6, sea surface temperature (SST) increased steadily from  $\sim 15^\circ C$  to peak values of  $25^\circ C$  (Fig. 4 and 5) observed on August 3. Sea surface  $pCO_2$  was already as low as  $\sim 100 \mu atm$  at the beginning of July (Fig. 5a) and decreased further to the lowest values of  $\sim 70 \mu atm$  on July 24. The drop in  $pCO_2$  and the simultaneous increase in SST correspond to a decrease of  $C_T^*$  of almost  $90 \mu mol kg^{-1}$  (Fig. 4). During this period of intense primary production, the regional variability of SST,  $pCO_2$ , and  $C_T^*$  across stations was low compared to their temporal change (Fig. 5a–b; Fig. C3). The regional variability is slightly higher when including the coastal stations 01, 13, and 14 (results not shown), but is generally lower than suggested by the bloom patchiness typically observed through remote sensing (Fig. 1a). With respect to  $pCO_2$  dynamics, it should be noted that (i) the observed temperature increase and  $C_T^*$  drawdown have opposing effects on  $pCO_2$  and (ii) the change of  $pCO_2$  per change in  $C_T^*$  is generally low at low absolute  $pCO_2$ . The observed  $C_T^*$  dynamics in surface waters are clearly attributable to the primary production activity of phytoplankton and go along with an observed increase of the biomass of *Nodularia* sp. (Fig. B2), which also peaked on July 24.

285 Between the extremes of  $pCO_2$  and  $C_T^*$  (minimum on July 24) and SST (maximum on August 3), a noticeable increase of surface  $C_T^*$  was observed on July 31, which was accompanied by a higher regional variability across the station network

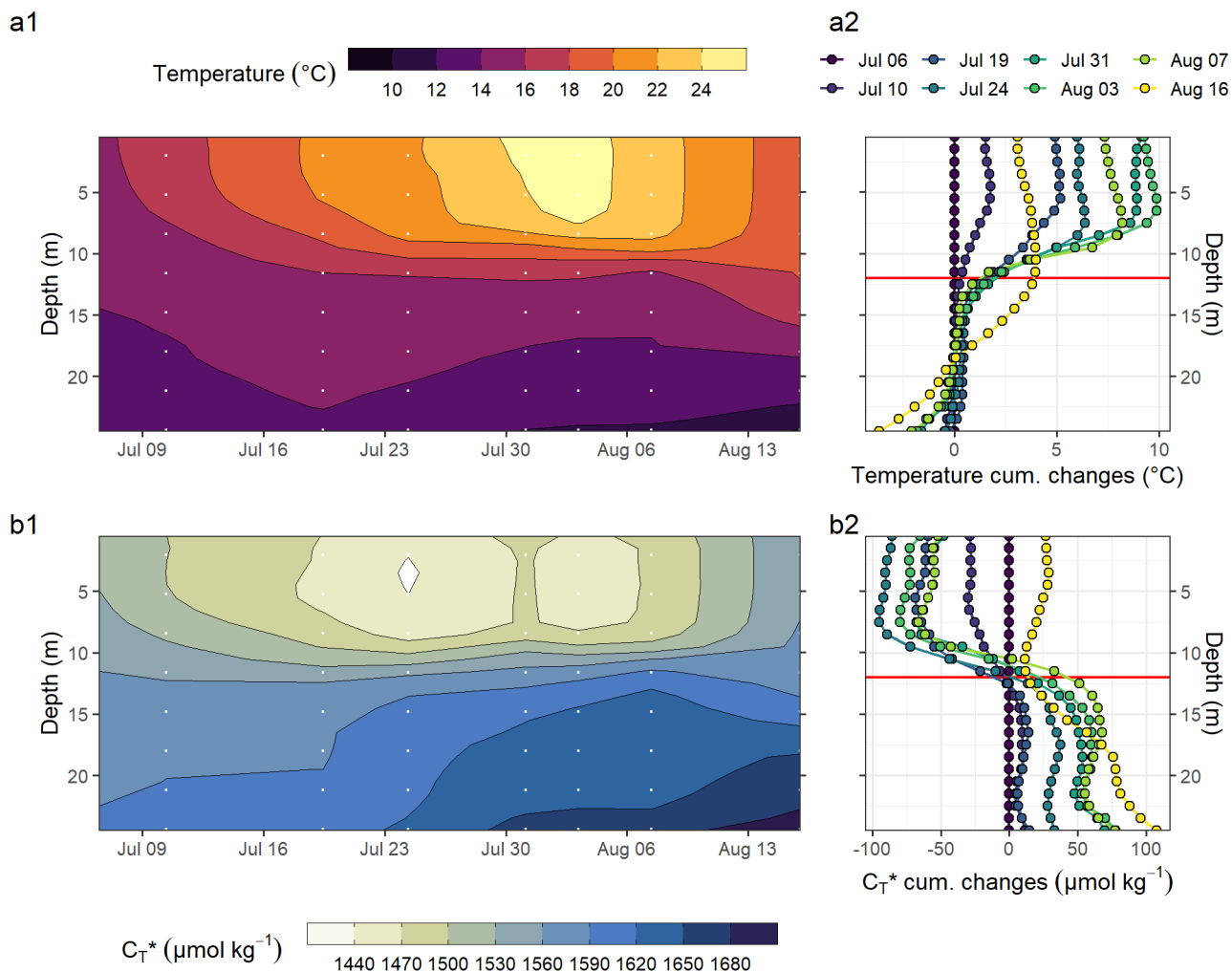


**Figure 3.** Overview of (a) temperature, (b)  $p\text{CO}_2$  and (c)  $C_T^*$  profiles recorded throughout the BloomSail field sampling campaign on board SV *Tina V*.

290 (Fig. 5a,c). The temporary  $C_T^*$  increase was limited to the north-eastern stations 07 – 10 (Fig. C3) and paralleled by a drop in salinity and elevated  $A_T$  at the same stations (Fig. B1). It is therefore attributable to the lateral exchange of water masses. All signals of this lateral intrusion vanished within a week. At the other stations (02 – 06 and 11 – 12), no noticeable signs of water mass exchange or  $C_T^*$  changes were observed between July 24 and August 3, indicating that NCP had ceased during this period. During the first two weeks of August the study area was affected by increased wind speeds, causing a decrease of SST  
295 back to  $\sim 18^\circ\text{C}$ . The simultaneous return of surface  $p\text{CO}_2$  to  $\sim 150 \mu\text{atm}$  corresponded to a  $C_T^*$  increase of  $\sim 100 \mu\text{mol kg}^{-1}$ .

The observed surface warming and  $C_T^*$  drawdown extended vertically to a water depth of  $\sim 10$  m (Fig. 4). On the first cruise day (July 6), the vertical distribution of  $C_T^*$  and temperature was still relatively homogenous.  $C_T^*$  at 25 m water depth was  $\sim 70 \mu\text{mol kg}^{-1}$  higher than at the surface. Likewise, the temperature gradient covered only  $\sim 3^\circ\text{C}$  from  $16^\circ\text{C}$  at the surface to  $13^\circ\text{C}$  at depth. The warming of surface waters caused an increasingly stable thermocline to be established at around 10 m  
300 water depth, reaching a temperature gradient of  $\sim 10^\circ\text{C}$  across 5 m on August 3. Continuous and uniform consumption of  $C_T^*$  within the surface layer enhanced the vertical  $C_T^*$  gradient to  $>150 \mu\text{mol kg}^{-1}$  between the surface and 25 m water depth. The  $C_T^*$  drawdown was observed to a maximum depth of 12 m.

