BALTSEM - a marine model for decision support within the Baltic Sea Region

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Baltic Nest Institute

The Baltic Nest Institute

The Baltic Nest Institute host the Nest model, a decision support system aimed at facilitating adaptive management of environmental concern in the Baltic Sea.

Nest can be used to calculate required actions needed to attain politically agreed targets for the Baltic Sea ecosystem. By modeling the entire drainage area, Nest is a novel tool for implementing the ecosystem approach in a large marine ecosystem. The main focus of the model is on eutrophication and the flows of nutrients from land to sea.

Reducing the nutrient input to the sea and thus decreasing the negative environmental impacts is a politically prioritized area of international cooperation. Baltic Nest Institute can contribute to this process by formulating policies that are fair, transparent and cost-efficient. The main target group for the Nest Decision Support System is HELCOM and regional water directors in the riparian countries.

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1 Introduction

A longstanding recognition of eutrophication as the most common threat to the entire Baltic Sea (see *e.g.* Voipio, 1981; Larsson *et al.*, 1985; HELCOM, 1993, Wulff *et al.*, 2001c) has led to the international agreement on nutrient load reductions within the Baltic Sea Action Plan (BSAP, 2007; Backer *et al.* 2010). The nutrient load reductions were based on quantitative estimates of the "maximum allowed nutrient inputs" evaluated with a help of the decision support system (DSS) Baltic Nest (http://nest.su.se) developed within the MARE (Marine Research on Eutrophication) program (Wulff *et al.*, 2001a; Johansson *et al.* 2007). As demonstrated by a comparison to available data derived from observations, the marine biogeochemical model SANBALTS (Simple As Necessary Baltic Long-Term large-Scale) used in this evaluation is capable to realistically simulate both contemporary and pre-industrial trophic states of the Baltic Sea (Savchuk and Wulff, 2007, 2009; Savchuk *et al.* 2008). A key to successful performance of SANBALTS lays in accounting for major sources and sinks that determine the size of internal nutrient pools and, thus, govern the large scale Baltic Sea eutrophication. Particularly, the most important phenomena that have to be reproduced by eutrophication models are a) spatial gradients of environmental conditions and limiting nutrients, b) interconnectivity of the major Baltic Sea basins, c) sporadic ventilation of the hypoxia prone deep-water layers with saltwater inflows, d) redox alterations of the coupled nitrogen and phosphorus biogeochemical cycles, and d) nitrogen fixation by cyanobacteria.

At the same time, both a rather high aggregation of ecosystem variables (organic and inorganic forms of nutrients without explicit description of biota) and their correspondent spatial-temporal averaging (annual within homogeneous basins) implemented in SANBALTS make this model not appropriate enough for further revision and elaboration of the BSAP. Because such revision has also to take into consideration indicators required by the Marine Strategy Framework Directive (MSFD) of the European Union (Anonymous, 2010; Ferreira *et al.* 2011) and characterized by higher spatial and temporal resolution, *e.g.* basin-wise winter surface nutrient concentrations and summer phytoplankton biomasses, and because of a necessity to factor in the possible effects of climate fluctuations, the appropriate model must simulate changes in ecosystem seasonal dynamics occurring over tens of years in response to both nutrient load reductions and climate changes.

In principle, the continuing development of computing resources has made it feasible to implement for such purposes three-dimensional coupled physical-biogeochemical models with a relatively high resolution (*e.g.,* Neumann and Schernewski, 2008; Almroth and Skogen, 2010; Neumann, 2010; Eilola *et al.*, 2011a; b; Meier *et al.*, 2011a; 2012). However, with such models a simulation of the entire Baltic Sea over several decades still requires many days of computation even at supercomputer centers, which greatly hinders numerical experimentation needed for both model calibration and sensitivity analysis, including scenario responses. Therefore, there is a need for the model that is both reliable and convenient enough to be used for the revision of BSAP and implementation of MSFD, as well as for similar managerial tasks within an ecosystem approach. To serve this need, the

model should be computationally fast for allowing multiple numerical runs necessary for finding and testing suitable distributions of the water-protection measures. Furthermore, for a building of credibility necessary in the national deliberations and international negotiations it should also be publicly accessible through the decision support system Nest allowing to any interested party running hindcast and scenario experiments as well as visualize its results. For these purposes, we present here the latest developments of the BAltic sea Long-Term large Scale Eutrophication Model (BALTSEM), which captures the main features of the Baltic Sea eutrophication, and now serves as a next generation marine model in the Baltic Nest system (http://nest.su.se). These results as well as hindcast for 1850-2006 and future scenarios can be reproduced and analyzed on-line. Since BALTSEM performance at long-term scales has already been presented by Eilola *et al.* (2011a) and Gustafsson *et al.* (2012), this paper is especially focused on a seasonal scale.

2 Methods and data

2.1 The model

The principal foundations of BALTSEM were laid down in the Baltic Sea System Study project (BASYS, Gustafsson, 1999; Savchuk 1999), where biogeochemical models, previously developed for the Baltic Proper (Stigebrandt and Wulff, 1987; Savchuk and Wulff 1996; 2001), were modified and combined with a new physical model (Gustafsson, 2000a; 2000b; 2003), and ultimately extended over the entire Baltic Sea. The specifics of BALTSEM are that it divides the Baltic Sea into 13 interconnected marine basins (Fig. 1) each of which is assumed horizontally homogeneous but is described with a high vertical resolution. The transports of state variables both within and between these basins are simulated by hydrodynamical module, and translocations of nutrients between ecosystem variables are described by biogeochemical module. Although the mathematical formulations of both modules have been presented in detail in previous publications, here we briefly repeat and explain all the essential features for the sake of wider audience involved into decision-making and adaptive management processes.

2.1.1 Hydrodynamical module

The hydrodynamical module is described at length by Gustafsson (2003), however, at that time the model did not sub-divide the Gulf of Finland and Gulf of Riga from the Baltic proper. The water exchange between 13 basins is dynamically regulated at horizontal contractions and/or sills separating the basins. The parameterizations of flows between basins and through open boundary in the northern Kattegat differ due to different dynamic characteristics. The flow dynamics are forced by wind, varying sea level (Carlsson, 1998) and density differences between the basins and are controlled by frictional resistance and dynamical flow contraction due to Bernoulli and Coriolis effects (Stigebrandt, 1990; Gustafsson, 2000a; 2003). The vertical stratification is resolved by a variable number of layers where the layers are created by inflows of waters with differing density, while a total amount of layers is kept below a prescribed maximum by fusion (Gustafsson, 2000a). Vertical mixing is described by a mixed layer model for the Baltic Sea (Stigebrandt, 1985) and a deep water mixing parameterization where the coefficient of vertical diffusion varies

with the stratification (Stigebrandt, 1987) and mixing wind (Stigebrandt and Aure, 1989; Axell, 1998). The sea-ice model follows the model of the Arctic sea ice by Björk (1992; 1997), with dynamics adapted to the Baltic Sea (Nohr *et al.*, 2009). Heating/cooling and evaporation at the sea surface is calculated using bulk formulas (Björk, 1997; Gustafsson, 2003). The deep-water inflows are described by a mixing sub-model of dense gravity currents following Stigebrandt (1987). At the open boundary in the Kattegat the boundary conditions in form of concentration profiles are implemented.
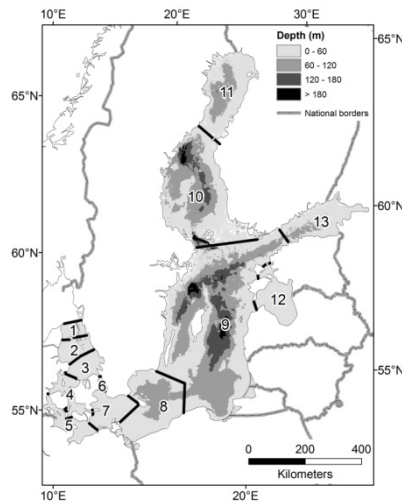

Fig. 1. The Baltic Sea partitioning into thirteen BALTSEM basins.
1 – Northern Kattegat (NK), 2 – Central Kattegat (CK), 3 – Southern Kattegat (SK),
4 - Samsø Belt (SB), 5- Fehmarn Belt (FB), 6 – Öresund (OS),
7 – Arkona basin (AR), 8 – Bornholm basin (BN), 9 – Gotland Sea (GS),
10 – Bothnian Sea (BS), 11 – Bothnian Bay (BB), 12 – Gulf of Riga (GR),
13 – Gulf of Finland (GF); hereafter Kattegat (KT) comprises NK, CK, and SK,
Danish Straits – SB, FB, and OS, Baltic Proper – AR, BN, and GS.
Digit "9" also indicates an approximate location of the monitoring station BY-15

2.1.2 Biogeochemical module

All basic principles used in BALTSEM's biogeochemical module mostly follow those developed in the marine ecosystem modelling practice over decades (*e.g.* Riley, 1946; Patten, 1968; Kremer and Nixon, 1978; Nihoul, 1998; Blackford *et al.* 2010; St. John *et al.* 2010). The exact specific formulations are presented in full mathematical detail with relevant references by Savchuk and Wulff (1996) and Savchuk (2002). Here, we give a qualitative description of major rationales, which might be useful for a proper interpretation of simulations, and introduce a few modifications required by the expansion of the model, initially developed and calibrated for the Baltic Proper and Gulf of Riga, to the north-east over the Gulfs of Bothnia and Finland, and to the west over the Baltic Sea entrance area.

Within every of the thirteen model basins the internal nutrient dynamics are driven by biogeochemical processes and interactions in the coupled pelagic and benthic systems (Fig. 2). The pelagic system is represented by three phytoplankton functional groups (diatoms,
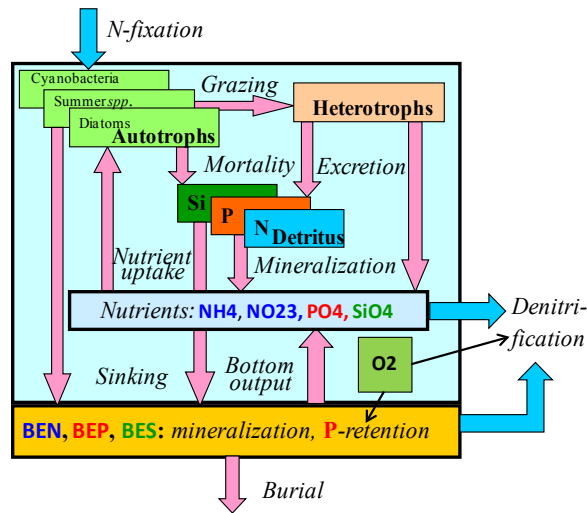
Fig. 2 Generalized scheme of the main biogeochemical fluxes between state variables

cyanobacteria, and others), heterotrophs, detritus nutrients (nitrogen, phosphorus, and silica), inorganic nutrients (ammonium, nitrate, phosphate, and silicate), and dissolved oxygen. By definition, the "cyanobacteria" state variable represents the entire cyanobacterial community, that is, comprises not only the most conspicuous diazotrophic *Nodularia* and *Aphanizomenon* spp., but also the smaller cyanobacteria that constitute a large proportion of cyanobacterial biomass and are responsible for a significant share of their primary production (*e.g.* Stal *et al.*, 2003). This share may be supported either by direct nitrogen fixation (Wasmund *et al.*, 2001; Farnelid *et al.*, 2009) or by fast utilization of nitrogen fixed by larger diazotrophs (Ohlendink *et al.*, 2000, 2007; Ploug *et al.* 2010). Heterotrophs represent the entire pelagic community of phytoplankton and detritus consumers, including both micro- and mesozooplankton. In contrast to some other Baltic models (*e.g.* Eilola *et al.* 2009; Neumann, 2010), the "splitting" of detritus into individual nutrient variables decouples nutrient cycling from the Redfield ratio and allows us, for example, to account for different stoichiometric composition of phytoplankton and zooplankton, to simulate preferential mineralization of one nutrient over another, and requires no "Redfield ratio" adjustments of the external nutrient loads. Following the convenient Baltic tradition (Fonselius, 1969) hydrogen sulfide is considered as negative oxygen: 1 mL of H_2S L^{-1} = -2 mL O_2 L^{-1}. Three sediment state variables are formulated as pools of bioavailable nitrogen, phosphorus, and silica in the active top layer of sediments. Such vertically integrated bulk parameterization is considered a best compromise between computational demand and attained accuracy for large-scale modeling (Soetaert *et al.*, 2000).

