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A scalable dynamic characterisation approach for water quality management in semi-enclosed seas and archipelagos

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ABSTRACT

In semi-enclosed seas, eutrophication may affect both the coastal waters and the whole sea. We develop and test a modelling approach that can account for nutrient loads from land as well as for influences and feedbacks on water quality across the scales of a whole semi-enclosed sea and its coastal zones. We test its applicability in the example cases of the Baltic Sea and one of its local archipelagos, the Archipelago Sea. For the Baltic Sea scale, model validation shows good representation of surface water quality dynamics and a generally moderate model performance for deeper waters. For the Archipelago Sea, management scenario simulations show that successful sea measures may have the most important effects on coastal water quality. This highlights the need to consistently account for whole-sea water-quality dynamics and management effects, in addition to effects of land drivers, in modelling for characterisation and management of local water quality.

1. Introduction

Eutrophication is a major environmental issue, often caused by an increase in anthropogenic nutrient inputs (Nixon, 1995). Coastal areas, which receive most of the land-based nutrient inputs, are therefore particularly vulnerable to eutrophication. This can lead to oxygen depletion, toxic algae blooms and fish kills, thereby damaging essential coastal ecosystem services (Smith and Schindler, 2009). As nutrients dilute into the ocean, these effects become less visible. However, in the case of semi-enclosed seas, increased nutrient inputs can substantially affect the whole sea. These systems are often characterised by a large catchment area on land compared with their sea-water surface area and a limited water exchange with the ocean (Martin et al., 1981). The properties of such systems lead both to stronger impacts from the land catchment and their anthropogenic pressures, and to more sensitive internal dynamics than in oceans (Caddy, 1993; Newton et al., 2014). For example, the Black Sea is subject to regional-scale eutrophication (Kideys, 2002), while in the Baltic Sea and Yellow Sea such conditions are in progress (Voss et al., 2011; Liu et al., 2013).

Furthermore, various policy and management frameworks may overlap in regulating and/or affecting coastal water quality. For example, the Water Framework Directive (WFD) implemented in the European Union (EU), requires a good ecological status for both inland and coastal waters by 2021 (Borja et al., 2010). Moreover, the EU Marine Strategy Framework Directive (MSFD) regulates water quality up to 200 nm from the coast (corresponding to the Exclusive Economic Zone) (Borja et al., 2010). For the Baltic Sea, the Helsinki Commission (HELCOM) Baltic Sea Action Plan (BSAP) has also been agreed and implemented among the Baltic countries and sets targets for their required reductions of nutrient loads from land into the sea (HELCOM, 2007). Such transboundary policies and agreements foster collaboration among countries, are useful in efforts to meet major challenges, such as climate change and its effects on regional coastal and marine eutrophication, and may overlap with and/or complement the coastal policies and management practices of the involved countries. In terms of policy overlaps, for example in the case of the Baltic Sea, the BSAP, focusing on the whole sea, overlaps with the MSFD for water quality up to 200 nm from the coast, and both in turn overlap with the WFD for coastal waters.

Conceptualisation and modelling approaches that can support effective and efficient water quality management based on different overlapping regulations are lacking in various ways. For instance, approaches that focus on coastal zones may not explicitly model the coupling of the coastal waters with the open sea conditions (Li et al., 2015; Fennel et al., 2011). Furthermore, large-scale management-support models, such as the BALTSEM for the Baltic Sea (Savchuk et al.,

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2012), may not be adaptable to explicitly consider and model key processes in the coastal zones with sufficient resolution. More detailed modelling approaches, developed for process understanding, may be able to account for regional sea and coastal conditions (e.g., ERGOM (Neumann, 2000) and RCO-SCOBI (Eilola et al., 2009) for the Baltic Sea). However, such models are often computationally and data expensive, and thus are not suited for exploratory and scenario-based analysis, and assessment methodology commonly required for decision making (de la Mare et al., 2012).

Environmental changes in coastal zones and archipelagos may require dynamic model coupling with conditions in the host semi-enclosed sea using suitable modelling approaches that can support effective water-quality management across spatial and temporal scales. A suitable conceptualisation and modelling approach should then support multi-variable water quality management (Chen et al., 2013), and be coherent across the whole sea in order to consistently simulate coupling effects between the sea and its archipelagos, as required by different regulatory frameworks. Furthermore, a suitable approach should be relatively simple to implement in order to explore different land and/or sea management alternatives (de la Mare et al., 2012) as well as different climate change scenarios. Finally, a suitable approach should be scalable dynamically in space and time, such that influences on coastal water quality from mitigation efforts in the sea or on land can be resolved, and possible synergies and conflicts can be identified among different possible efforts to reach the targets of overlapping marine, inland and coastal water regulations.

In this study, we develop and test the application of a conceptualisation and modelling approach that may be suitable according to the above criteria. We use the Baltic Sea, a semi-enclosed sea situated in Northern Europe, and one of its many archipelagos, the Archipelago Sea, as concrete cross-scale case examples for this testing. Baltic Sea is subject to increasing coastal and open sea eutrophication (Conley et al., 2009a), while significant improvements from management practices toward reaching regulatory goals have yet to be observed (Conley et al., 2009b; Destouni et al., 2017). As discussed above, several environmental regulatory frameworks for the coastal waters of the Baltic Sea may overlap, including the BSAP, the MSFD and the WFD. Moreover, the Baltic Sea is characterised by a complex bathymetry and flow structure, and approximately 25% of its surface area comprises coastal waters and archipelagos (less than 20 m depth) (Leppäranta and Myrberg, 2009). These characteristics, together with a relatively good data availability, make the Baltic Sea and the Archipelago Sea interesting cross-scale and cross-environment case examples for applying and testing the proposed conceptualisation and modelling approach.

2. Problem formulation and conceptualisation

Evolution of coastal and marine water quality in semi-enclosed seas depends on hydroclimatic and anthropogenic influences (e.g., changes in temperature, freshwater inputs, land-uses and associated nutrient loading from land). In addition, coastal and marine water quality also depends on various processes within the sea and its coastal waters. Modelling of the different change drivers, cause-effect relationships and feedbacks is subject to considerable uncertainty (Bring et al., 2015a; Conley et al., 2009a; Destouni et al., 2008). Such uncertainty can be accounted for by considering and simulating different evolution scenarios, representing a range of plausible futures (Bring et al., 2015b).

The specific methodological and scientific question this work addresses is how to link large-scale processes of water quality change with local-scale impacts from alternative measures in archipelagos of semi-enclosed seas, in an efficient, transparent and coherent manner. The key challenge is to develop a methodology capable of characterising water quality conditions based on available data and efficiently simulating reliable projections of water quality evolution under alternative scenarios. The methodology also needs to incorporate management performance assessment by comparison of projected water quality conditions with monitoring data.

Key components and workflow for such a general and flexible methodology referred to as a Scalable Dynamic Characterisation (SDC) approach, are presented in Appendix A; SDC is specifically designed for exploring scenarios to manage water quality in archipelagos and semi-enclosed seas. As its main feature, the spatial resolution in the SDC approach can vary within the system, depending on management focus and various zone properties. Furthermore, SDC provides for a dynamic description of water quality processes to simulate time-dependent management and climate-change scenarios. An important simplification within SDC is achieved by decoupling the hydrodynamics from water quality modelling; such decoupling is motivated by the fact that hydrodynamics controls transport and biogeochemical processes without being significantly influenced by them (Lehtoranta et al., 2009). Finally, the model representation of water quality processes in SDC is tested against available observation data across relevant scales.

The proposed SDC approach will be illustrated for the Baltic Sea. Although implemented on a specific semi-enclosed sea, the illustration example is generic in the sense that no specific management task is predefined. Thus, step 7 in Fig. 7 should be considered as being outside the scope of the present study. Likewise, selected archipelago locations (step 1, Fig. 7) are arbitrary and for illustration purpose only, i.e., without direct reference to a specific regulatory framework. The next section outlines the investigated model implementation as defined by steps 2 to 6 for the selected examples (Fig. 1). Characterisation and model result testing with validation are done over periods 2003–2008 and 2001–2005, for the Baltic Sea and Archipelago Sea, respectively. To also test and illustrate the scenario formulation and analysis included in step 2 of the SDC, we consider here three scenarios corresponding to different types of nutrient-load mitigation measures as given in Table 1.

3. Materials and methods

3.1. The Baltic Sea and Archipelago Sea

The Baltic Sea is a semi-enclosed sea, situated between central and northern Europe and one of the world's largest brackish water bodies. It is characterised by a long average residence time (greater than 20 years) (Wulff and Stigebrandt, 1989), and a large catchment area relative to the sea surface area, with a total population of 85 million people (HELCOM, 2010). Increased nutrient loads from the catchment to the Baltic Sea have led to growing regional-scale water-quality and eutrophication issues over the last century (Savchuk et al., 2008). Moreover, due to the strong vertical stratification in the Baltic Proper, increased primary production enhances internal loading of phosphorus from anoxic sediments, which in turn reinforces and maintains the Baltic Sea eutrophic situation (Stigebrandt, 2018; Vahtera et al., 2007).

Coastal zones are the main pathway for nutrients from land toward the sea and the Baltic Sea is characterised by a high diversity of coasts, with sandy coasts, cliffs, estuaries and major archipelagos (Schiewer, 2008). Among these, the Archipelago Sea is situated in the south-west of Finland, between the Gulf of Bothnia, the Baltic Proper and the Gulf of Finland. It is characterised by a complex topography (around 17,700 isles, forming clusters), and a shallow and irregular bathymetry (average depth of 23 m, with some trenches reaching 100 m). This archipelago is considered to act as a nutrient load buffer between land and the open sea (Bonsdorff et al., 1997). Eutrophied conditions have become more common here due to increased nutrient loads from agricultural runoff, fish farming and other industries, but also due to increased nutrient concentrations in inflowing waters from the Baltic Proper and the Gulf of Finland (Peuhkuri, 2002).

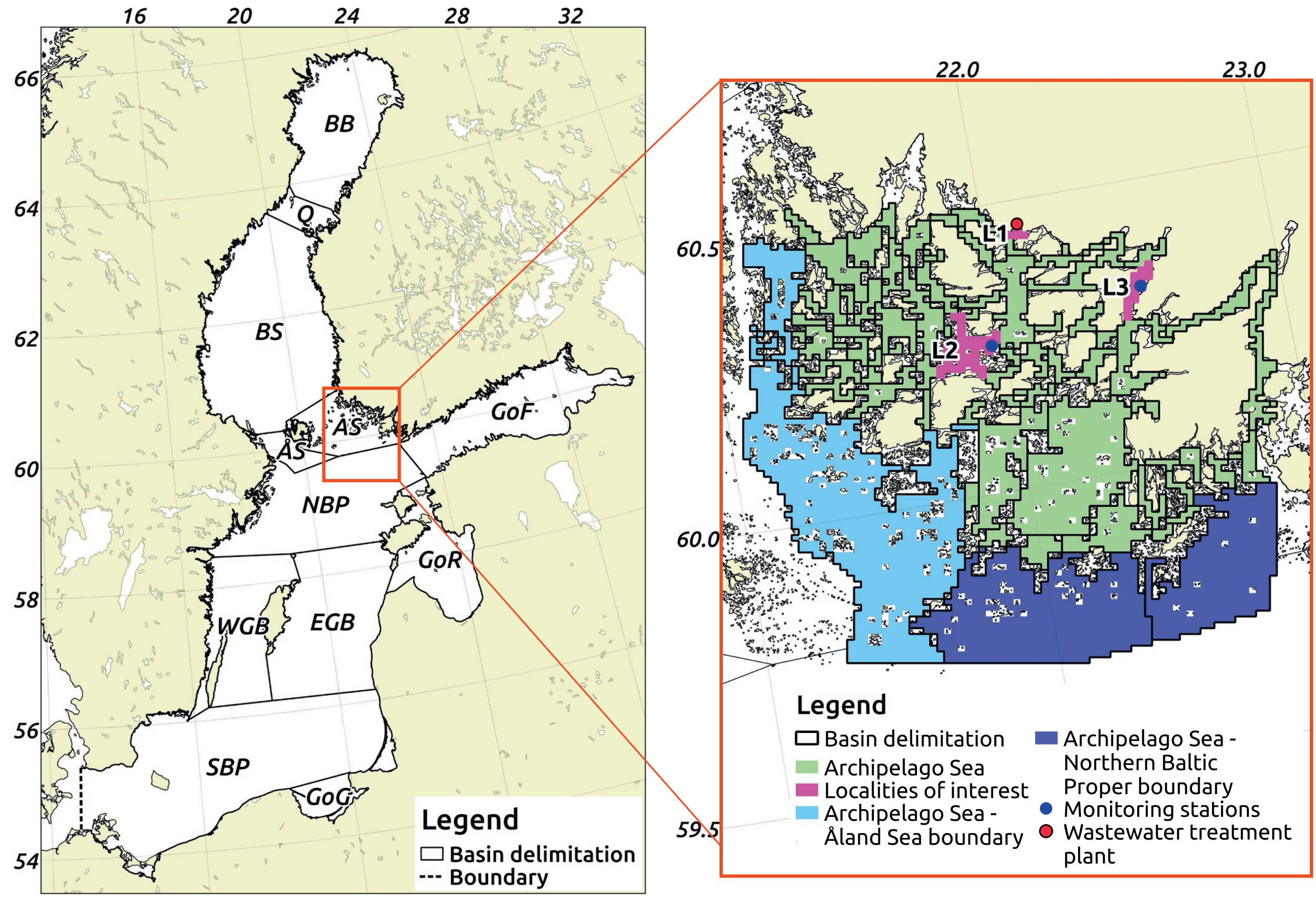

Fig. 1. Left: Baltic Sea system and its basin definition. BB: Bothnian Bay; Q: the Quark; BS: Bothnian Sea; AS: Archipelago Sea; ÅS: Åland Sea; GoF: Gulf of Finland; NBP: Northern Baltic Proper; GoR: Gulf of Riga; EGB: Eastern Gotland Basin; WGB: Western Gotland Basin; SBP: Southern Baltic Proper; GoG: Gulf of Gdansk. Right: Archipelago Sea sub-basin definition. Boundary conditions are represented in brown (dark: AS–ÅS and light: AS–NBP). Localities of interest are delimited in red. Red dots: monitoring stations and green dot: Turun Kaupuni Waste Water Treatment Plant (WWTP). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3.2. Hydrodynamics