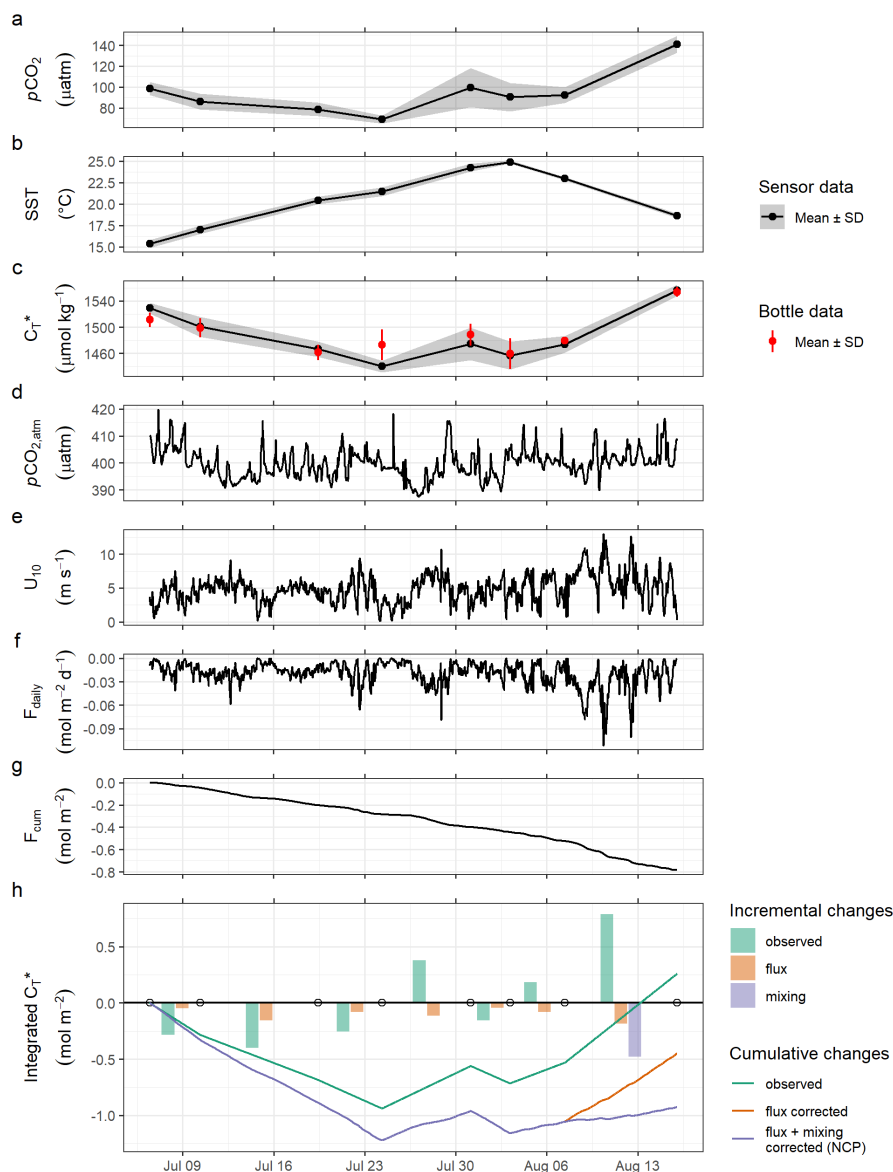
Between August 7 and 16 the SST drop of  $\sim 6^\circ\text{C}$  was accompanied by a temperature increase in deeper water layers (11 – 17 m) of up to  $5^\circ\text{C}$ . This vertical redistribution of heat indicates vertical mixing of water masses, which was also reflected in  
305 a steep increase of  $C_T^*$  in the surface water and a loss of  $C_T^*$  between 11 – 17 m (Fig. 3 and 4).



**Figure 4.** (a) Temperature and (b)  $C_T^*$  between July 6 and August 16 displayed as (1) Hovmoeller plots and (2) profiles of cumulative changes since the first cruise on July 6. Mean cruise dates are indicated by white dots in (1) and the integration depth of 12 m is indicated as a red, horizontal line in (2).

### 3.2 NCP best-guess based on profiling measurements

Net community production (NCP) was determined through vertical integration of the observed consumption of  $C_T^*$  from the surface to a water depth of 12 m. The chosen integration depth reflects the maximum penetration depth of the incremental (i.e. between cruise days), as well as the cumulative (i.e. from July 6 – 24)  $C_T^*$  drawdown (Fig. 4). Likewise, about 95% of the cumulative warming signal, which refers to positive temperature changes integrated over depth, occurred above 12 m.



**Figure 5.** Time series displaying from top to bottom: Surface water observation of (a)  $p\text{CO}_2$ , (b) temperature, (c)  $C_T^*$  with grey ribbons indicating the standard deviation across stations; atmospheric observations of (d)  $p\text{CO}_{2,atm}$ , (e) wind speed at 10 m, (f) daily and (g) cumulative air–sea fluxes of  $\text{CO}_2$ ; as well as (h) the derived water column inventory changes of  $C_T^*$ . In (h), bars represent incremental changes between cruise events (open circles), whereas lines represent cumulative changes since the first cruise. Colours distinguish observed  $C_T^*$  changes from values referring to the applied air–sea  $\text{CO}_2$  flux and mixing correction. Net community production (NCP) is equal to the flux and mixing corrected cumulative changes of  $C_T^*$  (purple line) and reaches its peak value on July 24.



Until July 24, the depth-integrated  $C_T^*$  consumption amounted to  $\sim 0.9 \text{ mol m}^{-2}$  (Fig. 5H). This observed  $C_T^*$  consumption was corrected for air-sea fluxes of  $\text{CO}_2$  ( $F$ ). Between July 6 and August 7, the cumulative flux ( $F_{cum}$ ) amounted to around  $-0.5 \text{ mol m}^{-2}$  (Fig. 5G), with a negative sign representing  $\text{CO}_2$  uptake from the atmosphere. In the absence of noticeable vertical mixing, this flux was entirely added to the observed  $C_T^*$  consumption. Only between August 7 and 16, when mixing to about  
315 17 m water depth was observed, a significant fraction of the  $\text{CO}_2$  taken up from the atmosphere was transported below 12 m water depth. To account for the partial loss of airborne  $\text{CO}_2$  to deeper waters during this 9 day-period, only 12/17 of  $F_{cum}$  during this time ( $-0.2 \text{ mol m}^{-2}$ ), which is the fraction that would remain in the upper water column, was added to the observed  $C_T^*$  consumption. In addition, a significant amount of  $C_T^*$  entrainment ( $\sim 0.5 \text{ mol m}^{-2}$ ) into the surface layer was caused by the vertical mixing between August 7 and 16 (Fig. 5H and C2).

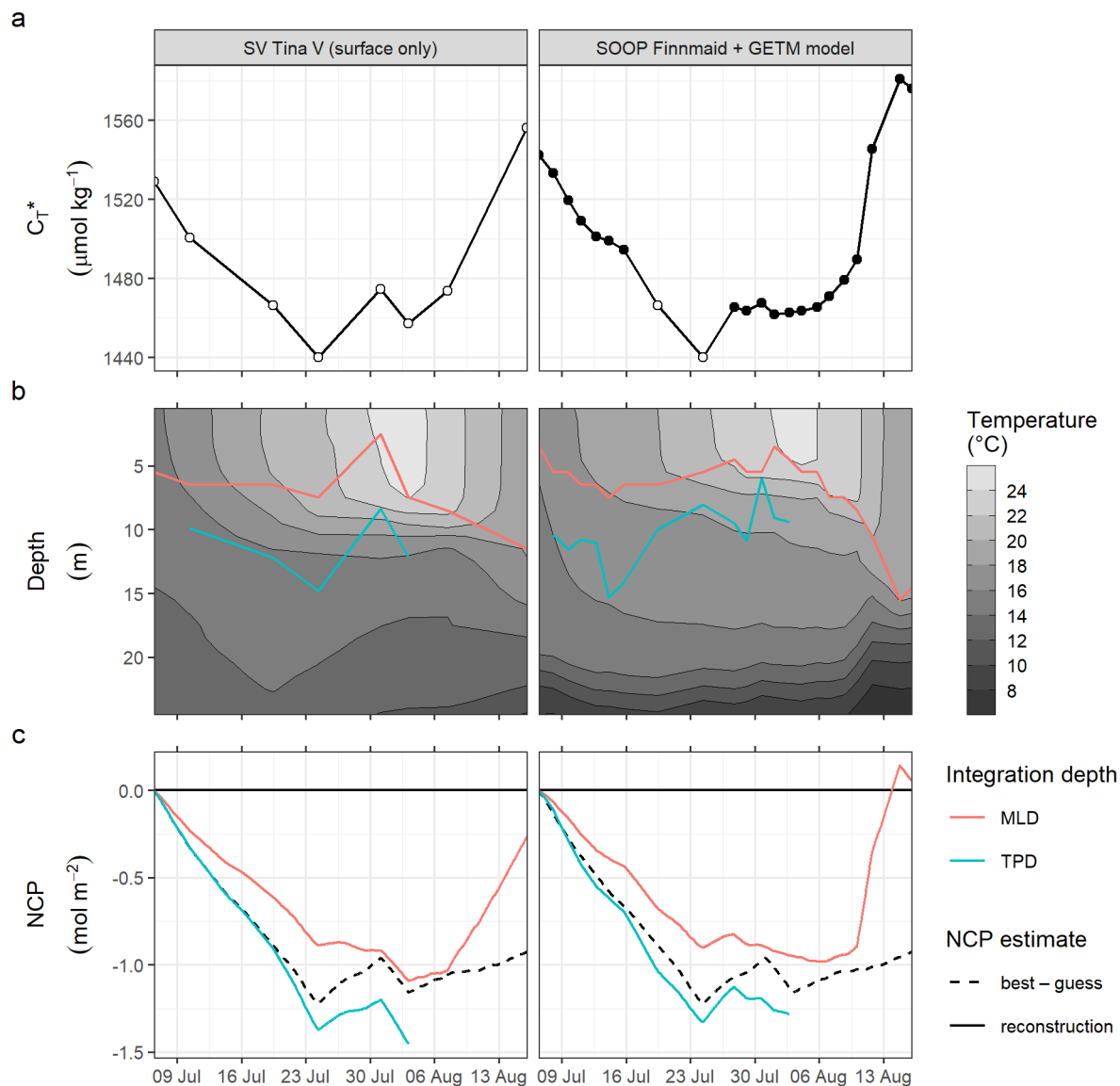
320 After correction for air-sea fluxes and vertical entrainment of  $\text{CO}_2$ , the cumulative changes of depth-integrated  $C_T^*$  represent the NCP between 0 – 12 m water depth (Fig. 5H). The peak NCP value of  $\sim 1.2 \text{ mol m}^{-2}$  was observed on July 24 and is of primary interest because it reflects the amount of organic matter that was produced and is potentially available to be either exported or remineralised. After July 24, no signs of continued NCP were observed. Accordingly, the following attempt to reconstruct NCP based on surface  $p\text{CO}_2$  observations focuses on the period July 6 – 24.