Filtration rate, determining food consumption by heterotrophs, depends on both water temperature and availability of food consisting of both autotrophs and detrital suspended particles. A part of the consumed food is assimilated, while unassimilated particles are added to the detritus pool. The heterotrophs' biomass decreases due to mortality and excretion. To mimic the top-down control by higher trophic levels, the mortality of heterotrophs is density-dependent. The temperature-dependent excretion of ammonium and phosphate by the heterotrophs is used for coupling and stoichiometric adjustment of the nitrogen and

phosphorus cycles. This parameterization accounts for the lower and variable N: P ratio of the ingested food compared to that of consumers and results in faster recycling of phosphorus compared to nitrogen.

Light and concentrations of inorganic nutrients control the temperature-dependent growth rate of all phytoplankton groups according to Liebig's "minimum law" concept. Photo-inhibition at high light intensities and a fast adaptation at low levels are included into the parameterization of the light effect. Limiting effects of nutrient concentrations are described by saturation curves (equivalent to the Michaelis-Menten, Monod, and Langmuir equations); including also the ammonium-induced inhibition of nitrate uptake. The mortality rates and sinking velocities of all autotrophs are temperature dependent and inversely related to the same limiting functions that are used to describe their growth rate. Therefore, these losses increase when the growth limitation intensifies. At a water temperature higher than 14 C° and an ambient inorganic N:P molar ratio lower than the Redfield ratio of 16, the "cyanobacteria" state variable is enabled to fix molecular nitrogen. The nitrogen fixation rate is then dependent on temperature, ambient N:P ratio, and concentration of phosphate. Thus, in BALTSEM cyanobacteria have negative buoyancy and are capable of utilizing dissolved inorganic nitrogen compounds (see *e.g.* LaRoche and Breitbarth, 2005; Kangro *et al.* 2007; Vintila and El-Shehawy, 2010), in contrast to some other models (Tyrell, 1999; Fennel *et al.,* 2002; Neumann and Schernewski, 2008;).

The detrital nitrogen, phosphorus, and silica concentrations increase due to plankton mortality and are decreased by consumption of heterotrophs as well as by temperature-dependent mineralization and sedimentation. Assuming preferential nutrient regeneration, the specific phosphorus mineralization rate is set 50% higher than that of nitrogen, which, in turn is twice of the dissolution rate of biogenic silica. The sinking velocity of all detritus variables is proportional to the variable ratio between simulated detritus silica and nitrogen, to mimic a faster sedimentation of "diatom remnants", compared to other sources of detritus.

Mineralization of detritus and excretion by heterotrophs increase ammonium and phosphate concentrations. Ammonium is nitrified to nitrate under aerobic conditions. At low oxygen concentration, nitrate is denitrified to molecular nitrogen due to all the processes that lead to transformation of combined nitrogen into gaseous end products (Devol, 2008). This pelagic denitrification starts at a "threshold" oxygen concentration and its rate depends on temperature and nitrate concentration.

Oxygen is produced by autotrophs and is subject to exchange with the atmosphere according to the parameterization described below, in Sect. 2.1.3. Oxygen consumption is determined by respiration of heterotrophs, mineralization of detritus and sediment organic matter, and nitrification. The anaerobic decomposition of organic matter in the anoxic layers produces hydrogen sulfide. Under hypoxic conditions in the vicinity to redoxcline, oxygen utilization is doubled, mimicking consumption by reduced forms of manganese, iron, and sulfur diffusing upwards from the anaerobic zone (Morse and Eldridge, 2007; Yakushev *et al.,* 2007; Kuznetsov, 2008). At the same time, an oxygen equivalent of nitrate denitrified for the

oxidation of organic matter in the pelagic and benthic systems is returned to the dissolved oxygen pool.

Sediment pools of nutrients are increased by sedimentation of autotrophs and detritus, and are decreased due to mineralization and burial. Mineralization fluxes are split into several pathways, the proportions depending on oxygen concentration in the overlying water. In the presence of oxygen, a fraction of nitrate produced by mineralization and nitrification is released into the overlying water, while the remaining fraction is denitrified. Under anaerobic conditions the entire mineralized nitrogen is released as ammonium. Likewise, under aerobic conditions one part of phosphate produced by mineralization is retained (sequestered) in the sediments, mimicking adsorption and complexation. The remaining fraction is released into the overlying water. Under anaerobic conditions no phosphorus retention occurs and even some of the previously sequestered phosphorus is released into the water column. Concurrently with oxygen conditions, the phosphorus retention capability of the sediments also inversely depends on simulated salinity, which is considered a proxy of both the sulfate concentration (*e.g.* Blomquist *et al.*, 2004) and the contribution of iron- and humus-enriched fresh waters (*e.g.* Golterman, 2004), especially those draining the wetlands, forests, and rocks of the north-eastern watersheds. All mineralized silica is released into the water. Finally, the sediment nutrients are buried with a constant rate.

In this large scale model with rather aggregated biotic and sediment variables, the water temperature dependencies are used for representation of seasonal changes in ecosystem structure and functioning (*e.g.* Hällfors *et al.*, 1981; Hagström *et al.*, 2001; Wasmund and Siegel, 2008). In contrast to the growth rates of "diatoms" and "cyanobacteria" with a temperature coefficient Q_{10} of 1.9, "others" autotrophs are assigned a higher Q_{10} of 3.3, to reflect the seasonal succession from spring dinoflagellates to a diverse summer community of small, fast growing species. The summer nutrient recycling is performed by a developed heterotrophic community, comprising a wide spectrum of organisms from bacteria to zooplankton. In BALTSEM, a fast development of such community is simulated with a sharply increasing filtration rate ($Q_{10} = 12$) and decreasing net growth efficiency ($Q_{10} = 5.5$). To mimic the higher lability of freshly deposited organic matter in summer at shallower bottoms, the sediment mineralization rates are assumed dependent on the square of water temperature.

2.1.3 Coupling of transport and transformation processes

Detritus and phytoplankton are sinking with a vertically varying velocity dependent on the local environmental conditions, as described above. A special routine is developed to cope with high sinking speeds and thin layers based on a Lagrangian approach (Gustafsson, 2003). In principle, the particles from a layer are sinking through the layers below until either the time of the time-step is used up or the particles have hit the sediment surface.

The vertical distribution of sediments is described by a fixed grid of 1 m resolution. The area of bottoms within that vertical distance then gives the area of each segment of sediment surface. However, since the water column is divided into layers of variable thickness,

interaction between the water column and the sediment needs to be done on each coinciding interval of specific layers and sediment surfaces (see Gustafsson, 2003). The areas of these surfaces are computed assuming a linear change of bottom area with depth within every sediment surface segment.

In the shallow Baltic Sea, a significant spatial redistribution of sediment nutrients occurs due to the erosion and resuspension processes (*e.g.* Struck *et al.*, 2004; Hille, 2005; Danielsson *et al.*, 2007). Description of bottom erosion followed by near bottom lateral transport and eventual settling of suspended nutrients seems to be rather straightforward in three-dimensional models (*e.g.* Almroth-Rosell *et al.*, 2011 and references therein). In BALTSEM, the sediment domain in every basin can be visualised as a terraced inner surface of inverted cone, with a 1 m vertical distance between terraces and their areas determined by the hypsographic curves. In such setting, the conventional description of resuspension is senseless by definition both because there are no horizontal intra-basin currents necessary for a subsequent near bottom transportation of resuspended particles, and because the particles, once lifted up from the bottom, must be instantly and evenly dispersed within corresponding water layer extending over the entire basin. Instead, the resulting downward movement of sediment nutrients is parameterized with a resuspension rate exponentially decreasing with depth. Nutrients lifted up from each sediment terrace are then immediately transported into the next terrace, simultaneously for all terraces and mimicking for faster transports over steeper bottom slopes.

Nutrients released from and oxygen consumed by the sediments are accumulated for each water layer in proportion to the sediment surfaces that the layer interfaces to.

Approximation of the Baltic Sea with a chain of rather spacious but horizontally homogeneous water columns results in the instant spreading of the changes caused by inter-basin transports over the entire basins. Particularly undesirable this effect is in the case of oxygen transport with the major saltwater inflows. In the model, the instant arrival of oxygen-enriched waters into the deeper layers results in an overestimated oxygen concentration with associated biogeochemical consequences (Savchuk and Wulff, 1996; 2001). In reality, it takes two to five months for saline waters to arrive into the Gotland Deep from the Danish Straits (Matthäus, 2008), during which time the propagating water loses oxygen due to its consumption both within the water column and by the sediments. In parameterization of the mixing in dense gravity currents (Stigebrandt, 1987), the velocity and thickness of currents are computed. Together with provided width of the currents and prescribed rates of pelagic and benthic oxygen consumption, these parameters are used in the present version of BALTSEM to compute reduction of oxygen concentrations during propagation in the dense gravity currents.

Oxygen flux through the sea surface is computed using a wind and temperature dependent piston velocity (Liss and Merlivat, 1986) and assuming a 2.5% oversaturation due to effects of bubbles (Stigebrandt, 1991). Oxygen exchange through the sea surface is only taking place

for the open water fraction of the basin, not covered by ice. Details are given by Gustafsson (2003).

The model takes into account conservation of pelagic state variables in snow and sea ice. Thus, all constituents are captured into ice brine pockets in proportion to salt. Additional nutrients are stored in primarily snow but also in ice because of atmospheric deposition, which leads to a pulse of nutrients in the spring melt water.

Temporal and spatial changes of the photosynthetically active radiation (PAR) penetrated under the sea surface are described by the Beer's law with a light extinction coefficient (k_d, m^{-1}) dependent on both the background and dynamical attenuation. The latter is calculated from the simulated distribution of particulate plankton and detritus variables. In the brackish Baltic Sea, the background attenuation is determined not only by suspended inorganic matter but also by characteristically high concentration of colored dissolved organic matter (CDOM) that is to a large extent introduced with the freshwater runoff (Bowers and Brett, 2008) and displays quite pronounced gradient from the norther and eastern gulfs to the entrance area (*e.g.* Poryvkina *et al.*, 1992; Pettersson *et al.*, 1997; Hagström *et al.*, 2001). In BALTSEM, this gradient is reproduced with the background attenuation dependent on simulated salinity in such a way that in January, with a negligible effect of the modeled particulates, k_d decreases from 0.33 in the Bothnian Bay to 0.22 in the Gotland Sea to 0.16 in the Central Kattegat. Assuming the relationship between Secchi depth (scd) and extinction coefficient in a form of scd = $1.7/k_d$ (*e.g.* Raymont, 1980; Kratzer *et al.*, 2003), the water transparency increases from 5.2 m to 7.7 m to 10.5 m, respectively.

2.2 Initial and boundary conditions

2.2.1 Initial conditions

Vertical distributions of hydrographic variables and inorganic nutrients were extracted from the Baltic Environmental Database (BED) with the SwingStations tool (Sokolov and Wulff, 1999) as horizontal averages within the model basins. For the basins with sufficient data coverage, the averaging was made over January-March, 1970, while for the gulfs their winter vertical structure was reconstructed from measurements available for the mid 1970s and extrapolated backwards to 1970 according to the results of linear trend analysis (HELCOM, 1996). Low and vertically homogeneous values were prescribed for detritus variables (1 mg N m^{-3}, 0.1 mg P m^{-3}, and 1.0 mg Si m^{-3}), autotrophs (0.0001 mg N m^{-3} each group), and heterotrophs (1 mg N m^{-3}).