The underlying hydrodynamic forcing used in this study is based on previous modelling work of Dargahi et al. (2017) for the period 2000–2009. For this modelling, they have used GEMSS® (Generalized Environmental Modelling System for Surface waters), a multi-purpose, time-dependent, 3D hydrodynamic model. This model has been verified and used for similar studies worldwide, and an exhaustive description of the modelling methodology is found in Dargahi et al. (2017). It is set up with a horizontal resolution of 5 km and 47 vertical layers of fixed thickness which increases with depth. The model is forced by the open sea boundary at the south-western part of the Southern Baltic Proper, by surface heat fluxes and wind stresses, and by freshwater discharges and associated temperatures from 69 main rivers draining into the Baltic Sea.

This model has been validated for 10 years (2000–2009) of simulation. Salinity and temperature plots (Fig. 2) illustrate the model ability to reproduce the temporal variations and the stratification for the station BY15 (EGB). For each monitoring station, the mean relative errors for temperature and salinity range between 4% and 10% (Dargahi et al., 2017).

In our study, the hydrodynamic results of Dargahi et al. (2017) are aggregated for a division of the Baltic Sea (excluding the western part) into 12 main basins (Fig. 1). This delimitation follows the Baltic Sea bathymetry (HELCOM, 2013a). Even though the Baltic Sea is relatively shallow (mean depth of 54 m), it is also characterised by significant depth variations and the presence of sills. These sills largely govern the Baltic Sea flow and transport processes (Leppäranta and Myrberg, 2009) ensuring that the horizontal mixing is greater within each delimited basin than between them.

Each basin is further divided into two vertical layers. The division is done at the pycnocline of each basin, which is the zone of maximum density gradient and lowest vertical mixing, thereby ensuring a mixed surface layer (Reissmann et al., 2009). The two layers are mixed together at times when pycnocline is weak or unstable. Our division into just two layers is a strong simplification for deep waters, where gradients of nutrient concentrations can be high (Conley et al., 1997). With around 70% of the Baltic Sea volume being above the perennial halocline (65 m), while deep water below 130 m occupies only around 5% (Stigebrandt and Wulff, 1987) however, a two-layer structure is suitable for the major part of the Baltic Sea, and especially for its surface waters, which are the main focus of management efforts (HELCOM, 2009). With a two-layer structure, the horizontal and vertical flows, and nutrient and algae transport between the basins and their layers, can be calculated and volume-averaged physical properties (salinity and temperature) aggregated over each layer. Thus, the simplified structure is used for water quality computations only, whereas the hydrodynamic/physical variables are computed with a full three-dimensional resolution and then suitably aggregated.

Hydrodynamics of the Archipelago Sea is obtained by downscaling of the GEMSS® Baltic Sea model (Dargahi and Cvetkovic, 2014). The downscaled model simulates the Åland and Archipelago Seas with a medium resolution of 1.3 km for the period 2001–2005. Boundary conditions are derived from the Baltic Sea model results using a cascade approach. The Archipelago Sea is divided into 82 sub-basins with different horizontal extents (Fig. 1), according to the coastal bathymetry. As in the Baltic Sea case, these sub-basins are also vertically divided into two layers at 10 m depth, which corresponds to the management-relevant surface water delimitation and approximates the euphotic depth (HELCOM, 2009; Aarup, 2002). Using the 3D hydrodynamics results, transport between the archipelago sub-basins and their layers is calculated and volume-averaged physical properties are aggregated for each layer.

3.3. Water quality

To represent water quality conditions of the Baltic Sea and the Archipelago Sea, a simple carbon-based biogeochemical model developed by Kiirikki et al. (2001, 2006) is applied in each (sub-)basin (see Appendix B for the model structure). The ecosystem part of the model, based on the oceanic phytoplankton model of Tyrrell (1999), accounts for the cyanobacteria, the other phytoplankton, the concentrations of dissolved inorganic nitrogen (DIN: ammonium, nitrite and nitrate) and phosphorus (DIP: phosphate), and organic nutrients (nitrogen (N), phosphorus (P) and carbon (C) in detritus) (Kiirikki et al., 2001). The sediment part represents the nutrients (N, P and C) in volatile sediments and the iron-bound P, and describes rates of detritus sedimentation, sediment mineralization and denitrification, and release of iron-bound P (internal loading) that is modelled as a function of the CO_2 efflux from the sediments (Kiirikki et al., 2006). The CO_2 efflux is used as a proxy of oxygen consumption and microbial reduction pathways at the sediment-water interface (Kiirikki et al., 2006; Lehtoranta et al., 2009). The biogeochemical model has been validated for the Gulf of Finland and internal loading has been found to have a higher correlation to the sediment CO_2 flux than to the near-bottom oxygen concentration in the Gulf of Finland (Kiirikki et al., 2006). Moreover, oxygen concentrations can present strong vertical gradients (Conley et al., 1997), making the carbon-based approach more robust given the underlying aggregated hydrodynamics.

The choice of a carbon-based model, which does not explicitly represent oxygen conditions, is also supported by the study of Lehtoranta et al. (2009), showing that the quantity and quality of organic matter (OM) in the sediments govern internal loading. Moreover, the study of Conley and Johnstone (1995) indicates that the OM flux plays a significant role for P mineralization in sediments. Indeed, in their study, local anoxia prevailed while aerobic conditions were maintained. Furthermore, a relatively constant oxygen influx is maintained in well mixed coastal and shallow sea zones, as the influence of the atmospheric forcing makes the oxygen concentration less stratified (Reissmann et al., 2009). While the carbon-based model has limited applicability in deeper waters where extended anoxic conditions prevail, its assumptions are applicable for most parts of the relatively shallow Baltic Sea and especially in its coastal zones. Therefore, the SDC approach has been implemented using the carbon-based model to quantify the main management-relevant variables in the Baltic Sea and its coastal waters, due to its robustness and simplicity.

For the Baltic Sea application, the only boundary condition with the open sea is situated in the south-west of the Baltic Sea. The influence of the North Sea is accounted for by use of actual monitoring data from the station BY2 (flow to and from Kattegat). For the Archipelago Sea, a one-way nesting approach is implemented for simplicity, where the boundary conditions are determined by the Baltic Sea model results at the Archipelago Sea – Northern Baltic Proper and the Archipelago Sea – Åland Sea interfaces (Fig. 1).

3.4. Data and scenarios

The hydrodynamic model of the Baltic Sea and Archipelago Sea requires various input data, such as shoreline and bathymetry, daily or monthly river flows and temperatures, meteorological forcing, and wave height. These data are described and analysed in Dargahi et al. (2017). The corresponding water quality models require nutrient loads, solar radiation and the underlying hydrodynamic inputs. For the Baltic Sea water quality model, nutrient loads have been obtained from the Fifth Baltic Sea pollution load compilation of HELCOM (PLC-5.5), which comprises total N and P inputs (1994–2010) for atmospheric, point source and riverine loads (HELCOM, 2013b). A detailed methodological description of this data account is given in Supplementary Materials S2. Boundary conditions for DIN, DIP and algae concentrations have been obtained from the BY2 HELCOM monitoring station, located in the south-west Baltic proper. Daily solar radiation data have been extracted from the SMHI mesoscale solar radiation model (STRÅNG, Landelius et al., 2001) at the centre of each basin. For the Archipelago Sea water quality model, spatially uniform daily solar radiations have been extracted from the STRÅNG model at the centre of the Archipelago Sea basin. A baseline scenario (without any mitigation, Table 1) has been defined, for which nutrient loads are based on repeated data for the year 2000, as obtained from Finland's environmental administration (http://www.ymparisto.fi), including loads from industries at point sources, wastewater treatment plants (WWTPs), fish farms, and rivers. This baseline scenario is unlikely to represent actual conditions of the Archipelago Sea over the whole period 2001–2005, but is used here for comparison with the alternative, yet related, scenarios of mitigating these repeated loads (Table 1).

For calibration-validation of the Baltic Sea model in the baseline scenario, monitoring data for DIN, DIP and chlorophyll a (Chla) are obtained from the SHARK (Havs- och vattenmyndigheten och SMHI) and ICES databases (The International Council for the Exploration of the Sea, 2015). For most Baltic Sea basins, one to three non-coastal monitoring stations are available and used for the calibration-validation process (Supplementary Materials S3 Fig. S1). For calibration-validation of the Archipelago Sea model, DIN, DIP and Chla monitoring data are obtained from the Finnish Environmental Institute (SYKE, http://www.syke.fi/en-US/Open_information) at the stations Nau 2361 Seili

Table 1
Assumed mitigation levels on land and in the sea for scenarios S1–3 and relative reduction (%) compared to the baseline scenario in nutrient loads from land and concentrations given as boundary conditions.

Scenarios	Assumed mitigation in each scenario	Reduction in Turku WWTP DIN and DIP loads (%)	Reduction in given sea boundary condition concentrations (%)		
			DIN	DIP	Chla
Baseline	No mitigation	0	0	0	0
Land mitigation (S1)	50% decrease in Turku WWTP nutrient load	50	0	0	0
Sea mitigation (S2)	DIN, DIP and Chla concentrations assumed to have been reduced close to good ecological status at the boundary	0	50	30–50	63
Combined mitigation (S3)	Combination of S1 and S2	50	50	30–50	63

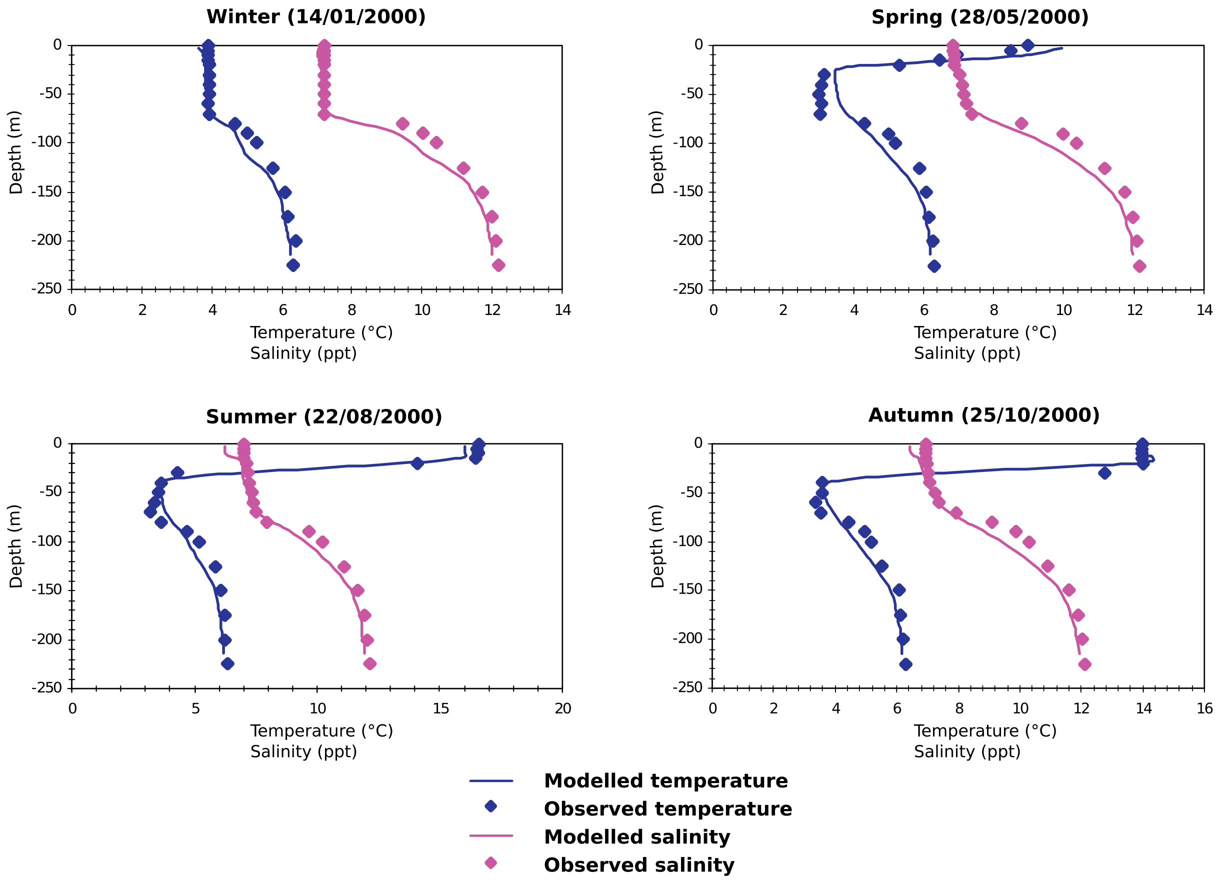

Fig. 2. Comparison of modelled seasonal salinity (S) and temperature (T) with corresponding observations at the monitoring station BY15 (Eastern Gotland Basin) in year 2000 at different dates. (Modified from Dargahi et al., 2017.)

intens (corresponding to location L2 in Fig. 1) and Pala 115 Tryholm (location L3 in Fig. 1).