### 325 3.3 NCP reconstruction based on surface $p\text{CO}_2$ and hydrographical profiles

The reconstruction of depth-integrated NCP was tested for two data sets containing the same type of information, namely the observed changes in surface  $p\text{CO}_2$  and vertical profiles of seawater salinity and temperature. The first data set “SV Tina V (surface only)” contains the surface  $p\text{CO}_2$  data recorded during the BloomSail expedition, as well as the complete CTD profiles. The second data set (“SOOP Finnmaid + GETM model”) combines surface  $p\text{CO}_2$  observations from SOOP *Finnmaid*  
330 with seawater salinity and temperature as estimated with the GETM model. For both data sets  $C_T^*$  time series were calculated based on the same mean  $A_T$ .

An almost identical decrease of surface  $C_T^*$  of  $\sim 50 \mu\text{mol kg}^{-1}$  was determined between July 6 and 16 (Fig. 6A), based on the completely independent  $p\text{CO}_2$  data recorded on SOOP *Finnmaid* and SV *Tina V*. Likewise, a very similar increase in  $C_T^*$  between August 6 and 15 was determined from both independent observational data sets. The good agreement between the  
335 independent observations justifies that a data gap due to failure of instrumentation on the SOOP was filled with two observations from SV *Tina V* on July 19 and 24 (open circles in (Fig. 6A).

Good agreement was also found for the spatio-temporal dynamics of observed and modelled seawater temperature (Fig. 6B). Observed and modelled SST agreed within  $1^\circ\text{C}$  over the entire observation period, despite an absolute change spanning almost  $10^\circ\text{C}$ . Slightly higher deviations between observed and modelled temperature were found around the thermocline, where the  
340 observational record revealed a stronger temperature gradient. This difference is likely due to an imperfect representation of Langmuir circulation in the model (Axell, 2002), whereas the absence of increased light attenuation caused by phytoplankton particles was previously found to have only minor impacts on modeled SST dynamics (Löptien and Meier, 2011). Most importantly, the mean temperature penetration depths (TPD) derived from the observational and model data differ less than 1 m, indicating that surface warming and the integrated heat uptake are accurately represented by the model. The TPD (mean



**Figure 6.** Time series illustrating the reconstruction of depth-integrated NCP from surface  $C_T^*$  and vertically resolved hydrographical parameters. Displayed are results based on two test data sets, namely observations from SV *Tina V* without  $C_T^*$  data at depth (left panels) and a combination of SOOP  $C_T^*$  and modelled hydrographical data (right panels). From top to bottom, panels represent (a) surface  $C_T^*$ , (b) the vertical distribution of temperature together with the mixed layer depth (MLD) and temperature penetration depth (TPD) for each cruise day, and (c) depth-integrated NCP comparing the reconstruction approaches (solid lines) with the best-guess estimate (dashed black line) according to Fig. 5. Please note that a data gap in the SOOP record was filled with two observations from SV *Tina V* (open circles in a).





345  $\pm$  SD) across the observed productive period between July 6 and 24 was determined as  $12.3 \pm 2.5$  m and  $11.4 \pm 2.3$  m for the observational and model data, respectively (Fig. 6B). The TPD estimates are considerably higher than the respective mixed layer depth (MLD) estimates ( $6.0 \pm 1.9$  m and  $5.5 \pm 1.2$  m) and agree better with the observed penetration depth of  $C_T^*$  drawdown, indicating that TPD is the favourable approximation of the integration depth.

The NCP reconstruction based on TPD is generally higher than the MLD-based estimate (Fig. 6C). Comparing peak cumulative NCP estimates for July 24, the TPD-approach results in a  $\sim 10\%$  overestimation compared to the best-guess estimate, i.e. the value derived from vertically resolved measurements. In contrast, the MLD-based NCP estimate is  $\sim 30\%$  lower than this best-guess estimate. The reconstructed NCP estimates are very similar for both test data sets, as the good agreement between the underlying  $C_T^*$ , MLD and TPD time series suggests.

355 Comparing the deviation between the best-guess and reconstructed NCP estimates in the light of the lateral variability observed within the study area, it must be emphasised that between July 6 and 24, the mean standard deviation of  $pCO_2$  and  $C_T^*$  across stations amounted to  $\pm 6 \mu\text{atm}$  and  $\pm 11 \mu\text{mol kg}^{-1}$ , respectively. This is higher than the likely uncertainty associated with the  $pCO_2$  measurements (see Methods), as well as its response time correction (see Methods and Appendix A4) or conversion to  $C_T^*$  (see Appendix C1). Therefore, the lateral variability of seawater chemistry and the production signal are generally considered the highest source of uncertainty to our NCP estimates. Still, this lateral variability is small compared to the signal to be resolved (i.e. the  $C_T^*$  consumption of  $\sim 90 \mu\text{mol kg}^{-1}$ ), but on a relative scale ( $\sim 10\%$ ) in about the same order of magnitude as the difference between the best-guess and the TPD-based, reconstructed NCP estimates. In contrast, the lateral variability is smaller than the deviation between the best-guess and the MLD-based, reconstructed NCP estimates.

All reconstructed NCP estimates include the correction of air-sea fluxes of  $CO_2$ , but it is impossible to quantify and correct vertical entrainment fluxes due to mixing, because the vertical distribution of  $C_T^*$  across the water column can not be resolved. 365 The strong deviation between the best-guess NCP and the MLD-based reconstruction on August 16 is due to this missing correction of vertical mixing. This deviation highlights that the reconstruction approach is only applicable to production periods with a stable or shoaling thermocline. The TPD-based approach does not allow for any estimate during the last two weeks of the observations period, as the TPD is per definition only applicable to periods of warming surface waters.