The prescription of initial conditions in the benthic system is more problematic. The depth distributions of model sediment variables must be given as areal concentrations (g N (P, Si) m^{-2}) , horizontally averaged within every basin at each depth step over a mosaic of bottom types and sediment conditions occurring within this sediment "strip". The typical levels of such concentrations can be estimated from results of several studies (Carman and Cederwall, 2001; Jansen *et al.*, 2003; Conley *et al.*, 2008). Unfortunately, the trend analysis in the dated sediment cores (see *e.g.* Emeis *et al.*, 2000; Christiansen *et al.*, 2002; Kotilainen *et al.*, 2002;

Hille, 2005; Dähnke *et al.*, 2008) covers mostly the accumulation bottoms, i.e. only 30-40% of the total sediment area and its results are neither conclusive nor resolved enough for a consistent reconstruction of sediment nutrient pools in the narrow time window at the turn of the 1960s. Therefore, we have used two approaches resulted in quite different initial sediment nutrient pools. In the first one, BALTSEM was first run over 1970-2006 from some conventional initial conditions and the final sediment distribution was prescribed as new initial conditions. The sediment dynamics emerged in a subsequent simulation is presented and discussed by Eilola *et al.* (2011a). In the present study, we picked the sediment distributions up from the long-term hindcast simulation over 1850-2006 (Gustafsson *et al.*, 2012), and consequences of such a choice are presented in this paper.

2.2.2 Hydrophysical forcing

The meteorological forcing originates from a dynamic downscaling of the ERA40 reanalysis with the Rossby Centre Atmospheric model (RCA) (see Meier *et al.*, 2011b). The meteorological forcing is given with 3h resolution. In addition, observed sea levels from Hornbaek and Viken are combined into a daily average time-series that force exchange through the Entrance area. Monthly river discharge time-series to each basin were obtained primarily from SMHI (see Gustafsson *et al.*, 2012). Solar radiation is computed (Gustafsson, 2003) using cloudiness from the atmospheric forcing data set.

2.2.3 Nutrient inputs

Reconstruction of the nutrient land loads (monitored and non-monitored rivers, diffusive and direct point sources from coastal areas) was based on the data both found in BED and provided by HELCOM, and is described in detail by Wulff *et al.* (2009) and Savchuk *et al.* (2012). For silicate, the reconstruction over the 2000s was made from the regressions with the freshwater discharge, estimated from 1970-2000 monthly time series. Organic fractions were calculated as a difference between total and inorganic concentrations of nutrients. Finally, only 30% of organic nitrogen in the riverine loads has been assumed bioavailable (Seitzinger *et al.*, 2002; Stepanauskas *et al.*, 2002; Wiegner *et al.*, 2006; Ptacnik *et al.*, 2010). Organic content of both TN and TP inputs from the point sources was assumed 50% and completely bioavailable.

Atmospheric deposition of inorganic nitrogen was reconstructed from estimates obtained by Granat (2001) and from simulations made by the Cooperative Programme for Monitoring and Evaluation of the Long-range Transmissions of Air Pollutants in Europe (EMEP, see *e.g.* Bartnicki *et al.*, 2008) and available through "EMEP data" module of the DSS Baltic Nest (Savchuk *et al.*, 2012). Additionally, the deposition of organic nitrogen was assumed to be 20% of DIN wet deposition, or 12-13% of the total bioavailable nitrogen (*e.g.* Cornell *et al.*, 2003; Rahm *et al.*, 2005; Rolff *et al.*, 2008). The phosphorus deposition data are rather fragmentary (Mahowald *et al.*, 2008; Rolff *et al.* 2008; Savchuk, 2005; 2009; and references therein) and, for the sake of simplicity, a 15 kg P km^{-2} yr^{-1} were assumed invariably and evenly deposited over the entire Baltic Sea.
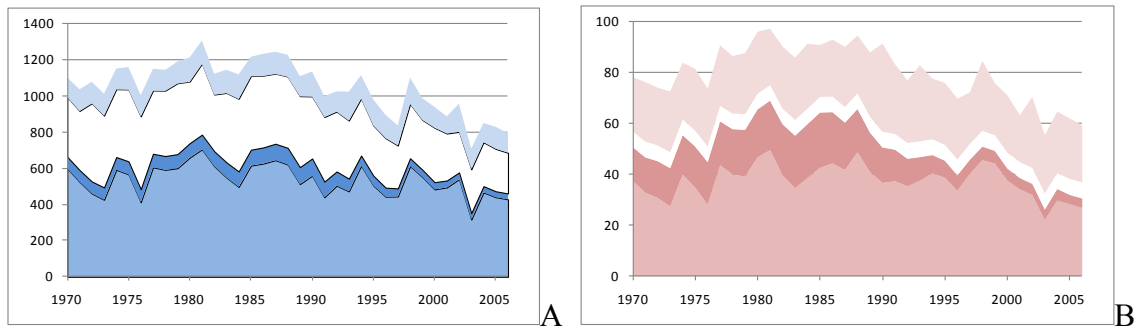
Fig. 3 External inputs (10^3 tonnes yr^{-1}) of bioavailable nitrogen (A) and phosphorus (B) to the entire Baltic Sea. The sources are (from bottom to top): riverine loads, direct point sources, atmospheric deposition, and import from the Skagerrak

The described reconstruction of external nutrient inputs yielded rather distinctive long-term dynamics illustrated here by the integral fluxes (Fig. 3), while basin-wise averages can be found in the nutrient budgets (see Tables 7 and 8 below). Relative contribution of different sources follows well-known patterns. The most important sources for both nitrogen and phosphorus are the land loads that supply about half of the total inputs. The significance of other sources differs between nutrients: the point sources, atmosphere, and the Skagerrak on average supply respectively 6, 31, and 12% of the bioavailable nitrogen input, while contributions of these sources to the phosphorus input are 15, 8, and 30%, respectively. The pronounced decrease of inputs from the 1980s towards the 2000s is caused not only by a naturally-driven decline in freshwater discharges but also by the reduction of nitrogen atmospheric emissions and phosphorus removal at the waste water treatment plants.

At the open boundary to the Skagerrak observed profiles of nutrients and hydrographic variables from the innermost stations of the monitoring section between Torungen, Norway and Hirtshals, Denmark are used. This section is monitored approximately every second week, but interpolated to daily resolutions. In case of long gaps, the average annual cycle is used instead of linear interpolation.

2.3 Model-data comparison

Despite ever increasing demand in the quantitative model validation (*e.g.* Arhonditsis and Brett, 2004; Lynch *et al.*, 2009), particularly important for the models aimed at a decision support with expensive consequences (*e.g.* Fitzpatrick, 2009; Stow *et al.*, 2009), there are surprisingly few commonly accepted methods and procedures for quantification of model performance, while even the corresponding theory and terminology are full of confusions and disagreements (*e.g.* Oreskes *et al.*, 1994; Arhonditsis *et al.*, 2006; Lynch *et al.*, 2009; Stow *et al.*, 2009). One common misconception, especially outside of a narrow circle of modelers is that "data are truth", whereas already under-sampling and imperfect methods of observations alone generate unknown truth-data errors (Lynch *et al.*, 2009). Moreover, "we do not model what we measure, and we do not measure what we model" (Franks, 2009), intentionally simplifying reality by aggregation of natural prototypes, which is at best made with an accounting for a chosen window of spatial-temporal domain. Therefore, before any model-data comparison, the raw measurements should be converted into "data", *i.e.* be pre-

processed by aggregation and necessary averaging, thus securing as close resemblance to model variables as possible.

Evaluation of BALTSEM capability to realistically reproduce the major mechanisms of the Baltic Sea eutrophication is further impeded by the following. The simulation represents continuous dynamics of variables assumed homogeneous (averaged) over thousands of square kilometres, whereas observational statistics are based on sparse and infrequent sampling from natural fields subject to multi-scale spatial and temporal variability, from diurnal rhythms and synoptic patchiness to interannual variations of seasonal cycles. Such differences are most pronounced for the Gotland Sea basin, considered horizontally homogeneous in BALTSEM settings but in reality covering large area extending from the Gdansk Deep to the Northern Baltic Proper (cf. Fig. 1).

2.3.1 Data sources and preparation

All the original oceanographic observations were taken from the BED and other major data sources around the Baltic Sea such as IOW (Germany), NERI (Denmark), SYKE-FMI (Finland), and SHARK (SMHI, Sweden) databases. The full list of the data contributors can be found at http://nest.su.se/bed/acknowle.shtml. This information has been accessed and pre-processed either directly (*e.g.* Gustafsson and Rodriguez Medina, 2011) or with the Data Assimilation System (DAS) and "Riverine and marine data" module of the Baltic Nest system.

Particularly, time-depth contour plots for specified time and depth intervals at chosen locations as well as some seasonal statistics were prepared with the Baltic Nest; basin-wide average nutrient pools were computed from three-dimensional gridded fields reconstructed with DAS (Sokolov *et al.*, 1997). In order to somewhat reconcile infrequent and sparse observations with simulated dynamics representing large basins assumed horizontally homogeneous, the basin-wide monthly time-series were prepared from available long-term observations in the following way. All the measurements found in monthly intervals over 1970-2006 for all frequently sampled water layers within every BALTSEM basin, i.e. usually at 5 m intervals for the top 20 m of the water column and 10 – 25 m intervals for the deeper parts of basins, were pooled together and averaged. Coastal measurements, defined as being sampled within 12 nautical miles from the shore, were excluded for all basins except the three Danish Straits basins, where the 12 nm coastal strip covers almost the entire basins. In the Bothnian Sea, the Understen-Märket trench, which provides the deepest connection between Baltic Proper and Bothnian Sea (about 90 m, Hietala *et al.*, 2007), was excluded from the compilation, since conditions in this transition area are not representative for the Bothnian Sea as a whole. Similarly, measurements from several isolated depressions in the northern part of the Gotland Sea (north of 59.35 N) were excluded as they often display their own dynamics, asynchronous to that in the larger basin's domain.

In addition to the imminent uncertainty of comparison between field observations and BALTSEM simulations of abiotic variables, already mentioned above, the quantitative comparison of simulated plankton dynamics to available data is further hampered by

uncertainties of conversion between measured quantities and simulated variables, which are expressed in nitrogen units. The ratios of nitrogen density in living cells to their carbon or chlorophyll density vary both between and within species in dependence on ambient environment and the recent history of the populations (*e.g.* Menden-Deuer and Lessard, 2000; Geider and La Roche, 2002; Wasmund and Siegel, 2008; Finkel *et al.*, 2010). Therefore, we consider an elaborate search for the "precise" species- and site-specific coefficients futile and restrict ourselves to rather simple and straightforward conversions suitable for rough, order of magnitude comparisons. Namely, we assume a C:N weight ratio in plankton of 6, a carbon to wet weight (C:ww) ratio of 0.04 and 0.11 in diatoms and other protist plankton, respectively (Menden-Deuer and Lessard, 2000), and a C:Chl *a* ratio of 30 in spring and 60 in summer or during generally unfavourable conditions (*e.g.* Wasmund and Siegel, 2008). Similarly, the weight ratio C:N = 6 is used to convert some biogeochemical fluxes from simulated nitrogen units into more commonly used carbon units.