In addition to the baseline scenario, three comparative scenarios are considered for possible mitigation of nutrient inputs to the Archipelago Sea. Scenario 1 (S1) assumes a reduction of land-based nutrient loads from the Turku WWTP by 50%. Scenario 2 (S2) assumes that improved water quality conditions (close to good ecological status (GES)) have been maintained as the Baltic Sea boundary conditions to the Archipelago Sea. The maximum winter DIN and DIP are cut to 28 $mg \cdot m^{-3}$ and 7.8 $mg \cdot m^{-3}$, respectively and the average Chla concentration is divided to amount to 2 $mg \cdot m^{-3}$, which corresponds to a reduction of winter DIN and DIP concentrations, and summer Chla, by approximately 50%, 30–50 % and 63%, respectively. This scenario does not suggest that reaching conditions close to GES in the Baltic Sea is straightforward. Indeed, due to complex internal processes (such as internal loading), decreasing eutrophication in the Baltic Sea is not only a matter of reducing land-based nutrient inputs (Stigebrandt, 2018). Finally, Scenario 3 (S3) is the combination of S1 and S2. The effects of these scenarios, relative to the baseline scenario conditions, are studied on three coastal localities, L1, L2 and L3 (Fig. 1). Locality 1 (L1) is a coastal sub-basin, where the Turku WWTP discharges (S1). Locality 2 (L2) is a coastal sub-basin in the middle of the archipelago, situated between L1 (affected directly by scenario S1) and the boundary conditions (S2). Locality 3 (L3) is also a coastal sub-basin, situated at a comparable distance from L1 as from L2.

3.5. Setup and calibration-validation of the water quality model

To simulate water quality conditions, a Python code has been developed, based on the eutrophication model from Cerco and Cole (1993). Firstly, this code processes the hydrodynamic results into a file that describes the time-dependent horizontal flow and transport between basins and vertical flow and transport between layers. This file can be reused if the hydrodynamic results and the basin definitions are not modified. Secondly, the transport and biogeochemical equations are solved for each time step. The time steps are kept smaller than both the residence time in the basin and a daily maximum time step. The Python code was used to simulate water quality in the Baltic Sea for the period April 2001 to December 2009 and the Archipelago Sea for the period April 2001 to January 2005.

For the Baltic Sea simulations, initialization and calibration is done simultaneously. Due to the absence of data for some variables, initial conditions are obtained by a 20-year spin up of the model with repeated forcing of the years 2001 and 2002. This allows sediment pools to build up such that the main simulation can start from an equilibrium state (Gustafsson et al., 2012). Calibration is done iteratively, simultaneously with the initialization, by varying parameter values to minimise the error between model results and observations data for DIN, DIP, and biomass. The short-term variations are calibrated for the years 2001 and 2002, while the year 2009 is used to ensure stable representation of sediment pools. Parameter values represent averaged basin conditions

Table 2
Model cost function results per Baltic Sea basin for the validation period (good: green; reasonable: orange; poor: red). See Appendix C for further explanation of the model cost function.

Basin	DIN		DIP	
	Surface	Deep	Surface	Deep
BB	0.23	0.47	0.85	0.92
Q	NaN	NaN	NaN	NaN
BS	0.09	0.59	0.17	1.20
GoF	0.18	0.50	0.21	1.52
ÅS	NaN	NaN	NaN	NaN
AS	0.06	0.85	0.19	1.88
NBP	0.40	1.84	0.19	4.84
GoR	0.12	0.53	0.69	0.37
EGB	0.21	1.85	0.18	2.92
WGB	0.31	1.20	0.05	4.18
SBP	0.17	1.43	0.26	1.42
GoG	0.25	0.92	0.39	0.99

for sediment types, food-web relations, and species compositions, which vary throughout the Baltic Sea (Gogina and Zettler, 2010); these are therefore calibrated specifically for each (sub-)basin. The Archipelago Sea simulations are calibrated and initialized using parameter values and initial conditions for the Archipelago Sea basin from the Baltic Sea model.

Validation of the Baltic Sea model is carried out for the period 2003–2008 by comparison with monitoring data. Furthermore, cost functions and Taylor diagrams, as described in Appendix C, are used to quantify model performance for DIN and DIP in the surface and deep layer of each basin. Validation of the Archipelago Sea model is carried out for the baseline scenario, by comparison with monitoring data from stations L2 and L3 (Fig. 1).

4. Results

4.1. Validation of modelling approach

Cost function results for the water quality model applied to each Baltic Sea basin and layer are given in Table 2. The overall mean cost of our, relatively simple, modelling approach is 0.89, similar to the score of the RCO-SCOBI model for the Baltic Sea (Eilola et al., 2011). For surface DIN and DIP, averaged model results for all basins are good (less than a standard deviation difference from the observations). For the deep layer, the model exhibits good or reasonable results for DIN, and for DIP with the exception of the Baltic Proper, where the model performance is generally poor.

Taylor diagrams in Fig. 3 show that, for surface DIN, the model result correlation with available monitoring data is good, greater than 0.8 for most of the Baltic Sea basins, with normalized standard deviations close to 1, meaning that the system variations are well explained by the model except for the Gulf of Riga and the Bothnian Bay. Deep DIN representation is acceptable, with most of the basins having a correlation around 0.5 and a normalized standard deviation around 0.5. The surface DIP results exhibit good correlation with the monitoring data (between 0.7 and 0.9) apart from the Bothnian Bay, even though the standard deviation is underestimated by the model. The Taylor diagram for deep DIP shows that the model performs poorly in representing the DIP variability, with a low correlation and normalized standard deviation.

Overall, the cost functions combined with the Taylor diagrams for surface DIN and DIP show that the simple water quality model performs well in its representation of both nutrients levels and their dynamics for most Baltic Sea basins. Moreover, the algal levels and dynamics are in accordance with the monitoring data, showing that the water quality representation also facilitates a good ecosystem description. Further system dynamics validation for the Baltic Sea (see more details and results in Appendix D) is in agreement with the conclusions from the Taylor diagrams and cost functions. Comparison with the model ensemble analysis by Eilola et al. (2011) (Supplementary Materials S4) shows performances comparable to other Baltic Sea models but suggests an underestimation of pelagic pools.

Furthermore, validation results also show (Supplementary Materials S4 Fig. S2) that our modelling approach captures the typical North-South gradient of water quality characteristics in the Baltic Sea, with high DIN and low DIP concentrations in the Bothnian Bay, due to limited denitrification and land-based P loading (Kuparinen et al., 1996), and lower DIN and higher DIP concentrations in southern basins. Comparison with monitoring data indicates that considerable discrepancies occur mainly in the deep part of the Baltic Proper for DIP, and to a lesser extent for DIN. The Baltic Proper basins are characterised by their great depth and relatively large, permanently anoxic areas (Conley et al., 2009a). Satisfactory results in other parts of the Baltic Sea suggest that processes specific to permanently anoxic areas are responsible for the main discrepancies, as these processes are not accounted for in the carbon-based model, but can also create strong concentration gradients that are not captured by the simple two-layer approach. For surface water quality, however, our relatively simple approach performs well, which may be due to calibration reduction of forcing uncertainties and model biases. Overall, the validation results supports the ability of the Baltic Sea model to represent short- to medium-term water quality conditions and variations for management purposes, with surface conditions as a primary focus, and for providing nested boundary conditions for local-scale model applications to coastal zones.

For the Archipelago Sea, a rigorous validation cannot be carried out, as nutrient load data represent the year 2000, while the simulation has been performed for the period 2001–2005. Model results are nevertheless compared with available data to check whether and how well the main characteristics of the system dynamics are captured by the model. Fig. 4 exemplify system dynamics for the sub-basins L2 and L3. Results for the centre of the archipelago (L2) display characteristics of effects from both the coastal nutrient loading from land and the open sea conditions. The eastern inner sub-basin (L3) is adjacent to coastal waters receiving high nutrient loads from land (mainly from the Paimionjoki River), which makes it representative of such recipient coastal waters. For the westernmost part of the archipelago, only scarce monitoring data are available for comparison, and the model displays low primary production due to lower nutrient loading and possibly also due to higher prevailing hydrodynamic flow rates.

The central archipelago sub-basin (L2) is relatively deep and divided into two layers (Fig. 4, red curve). Algal dynamics here is in good accordance with the Chla measurements. Surface DIN and DIP levels and dynamics also show good agreement with the monitoring data. The phase shift in the DIN and DIP increase during late autumn indicates delayed modelled that organic N and P mineralization. Deep DIN simulation shows good accordance with the data, but deep DIP is underestimated, which could be partly explained by too high vertical mixing. No anoxic conditions result for this sub-basin, agreeing with the measurements of oxygen concentration.

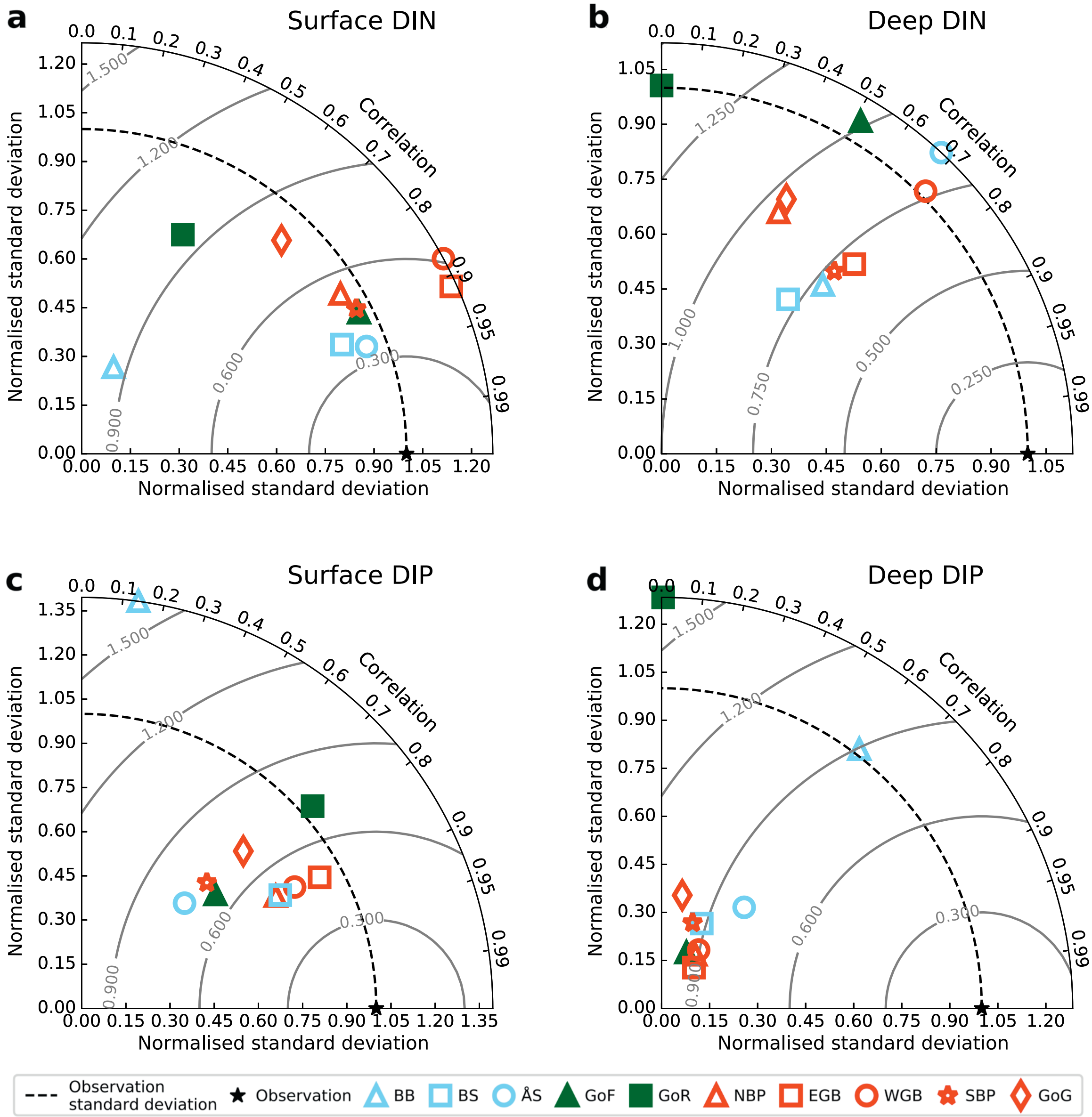

Fig. 3. Taylor diagrams of modelled (a) surface DIN, (b) deep DIN, (c) surface DIP and (d) deep DIP for the validation period (2002–2008). Standard deviations of model result are normalized with the observation standard deviation. The solid lines show equidistance to the observation point on the x-axis, which is proportional to the model root mean square error relative to observations. More information on Taylor diagrams is provided in Appendix C.