## 4 Discussion

### 370 4.1 Comparison to previous studies

Having in mind the application of our NCP reconstruction approach to other surface  $pCO_2$  observation, it is important to examine if the biogeochemical dynamics of the 2018 cyanobacteria bloom investigated in this study is representative for those in other years. Unfortunately, only a few previous studies aimed at the quantification of cyanobacteria growth as a component of the Baltic Sea carbon budget. One exception is the interpretation of SOOP *Finnmaid* data by Schneider et al. (2014). Focusing 375 on the period from June to August and taking into consideration individual production pulses observed in the years 2005, 2008, 2009 and 2011, the authors found average daily rates of  $C_T^*$  consumption ranging from 3 to  $8 \mu\text{mol kg}^{-1} \text{d}^{-1}$ , which is comparable to the mean rate of  $4.4 \mu\text{mol kg}^{-1} \text{d}^{-1}$  determined in this study (i.e. the average  $C_T^*$  drawdown of  $\sim 90 \mu\text{mol kg}^{-1}$



over 12 days, Fig. 4). The individual production events identified by Schneider et al. (2014) lasted 1 to 5 weeks, similar to the duration described in this study. Finally, Schneider et al. (2014) also provided a depth-integrated NCP estimate based on a daily modelled mixing depths, which ranged from 3 – 20 m and were derived from the vertical distribution of a tracer one day after its injection into the surface. Although this approach is primarily useful to estimate the vertical distribution of air-sea CO<sub>2</sub> fluxes and does not necessarily reflect the vertical extent of net community production, their determined midsummer NCP estimates (1 – 2.1 mol m<sup>-2</sup>) are in the same order of magnitude as the best-guess estimate derived in this study. It should be noted that the NCP estimates by Schneider et al. (2014) refer to the cumulative NCP of one to three production pulses per years, whereas our estimate of ~1.2 mol m<sup>-2</sup> refers to a single bloom event.

Wasmund et al. (2001) conducted <sup>14</sup>C incubation experiments at different water depths to determine instantaneous rates of primary production during a cyanobacteria bloom. The obtained daytime carbon fixation rates in surface waters (0.4 – 0.8 mmol C m<sup>-3</sup> h<sup>-1</sup>) are in the same order of magnitude as the mean rate found in this study. More importantly, the authors also found significantly lower fixation rates below 10 m water depth (< 0.2 mmol-C m<sup>-3</sup> h<sup>-1</sup>), which agrees with the depth distribution of NCP observed in this study.

Furthermore, the succession of different cyanobacteria genera observed in 2018, with the *Nodularia* dominated bloom following an earlier presence of *Aphanizomenon* (Fig. B2), was previously described as a typical pattern (Wasmund, 2017), as well as the fact that increased wind speed and turbulence can inhibit N-fixation of cyanobacteria and cause the termination of the bloom (Wasmund, 1997).

In conclusion, the bloom event duration, C<sub>T</sub>\* drawdown, and NCP, as well as the vertical extend of carbon fixation and the succession of the bloom observed in this study agree well with observations in previous years, and distinct differences cannot be found. We therefore conclude that the findings of this study are representative for Baltic Sea cyanobacteria blooms in general, although the SST and pCO<sub>2</sub> levels in 2018 were at the upper and lower end, respectively, of the conditions observed in previous years (Schneider and Müller, 2018).

#### 4.2 Recommendations and caveats for NCP reconstruction from SOOP and model data

The good agreement between our best-guess and the reconstructed, TPD-based NCP estimate of the production peak on July 24 (Fig. 6C) indicates that it is possible to determine NCP from surface pCO<sub>2</sub> observations and vertically resolved seawater temperature with little uncertainty. For the NCP calculation based on surface pCO<sub>2</sub> observations from SOOP and modelled temperature profiles, we recommend to:

1. Convert surface pCO<sub>2</sub> to C<sub>T</sub>\* based on a mean A<sub>T</sub> estimate for the region under consideration.
2. Identify production pulses dominated by cyanobacteria as periods characterised by a decrease in C<sub>T</sub>\* that occurs between June and August.
3. Integrate observed surface C<sub>T</sub>\* changes to the temperature penetration depth (TPD) estimated from modelled temperature profiles, rather than using a mixed layer depth (MLD) estimate.



- 410 4. Perform the integration individually for each production pulse and limit NCP reconstruction to periods characterised by a stable or shoaling thermocline.

It should be emphasised that lateral variability and water mass transport are critical for observation-based NCP estimates and constitute the largest source of uncertainty in our estimates. However, SOOP observations allow averaging of observations across large regions, which reduces the impact of lateral water mass transport (Schneider and Müller, 2018). The region for spatial averaging should be chosen large enough to avoid as much as possible the influence of lateral perturbations which depend on the surface dynamics and the biogeochemical gradients in the surrounding area. Yet, the region for spatial averaging should be chosen small enough to ensure that variations of  $p\text{CO}_2$  within the region are small compared to the temporal changes of interest. Another critical aspect of the recommended NCP reconstruction approach is the restriction to periods of a stable or shoaling thermocline. While in principle it is possible that net organic matter production could occur also during periods of a deepening thermocline, this process was observed neither in this study nor previous years (Schneider and Müller, 2018), and is in line with the planktological finding that increased wind speed causes the termination of the bloom (Wasmund, 1997).

The NCP reconstruction approach presented in this study was derived from observations covering a single bloom event within the Central Baltic Sea. In the lack of comparable comprehensive observational data that underlie our best-guess estimate, the applicability of this approach could not be tested for other regions or bloom events. However, the dynamics and intensity of the bloom event described here are comparable to previous, independent descriptions of cyanobacteria blooms. Therefore, it is assumed that underlying biogeochemical mechanisms are representative and that the NCP reconstruction approach can be applied to other cyanobacteria bloom events. Specifically, we assume that the findings represented here can be applied to evaluate past and future  $p\text{CO}_2$  observations made on *Finnmaid* and other SOOP in the Central Baltic Sea without compromise. Larger uncertainties should be expected when applying the approach to other basins of (or even outside) the Baltic Sea.

## 430 5 Conclusions

In this study, the depth-integrated quantification of NCP that occurred during a cyanobacteria bloom in the Baltic Sea in 2018 is achieved through the interpretation of profiling measurements of  $p\text{CO}_2$  that covered the entire bloom event. Furthermore, it is demonstrated that this best-guess estimate can be reconstructed with small bias from SOOP  $p\text{CO}_2$  observations and modelled temperature profiles. Recommendations to apply our reconstruction approach to the comprehensive long-term record of surface  $p\text{CO}_2$  data available for the Baltic Sea are given. The application of this approach will allow for the detection and attribution of trends in cyanobacteria NCP across decades. In particular the comparison of NCP estimates of bloom events that occurred under different environmental conditions will provide a better understanding of the controlling factors. Ultimately, this knowledge will inform the design and monitoring of conservation measures aiming at a Good Environmental Status of the Baltic Sea and potentially other regions.



440 *Code and data availability.*

**Website:** Following the concept of literature programming and relying on the R package workflowr (Blischak et al., 2019), the code, plain text comments, and graphical output of this study are compiled as a website available at: <https://jens-daniel-mueller.github.io/BloomSail/>.

**Code and raw data:** A release of the Github repository underlying the website and containing all code was tagged as "os-2020-120\_submission" and archived on <https://zenodo.org/>. All raw data required to run the analysis were uploaded manually to this archive.

445 Thus, the combined code and data are available under doi: <https://doi.org/10.5281/zenodo.4553314>.

**Processed environmental data:** Processed in situ observation of this study will be made available through <https://www.pangaea.de/> upon acceptance of the manuscript.



## Appendix A: $p\text{CO}_2$ sensor measurements

### A1 Sensor calibration

450 The CONTROS HydroC®  $\text{CO}_2$  sensor used in this study (serial number  $\text{CO}_2$ -0618-001) was calibrated in water by the manufacturer at 15 °C before (June 2018) and after (October 2018) the deployment for a measuring range of 100 to 500  $\mu\text{atm}$ . The pre- and post-deployment calibration polynomials met the 6 steps per calibration with an  $R^2$  of 0.999999 (pre) and 0.999993 (post) at an RMSE of 0.13  $\mu\text{atm}$  (pre) and 0.43  $\mu\text{atm}$  (post). The time between the calibrations was about 107 days and the sensor runtime during this interval was about 506 hours or little more than 21 days. The zero drift observed between the two  
455 calibrations was only 0.89  $\mu\text{atm}$ .

### A2 Sensor configuration and operation

The instrument periodically records zeroing values, during which the  $\text{CO}_2$  within the gas stream is scrubbed by a soda lime cartridge. Zeroings of two minutes duration were recorded every five hours during the field deployment. A period of 600 seconds after the zeroing was flagged as a flush period, during which the sensor signal recovers to environmental conditions.  
460 Recordings during the flush and zeroing period were removed before further biogeochemical interpretation.

For the majority of the measurements, the sensor was operated with a 8W-pump (SBE-5T; Sea-Bird Electronics, Bellevue, USA) and the logging interval was set to 1 second. Only for the first two cruise days on July 6 and 10, a 1W-pump (SBE-5M, Sea-Bird Electronics) was used and the logging interval set to 10 seconds.