2.3.2 Model performance measures

Taylor diagrams (Taylor, 2001) were used to assess how well the model matches the seasonal pattern of nutrient concentrations in the surface layer of each basin. Taylor diagrams are polar plots where the angular coordinate is a measure of the correlation coefficient R between model results and observations, while the radial distance to the origin displays how well the model represents the variability of the field data. We have normalized the standard deviation of the model results by the standard deviation of the observations, so that a radial distance equal to one means that the variability of the modelled and observed fields are equal, whereas a radial distance < 1 (or > 1) means that the model results are less (or more) variable than the observations. The displayed pattern statistics are computed from long-term monthly means of simulated and observed data in the surface layer (0 – 10 m) of each basin.

Taylor diagrams assess how well model represents patterns in the field data without accounting for the model bias, i.e. the differences between the general levels of simulated and observed time-series (Taylor, 2001; Venkatram, 2008; Andersson, 2009; Joliff, 2009). Therefore, we define here a measure for the relative bias. Similarly to Eilola *et al.* (2011a), we compare model-data difference with the data variability. However, to emphasize both long-term changes and seasonality of variables, we use time series of a model-data difference of pairwise monthly means. Because seasonal cycle is also reflected in monthly standard deviations, especially in the upper part of the water column we scaled these differences with month-specific standard deviation SD_m. SD_m was calculated as the standard deviation of data collected in month *m* during the period 2000 – 2006 for each available sampling depth. Pooling the data collected during this seven-year period ensured that also at rarely sampled horizons enough data were available to reproduce fairly smooth seasonal cycles of data standard deviations in the upper part of the water column. At the same time, the period was small enough to reduce the impact of long-term changes in the observations on the monthly standard deviations. To remove any remaining outliers, the estimated monthly standard deviations were replaced by a spline smooth fitted by a GAM model. To avoid shifts due to some seasons being over-represented in the field data, in every basin the relative bias RB_i at each sampling depth was calculated as an average of the twelve months in the annual cycle.

$$RB_i = \frac{1}{12} \sum_{m=1}^{12} \left(\frac{1}{n_{im}} \sum_{j=1}^{n_{im}} \frac{abs\left(M_{imj} - D_{imj}\right)}{SD_{im}} \right)$$

where $m = 1..12$ denotes the month in the seasonal cycle, n_{im} is the number of monthly data averages D_{imj} available at depth i in month m of year j, and M_{imj} is the model averages computed at sampling depth i in month m of the same year j. Thus, being based on monthly values computed from available data over the entire simulated time interval, the relative bias simultaneously characterizes several time scales: seasonal, interannual, and decadal.

Similarly to the cost function used by Eilola *et al.* (2011a) and being based on just the 1970 – 2005 averages of observations and model outputs, the *RB* also indicates how the model-data disagreement compares to the natural variability of simulated parameters. However, by replacing absolute value of a difference between long-term averages with an average of absolute values of pairwise model-data differences our index also captures the model bias in representation of long-term trends. Furthermore, scaling the relative bias to a measure of data variability within each month instead of using the standard deviation of monthly averages assures that model-data misfits during the nutrient deplete summer period have a representative impact on the cost function. These distinctions allow us to consider *RB* index a significantly more rigorous measure of model skill than the cost function, but also make the two incomparable. For such a comparison, we have also calculated the cost function strictly according to Eilola *et al.* (2011).

For a model-data comparison of the annually averaged basin-integrated pools, which supposedly are more robust to sampling and measurement uncertainties, we have also used the Theil's inequality index:

$$TI = \frac{\sqrt{\Sigma(P_o - P_m)^2 / N}}{\sqrt{\Sigma P_o^2 / N} + \sqrt{\Sigma P_m^2 / N}}$$

where P_o and P_m are time series of annual means of the basin wide pools of variables, reconstructed with the DAS system from observations and computed from BALSEM simulation, respectively. Similarly to the relative bias, this index also measures the degree to which observed dynamics differ from simulated dynamics and emphasizes systematic deviations but is bounded to the interval 0 (perfect match) and 1 (no match) (Leuthold, 1975; Beck, 1987).

3 Results and discussion

3.1 Seasonal dynamics and its inter-annual variations

Long latitudinal extension of the Baltic Sea and different environmental conditions along the drainage basin create pronounced meridian gradients both in ecosystem seasonal dynamics and in nutrient limitation: the productive season starts earlier and lasts longer at the Baltic Sea entrance than in the Gulf of Bothnia, nitrogen limitation in the Baltic Proper changes into phosphorus limitation in the Bothnian Bay (*e.g.* Voipio, 1981; Granéli *et al.*, 1990; HELCOM, 2009). As shown by formal assessment of the model performance, in general these major regularities are captured reasonably by BALTSEM both at seasonal and long-term scales (See Figs. 6 and 13 below). Therefore, here we will mostly focus on some peculiarities in the 1970 – 2006 hindcast simulation and its discrepancies with the available data.

3.1.1 Abiotic pelagic variables

To illustrate model performance at the seasonal scale in more detail, we have chosen three BALTSEM basins representing the entire Baltic Sea environmental gradient, namely, the Central Kattegat (CK), the Gotland Sea (GS), and the Bothnian Bay (BB) (cf. Fig. 1). The extremes, amplitude, and timing of simulated seasonal cycles in the water temperature and nutrient concentration are very close to those of measured variations (Fig.4). A common feature of the simulated nutrient dynamics in the Gulf of Bothnia, annually experiencing ice coverage, is the late winter acceleration of nutrient accumulation (see, for instance, BB in Fig. 4 B, C) caused by combined nutrient input from the spring river flood and off-loading of melting ice (Rahm *et al.*, 1995; Granskog *et al.*, 2006), which is less pronounced in the monitoring data than in the model. Also, in calm conditions, the riverine water is captured into a quite thin fresh layer below the ice with rather high nutrient concentrations. This has been observed in the northern part of Bothnian Bay and happens occasionally in the model simulations.

The persistent and severe phosphorus limitation in BB changes into persistent nitrogen limitation in the Baltic Proper and towards the Skagerrak. In the Bothnian Sea separating these extremes, the nutrient limitation is almost balanced *sensu* Redfield both in the model and according to observations and experimental assays *(e.g.* Hagström *et al.*, 2001; Tamminen and Andersen, 2007).

The most pronounced discrepancy between simulations and available information is a considerable underutilization of DIN in the Bothnian Bay, even in spite of a slightly overestimated phosphate concentration in the model (cf. Fig. 4 B and C for BB). Whereas the median of observed nitrate concentration decreases from May to July by about 5 μM, the simulated decrease has hardly exceeded 2 μM. Both in BALTSEM and in some other models (cf. Eilola *et al.*, 2011a) this underutilization is caused by a strong phosphorus limitation of the nitrogen uptake by phytoplankton. This mismatch indicates a deficiency of the current model formulations in adequate reproducing of the stoichiometry and intensity of summer nutrient recycling in the Bothnian Bay (Andersson *et al.,* 1996; Hagström *et al.*, 2001; see also Sect. 3.1.3 below).
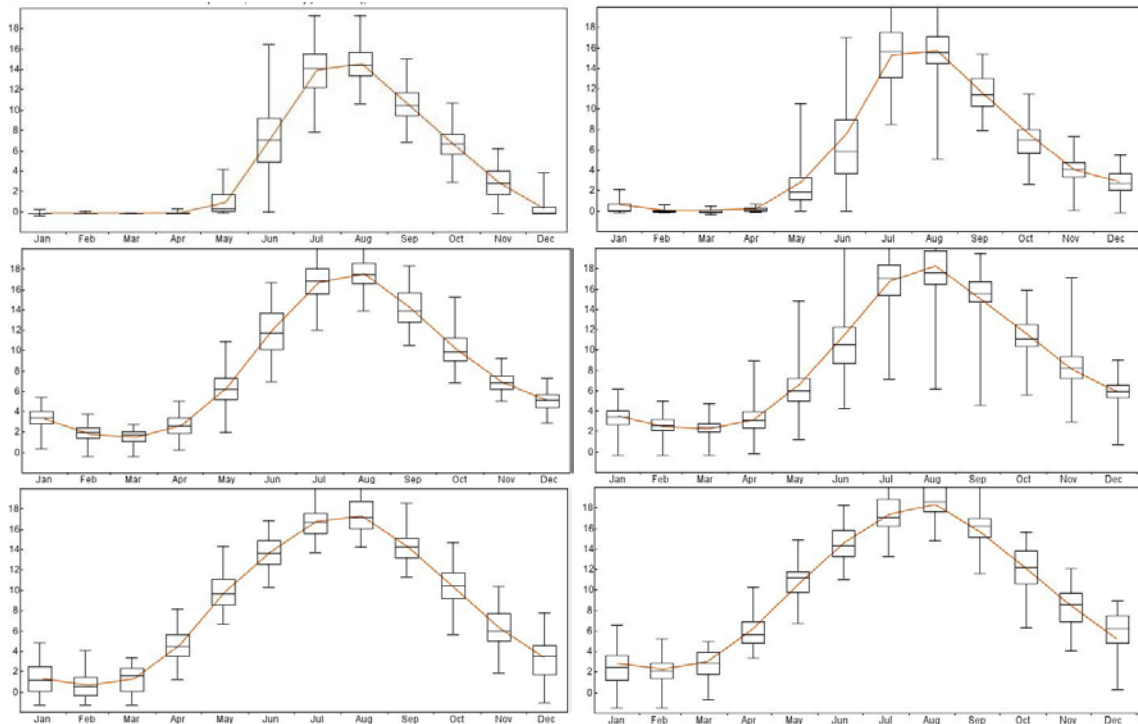
Fig. 4A. A comparison of simulated (left) and observed (right) seasonal variations of temperature (A), oxidized inorganic nitrogen (B), and phosphate (C) in the surface layers of the Bothnia Bay (upper rows), the Gotland Sea (middle rows), and the central Kattegat (bottom rows). Graphs of long-term (1994-2006) monthly averages (curves) and boxes-and-whiskers (median, 25% and 75% percentile, minimum and maximum values) were built with the Baltic Nest system both from the model outputs, and from the observations aggregated over the correspondent basins
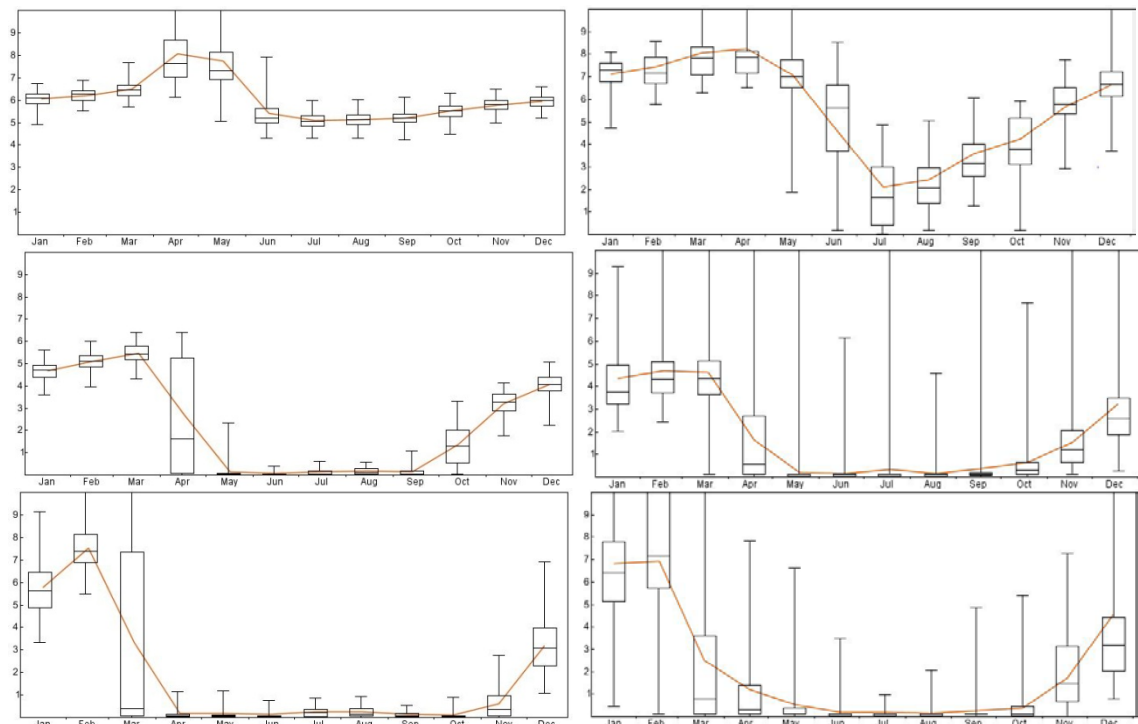