The eastern inner sub-basin (Fig. 4, green curve) is relatively shallow and thus only composed of a surface layer. It experiences higher algal densities than the central sub-basin L2, with higher phytoplankton spring blooms and summer cyanobacteria concentrations. Chla measurements indicate that the model overestimates the summer concentration, but the comparison is not conclusive due to the scarcity of data and uncertainties in conversion from biomass to Chla. The model simulation captures summer DIN deficiency, and DIP concentrations are also in the range of monitoring data. This sub-basin experiences seasonal anoxic events, which are also represented by the model (iron-bound P release), but slightly ahead in time (July–August) relative to observation (August–September). The P internal loading explains the magnitude of cyanobacteria blooms, by increasing summer DIP concentrations.

4.2. Scenario results

Fig. 5 shows the reduction of winter DIN concentration (Fig. 5a) and summer Chla (Fig. 5b) under the combined mitigation scenario S3 relative to the baseline scenario (Table 1). A clear gradient can be seen for both variables, with a decreasing effect of S3 with distance from the sea boundaries. The Chla results (Fig. 5b) exhibit a similar local gradient close to and decreasing with distance from the WWTP (L1). Due to dilution, effects of reduction in nutrient inputs from WWTP should commonly be stronger in the direct proximity to such mitigation implementation. However, non-trivial spatial variations may also occur depending on underlying hydrodynamics.

Fig. 6 shows how each simulated scenario affects the management variables for all three localities in focus, L1–3. S1 leads to a substantial

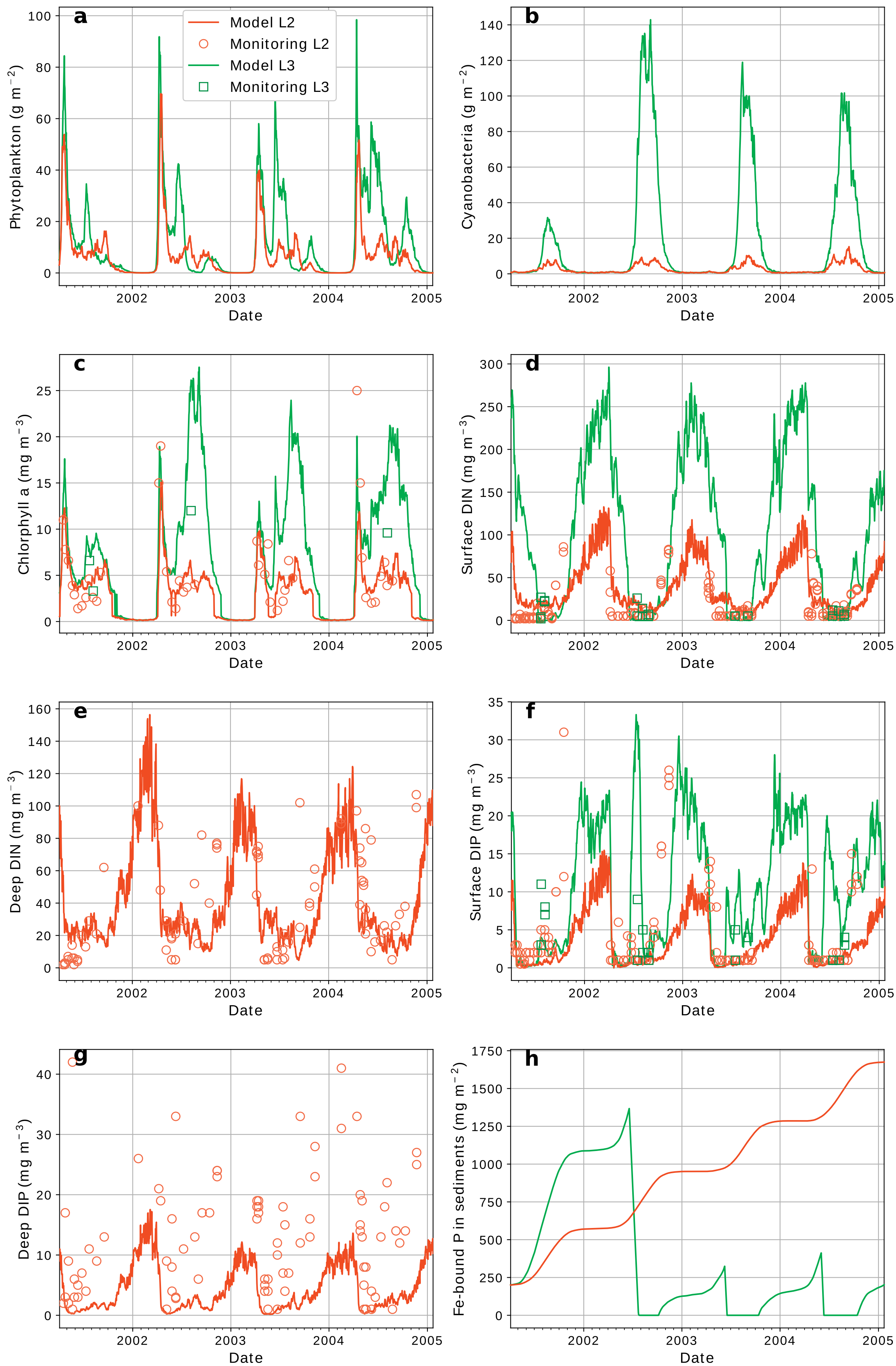

Fig. 4. Modelled water quality dynamics for the central archipelago sub-basin (L2) and eastern inner sub-basin (L3) for the simulation period (2001–2005) compared with observations from Nau 2361 Seili intens (L2) and Pala 115 Tryholm (L3). (a) Phytoplankton areal density, (b) Cyanobacteria areal density, (c) Chlorophyll a concentration, (d) Surface DIN concentration, (e) Deep DIN concentration, (f) Surface DIP concentration, (g) Deep DIP concentration, (h) Iron bound-P areal density in volatile sediments. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

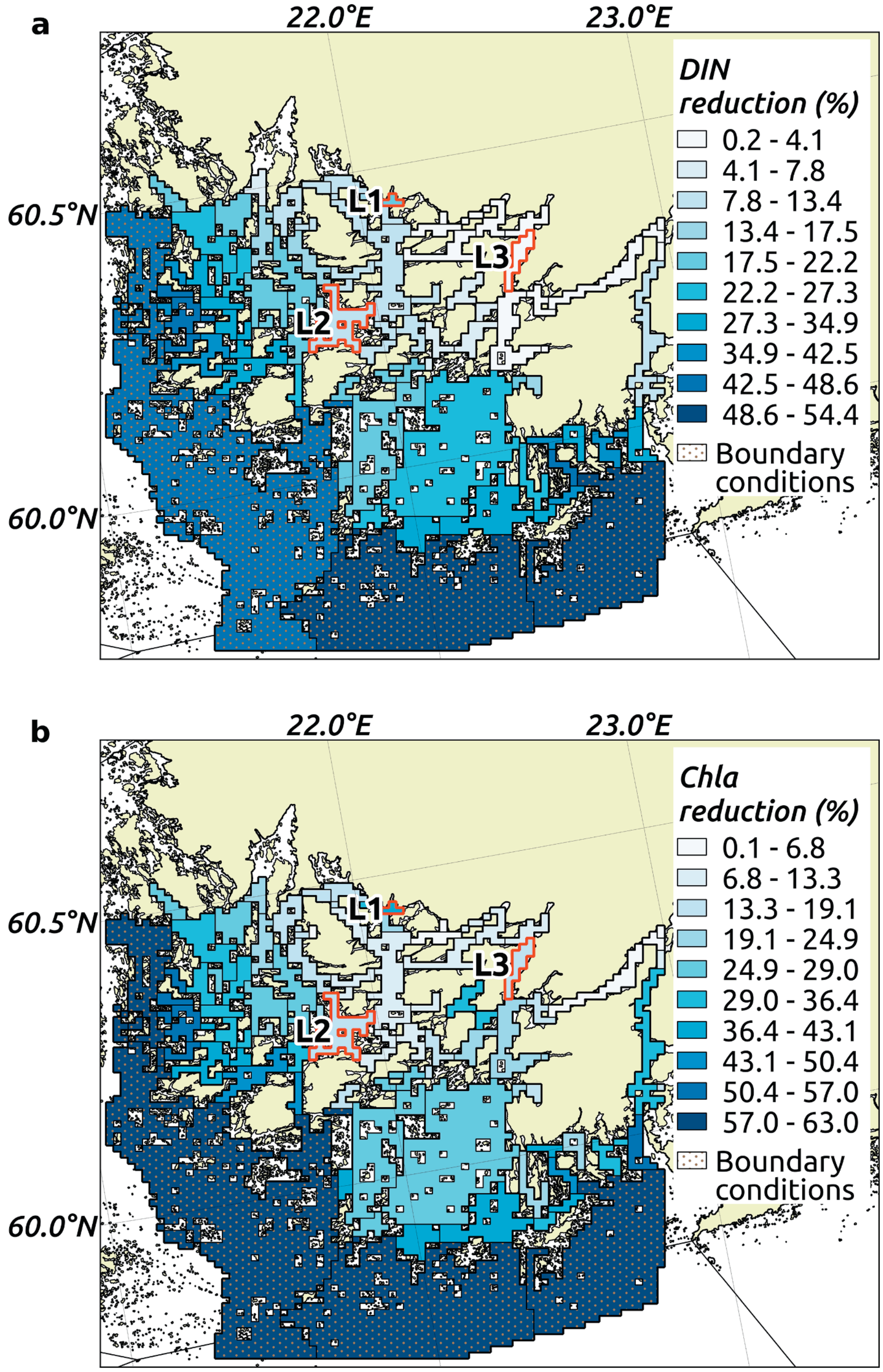

Fig. 5. Concentration reductions under mitigation scenario S3 relative to the baseline scenario (Table 1). (a) Results for winter surface DIN and (b) summer chlorophyll a.

decrease of winter nutrient and summer chlorophyll concentrations for L1, a moderate decrease of the winter DIN concentration for L2 and no significant effects for L3. While reducing DIN and DIP loadings by the same proportion, the scenario S1 affects more the winter DIN than the winter DIP concentrations at L1. This is likely due to stronger sediment feedbacks that affect P (Vahtera et al., 2007). The scenario S2 leads to a moderate decrease of DIN and DIP winter concentrations at L2 and a slight decrease of these concentrations at L1 and L3, whereas it substantially decreases summer chlorophyll concentrations at all three localities. These differences indicate that S2 affects summer algae conditions more than spring blooms, as the latter are more influenced by winter nutrient concentrations (Vahtera et al., 2007). Seasonal flow variations and changes in the internal dynamics are possible explanations for this influence, since they can change the amount of available nutrient during summer without affecting winter concentrations. As a combination of S1 and S2, the total effects of scenario S3 seem to be

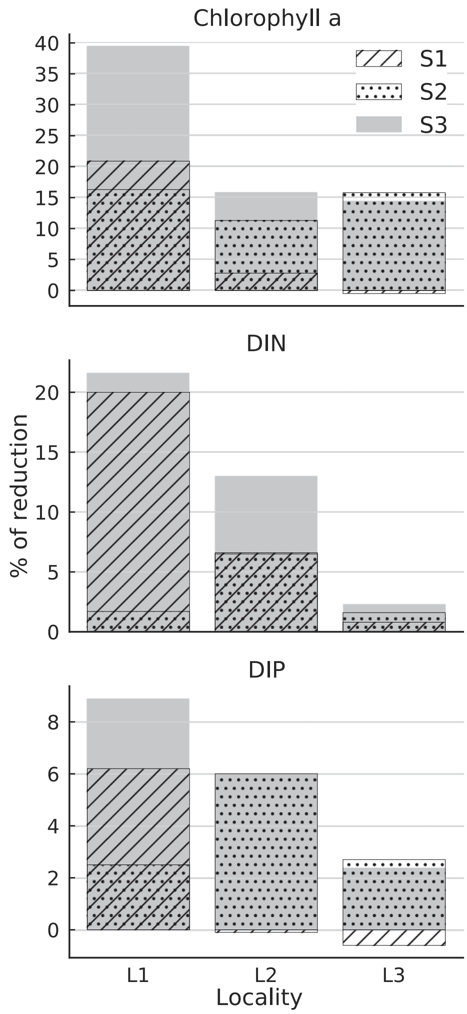

Fig. 6. Relative reduction (%) of winter (DJF) surface DIN and DIP and summer (JA) chlorophyll a compared to the baseline scenario under the three mitigation scenarios (S1–3) for the period September 2001–September 2004 at the three localities (L1–3).

additive for winter nutrient concentrations and be somewhat stronger for summer chlorophyll.