The downcast profiles were always recorded continuously and with a steady profiling speed of  $\sim 2 \text{ m min}^{-1}$ . The upcast  
465 profiles were either performed continuously as well, or with a stop to record an equilibrated reference  $p\text{CO}_2$  value at a desired depth. Only continuous downcast profiles were used for biogeochemical interpretation.

Zeroing signals were recorded by the CTD unit from the analogue sensor output, as well as in the internal sensor memory. Both records were used to ensure exact temporal match of the CTD and  $p\text{CO}_2$  time series. Only  $p\text{CO}_2$  data stored with higher temporal resolution in the internal memory were used during further analysis.

### 470 A3 Data post-processing

A drift correction as discussed in Fietzek et al. (2014) was applied to the field data to improve the data quality. This post-processing considers information from the pre- and post-deployment calibrations (i.e. concentration dependent or span drift) and the regular in situ zeroings (i.e. zero drift).

The first 60 seconds within every zeroing interval were discarded to only consider smooth zero-gas measurements that are  
475 not affected by the signal drop from ambient  $p\text{CO}_2$  to the zero value. Zero signals for every point of the deployment were obtained by linear interpolation of the zero measurements. In case of data gaps larger than 2 hours within the deployment data, the course of the 2 zero signals before or after the gap was linearly extrapolated forward or backward, respectively, instead of an interpolation over the time of the measuring gap. A concentration-dependent drift of the sensor was considered



by transforming the pre– into the post–deployment calibration polynomial according to the actual sensor runtime (and not  
480 according to the course of the zero measurements as applied within Fietzek et al. (2014)).

Approx. 100 unrealistic outliers were found within the sensor temperature record ( $T_{\text{sensor}}$  parameter) of the HydroC®. These  
were identified to be electronic artefacts and the values replaced by the constant temperatures recorded before and after these  
events that only lasted a few seconds at most.

Given the statistics of the pre– and post–deployment calibration, the small drift encountered throughout the deployment and  
485 the otherwise smooth performance of the sensor during the deployment, the accuracy of the measurements is considered to be  
1% of reading as also found within Fietzek et al. (2014).

#### A4 $p\text{CO}_2$ response time correction

The actual in situ response times ( $\tau$ ) of the sensor were determined by fitting an exponential function to the signal recovery  
following a zeroing (Fig A1; Fiedler et al. (2013); Fietzek et al. (2014)). The determined  $\tau$  values were used subsequently to  
490 correct the signal delay (Fiedler et al., 2013; Fietzek et al., 2014; Atamanchuk et al., 2015).

##### A4.1 Response time determination

In situ response times ( $\tau$ ) were determined from  $p\text{CO}_2$  data recorded during the flush period after each zeroing. Data recorded  
during the initial 20 seconds of each flush period were removed as those are affected by the mixing of residual gas volumes  
inside the sensor. Individual  $\tau$  values were determined by fitting the non–linear model

$$495 \quad p\text{CO}_2(t) = p\text{CO}_2(t_{\text{end}}) + (p\text{CO}_2(t_0) - p\text{CO}_2(t_{\text{end}})) \cdot e^{(-dt/\tau)} \quad (\text{A1})$$

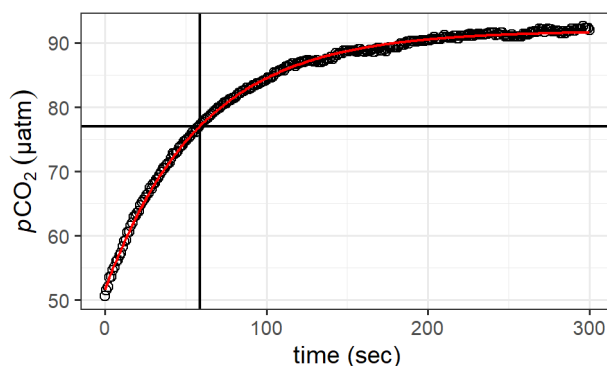
where  $p\text{CO}_2(t)$  is the recorded  $p\text{CO}_2$  at time  $t$ ,  $p\text{CO}_2(t_0)$  and  $p\text{CO}_2(t_{\text{end}})$  are the fitted  $p\text{CO}_2$  values at the beginning and the  
end of the equilibration process, and  $dt$  is the time since the beginning of the equilibration process. In situ  $\tau$  was determined  
for a fit interval length of 300 seconds. Flush periods were discarded when the mean of absolute residuals from the fit exceeded  
1% of the final  $p\text{CO}_2$ , a condition which indicated unstable environmental  $p\text{CO}_2$  (e.g. due to unintended heaving of the sensor  
500 package).

Similar to previous studies, a decrease of  $\tau$  with increasing in situ temperature was found. The dependence of  $\tau$  on temper-  
ature was fitted with linear regression models, separately for the deployments with the 1W– and 8W–pump. The sensor was  
carefully cleaned after each cruise and no signs of a changing sensor response time over time as an indicative of fouling on the  
sensor’s membrane were detected.

##### 505 A4.2 Correction procedure

For each recorded  $p\text{CO}_2$  value, the corresponding  $\tau$  was calculated from measured in situ temperature. The response time  
correction was then applied according to equation (S3) in the supplementary material of Bittig et al. (2018):

$$p\text{CO}_{2,\text{insitu}} = \frac{1}{2b} \cdot (p\text{CO}_{2,\text{obs}}(t_{i+1}) - a \cdot p\text{CO}_{2,\text{obs}}(t_i)); \quad a = 1 - 2b, \quad b = \left(1 + 2 \frac{\tau}{t_{i+1} - t_i}\right)^{-1} \quad (\text{A2})$$

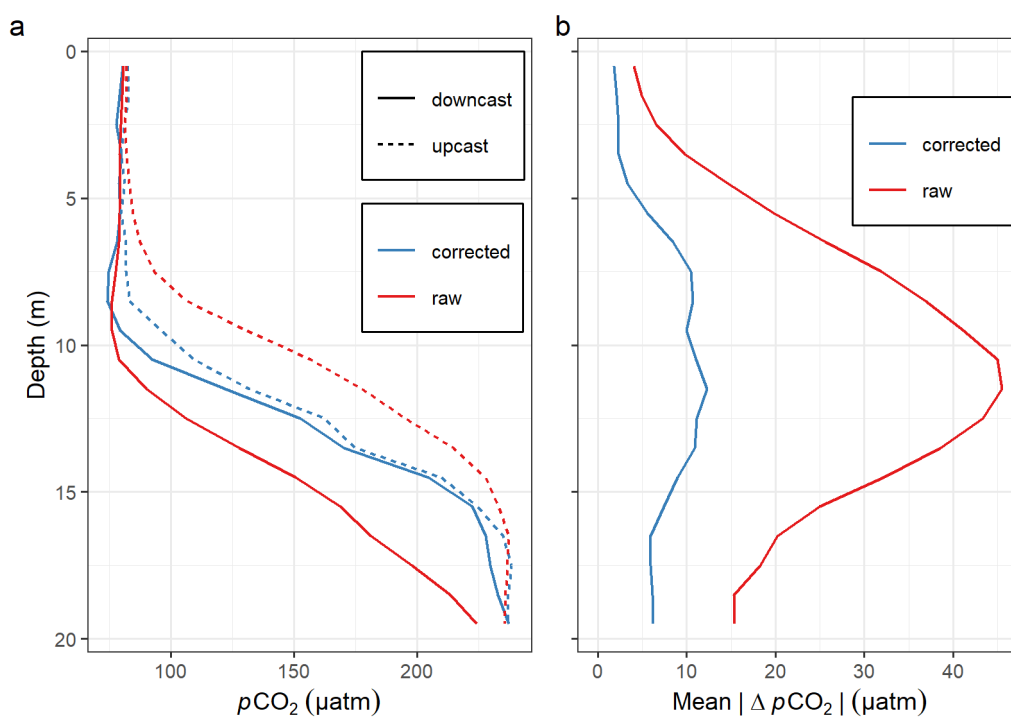


**Figure A1.** Exemplary determination of the response time  $\tau$  through fitting an exponential function (red curve) to the  $p\text{CO}_2$  signal recovery following a zeroing measurement. The determined response time  $\tau$  and  $p\text{CO}_2(t=\tau)$  are indicated by a vertical and horizontal line, respectively.

where  $p\text{CO}_{2,insitu}$  is the true in situ  $p\text{CO}_2$  time series,  $p\text{CO}_{2,obs}$  the  $p\text{CO}_2$  time series as recorded by the sensor, and  $\tau$  the  
510 response time for the interval between  $t_i$  and  $t_{i+1}$ . Due to the short interval between adjacent observations in our study, the  
calculated value from the right side of equation A2 was considered directly representative for  $p\text{CO}_{2,insitu}(t_{i+1})$ , although it  
is strictly the mean value between two adjacent observations, i.e.  $0.5 \cdot (p\text{CO}_{2,insitu}(t_i) + p\text{CO}_{2,insitu}(t_{i+1}))$ . Finally, a rolling  
mean with a window width of 30 sec was applied to the response time corrected  $p\text{CO}_{2,insitu}$  time series to remove short term  
noise. Please note that throughout the rest of the manuscript  $p\text{CO}_{2,insitu}$  is referred to as  $p\text{CO}_2$ .