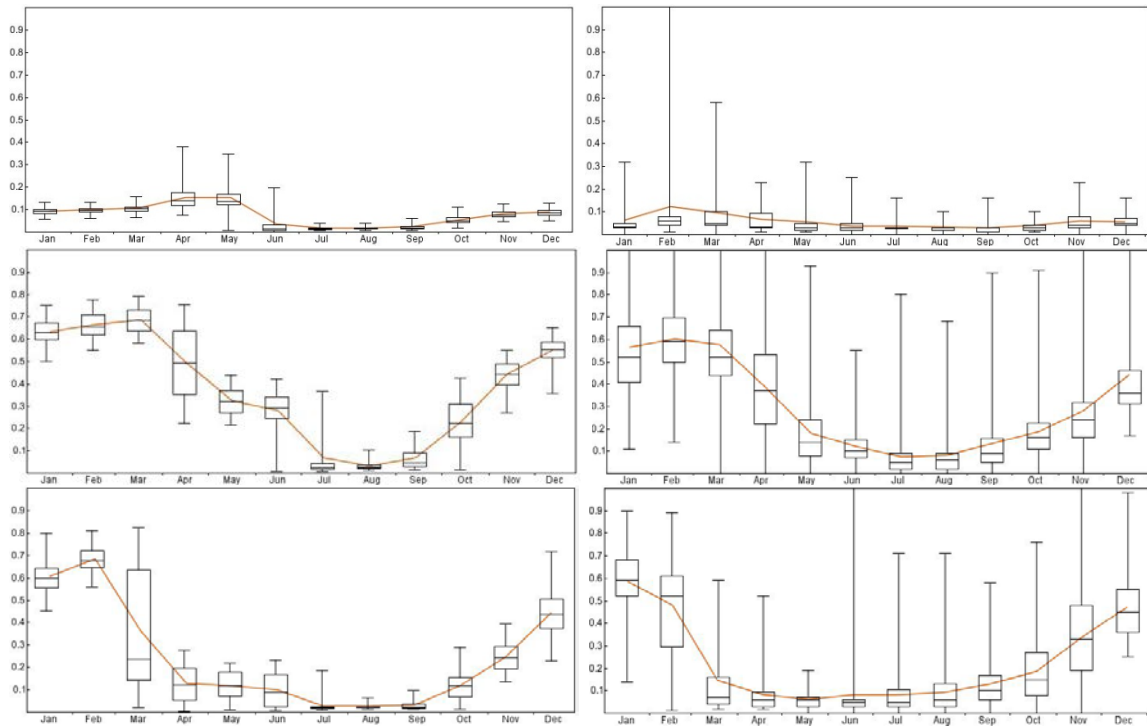Fig. 4B. (continuation: oxidized inorganic nitrogen)

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Fig. 4C (continuation: phosphate)

This weak nutrient consumption is also a reason for excessive accumulation of silicate in the model comparing to observations (not shown), especially in the Bothnian Bay (40-50 vs. 20-30 µM, respectively) and in the Bothnian Sea (ca. 30 µM vs. 10-20 µM, respectively). Silicate model-data comparability somewhat improves south of the Gulf of Bothnia, particularly regarding the amplitude of seasonal variations (see Figs 6 and 13 below). However, since silica has not become permanently limiting yet either in the Baltic Sea (Danielsson *et al.*, 2008) or in BALTSEM, the influence of these discrepancies on the performance of other model variables is assumed insignificant.

The early summer phosphate concentration in the surface layers of nitrogen limited basins is higher and more stable in the simulation compared to observations (see Fig. 4C and Fig. 5 below). In BALTSEM, with its fixed phytoplankton N:P ratio, the entire phosphorus pool left unutilized after spring bloom stays in the water as phosphate. In nature, the phosphorus pool is gradually building up both in cyanobacteria cells due to luxury consumption and in the water column as dissolved organic phosphorus (Larsson *et al.*, 2001; Naush *et al.*, 2004; 2008; Vahtera *et al.*, 2007b; 2010; Walve and Larsson, 2007; 2010). Neither cell phosphorus storage, nor dissolved organic phosphorus state variable are considered in BALTSEM. However, regardless of the provisional storage mechanisms, the eventual fate of these phosphorus reserves is the same both in the field and in the model – to support nitrogen fixation during cyanobacterial blooms (Raateoja *et al.*, 2011). Note also, that a more sophisticated accounting for variable C:N:P composition of cyanobacteria in another Baltic ecosystem model resulted in almost negligible changes in performance (Kuznetsov *et al.*, 2008).
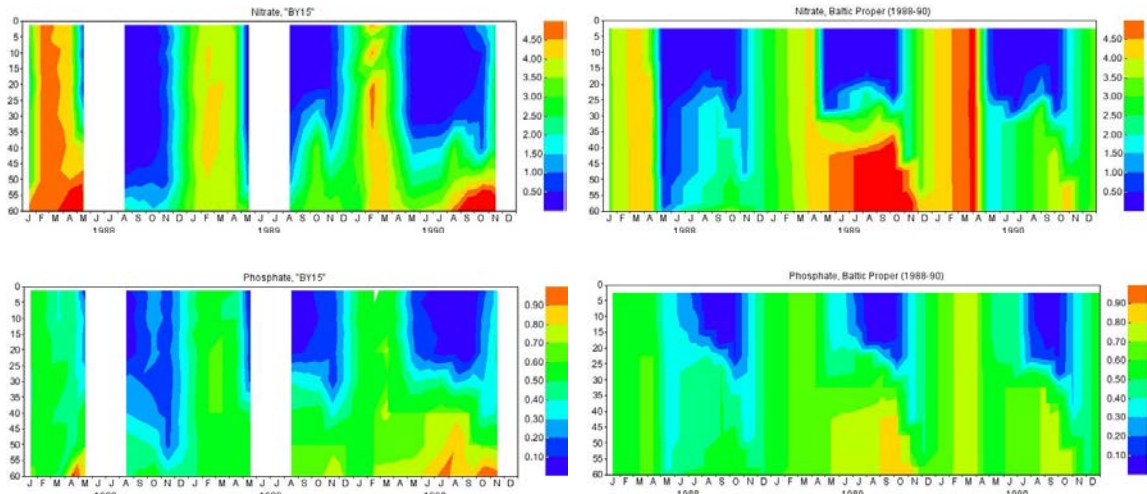
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Fig. 5. Dynamics of nitrate (top) and phosphate (bottom) concentrations (μM), observed at monitoring station BY15 9 (left) and simulated for the Gotland Sea basin (right) during 1988-1990. Measurements and model outputs are averaged over 30-day consecutive intervals; white strips indicate absence of measurements

Another discrepancy from the observed seasonal dynamics, occurring also at least in two other Baltic ecosystem models (Eilola *et al.*, 2011a), is a shallower depletion of nutrients associated with the spring bloom (Fig. 5). In contrast to this peculiarity, which is more pronounced in some years compared to others, in sub-thermocline water layers simulated nutrients accumulate faster than indicated by measurements. Taken together, both these features imply a possible underutilization of nutrients during vegetative season.
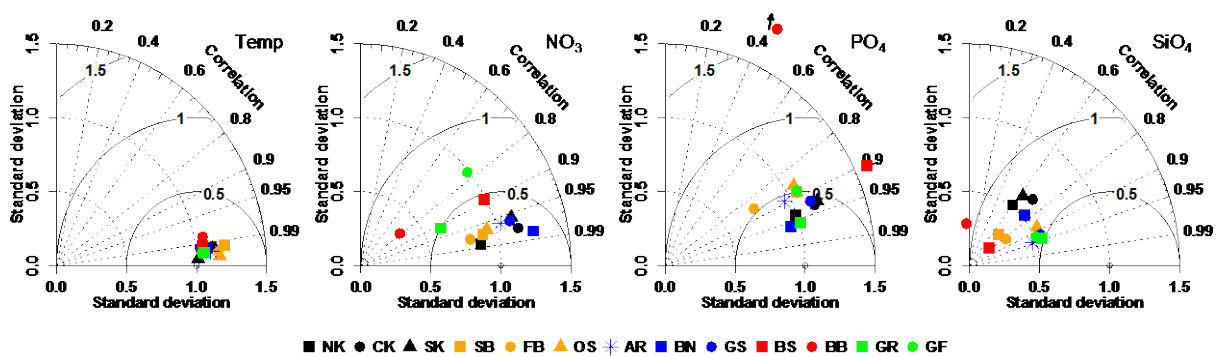

Fig. 6. Taylor diagrams built on long-term (1970-2006) monthly means of simulated and measured abiotic variables averaged over surface layer (0-10 m) of all the basins. For abbreviated basin names see Fig. 1

The overall BALTSEM capability in reproducing major spatial gradients in seasonal cycles over decades with a single set of constants is demonstrated by the Taylor diagrams (Fig. 6). As can be expected already from comparisons in Fig. 4A, BALTSEM perfectly reproduces the seasonal temperature pattern in the surface layer, with correlation coefficients higher than 0.95 and almost matching the variability of observations. The seasonal dynamics of phosphate are generally reproduced well in all the basins except for the Gulf of Bothnia, where, in an attempt to increase simulated nitrate utilization and primary production, the model was intentionally tuned to make winter accumulation of phosphate higher than

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indicated by measurements. The seasonal dynamics of nitrate is simulated less well than that of phosphate. In the Gulf of Finland and Bothnian Sea the magnitude of the seasonal cycle is captured well, but model-data linear correlation is lower than for other basins. In the Gulf of Finland, the model does not capture alteration of years with high and low winter nitrate concentrations. In the Bothnian Sea, the lower correlation is resulted from slightly delayed spring blooms and a too short productive season. The mediocre performance in the Gulf of Riga is caused by overestimated summer concentrations of nitrate during the high river load period in the 1980s. Finally, the model systematically underestimates silica consumption during the spring bloom, especially in the Gulf of Bothnia.

3.1.2 Biotic variables

Qualitatively, BALTSEM captures (Fig. 7) all the major features of seasonal dynamics of plankton communities (HELCOM, 1996; 2002; 2009; Hagström *et al.*, 2001; Wasmund and Siegel, 2008). The vegetation season expands from May-October in the Bothnian Bay to March-November in the Gotland Sea to February-December in the Kattegat. The trophogenic layer is deeper in the Gotland Sea, compared to the Bothnian Bay, where its depth is limited by lower water transparency, and to the Kattegat, where the permanent pycnocline restricts vertical mixing of phytoplankton to greater depths. However, the mixing is strong enough to sustain an upward flux of nutrients that supports a typical sub-surface phytoplankton maximum (*e.g.* Richardson and Christoffersen, 1991; Karlson *et al.*, 1996; HELCOM, 2002), which is being dominated in BALTSEM by diatoms in May, by "others" in May-June, and by cyanobacteria further onwards. In all basins except the Bothnian Bay, a diatom spring bloom segues into post bloom flagellate phase followed by the development of summer community and cyanobacteria blooms. The annual cycle ends with a more or less pronounced autumn development of larger diatoms. In the Bothnian Bay, all three groups bloom together in June with a greater contribution of the "others" species that increases even more during August-September, which resembles significant contribution of non-diatoms in observations (Andersson *et al.*, 1996; HELCOM, 1996). Heterotrophs reach their maximum everywhere in August, in sync with the temperature of surface water layer.