For L3, a slight increase of DIP and Chla can be noted under scenario S1. Even if this increased effect is not significant given the uncertainties, the lack of concentration reductions stresses that actual effects of management measure can be difficult to predict, due to complex dynamics and coupling effects, which cannot be just assumed without relevant system modelling.

5. Discussion

5.1. Result implications

For the Archipelago Sea, the simulation of water quality responses to the local mitigation scenario S1 shows that the effects are, as expected, stronger in the proximity to local measure implementation, but also spread unevenly over the whole archipelago and for different management variables. Regarding the latter aspect, equal land-source reduction for N and P (50%) leads to greater coastal-water quality reduction for N than for P (e.g. 20% and 6% reduction respectively, at L1), thereby reducing the DIN:DIP ratio and potentially increasing the risk of cyanobacteria blooms (Chen et al., 2013). The regional mitigation scenario S2, corresponding to improved conditions close to GES in neighbouring marine basins, leads to moderate and strong effects on winter nutrient concentrations and summer Chla, respectively, in the innermost archipelago sub-basins. These effects are also strong in the transitional sub-basins. For the combined scenario S3, with both local and regional mitigation measures, the effects are coupled, emphasizing the need to consistently consider and account for both types of effects in coastal water-quality management. Focused coastal modelling can potentially account for the sea influences by use of observation data to set the sea boundary conditions. However, sufficient availability and quality of such data, suitable for accurate assignment of sea boundary conditions, are commonly limited, with the data available often having poor spatiotemporal resolution and coverage, and/or being otherwise inconsistent with the model requirements. Therefore, a validated regional water-quality model may be necessary for dynamic characterisation of relevant sea boundary conditions for coastal water quality, while also allowing for consistent simulation of regional-scale water-quality changes. A two-way model coupling may also be necessary for longer time scales to simulate local effects on regional water quality. However, for the time period considered here, the one-way nesting influence is sufficient, as effects of local mitigation scenario S1 remain localised over the simulation period. At any rate, the proposed and exemplified modelling approach to simulating different management scenarios can be used for science-based identification of effective mitigation measures under multi-variate considerations (Chen et al., 2013) and in support of local-coastal and whole-sea compliance with various environmental regulations.

Furthermore, climate change can also affect the hydrodynamic and biogeochemical properties of the sea (e.g. internal loading), and the hydrological processes driving the land-based nutrient inputs to the sea. Changes in land-use may also strongly influence hydrological and runoff (Destouni et al., 2013; Jaramillo and Destouni, 2015), and associated nutrient loads to the sea and thereby coastal water quality (Törnqvist et al., 2015). Overall, hydrodynamic, biogeochemical and catchment processes are influenced by global, regional and local changes. Consistent integrated regional (whole sea) and local (coastal) water quality modelling is then needed to realistically, yet relatively simply, account for the whole range of such possible change influences at different scales and parts of the coastal-marine system. This paper has developed, and concretely exemplified and tested the application of such modelling in support of SDC and management of coastal-marine water quality across scales.

5.2. Generality and limitations of modelling approach

5.2.1. Basin-wise approach and hydrodynamics

In other parts of the world, basin-based modelling approaches have been used and found suitable for semi-enclosed coastal zones, lakes and estuaries that are characterised by a low tidal range and a limited water exchange with the open sea (Hagy and Murrell, 2007; Lam et al., 1987). Basin-wise aggregation and averaging of system and model properties can also be used for microtidal (e.g., Scottish inlets, Gillibrand et al., 2013) and macrotidal (e.g., Bay of Brest, Le Pape and Menesguen, 1997) areas. However, the present use of independent simulation results for the underlying hydrodynamics may not be suitable for such cases, as it is based on velocity profiles at fixed basin boundaries. Particle tracking and tide current filtering methods have instead been used to calculate flow exchange rates among basins in such cases (Lv et al., 2016; Salomon and Breton, 1991). Moreover, for macrotidal semi-enclosed coastal zones, with major water exchanges across their system boundaries, the model boundary has to be shifted from the entrance of the system toward the ocean to fit the coast-ocean discontinuity and avoid loss of nutrients and algae moved back and forth across the system entrance (Le Pape and Menesguen, 1997).

The pycnocline is used here for the separation into two vertical layers for water quality modelling, as this corresponds to the zone of least vertical mixing in the Baltic Sea application case. With the pycnocline being a widespread property of marine systems, this vertical delimitation method may have a general applicability for such regional systems. Open sea areas, however, may be considerably better represented by division into 3 to 5 vertical layers (Dargahi et al., 2017). The present two-layer vertical delimitation strongly simplifies the open sea system, which explains part of the discrepancies found in the present results for the deep waters of the Baltic Proper. In general, the choice of vertical model layering should depend on the physical properties of the modelled coastal-marine domain and the simplification required for scenario analysis in the SDC.

5.2.2. Water quality

The biogeochemical model used here together with the basin-wise hydrodynamic aggregation is primarily aimed to capture the surface water quality dynamics across the studied Baltic and Archipelago scales. Model representation of deeper water dynamics can then be improved by modelling preferential P remineralization (Jilbert et al., 2011) and implementing more vertical layers to reduce the modelled vertical mixing scale. The overestimation of the modelled vertical mixing scale gives too high supply of DIP in the surface layer that is compensated for by an underestimation of the calibrated sediment remineralization rates, keeping the deep DIP concentrations too low and yielding high P sediment densities (Supplementary Materials S4, Table S7). While the model-observation discrepancies for deep waters constitute a limitation for long-term regional simulations, they have a limited impact for medium-term coastal management studies, where the surface water quality plays a more important role (HELCOM, 2009).

The ecosystem part of the biogeochemical model used here is based on a general oceanic model developed by Tyrrell (1999). The sediment part uses carbon as the main driving variable and has been developed for the Baltic Sea by Kiirikki et al. (2006). While carbon has been shown to play an important role for the sediment release of P in other parts of the world (e.g., Gulf of Mexico, Fennel et al., 2011), to our best knowledge, this model has so far only been verified for the Baltic Sea. Application of this water quality modelling to other coastal-marine systems would require site-specific calibration and adaptation to capture the prevailing dominant processes at each site.

6. Conclusions

In this study, we have developed and tested the applicability of a relatively simple SDC approach to water quality modelling as designed in Appendix A, which can support cross-scale and cross-environment analysis of management scenarios for semi-enclosed seas and their coastal zones. The main findings of this study are summarised as follows:

- The proposed SDC approach (Appendix A) is applicable for the illustration examples of the Baltic Sea and Archipelago Sea within it, with spatial scales between the sea and archipelago differing by an order of magnitude in terms of resolution and typical basin dimension. Further downscaling within the archipelago following the SDC steps (Appendix A) would in principle also be possible if needed for more spatially refined management and/or regulatory considerations.
- The developed, readily implemented, carbon-based water quality model (Appendix B) adequately represents surface water quality dynamics in the Baltic Sea basins. For the deeper waters, model performance is moderate, with the Baltic Proper displaying the greatest discrepancies in comparison with observation data. Comparison of the SDC results with other modelling studies in the literature shows similar model performance of other models applied to the Baltic Sea.
- A general-purpose tool for three-dimensional hydrodynamic modelling with a relatively coarse resolution provides a suitable representation basis for the physical processes affecting water quality in the Baltic Sea. In this model tool, division into basins and aggregation of flow variables over each basin can suitably follow the shoreline/bathymetry structure of a given semi-enclosed sea and its archipelago or coastal zone.
- As illustrated for the scale and local environment of the Archipelago Sea within the Baltic Sea, different scenarios of environmental management measures and outcomes on land and in the open sea show that effective sea measures may yield the most important coastal effects, in this case for the summer concentration of algae. This highlights the need to realistically account for variations and changes in the overall water quality conditions of the semi-enclosed sea for relevant assessment of corresponding local coastal conditions.

The relative simplicity of the presented modelling approach for SDC makes it suitable for comparative simulation and analysis of various management and/or hydroclimatic scenarios for both land and the sea. The simplicity is mainly achieved by aggregating eutrophication conditions on management-relevant basin scales for each considered sea environment, and by decoupling the water quality modelling part from the hydrodynamics part. The positive model results in this study call for further research efforts to test this SDC approach for different scenario conditions and other coastal locations and scales in the Baltic Sea, as well as for other semi-enclosed seas, and their coastal zones and archipelagos across the world.

Acknowledgments

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- STRÅNG data used here are from the Swedish Meteorological and Hydrological Institute (SMHI), and were produced with support from the Swedish Radiation Protection Authority and the Swedish Environmental Agency.
- The Swedish Agency for Marine and Water Management (SHARK), the Swedish Meteorological and Hydrological Institute (SMHI) and the Finnish Environmental Institute (SYKE) kindly provided monitoring data.
- The International Council for the Exploration of the Sea (Copenhagen) kindly provided datasets on Ocean hydrography.
- The Global Runoff Data Centre (56068 Koblenz, Germany), SMHI kindly provided river discharges datasets.
- Finland's environmental administration kindly provided river discharges datasets and nutrient load data.

Appendix A. The scalable dynamic characterisation (SDC) approach

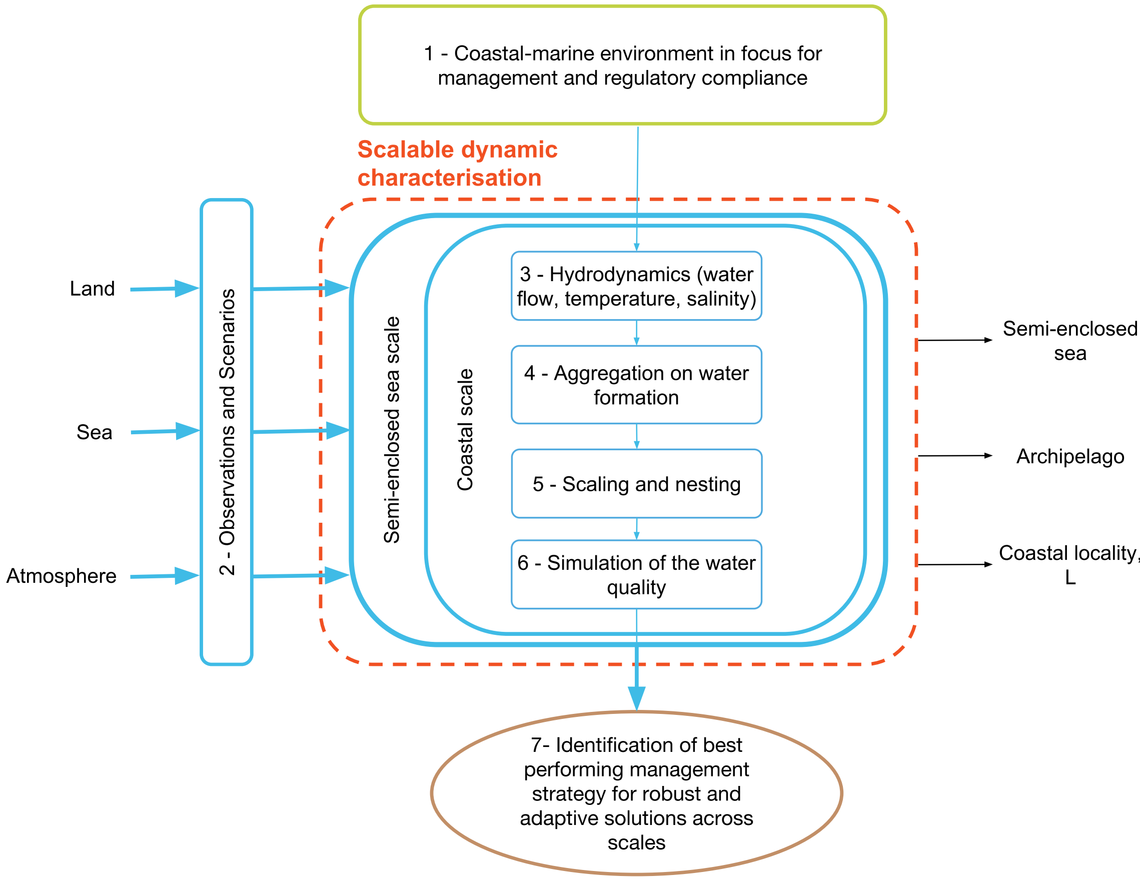


Fig. 7. Schematic representation of a scalable dynamic characterisation (SDC) main components, numbered 1–7, in the proposed work flow order.