#### 515 A4.3 Quality assessment

The improvements by the response time correction were investigated based on the difference between up- and downcast  $p\text{CO}_2$   
profiles vertically gridded into 1m depth intervals. To focus this quality assessment on the conditions in near surface waters  
which are subject of this study, profiles were discarded which exceeded a maximum depth of 30 m and/or a maximum  $p\text{CO}_2$   
of 300  $\mu\text{atm}$ . Those profiles were excluded only for the quality assessment (not for the biogeochemical interpretation) to avoid  
520 a bias through exposure to very high  $p\text{CO}_2$  at greater depth. Furthermore, profiles were removed with a maximum number  
of missing observations from two or more depth intervals, which occasionally occurred when a sensor zeroing started while  
profiling. Based on this subset of response time corrected  $p\text{CO}_2$  profiles it was found that the mean absolute  $p\text{CO}_2$  difference  
between the up- and downcast profile was  $<2.5 \mu\text{atm}$  averaged across the upper 5 m of the water column and  $<7.5 \mu\text{atm}$  across  
525 the upper 20 m. The highest offset was found at around 10 m water depth and results from the steep environmental  $p\text{CO}_2$   
gradient around the thermocline.



**Figure A2.** Comparison of  $p\text{CO}_2$  profiles before (raw) and after (corrected) response time correction: (a) Exemplary up- and downcast  $p\text{CO}_2$  profiles at one station and (b) mean absolute  $p\text{CO}_2$  difference between up- and downcast profiles across all profiles included in the quality assessment.





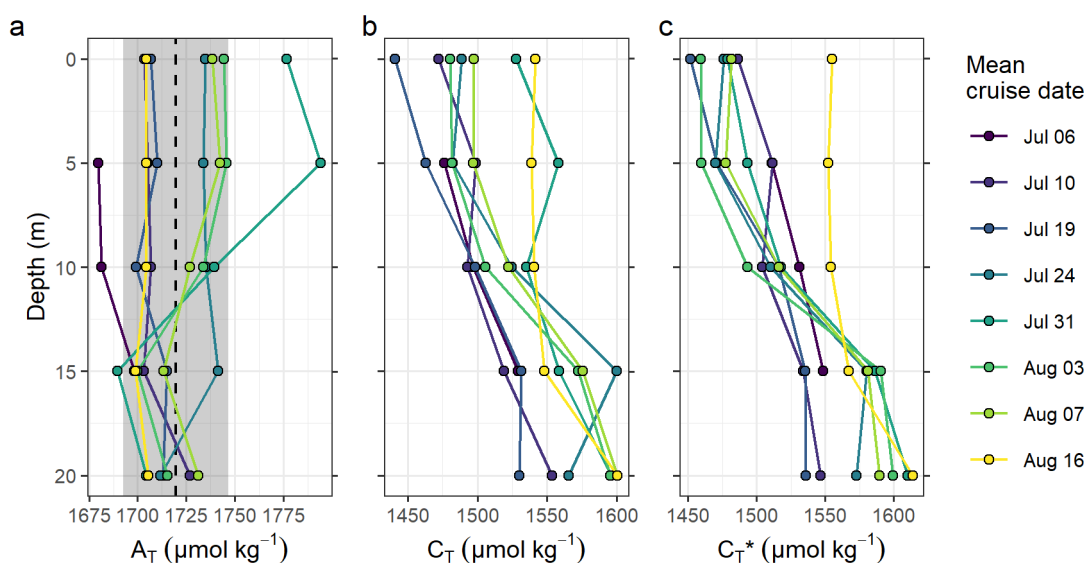
## Appendix B: Discrete samples

### B1 $C_T$ and $A_T$

Dissolved inorganic carbon ( $C_T$ ) was determined from discrete bottle samples with an Automated Infra Red Inorganic Carbon Analyzer (AIRICA, MARIANDA, Kiel, Germany). The analysis relies on the stripping of  $CO_2$  through acidification. The released  $CO_2$  is transported with a nitrogen carrier gas stream to an infrared detection unit (LI-7000, LI-COR Biosciences, Lincoln, USA), where the peak area is determined. Comparison to measurements performed on certified reference materials (CRM Batch 173; Dickson et al., 2003) allows for the calculation of  $C_T$ . Triplicated measurements were performed on each sample and a precision of  $2 \mu\text{mol kg}^{-1}$  was achieved.

Total alkalinity ( $A_T$ ) was analysed by open cell titration of 125 – 140 g of sample. The method involves a two-stage titration. After a first, single addition of hydrochloric acid to achieve a pH 4 – 3.5,  $A_T$  is determined during a continued, stepwise titration to pH 3, during which pH is recorded potentiometrically (Dickson et al., 2007). Measurements were referenced to CRM batch 173 (Dickson et al., 2003).

$C_T^*$  calculated for discrete samples refers to a classical alkalinity-normalised  $C_T$ , and was defined as  $C_T^* = C_T \cdot A_{T,\text{mean}} / A_T$ .  $C_T^*$  derived from discrete samples or  $pCO_2$  sensor data are directly comparable (Fig. 5c) because they are referenced to the same mean  $A_T$  of the discrete samples ( $1720 \mu\text{mol kg}^{-1}$ ).

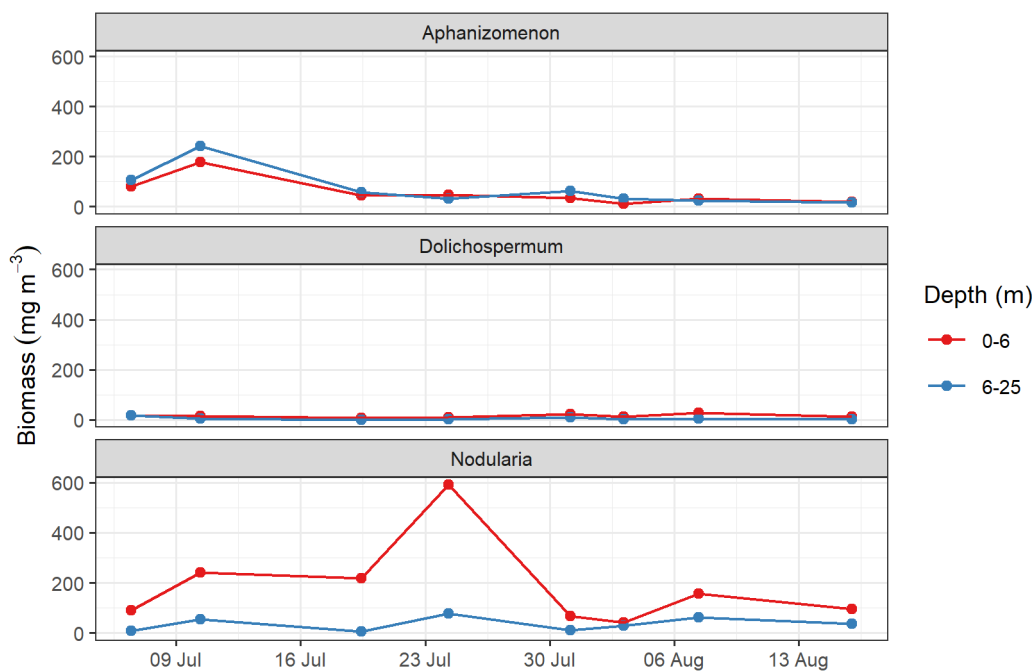


**Figure B1.** Vertical profiles of (a)  $A_T$ , (b)  $C_T$ , and (c)  $C_T$  normalised to the mean alkalinity ( $C_T^*$ ). Shown are cruise mean values for discrete samples taken at stations 07 and 10. The dashed line and grey area in (a) indicate the mean  $\pm 1$  standard deviation of  $A_T$  across the upper 20 m of the water column.