In BALTSEM, the general pattern of cyanobacteria dynamics is similar everywhere southwards of the Gulf of Bothnia. Cyanobacteria slowly start growing in spring together with the "others" species but reach the bloom proportions only in July, then go through an intermediate minimum in August, being complemented and partly replaced by the "others", and, finally, develop the second maximum (cf. Fig. 7A and B). Although cyanobacteria, especially small species are found everywhere in the Baltic Sea (*e.g.* Andersson *et al.*, 1996; Yurkovskis *et al.*, 1999; Kahru *et al.*, 2000; Wasmund *et al.*, 2011), including Kattegat and Skagerrak (Kuylenstierna and Karlson, 1994; Karlson *et al.*, 1996; Ærtebjerg *et al.* 2003; Henriksen, 2009), their dominating contribution in September could partly be a model artefact produced by the strong similarity between parameterizations of cyanobacteria and "others" species. Except for the nitrogen-fixing capability, the only differences between these two variables are a higher availability of "others" as food source for heterotrophs and a steeper temperature dependence of their growth rate. Consequently, when cyanobacteria develop in the model without a significant contribution nitrogen fixation, their dynamics

could also be interpreted as the dynamics of "others" species, especially in the Bothnian Bay, where nitrogen fixation does not occur at all.
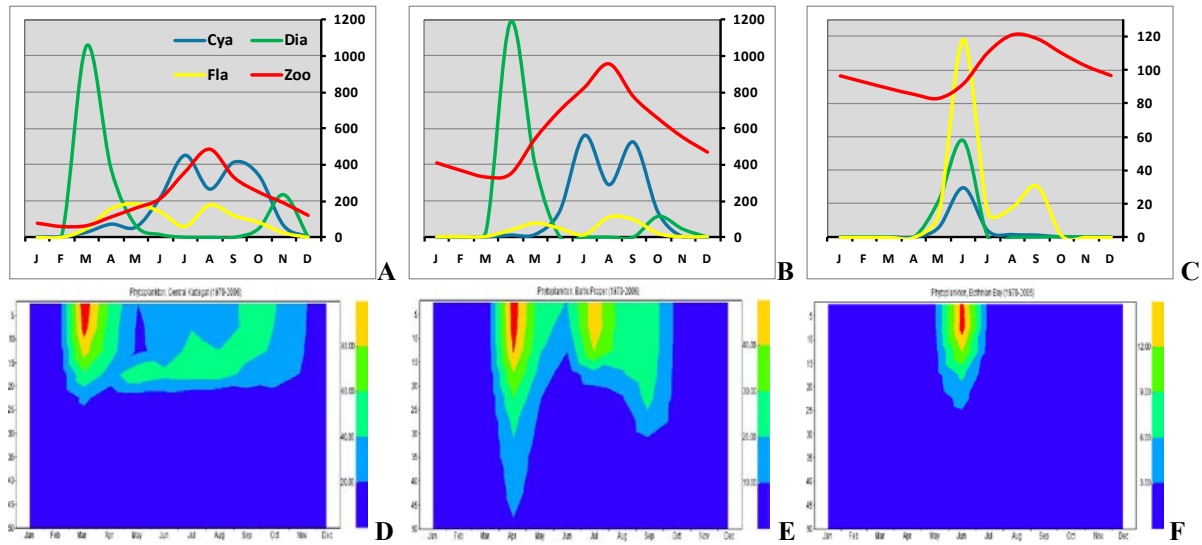

Fig. 7. Long-term (1970-2006) average seasonal dynamics of plankton variables in the Central Kattegat (A, D), Gotland Sea (B, E), and Bothnia Bay (C, F) presented as a vertically integrated seasonal succession (top, mg C m^{-2}) and vertically resolved total phytoplankton (bottom, mg C m^{-3}) monthly averages. Note differences in scales.

Table 1 Typical characteristics of plankton biomass simulated for 1970-2006 in the surface layer of selected basins

BALT-SEM basin	Spring phytoplankton				Summer phytoplankton				Heterotrophs (g ww m^{-3})	
	mg chl"a" m^{-3}		g ww m^{-3}		mg chl"a" m^{-3}		g ww m^{-3}			
	mean	max	mean	max	mean	max	mean	max	mean	max
BB					0.5	2.2	0.2	1.0	0.05	0.07
GF	5.0	40	3.5	30	3.0	8.0	0.8	4.0	0.9	1.9
GR	6.0	40	4.5	30	0.5	4.0	0.3	2.0	0.5	1.2
GS	3.0	15	2.0	12	1.0	5.7	0.5	2.7	0.4	1.1
CK	5.6	25	4.2	25	0.8	2.8	0.4	1.4	0.6	1.1

Note: Heterotrophs' biomass in August

Quantitatively, simulated plankton biomasses presented in conventional units (Table 1) are quite comparable to the typical levels estimated from observations (*e.g.,* HELCOM 1996, 2002; Möllmann *et al.*, 2000; Fleming and Kaitala, 2006; ICES, 2007; Suikkanen *et al.*, 2007; Wasmund and Siegel, 2008; Henriksen, 2009; Wasmund *et al.*, 2011). BALTSEM has also captured those conspicuous cyanobacterial blooms that occurred in the 1970s and 1980s as well as in 1992 and 2005 (see *e.g.* Edler *et al.*, 1985; Niemisto *et al.*, 1989; Kahru, 1997; Kahru *et al.*, 2007), but missed the bloom in 1999 that was "replaced" in simulation by the bloom in 2000. Satellite images characterize mostly the surface distribution of *Nodularia spumigena*, thus largely disregarding the contribution of other species included in the model "cyanobacteria" variable. Correspondingly, we could not find a meaningful consistency between simulated biomasses and the frequency of cyanobacterial accumulations both on

monthly and regional scales (Kahru *et al.*, 2007). However, the total annual amounts of fixed nitrogen obtained in the BALTSEM simulation are related to the total cumulative areas covered by cyanobacterial blooms estimated over June-August in 1979-1984 and 1998-2008 from satellite data (Kahru *et al.*, 2007) with a coefficient of linear correlation of 0.77, mainly because of the marked increase in both quantities from the 1980s to the 2000s.

3.1.3 Pelagic and sediment fluxes

Nutrient uptake by autotrophs is the major mechanism that converts external nutrient inputs into primary production of organic matter. In the BALTSEM basins, spring utilization of the oxidized nitrogen and phosphorus depletes their surface pools accumulated during winter (see also Fig. 4). Afterwards, nutrient utilization is increasingly supplemented by uptake of the ammonium nitrogen and phosphate, mostly regenerated by heterotrophs as well as from mineralizing organic matter, including organic matter produced due to nitrogen fixation (Fig. 8). Being presented in comparable to published per volume units, the simulated maximal rates of inorganic nitrogen uptake ranging from 30-40 mg N m^{-3} d^{-1} in spring with dominant contribution of nitrate to 5-10 mg N m^{-3} day^{-1} sustained by nitrogen compounds regenerated during summer are similar to the rates measured in the Skagerrak (Karlson *et al.*, 1996), Kattegat (Sahlsten *et al.*, 1988), Gulf of Riga (Berg *et al.*, 2001) and other marine areas similar to the Baltic Sea (Mulholland and Lomas, 2008). Simulated typical rates of nitrogen fixation of 5 – 25 mg N m^{-2} d^{-1} (Fig. 8) with occasional peak values up to 260 mg N m^{-2} d^{-1} (not shown) are fully comparable to the rates measured and compiled for the Baltic (Savchuk and Wulff, 2001; 2009; Wasmund *et al.*, 2001b; 2005b; Kangro *et al.*, 2007; Ohlendieck *et al.*, 2007; Degerholm *et al.*, 2008), including the maximum cyanobacteria occurrence from late June to early August (Kahru *et al.*, 2007) without significant regional differences from the Danish Straits to the Gulf of Finland (Wasmund *et al.*, 2001b; Ohlendieck *et al.*, 2007;). Although we are not aware about measurements of nitrogen fixation in the Kattegat, the cyanobacterial species that are found there, *e.g. Synechcoccus* type (*e.g.* HELCOM, 1996; Karlson *et al.*, 1996), are able to fix molecular nitrogen (*e.g.* Phlips *et al.*, 1989; Huang *et al.*, 1999) as, for instance, in the North Sea and English Channel (OSPAR Commission, 2000; Rees *et al.*, 2009).
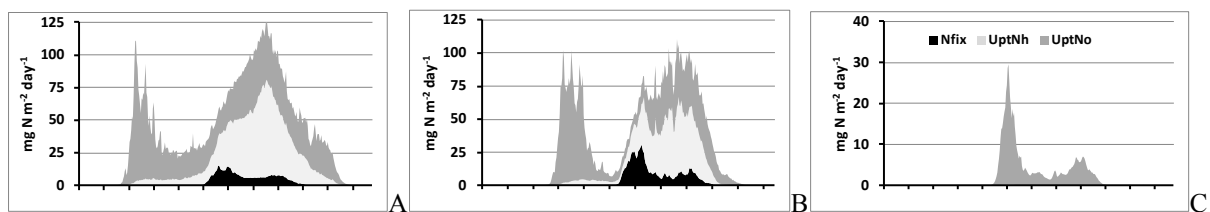

Fig. 8. Long-term average (1970-2006) seasonal cycle of daily nitrogen uptake in the water column of the Central Kattegat (A), Gotland Sea (B), and Bothnian Bay (C). *Nfix* – nitrogen fixation, *UptNh* – ammonium uptake, *UptNo* – nitrate uptake. Note differences in scale. Peak daily values are reaching 60-80 mg N m^{-2} d^{-1} in the Bothnian Bay, 300-500 mg N m^{-2} d^{-1} in the Baltic Proper and Entrance area, and up to 600-800 mg N m^{-2} d^{-1} in the Gulfs of Finland and Riga.

In contrast to the nutrient uptake and nitrogen fixation rates that have been measured rather seldom, the rates of primary production expressed in carbon units are measured on a more routine basis within many long-term monitoring programmes. The coverage of accumulated

data would even allow a systematic basin-wise model-data comparison. However, a direct comparison of simulated primary production with these measurements is complicated by two circumstances. The inter-calibrations repeatedly indicate large uncertainties of the measurements that often differ by a factor of 2-3 (*e.g.* Richardson, 1991; Rydberg *et al.*, 2006; Andreasson *et al.*, 2009; Larsson *et al.*, 2010). Further uncertainty arise from differing nature of the entities under comparison: the simulated phytoplankton growth rate expressed in nitrogen units corresponds to net primary production by definition (Platt *et al.*, 1989), whereas routine measurements, especially the historic observations represent values varying somewhere in between the gross and net primary production (*e.g.* Beardall *et al.*, 2009). The difference between the two is determined by extracellular excretion of dissolved organic substances, including the release of nitrogen-containing compounds (Bronk and Steinberg, 2008), and possible miscounting of respiration (*e.g.* Marra, 2009; Quay, 2010). Typically, this difference reaches up to 25-50% of gross production both in the Baltic Sea (*e.g.* Donali *et al.*, 1999; Sandberg *et al.*, 2000, 2004; Wasmund *et al.*, 2005a) and elsewhere (*e.g.* Bronk and Steinberg, 2008; Beardall *et al.*, 2009), generally increasing with deterioration of phytoplankton growth conditions (*e.g.* Lancelote, 1983; Morán *et al.*, 2002 and references therein; Borsheim *et al.*, 2005).