Based on the functional requirements presented in Section 2, the Scalable Dynamic Characterisation (SDC) approach is set in a management context with the following main components and workflow as illustrated in Fig. 7:

1. The coastal-marine environment and spatiotemporal scales in focus are chosen depending on regulation and management focus.
2. The relevant available observation data and scenarios to simulate are identified and formulated depending on regulation and management requirements, and associated model variables are quantified and validated.
3. Hydrodynamic modelling of, e.g., flow structure, temperature and salinity, are carried out independently (Le Pape and Menesguen, 1997) (e.g., Dargahi et al., 2017) and used as a basis for further simulation of nutrient and algae transport, and other water quality processes (e.g., Kiirikki et al., 2001).
4. To simplify the model system, the spatial domain of the coastal-marine environment in focus, determined in step 1, are partitioned into management-relevant subsystems (such as marine or coastal/archipelago (sub-)basins), which are further depth-divided in vertical layers. The horizontal and vertical sub-divisions depend on the hydrodynamic properties of the system. These properties are spatially averaged (aggregated) over each sub-basin and each associated depth-layer to more simply represent the horizontal and vertical flow and water quality processes.
5. The spatial scale relationships of hydrodynamics and water quality processes between a smaller scale of interest (e.g., a coastal zone or archipelago of the Baltic Sea) and a larger scale system (e.g., the whole Baltic Sea) are determined from larger-scale model results (depending on and validated against relevant available data for that scale), and used as boundary conditions for corresponding smaller-scale simulations.
6. A biogeochemical model (e.g., Kiirikki et al., 2001, 2006) is used to simulate water quality conditions for each sub-basin on the system scale. Such model implementation links the internal biogeochemical processes with the underlying internal hydrodynamics and the relevant external forcings (e.g., nutrient loads from land under each considered management scenario).
7. Water quality results for different scenarios (e.g., of various nutrient mitigation measures and/or climate-change projections), based on the SDC approach, are analysed and compared to identify best performing management strategies for regulatory compliance.

Appendix B. Water quality biogeochemical model

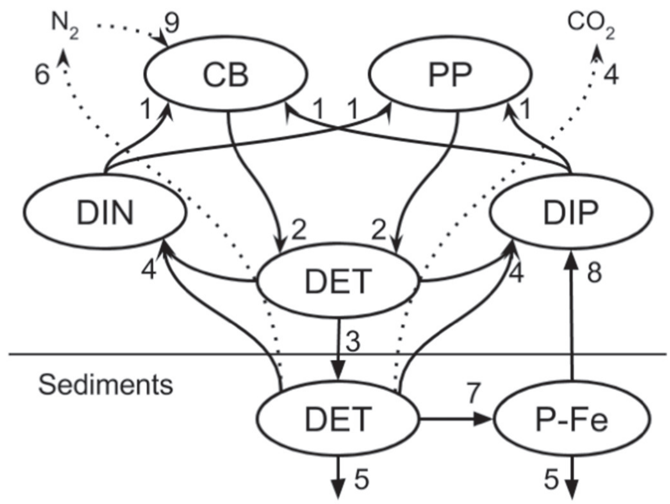


Fig. 8. Structure of the water quality model (modified from Kiirikki et al., 2006). CB: cyanobacteria; PP: other phytoplankton; DET: N, P and C in detritus and in volatile sediments (Nv, Pv, Cv); P-Fe: iron bound P. 1: uptake; 2: loss; 3: sink and sedimentation; 4: mineralization; 5: burial; 6: denitrification; 7: P-binding; 8: internal P loading; 9: N-fixing.

The water quality biogeochemical model implemented is represented (Fig. 8) and divided in a pelagic and a sediment part. The variables, parameters and their calibration, and equations are given in the Supplementary Material S1.

A complete description of the ecosystem part is given in Kiirikki et al. (2001) and its main characteristics are summarised as follow:

- The model considers two competing groups of algae, the cyanobacteria (principally the genera *Nodularia* and *Aphanizomenon*) and the other phytoplankton (representing principally diatoms and flagellates), as well as inorganic and organic nutrient concentrations.
- Algal growth rates depend on solar radiation, nutrient availability according to Michaelis-Menten kinetics, temperature according to Frisk (1982), and is limited by a self-shading factor, representing the carrying capacity of the system. The other phytoplankton growth requires availability of both DIN and DIP, while cyanobacteria growth requires only DIP, as they can fix atmospheric nitrogen. Cyanobacteria have a lower maximal growth rate and a higher optimal growth temperature, as the nitrogen fixing process requires energy. Both algal groups take up nutrient according to the Redfield ratio (Redfield, 1958).
- Algal loss rates depend on temperature. Cyanobacteria are avoided by grazers due to their toxicity (Sellner et al., 1996), which is modelled by a lower loss rate. A minimal overwintering biomass is defined to avoid extinction.
- Dead algal biomass is injected in the detritus pool according to the Redfield ratio. Sinking detritus are partly mineralized into dissolved inorganic nutrients and detritus reaching the bottom are converted into sediments.

The sediment part is explained in details in Kiirikki et al. (2006) and accounts for the volatile sediments described by their areal density. Sediments are not vertically resolved and processes account for varying accumulation and release rates, fulfilling the mass conservation and corresponding to a level 3 sediment model from Soetaert et al. (2000) that has a vertically integrated dynamic representation. Two states of sediment processes are considered, modelled as a function of the CO_2 flux, which corresponds to the energy consumption of microbial reduction. When the flux is below a threshold, situated approximately at 200–470 $\mathrm{mg \cdot C \cdot m^{-2} \cdot day^{-1}}$ (Kiirikki et al., 2006), denitrification occurs and part of the phosphorus in sediment is bound to ferric iron, reducing the mineralization process. When the flux is above, iron bound phosphorus is released, and no denitrification occurs as sediments are considered anoxic, increasing the release of inorganic nutrients to the water column. In both states, mineralization is proportional to the CO_2 flux (carbon-based model).

Appendix C. Validation methods

Validation and quantification of model performances for the basins are carried out using the model cost function, developed by Eilola et al. (2009), along with Taylor diagrams. The former is defined as $C = \frac{|M-O|}{Sd}$, where the mean difference between model results (M) and observations (O) is normalized by the standard deviation of the observation (Sd). The cost function is used to interpret model performance with regard to the prevailing data variability and results are considered good if the cost is less than the standard deviation ($0 \le C < 1$), reasonable if $1 \le C < 2$, and poor if the cost is greater than two standard deviations ($C \le 2$).

Taylor diagrams are used to assess how well a model represents the observed system dynamics in term of standard deviation of observation data (Taylor, 2001). In this polar type of plot, the angular coordinate gives the correlation with observations, the abscissa and ordinate show standard deviation, and distance from the observation point on the x-axis to the reference is proportional to the root-mean square error of the model relative to observations. To study the different basins simultaneously, the modelled standard deviation is here normalized by the corresponding observation standard deviations.

Appendix D. Baltic Sea system dynamics

Resulting Baltic Sea system dynamics are exemplified for the Western Gotland Basin and shown in Fig. 9 compared to the monitoring data of stations BY32 and BY38 (see Supplementary Material S3 Fig. S1). In contrast to the model results, the displayed observation data are not spatially averaged yet show small horizontal surface water variability, thereby justifying the model division into basins. The deep water variability is greater due to the vertical stratification (Fig. 9 f and h).

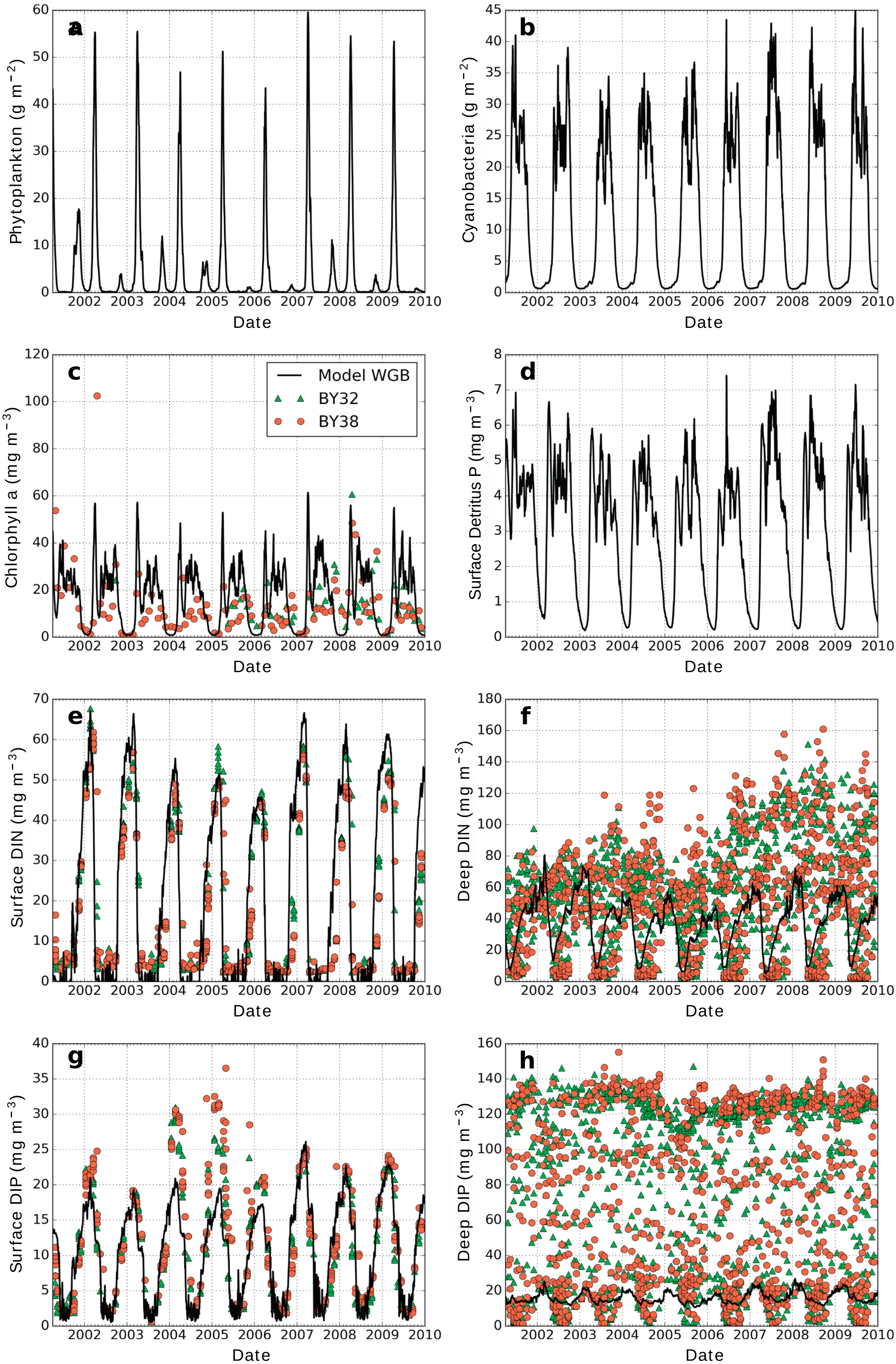
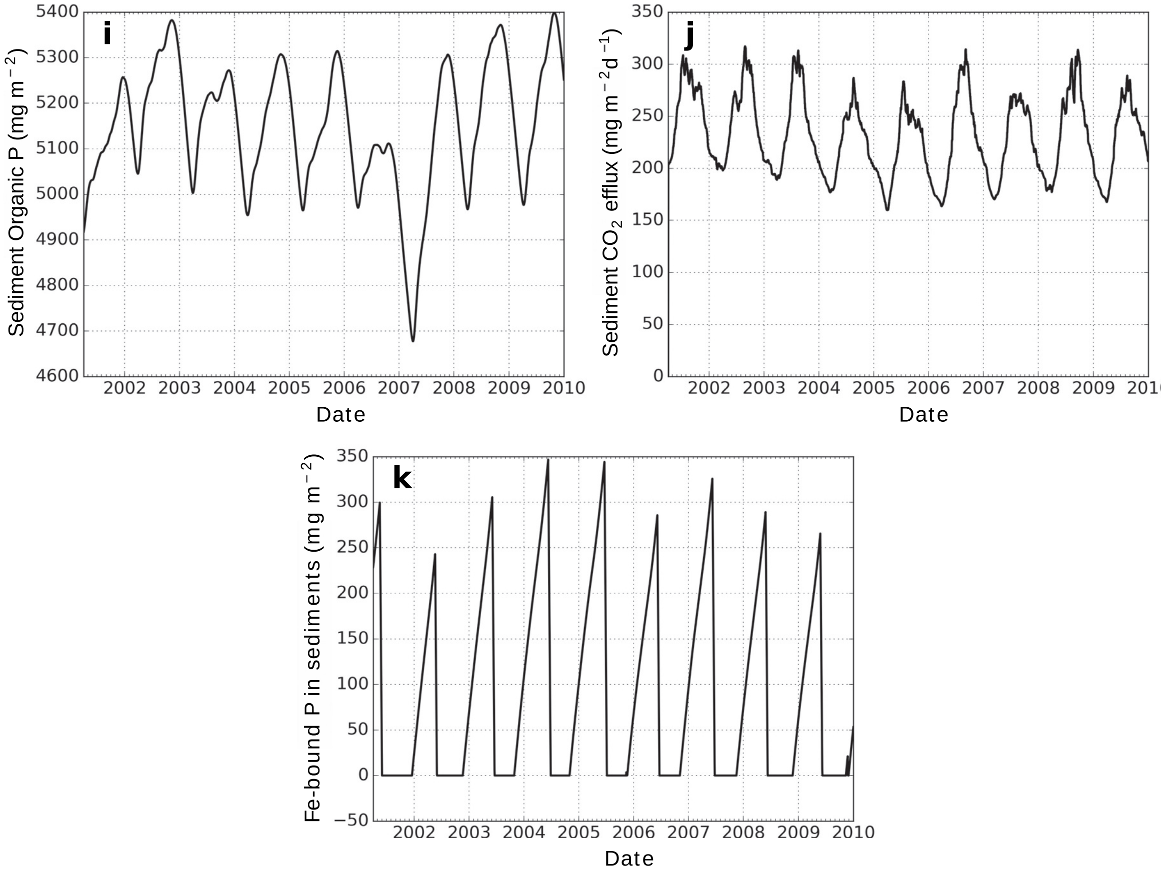