## B2 Phytoplankton

Phytoplankton samples were fixed with Lugol solution within no more than 24 hours after sampling. Samples were stored dark, before being transported to IOW and analysed in the laboratory within no more than 3 months after sampling. Phytoplankton community composition and biomass were determined by the Utermöhl method (HELCOM, 2017), which relies on microscope counts and the conversion of cell shape and size to biomass units.



**Figure B2.** Time series of cyanobacterial biomass, averaged for surface (0 – 6 m) and subsurface (6 – 25 m) water masses sampled from stations 07 and 10 (Fig. 1). Results are based on microscope counts and distinguish three genera (panels).

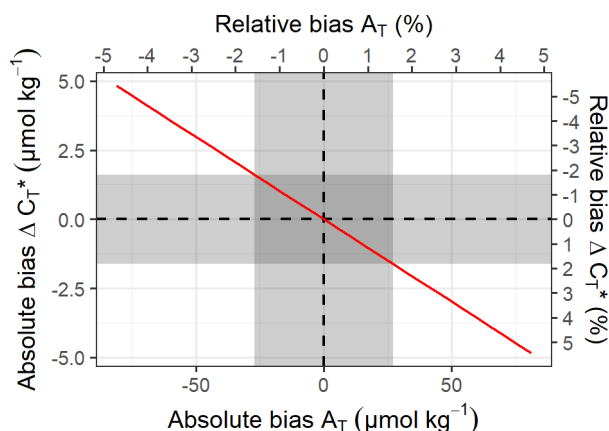


## Appendix C: Net community production estimation

### C1 Conversion from $p\text{CO}_2$ to $C_T^*$

The approach to estimate temporal changes (rather than absolute values) in the dissolved inorganic carbon concentration ( $C_T$ ) from a  $p\text{CO}_2$  time series was previously established and theoretically examined (Schneider et al., 2014, and references therein).  
550 It relies on a fixed estimate of alkalinity ( $A_T$ ) and is only applicable when noticeable internal changes in  $A_T$  can be excluded, as is the case in the Baltic Sea due to the absence of calcifying plankton (Tyrrell et al., 2008). To avoid confusion with measured or absolute  $C_T$  values and for consistency with previous studies, the calculated variable is referred to as  $C_T^*$ .

To evaluate the applicability of this approach under the specific  $p\text{CO}_2$  and temperature conditions observed in summer 2018, we calculated  $C_T^*$  changes between Jul 6 and 24 for a range of  $A_T$  values covering three times the standard deviation of  $A_T$   
555 observations (Fig. B1). For assumed  $A_T$  values of  $1747 \mu\text{mol kg}^{-1}$  and  $1693 \mu\text{mol kg}^{-1}$ , which is 1 standard deviation of the observations ( $27 \mu\text{mol kg}^{-1}$ ) higher and lower than the mean  $A_T$  ( $1720 \mu\text{mol kg}^{-1}$ ), the bias of the derived change in  $C_T^*$  amounts to  $\pm 1.6 \mu\text{mol kg}^{-1}$ . This bias is  $<2\%$  compared to the signal of interest, i.e. the absolute drawdown of  $C_T^*$  ( $89 \mu\text{mol kg}^{-1}$ ).



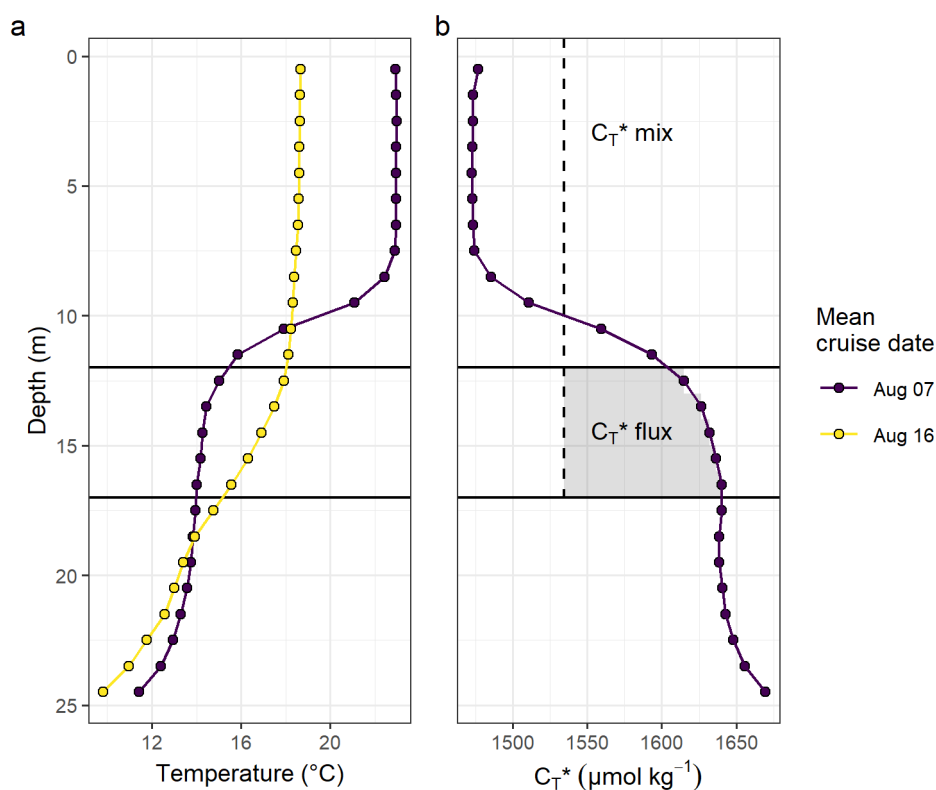
**Figure C1.** Bias of changes in  $C_T^*$  as a function of the bias in mean  $A_T$  used for calculation (see Fig. B1). Results correspond to the  $p\text{CO}_2$  and temperature conditions observed in this study and are expressed in absolute and relative units. Grey areas highlight  $\pm 1$  standard deviation around the mean  $A_T$ .

It should be noted that the bias assessment presented here reflects two types of errors, namely (i) the assignment of an  
560 erroneous mean  $A_T$  value for the calculation and (ii) the lateral exchange of water masses with different  $A_T$  but identical initial  $p\text{CO}_2$  during the observation period. The robustness of this approach to the latter aspect is the reason why  $p\text{CO}_2$  observations are more suitable to determine NCP than direct  $C_T$  measurements, when those are not normalised to corresponding  $A_T$  measurements.