Table 2   Primary production in the major Baltic Sea basins, simulated and compiled from published estimates for different time intervals

	BB	BS	BP[a]	GF	GR	DS[a]	KT[a]
Daily rates (mg C m^{-2} d^{-1}) simulated over 1970-2006 (mean ± s.d.) vs. literature data							
Spring[b]		May	April	May	April	March	March
Model		272 ± 469	408 ± 514	515 ± 985	530 ± 997	369 ± 493	411 ± 560
Data		350[c]	1000[d]	2500[e]	2000[g]	500-1000[h]	500-1200[h]
Summer[b]	June	September	August	August	September	August	August
Model	78 ± 129	145 ± 125	636 ± 556	1707 ± 1329	733 ± 457	1317 ± 535	706 ± 355
Data	100-300[c]	150[c]	600[d]-1000[c]	300-1300[f]	1500[g]	500-1000[h]	200-1000[h]
Annual integrals (g C m^{-2} yr^{-1}) simulated over two periods (mean ± s.d.) vs. literature data							
1970/82	4.7 ± 0.8	18 ± 3	52 ± 10	123 ± 39	59 ± 10	126 ± 22	87 ± 13
Data	12-20[i]	50-70[i]	40-140[d]	70-100[i]	90[i]	100-195[h]	90-125[h]
1994/06	4.6 ± 0.6	23 ± 3	98 ± 16	196 ± 67	132 ± 23	149 ± 18	103 ± 18
Data	16[j] – 17[i]	32[j] – 52[i]	65[j] – 200[i]	80[i] – 130[k]	200[g] – 250[i]	185-200[h]	116[l] -165[h]

[a] – aggregation weighted with basin areas; [b] – month of blooming in the model; [c] – Dahlgren *et al.*, 2010; [d] – Renk and Ochocki, 1999; [e] –Lignell, 1990; [f] – Silina, 1967; [g] – Savchuk, 2002 and references therein; [h] – Rydberg *et al.*, 2006; [i]- Wasmund *et al.*, 2001a and references therein; [j] – median value from Larsson *et al.*, 2010; [k] – Raateoja *et al.*, 2004; [l] - Carstensen *et al.*, 2003

Therefore, we should always expect simulated rates being systematically lower compared to those estimated from measurements, with larger differences under nutrient limitation that is

occurring during summer as well as northwards along the Gulf of Bothnia. However, even within these uncertainties the simulated primary production appears rather underestimated, especially in the Gulf of Bothnia (Table 2). How much of this underestimation is caused by the shallower and lesser depletion of nutrients during and after the spring bloom (cf. Fig. 5 above) remains a topic for future studies and further development of BALTSEM.

In BALTSEM, the entire multitude and variety of processes responsible for internal nutrient regeneration in marine environments is aggregated in three pathways: zooplankton excretion, pelagic detritus mineralization, and release of re-mineralized nutrients from the sediments (cf. Fig. 2 above). Unfortunately, there are no regional measurements of zooplankton excretion and detritus mineralization that would allow us to validate the simulated inter-basin differences (Table 3). The typical levels of these simulated fluxes are quite comparable to the ranges compiled in other coastal and estuarine environments for micro- and mesozooplankton taxa in (Corner and Davies, 1971; Ikeda *et al.*, 2001; Bronk and Steinberg, 2008; Steinberg and Saba, 2008; Sereda and Hudson, 2011).

Table 3 Typical and high (in brackets) rates of pelagic nutrient regeneration simulated in August (1970-2006) in the surface mixed layer

Basin	Heterotrophs' excretion				Mineralization	
	$mg\ N\ m^{-3}\ d^{-1}$	$\mu g\ N\ d^{-1}$ $mg\ dw^{-1}$	$mg\ P\ m^{-3}\ d^{-1}$	$\mu g\ P\ d^{-1}$ $mg\ dw^{-1}$	$mg\ N\ m^{-3}\ d^{-1}$	$mg\ P\ m^{-3}\ d^{-1}$
BB	0.04-0.08 (0.12)	10-20 (35)	0.005-0.01 (0.015)	1-3 (5)	0.04-0.1 (0.15)	0.01-0.02 (0.035)
BS	0. 2-0.8 (1.4)	20-60 (110)	0.05-0.15 (0.2)	3-8 (15)	0.1-0.15 (0.25)	0.02-0.03 (0.05)
GF	20-50 (100)	200-400 (600)	2-6 (14)	20-60 (100)	0.4-0.8 (1.7)	0.1-0.2 (0.35)
GR	5-20 (45)	100-300 (400)	0.5-5.0 (5.0)	10-40 (60)	0.3-0.6 (0.9)	0.05-0.15 (0.2)
GS	2-15 (25)	100-300 (500)	0. 2-2.0 (4.0)	10-40 (80)	0.2-0.4 (1.1)	0.03-0.1 (0.2)
FB	5-15 (30)	100-250 (350)	0.5-2.0 (4.0)	15-30 (50)	0.2-0.5 (0.9)	0.04-0.1 (0.18)
CK	5-15 (25)	100-200 (250)	0.5-1.5 (3.0)	15-30 (40)	0.15-0.4 (0.6)	0.04-0.08 (0.16)

Note: typical range and high value were eyeballed from corresponding time series graphs

In contrast to zooplankton excretion that has a strong seasonal signal (cf. Figs. 7 and 10 below), especially in the surface layers, the pelagic detritus mineralization occurs throughout the entire water column with a rather distinctive pattern governed by the detritus sinking and water temperature. As follows from comparison of Fig. 9A with Fig. 11A below, the subsurface maximum of mineralization in May is generated by a decaying spring bloom, whereas elevated mineralization in the deepest layers is associated with detritus produced during the previous vegetation season. With negligible diatom's contribution, remnants of

cyanobacteria and summer species sink slower, which results in a slower downward shifting of the deep-water maximum of mineralization flux.
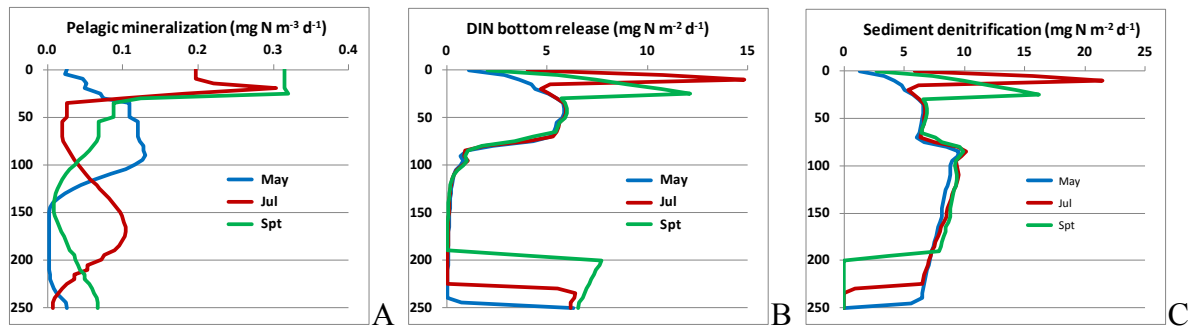

Fig. 9. Vertical distribution of mineralization in the water column (A) and in the sediments along the bottom slope, the later split into the DIN release into the water (B) and the loss by denitrification (C); exemplified for the Gotland Sea on three occasions during anoxia development in 2005 after the major saltwater inflow of 2003

Under suitable conditions, pelagic denitrification reached maximal rates of 1.4 and 10.4 mg N $m^{-3}d^{-1}$ in the Gotland Sea and Bornholm basin, respectively. In situation, exemplified with Fig. 9A, pelagic denitrification reached up to 0.005 – 0.015 mg N $m^{-3}d^{-1}$ in the hypoxic layer between about 100 and 150 m. These rates are well comparable to recently reported measurements, also exhibiting very high seasonal and spatial variations, from zero up to 11.3 mg N m-3 d^{-1}, albeit found almost exclusively in anoxic zone (Heitanen *et al.*, 2012).
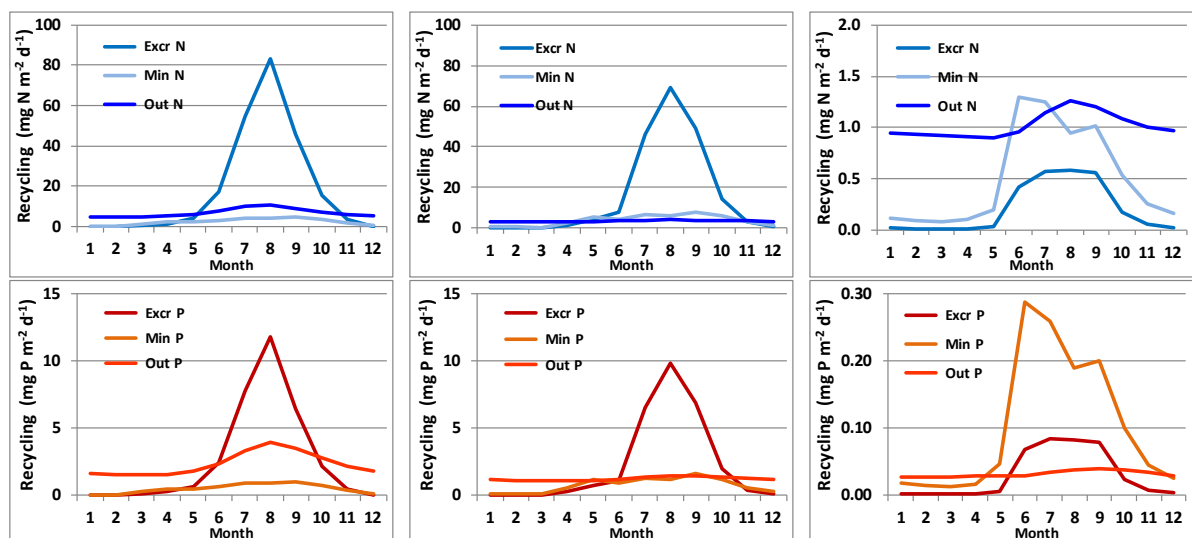

Fig. 10. Seasonal dynamics of nitrogen (top) and phosphorus (bottom) regeneration in the Central Kattegat (left), Gotland Sea (middle), and Bothnian Bay (right). *Excr* – zooplankton excretion, *Min* – detritus mineralization, *Out* – release from the sediments. Note differences in scale

In BALTSEM, contribution of zooplankton excretion into inorganic nutrient regeneration is comparable to the contribution from detritus mineralization only in the Bothnian Bay, and many-fold exceeds it farther southwards (Fig. 10). However, as assumed preferential mineralization of phosphorus (see Sect. 2.1.2) shifts grazer's diet closer to the zooplankton N:P stoichiometric demand, prescribed in BALTSEM equal to 24, the overall combined

effect of pelagic nutrient regeneration results in minor phosphorus enrichment of ambient waters characterized by the N:P molar range of 11 – 14, evaluated as long-term seasonal means. This result is in line with results of both the Baltic Sea (Walve and Larsson, 1999) and global (*e.g.* Elser and Hasset, 1994) studies, but somewhat contradicts to final conclusions by Pertola *et al.* (2002) about the Baltic Sea zooplankton being a phosphorus sink. Apparently, both more field data and specific sensitivity experiments with BALTSEM are needed to clear up this controversy.