Fig. 9. Modelled water quality dynamics for the Western Gotland Basin for the simulation period (2001–2010) compared with observations from BY32 and BY38. (a) Phytoplankton areal density, (b) Cyanobacteria areal density, (c) Chlorophyll a concentration, (d) Surface detritus P (e) Surface DIN concentration, (f) Deep DIN concentration, (g) Surface DIP concentration, (h) Deep DIP concentration. Modelled water quality dynamics for the Western Gotland Basin for the simulation period (2001–2010) compared with observations from BY32 and BY38. (i) organic P areal density in volatile sediments, (j) Sediments CO_2 efflux, (k) Iron bound-P areal density in volatile sediments.



The Western Gotland Basin follows the main pattern of water quality dynamics of the Baltic Proper, but there is still large variations among the basins. The northernmost areas have low primary production, limited by phosphorus, light availability and temperature, leading to different ecosystem characteristics than in the southern basins and making the northern basins less subject to anoxia (Conley et al., 2009a; Eilola et al., 2011). Denitrification and burial are also low in the northern basins, explaining the high nitrogen concentrations (Deutsch et al., 2010). The Bothnian and Archipelago Seas, influenced by both the Baltic Proper and the northern basins, have higher primary production than the Bothnian Bay and less anoxic conditions than the Baltic Proper. The Gulfs of Finland, Riga and Gdansk, on the eastern side of the sea, have relatively high primary production, due to high nutrient loads, and relatively high nutrient turnover rates due to higher than Baltic-average temperatures. These basins experience frequent seasonal hypoxia, but low permanent anoxia as they are relatively shallow and well mixed.

For the primary production, growth rates are functions of temperature, nutrient concentrations, light availability and maximal algal density, while death rates depend only on temperature. In the present study, net phytoplankton growth rates vary between $-0.23\,\text{day}^{-1}$ and $0.5\,\text{day}^{-1}$, which is in reasonable agreement with previous local studies by Pedersen and Borum (1996). In these studies, variation of phytoplankton growth rates was found to range from $-0.23\,\text{day}^{-1}$ to $0.39\,\text{day}^{-1}$ for the Roskilde fjord. Table 3 also compares our simulated net primary production results with previous estimations of gross primary production by Wasmund et al. (2001) and Larsson et al. (2010) (covering different periods). For further comparison, Meier et al. (2012) have more recently found a net primary production of $51.8\,\text{gC}\cdot\text{m}^{-2}$ for the period 1987–2007, which is consistent with our model results.

Table 3
North-South gradient of net primary production results in ($\text{gC}\cdot\text{m}^{-2}\cdot\text{year}^{-1}$) for 2002–2009 and data of gross primary production from Wasmund et al. (2001) (and references therein; periods: 1970s, 1980s and 1993–1997) and from [a] Larsson et al. (2010).

Basin	Model results	Data
Bothnian Bay	8	16[a]–17
The Quark	15	17–21[a]
Bothnian Sea	31	33[a]–52
Archipelago Sea	34	52
Å land Sea	60	52
Gulf of Finland	73	82
Northern Baltic Proper	85	162[a]–200

(*continued on next page*)

Table 3 (*continued*)

Basin	Model results	Data
Gulf of Riga	76	261
Eastern Gotland Basin	88	208
Western Gotland Basin	97	200
Southern Baltic Proper	89	64[a]–193
Gulf of Gdansk	96	283
Baltic Proper	**88**	**200**
Baltic Sea	**67**	**145**

References

Aarup, T., 2002. Transparency of the North Sea and Baltic Sea — a Secchi depth data mining study. Oceanologia 44, 323–337.

Bonsdorff, E., Blomqvist, E., Mattila, J., Norkko, A., 1997. Coastal eutrophication: causes, consequences and perspectives in the archipelago areas of the northern Baltic Sea. Estuar. Coast. Shelf Sci. 44, 63–72. https://doi.org/10.1016/S0272-7714(97)80008-X.

Borja, A., Elliott, M., Carstensen, J., Heiskanen, A.-S., van de Bund, W., 2010. Marine management — towards an integrated implementation of the European marine strategy framework and the water framework directives. Mar. Pollut. Bull. 60 (12), 2175–2186.

Bring, A., Asokan, S.M., Jaramillo, F., Jarsjö, J., Levi, L., Pietroń, J., Prieto, C., Rogberg, P., Destouni, G., 2015a. Implications of freshwater flux data from the CMIP5 multi-model output across a set of Northern Hemisphere drainage basins. Earth's Future 3 (6), 206–217. https://doi.org/10.1002/2014EF000296.

Bring, A., Rogberg, P., Destouni, G., 2015b. Variability in climate change simulations affects needed long-term riverine nutrient reductions for the Baltic Sea. AMBIO 44 (3), 381–391. https://doi.org/10.1007/s13280-015-0657-5.

Caddy, J.F., 1993. Toward a comparative evaluation of human impacts on fishery ecosystems of enclosed and semi-enclosed seas. Rev. Fish. Sci. 1 (1), 57–95. https://doi.org/10.1080/10641269309388535.

Cerco, C., Cole, T., 1993. Three-dimensional eutrophication model of Chesapeake Bay. J. Environ. Eng. 119, 1006–1025. https://doi.org/10.1061/(ASCE)0733-9372(1993)119:6(1006).

Chen, N., Peng, B., Hong, H., Turyaheebwa, N., Cui, S., Mo, X., 2013. Nutrient enrichment and N:P ratio decline in a coastal bay-river system in southeast China: the need for a dual nutrient (N and P) management strategy. Ocean Coast. Manag. 81, 7–13. https://doi.org/10.1016/j.ocecoaman.2012.07.013. Special Issue: Advancing Ecosystem Based Management.

Conley, D.J., Björck, S., Bonsdorff, E., Carstensen, J., Destouni, G., Gustafsson, B.G., Hietanen, S., Kortekaas, M., Kuosa, H., Meier, H.E.M., Müller-Karulis, B., Nordberg, K., Norkko, A., Nürnberg, G., Pitkänen, H., Rabalais, N.N., Rosenberg, R., Savchuk, O.P., Slomp, C.P., Voss, M., Wulff, F., Zillén, L., 2009a. Hypoxia-related processes in the Baltic Sea. Environ. Sci. Technol. 43 (10), 3412–3420. https://doi.org/10.1021/es802762a.

Conley, D.J., Bonsdorff, E., Carstensen, J., Destouni, G., Gustafsson, B.G., Hansson, L.-A., Rabalais, N.N., Voss, M., Zillén, L., 2009b. Tackling hypoxia in the Baltic Sea: is engineering a solution? Environ. Sci. Technol. 43 (10), 3407–3411. https://doi.org/10.1021/es8027633.

Conley, D.J., Johnstone, R., 1995. Biogeochemistry of N, P and Si in Baltic Sea sediments: response to a simulated deposition of a spring diatom bloom. Mar. Ecol. Prog. Ser. 122, 265–276. https://doi.org/10.3354/meps122265.

Conley, D.J., Stockenberg, A., Carman, R., Johnstone, R., Rahm, L., Wulff, F., 1997. Sediment-water nutrient fluxes in the Gulf of Finland, Baltic Sea. Estuar. Coast. Shelf Sci. 45 (5), 591–598. https://doi.org/10.1006/ecss.1997.0246.

Dargahi, B., Cvetkovic, V., 2014. Hydrodynamic and Transport Characterization of the Baltic Sea 2000–2009. TRITA-LWR Report 2014:03. KTH Royal Institute of Technology, Stockholm, Sweden. https://balsysproject.files.wordpress.com/2015/08/hydrodynamic-and-transport-characterization-of-the-baltic-sea-2000-2009.pdf.

Dargahi, B., Kolluru, V., Cvetkovic, V., 2017. Multi-layered stratification in the Baltic Sea: insight from a modeling study with reference to environmental conditions. J. Mar. Sci. Eng. 5 (1), 2. https://doi.org/10.3390/jmse5010002.

de la Mare, W., Ellis, N., Pascual, R., Tickell, S., 2012. An empirical model of water quality for use in rapid management strategy evaluation in southeast Queensland, Australia. Mar. Pollut. Bull. 64 (4), 704–711. https://doi.org/10.1016/j.marpolbul.2012.01.039.

Destouni, G., Fischer, I., Prieto, C., 2017. Water quality and ecosystem management: data-driven reality check of effects in streams and lakes. Water Resour. Res. 53. https://doi.org/10.1002/2016WR019954.

Destouni, G., Hannerz, F., Prieto, C., Jarsjö, J., Shibuo, Y., 2008. Small unmonitored near-coastal catchment areas yielding large mass loading to the sea. Glob. Biogeochem. Cycles 22 (4). https://doi.org/10.1029/2008GB003287.

Destouni, G., Jaramillo, F., Prieto, C., 2013. Hydroclimatic shifts driven by human water use for food and energy production. Nat. Clim. Chang. 3 (3), 213. https://doi.org/10.1038/NCLIMATE1719.

Deutsch, B., Forster, S., Wilhelm, M., Dippner, J., Voss, M., 2010. Denitrification in sediments as a major nitrogen sink in the Baltic Sea: an extrapolation using sediment characteristics. Biogeosciences 7 (10), 3259–3271. https://doi.org/10.5194/bg-7-3259-2010.

Eilola, K., Gustafsson, B.G., Kuznetsov, I., Meier, H.E.M., Neumann, T., Savchuk, O.P., 2011. Evaluation of biogeochemical cycles in an ensemble of three state-of-the-art numerical models of the Baltic Sea. J. Mar. Syst. 88 (2), 267–284. https://doi.org/10.1016/j.jmarsys.2011.05.004.

Eilola, K., Meier, H.E.M., Almroth, E., 2009. On the dynamics of oxygen, phosphorus and cyanobacteria in the Baltic Sea; a model study. J. Mar. Syst. 75 (1-2), 163–184. https://doi.org/10.1016/j.jmarsys.2008.08.009.

Fennel, K., Hetland, R., Feng, Y., DiMarco, S., 2011. A coupled physical-biological model of the northern Gulf of Mexico shelf: model description, validation and analysis of phytoplankton variability. Biogeosciences 8 (7), 1881. https://doi.org/10.5194/bg-8-1881-2011.

Frisk, T., 1982. An oxygen model for Lake Haukivesi. Hydrobiologia 86 (1-2), 133–139. https://doi.org/10.1007/BF00005800.