## C2 Calculation of the vertical entrainment flux of $C_T^*$

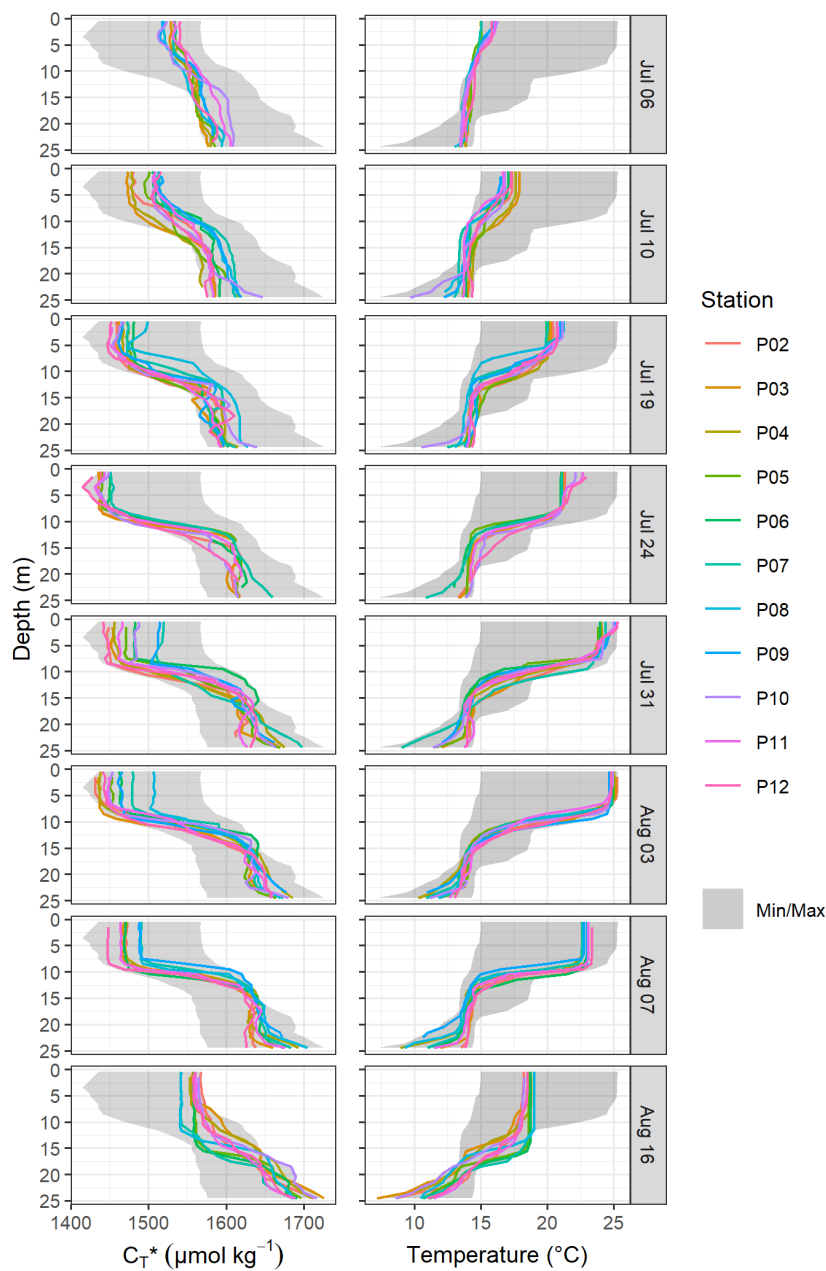
565 The vertical entrainment flux of  $C_T^*$  that occurred across the 12 m integration depth layer between Aug 7 and 16 was estimated assuming an instantaneous complete vertical mixing to 17 m water depth after Aug 7. For this scenario, the hypothetical homogeneous  $C_T^*$  concentration after the mixing event ( $C_T^*$ mix) equals the mean volume-weighted  $C_T^*$  concentration between 0 – 17 m (Fig. C2). Furthermore, the entrainment flux ( $C_T^*$ flux) into the surface water column (0 – 12 m) is equal to the concentration difference between observed  $C_T^*$  on Aug 7 and  $C_T^*$ mix, integrated from 12 to 17 m.



**Figure C2.** Illustration of the approximation of the entrainment flux of  $C_T^*$  due to vertical mixing. (a) The estimated deepening of the mixed layer from 12 to 17 m water depth between Aug 7 and 16 is based on the observed changes in the temperature profiles. (b) Assuming a complete, instantaneous mixing of the water column after Aug 7, the hypothetical homogeneous concentration of  $C_T^*$  ( $C_T^*$ mix) can be used to approximate the entrainment flux of  $C_T^*$  (grey area).



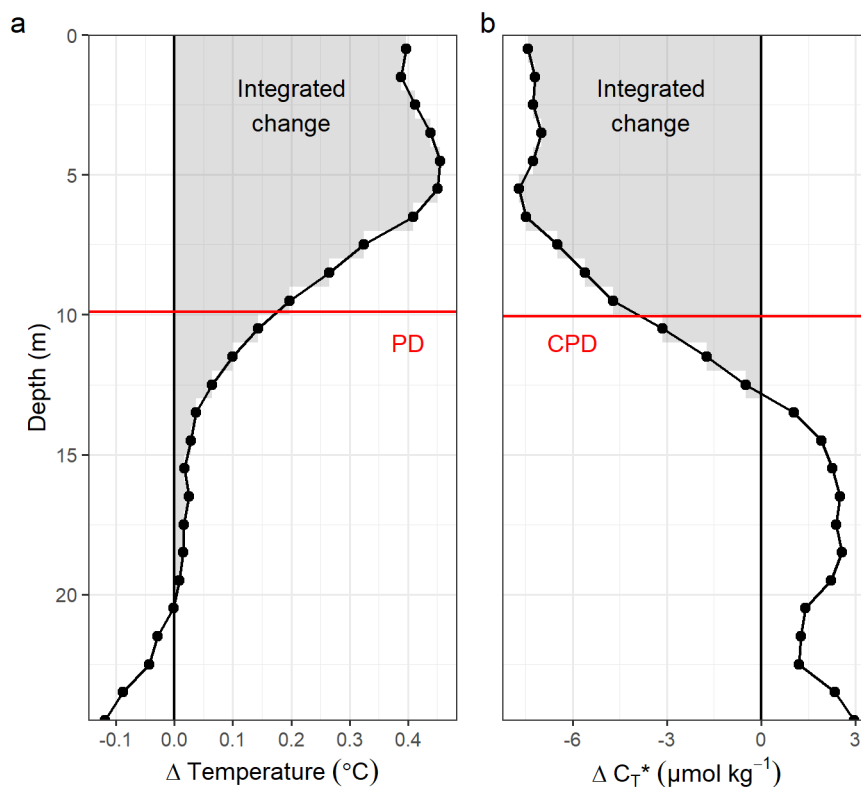
### 570 C3 Individual stations profiles



**Figure C3.** Individual profiles of  $C_T^*$  (left panels) and temperature (right) displayed separately for each cruise day (rows) and station (color). Grey ribbons indicate the minimum and maximum values observed across the entire study period.



#### C4 Temperature penetration depth (TPD) concept



**Figure C4.** Illustration of the temperature and  $C_1^*$  penetration depth concept, short TPD and CPD. Shown are exemplary profiles of incremental changes of (a) temperature and (b)  $C_1^*$  observed between the cruises on July 6 and 10. TPD and CPD (red horizontal lines) are defined as the depth-integrated positive (for temperature) and negative (for  $C_1^*$ ) changes (grey areas) divided by the change at the surface. TPD and CPD are expressed in units of metres.



#### Appendix D: SOOP *Finnmaid* $p\text{CO}_2$

For SOOP *Finnmaid* transects recorded between July 7 and July 16,  $p\text{CO}_2$  data were not available from the LI-COR system because of technical failure. Therefore, data generated by the Los Gatos (LGR) system were used to fill the gap. Unfortunately, the comparison of LI-COR and LGR measurements before July 7 indicated a small leakage in the LGR system, which was later also physically detected and fixed. The resulting difference between the two systems was clearly correlated with absolute  $p\text{CO}_2$ , as expected from contamination with ambient air. For data from the transect on July 5, the linear regression model  $p\text{CO}_{2,true} = p\text{CO}_{2,LGR} + 0.038 * p\text{CO}_{2,LGR} - 24.2$  was fitted, assuming that the LI-COR system had delivered the “true”  $p\text{CO}_{2,true}$  before its failure. Assuming further that the effect of the contamination remained constant, this relationship was then applied to reconstruct  $p\text{CO}_{2,true}$  from  $p\text{CO}_{2,LGR}$  for the period without LI-COR data. To validate this adjustment,  $p\text{CO}_{2,true}$  was also reconstructed from  $p\text{CO}_{2,LGR}$  on July 4 and compared to  $p\text{CO}_2$  directly measured with the LI-COR system. The mean difference was below  $2 \mu\text{atm}$  for the entire transect as well as for a data subset within the study region, giving confidence to the high accuracy of the adjusted  $p\text{CO}_{2,true}$ . It should be noted that the adjusted SOOP  $p\text{CO}_2$  data recorded between July 7 and July 16 agree well with the in situ  $p\text{CO}_2$  recorded by the sailing campaign, i.e. the standard deviations of all surface measurements in the study region overlap.



*Author contributions.* JDM was the lead author of this study and involved in all parts of it, in particular the conceptualization, funding acquisition, project administration, field sampling, data curation, visualisation and analysis, and manuscript writing. BS was involved in the conceptualization, formal analysis, and original draft preparation. UG generated and processed the GETM model data. PF supported the HydroC® sensor configuration and performed the data post processing. MBW and AR provided the atmospheric data and supported the field campaign logistically. NW was responsibly for the collection, analysis and interpretation of phytoplankton samples. SK designed and assembled the sensor package. GR was involved in the conceptualization, funding acquisition, and project administration and supervision. All authors contributed to the internal review and editing of the manuscript.

*Competing interests.* The authors declare that they have no conflict of interest.

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