Gillibrand, P.A., Inall, M.E., Portilla, E., Tett, P., 2013. A box model of the seasonal exchange and mixing in regions of restricted exchange: application to two contrasting Scottish inlets. Environ. Model. Softw. 43, 144–159. https://doi.org/10.1016/j.envsoft.2013.02.008.

Gogina, M., Zettler, M.L., 2010. Diversity and distribution of benthic macrofauna in the Baltic Sea: data inventory and its use for species distribution modelling and prediction. J. Sea Res. 64 (3), 313–321. https://doi.org/10.1016/j.seares.2010.04.005.

Gustafsson, B.G., Schenk, F., Blenckner, T., Eilola, K., Meier, H.E.M., Müller-Karulis, B., Neumann, T., Ruoho-Airola, T., Savchuk, O.P., Zorita, E., 2012. Reconstructing the development of Baltic Sea eutrophication 1850–2006. AMBIO 41 (6), 534–548. https://doi.org/10.1007/s13280-012-0318-x.

Hagy, J.D., Murrell, M.C., 2007. Susceptibility of a northern Gulf of Mexico estuary to hypoxia: an analysis using box models. Estuar. Coast. Shelf Sci. 74, 239–253. https://doi.org/10.1016/j.ecss.2007.04.013.

HELCOM, 2007. HELCOM Baltic Sea Action Plan. In: HELCOM Ministerial Meeting, Krakow, Poland, 15 November 2007, pp. 101.

HELCOM, 2009. Eutrophication in the Baltic Sea — an integrated thematic assessment of the effects of nutrient enrichment and eutrophication in the Baltic Sea region. In: Baltic Sea Environment Proceedings No. 115B, pp. 152.

HELCOM, 2010. Ecosystem health of the Baltic Sea 2003–2007: Helcom initial holistic assessment. In: Baltic Sea Environment Proceedings No. 122, pp. 63.

HELCOM, 2013a. Manual for Marine Monitoring in the COMBINE Programme of HELCOM. In: Helsinki Commission, Helsinki, Finland, pp. 406.

HELCOM, 2013b. Review of the Fifth Baltic Sea Pollution Load Compilation for the 2013 HELCOM Ministerial Meeting. In: Baltic Sea Environment Proceedings No. 141, pp. 54.

Jaramillo, F., Destouni, G., 2015. Local flow regulation and irrigation raise global human water consumption and footprint. Science 350 (6265), 1248–1251. https://doi.org/10.1126/science.aad1010.

Jilbert, T., Slomp, C.P., Gustafsson, B.G., Boer, W., 2011. Beyond the Fe-P-redox connection: preferential regeneration of phosphorus from organic matter as a key control on Baltic Sea nutrient cycles. Biogeosciences 8 (6), 1699–1720. https://doi.org/10.5194/bg-8-1699-2011.

Kideys, A.E., 2002. Fall and rise of the Black Sea ecosystem. Science 297 (5586), 1482–1484. https://doi.org/10.1126/science.1073002.

Kiirikki, M., Inkala, A., Kuosa, H., Pitkänen, H., Kuusisto, M., Sarkkula, J., 2001. Evaluating the effects of nutrient load reductions on the biomass of toxic nitrogen-fixing cyanobacteria in the Gulf of Finland, Baltic Sea. Boreal Environ. Res. 6, 131–146.

Kiirikki, M., Lehtoranta, J., Inkala, A., Pitkänen, H., Hietanen, S., Hall, P.O.J., Tengberg, A., Koponen, J., Sarkkula, J., 2006. A simple sediment process description suitable for 3D-ecosystem modelling — development and testing in the Gulf of Finland. J. Mar. Syst. 61, 55–66. https://doi.org/10.1016/j.jmarsys.2006.02.008.

Kuparinen, J., Leonardsson, K., Mattila, J., Wikner, J., 1996. Food web structure and function in the Gulf of Bothnia, the Baltic Sea. AMBIO 13–21.

Lam, D., Schertzer, W., Fraser, A., 1987. A post-audit analysis of the NWRI nine-box water quality model for Lake Erie. J. Great Lakes Res. 13 (4), 782–800. https://doi.org/10.1016/S0380-1330(87)71691-8.

Landelius, T., Josefsson, W., Persson, T., 2001. A System for Modelling Solar Radiation Parameters with Mesoscale Spatial Resolution. RMK No. 96. SMHI.

Larsson, U., Nyberg, S., Andreasson, K., Lindahl, O., Wikner, J., 2010. Phytoplankton production: measurements with problems. Havet 26–29 (in Swedish).

Le Pape, O., Menesguen, A., 1997. Hydrodynamic prevention of eutrophication in the Bay of Brest (France), a modelling approach. J. Mar. Syst. 12 (1-4), 171–186. https://doi.org/10.1016/S0924-7963(96)00096-6.

Lehtoranta, J., Ekholm, P., Pitkänen, H., 2009. Coastal eutrophication thresholds: a

matter of sediment microbial processes. AMBIO 38 (6), 303–308. https://doi.org/10.1579/09-A-656.1.
Leppäranta, M., Myrberg, K., 2009. Physical Oceanography of the Baltic Sea. Springer, pp. 378.
Li, K., Zhang, L., Li, Y., Zhang, L., Wang, X., 2015. A three-dimensional water quality model to evaluate the environmental capacity of nitrogen and phosphorus in Jiaozhou Bay, China. Mar. Pollut. Bull. 91 (1), 306–316. https://doi.org/10.1016/j.marpolbul.2014.11.020.
Liu, D., Keesing, J.K., He, P., Wang, Z., Shi, Y., Wang, Y., 2013. The world's largest macroalgal bloom in the Yellow Sea, China: formation and implications. Estuar. Coast. Shelf Sci. 129, 2–10. https://doi.org/10.1016/j.ecss.2013.05.021.
Lv, X., Liu, B., Yuan, D., Feng, H., Teo, F.-Y., 2016. Random walk method for modeling water exchange: an application to coastal zone environmental management. J. Hydro Environ. Res. 13, 66–75. https://doi.org/10.1016/j.jher.2015.07.001.
Martin, J., Burton, J., Eisma, D., 1981. River Inputs to Ocean Systems. United Nations Environment Programme.
Meier, H.E.M., Müller-Karulis, B., Andersson, H.C., Dieterich, C., Eilola, K., Gustafsson, B.G., Höglund, A., Hordoir, R., Kuznetsov, I., Neumann, T., et al., 2012. Impact of climate change on ecological quality indicators and biogeochemical fluxes in the Baltic Sea: a multi-model ensemble study. AMBIO 41 (6), 558–573. https://doi.org/10.1007/s13280-012-0320-3.
Neumann, T., 2000. Towards a 3D-ecosystem model of the Baltic Sea. J. Mar. Syst. 25, 405–419. https://doi.org/10.1016/S0924-7963(00)00030-0.
Newton, A., Icely, J., Cristina, S., Brito, A., Cardoso, A.C., Colijn, F., Riva, S.D., Gertz, F., Hansen, J.W., Holmer, M., Ivanova, K., Leppäkoski, E., Canu, D.M., Mocenni, C., Mudge, S., Murray, N., Pejrup, M., Razinkovas, A., Reizopoulou, S., Pérez-Ruzafa, A., Schernewski, G., Schubert, H., Carr, L., Solidoro, C., Viaroli, P.-L., Zaldvar, J.-M., 2014. An overview of ecological status, vulnerability and future perspectives of European large shallow, semi-enclosed coastal systems, lagoons and transitional waters. Estuar. Coast. Shelf Sci. 140, 95–122. https://doi.org/10.1016/j.ecss.2013.05.023.
Nixon, S.W., 1995. Coastal marine eutrophication: a definition, social causes, and future concerns. Ophelia 41 (1), 199–219. https://doi.org/10.1080/00785236.1995.10422044.
Pedersen, M., Borum, J., 1996. Nutrient control of algal growth in estuarine waters. Nutrient limitation and the importance of nitrogen requirements and nitrogen storage among phytoplankton and species of macroalgae. Mar. Ecol. Prog. Ser. 142, 261–272. https://doi.org/10.3354/meps142261.
Peuhkuri, T., 2002. Knowledge and interpretation in environmental conflict: fish farming and eutrophication in the Archipelago Sea, SW Finland. Landsc. Urban Plan. 61 (2-4), 157–168. https://doi.org/10.1016/S0169-2046(02)00110-X.
Redfield, A.C., 1958. The biological control of chemical factors in the environment. Am. Sci. 46 (3), 205–221.
Reissmann, J.H., Burchard, H., Feistel, R., Hagen, E., Lass, H.U., Mohrholz, V., Nausch, G., Umlauf, L., Wieczorek, G., 2009. Vertical mixing in the Baltic Sea and consequences for eutrophication — a review. Prog. Oceanogr. 82, 47–80. https://doi.org/10.1016/j.pocean.2007.10.004.
Salomon, J., Breton, M., 1991. Numerical study of the dispersive capacity of the Bay of Brest, France, towards dissolved substances. Environmental Hydraulics. Balkema, Rotterdam, pp. 459–464.
Savchuk, O.P., Gustafsson, B.G., Müller-Karulis, B., 2012. BALTSEM: A Marine Model for Decision Support Within the Baltic Sea Region. Technical Report Series, No. 7. Baltic Nest Institute.
Savchuk, O.P., Wulff, F., Hille, S., Humborg, C., Pollehne, F., 2008. The Baltic Sea a century ago — a reconstruction from model simulations, verified by observations. J. Mar. Syst. 74 (1-2), 485–494. https://doi.org/10.1016/j.jmarsys.2008.03.008.
Schiewer, U., 2008. The Baltic coastal zones. In: Ecology of Baltic Coastal Waters. Springer, pp. 23–33.
Sellner, K., Olson, M., Olli, K., 1996. Copepod interactions with toxic and non-toxic cyanobacteria from the Gulf of Finland. Phycologia 35, 177–182.
Smith, V.H., Schindler, D.W., 2009. Eutrophication science: where do we go from here? Trends Ecol. Evol. 24, 201–207. https://doi.org/10.1016/j.tree.2008.11.009.
Soetaert, K., Middelburg, J.J., Herman, P.M., Buis, K., 2000. On the coupling of benthic and pelagic biogeochemical models. Earth Sci. Rev. 51 (1-4), 173–201. https://doi.org/10.1016/S0012-8252(00)00004-0.
Stigebrandt, A., 2018, Feb, Feb. On the response of the Baltic Proper to changes of the total phosphorus supply. Ambio 47 (1), 31–44. https://doi.org/10.1007/s13280-017-0933-7.
Stigebrandt, A., Wulff, F., 1987. A model for the dynamics of nutrients and oxygen in the Baltic Proper. J. Mar. Res. 45 (3), 729–759. https://doi.org/10.1357/002224087788326812.
Taylor, K.E., 2001. Summarizing multiple aspects of model performance in a single diagram. J. Geophys. Res.-Atmos. 106 (D7), 7183–7192. https://doi.org/10.1029/2000JD900719.
The International Council for the Exploration of the Sea, 2015. ICES Dataset on Ocean Hydrography. Copenhagen.
Törnqvist, R., Jarsjö, J., Thorslund, J., Rao, P.S.C., Basu, N.B., Destouni, G., 2015. Mechanisms of basin-scale nitrogen load reductions under intensified irrigated agriculture. PloS one 10 (3), e0120015. https://doi.org/10.1371/journal.pone.0120015.
Tyrrell, T., 1999. The relative influences of nitrogen and phosphorus on oceanic primary production. Nature 400, 525–531. https://doi.org/10.1038/22941.
Vahtera, E., Conley, D.J., Gustafsson, B.G., Kuosa, H., Pitkänen, H., Savchuk, O.P., Tamminen, T., Viitasalo, M., Voss, M., Wasmund, N., Wulff, F., 2007. Internal ecosystem feedbacks enhance nitrogen-fixing cyanobacteria blooms and complicate management in the Baltic Sea. AMBIO 36 (2/3), 186–194. https://doi.org/10.1579/0044-7447(2007)36[186:IEFENC]2.0.CO;2.
Voss, M., Dippner, J.W., Humborg, C., Hürdler, J., Korth, F., Neumann, T., Schernewski, G., Venohr, M., 2011. History and scenarios of future development of Baltic Sea eutrophication. Estuar. Coast. Shelf Sci. 92 (3), 307–322. https://doi.org/10.1016/j.ecss.2010.12.037.
Wasmund, N., Andrushaitis, A., Łysiak-Pastuszak, E., Müller-Karulis, B., Nausch, G., Neumann, T., Ojaveer, H., Olenina, I., Postel, L., Witek, Z., 2001. Trophic status of the south-eastern Baltic Sea: a comparison of coastal and open areas. Estuar. Coast. Shelf Sci. 53, 849–864. https://doi.org/10.1006/ecss.2001.0828.
Wulff, F., Stigebrandt, A., 1989. A time-dependent budget model for nutrients in the Baltic Sea. Glob. Biogeochem. Cycles 3 (1), 63–78. https://doi.org/10.1029/GB003i001p00063.