According to the basin-invariant parameterization of detritus sedimentation (see Sect. 2.1.2), the sinking velocity of detritus displays rather distinctive seasonal time-depth variations (Fig. 11B), exceeding at maximum 2 m d^{-1} in the warm surface layers (cf. Fig. 4A). This value may seem greatly underestimated in comparison to sinking velocities of diatom aggregates and faecal pellets of 50 – 100 m d^{-1} (*e.g.* Sarthou *et al.*, 2005) that, however, are considered to be a minor component of the total downward flux of organic matter in the Baltic Sea (Blomqvist and Heiskanen, 2001 and references therein). One also should bear in mind that the detritus variables in BALTSEM represent all the variety of the "dead" particulate organic nutrients, covering the entire size spectrum and partly accounting also for the bioavailable dissolved fraction. Therefore, the BALTSEM performance is better to be evaluated from sedimentation fluxes (Fig. 11C) that are a product of concentration (Fig. 11A) and sinking velocity (Fig. 11B).
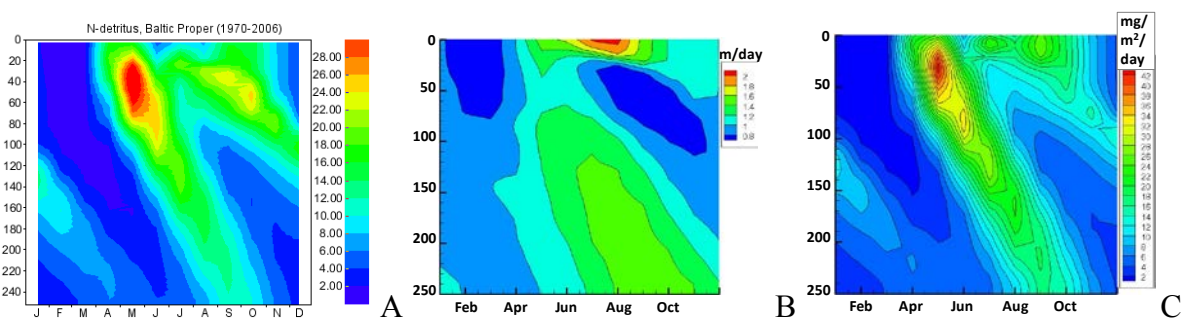

Fig. 11. Average (1970-2006) seasonal time-depth distribution of detritus nitrogen DN (A, mg N m^{-3}), its sinking velocity (B, m day^{-1}) and sedimentation flux (C, mg N m^{-2} day^{-1})

As has already been shown by a comparison to available fragmentary measurements in different basins, the sedimentation fluxes simulated with similar parameterizations were a good match to fluxes estimated from sediment traps (Savchuk, 2000; 2002; Savchuk and Wulff, 2001). Here we extend this comparison with unique time series of measurements made in 1995-2003 at 180 m in the Gotland Deep (Leipe *et al.*, 2008). Similarly to long-term monthly means of measurements (see Fig. 14.12 in Liepe *et al.*, 2008), the simulated flux (cf. Fig. 11C) also displays a bimodal seasonal distribution with the spring peak of 6 – 8 mg N m^{-2} d^{-1} being less than half of the summer peak of 18 – 20 mg N m^{-2} d^{-1}. However, the fluxes estimated from measurements are only a third of the simulated fluxes: about 3 and 7 mg N m^{-2} d^{-1} in April and August, respectively. Another important difference is the origin of these maxima. In the model, the summer peak at 180 m depth is generated by the spring bloom, while the spring peak can actually be traced to the summer-autumn blooming in the

previous year (cf. Fig. 11C). According to isotopic signature of particulate nitrogen in measurements, the summer peak reflects input of atmospheric molecular nitrogen (Leipe *et al.*, 2008), thus implying a vertically averaged sinking velocity of the cyanobacterial bloom products of about 6 m d^{-1}.

The sedimented nutrients are partly released back into the water column. In addition to temperature dependence of the sediment nutrient mineralization rates, the sediment processes are also governed by redox alterations. Therefore, a contribution of resulting nutrient release into the total regeneration differs between basins and nutrients (Fig. 10). As exemplified by comparing Fig. 9B and 9C, at the shallow bottoms the release of DIN, mostly as nitrate is quite comparable to the sediment denitrification; in the intermediate hypoxic layers deeper than ca. 100 m almost all mineralized nitrogen is denitrified and very little is returned to pelagic system, while in the expanding upwards anoxic zone the denitrification is shutting down and almost all regenerated nitrogen is released as ammonium. The augmentation of phosphate release by anoxia is less drastic, in this example from about 0.8 to 1.0 mg P m^{-2} d^{-1}.

As in our other models using similar parameterizations (Savchuk, 2000; 2002; Savchuk and Wulff, 1996; 2001), simulated fluxes (Table 4) are fully comparable to the ranges found in literature, including some recent studies in the Baltic Sea (*e.g.* Heitanen and Kuparinen, 2008; Almroth *et al.*, 2009; Lukkari *et al.*, 2009; Deutsch *et al.*, 2010; Mort *et al.*, 2010; Jäntti and Hietanen, 2012; Viktorsson *et al.*, 2012).

Table 4 Simulated rates (mean ± sd for 1970-2006; max in brackets) of sediment processes

	DIN release (mg N m^{-2} d^{-1})	Denitrification (mg N m^{-2} d^{-1})	DIP release (mg P m^{-2} d^{-1})	SiO$_4$ release (mg Si m^{-2} d^{-1})	BOD (g O$_2$ m^{-2} d^{-1})
Bothnian Bay	1.1 ± 0.3 (2.8)	1.2 ± 0.4 (3.8)	0.05 ± 0.06 (0.57)	0.43 ± 0.22 (1.03)	0.04 ± 0.01 (0.10)
Gulf of Finland	6.4 ± 3.5 (30.7)	10.8 ± 4.3 (48.1)	2.4 ± 0.9 (8.8)	11.2 ± 6.0 (32.1)	0.25 ± 0.10 (1.18)
Gotland Sea	2.9 ± 2.9 (21.6)	5.6 ± 3.1 (33.5)	1.0 ± 0.4 (6.2)	5.6 ± 3.4 (28.5)	0.12 ± 0.05 (0.83)
Gulf of Riga	7.7 ± 3.5 (31.5)	10.0 ± 5.2 (48.9)	2.3 ± 1.2 (9.6)	12.7 ± 9.5 (52.7)	0.27 ± 0.13 (1.20)
Central Kattegat	3.5 ± 2.1 (15.5)	5.9 ± 3.9 (29.3)	1.2 ± 0.8 (5.5)	8.6 ± 2.3 (20.5)	0.14 ± 0.09 (0.63)

3.2 Long-term developments

The long residence times of nutrients in the major basins of the Baltic Sea as well as long-term trends and variations in natural and societal driving forces determine slow system's responses in the range from several years to decades (*e.g.* Wulff *et al.*, 1990; 2001b; Savchuk, 2005). Some deficiencies of the model performance at seasonal and regional scales discussed above may accumulate in time and propagate into the neighbouring basins. Therefore, in this

Section we evaluate how plausibly BALTSEM can simulate the simultaneous long-term evolution of all the Baltic Sea basins.

3.2.1 Multi-scale dynamics of abiotic pelagic variables

BALTSEM's capability in simulating the long-term dynamics of the pelagic system is exemplified here for the Gotland Sea basin (Fig. 12) that experiences very conspicuous redox alterations of biogeochemical cycles determined by the oxygen dynamics in its deep layers (*e.g.* Savchuk, 2010 and references therein) and greatly affects the neighboring basins (*e.g.* Savchuk, 2005).
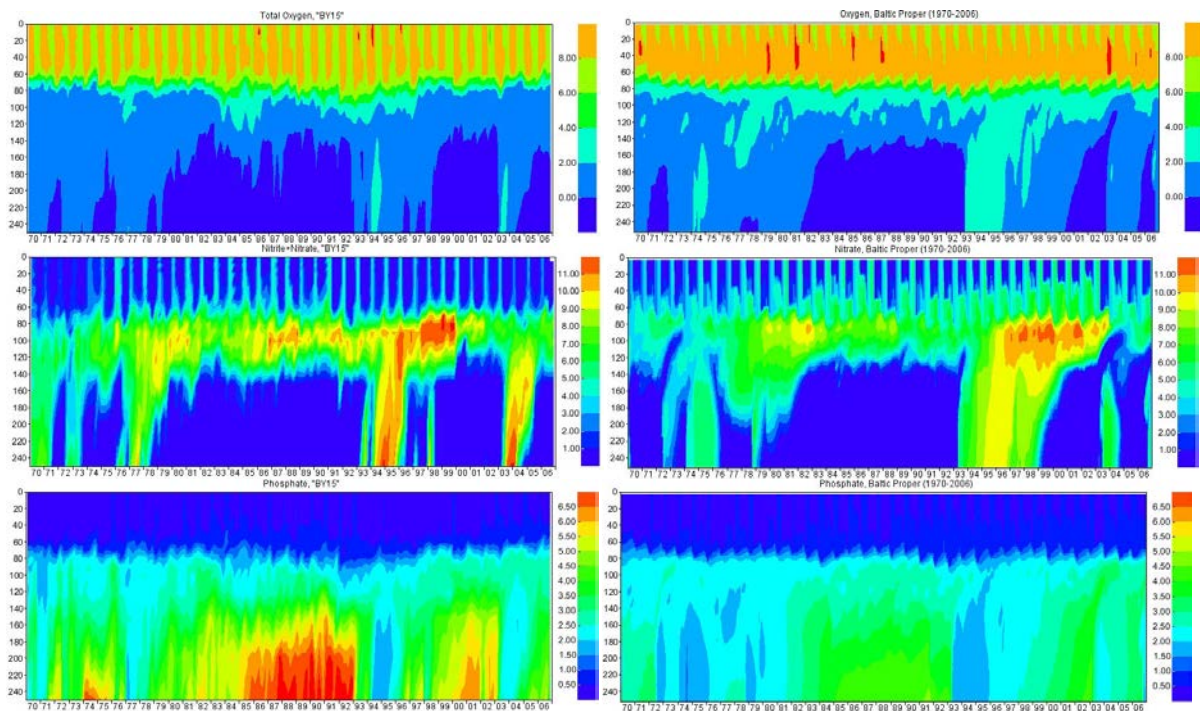

Fig. 12. Comparison of observed (left, BY15 in the Gotland Deep) and simulated (right, Gotland Sea basin) long-term time-depth dynamics of oxygen (top, mL O_2 L^{-1}), nitrate (middle, μM N), and phosphate (bottom, μM P)

Bearing in mind the inherent distinction between oxygen and nutrient dynamics simulated over the vast Gotland Sea and observed at a single monitoring station BY-15, the visual resemblance between the two can be considered as quite satisfactory. However, a more close inspection reveals some important differences. Comparison of oxygen dynamics shows that the simulated sporadic ventilation of deep water layers by the major inflows does not exactly follow the same pattern in chronology and intensity as indicated by observations. For instance, in BALTSEM the water is renewed all the way to the bottom in 1974, when only a minor inflow was observed, while the famous large inflow of 1976 aerated the entire water column in reality but does not penetrate deeper than about 180 m in the model. Furthermore, the inflows in 1993 – 1994 and 2003 produced in the model more and less intense oxygenation than observed, respectively. There is a range of reasons why the chronology and magnitude of deep-water renewals are not captured perfectly. The primary reason being the complex sequence of flow and mixing events that in the end product needs to be accurate within less than 1/10th of a *per mille* in salinity. Errors in forcing and simplifications in

description of dynamics as well as the limited spatial resolution put thus a limit on the possible accuracy. The integrated consequences of these model-data differences are also found in a comparison of hypoxic area and cod reproductive volume computed from simulations and reconstructed from observations (see Fig. 18 below).

As can be expected from the tight cause-effective relationships between oxygen and nutrient dynamics (*e.g.* Savchuk, 2010), these discrepancies in timing and duration of the redox alterations can also be seen in time-depth variations of nutrients because the decrease of oxygen concentration induces reduction of the nitrate pool due to denitrification and increase of the phosphate pool by the phosphorus released from anoxic bottoms. However, despite of multiple tuning experiments we still cannot overcome an almost two-fold difference between simulated and observed phosphate concentrations in the deepest layers of this basin.

This comparison of picturesque contour plots is also meant to give a better understanding of what might lay behind the relative biases computed as a quantitative measure of model-data disagreement for all abiotic variables in all basins at seasonal to decadal scales (Fig. 13).
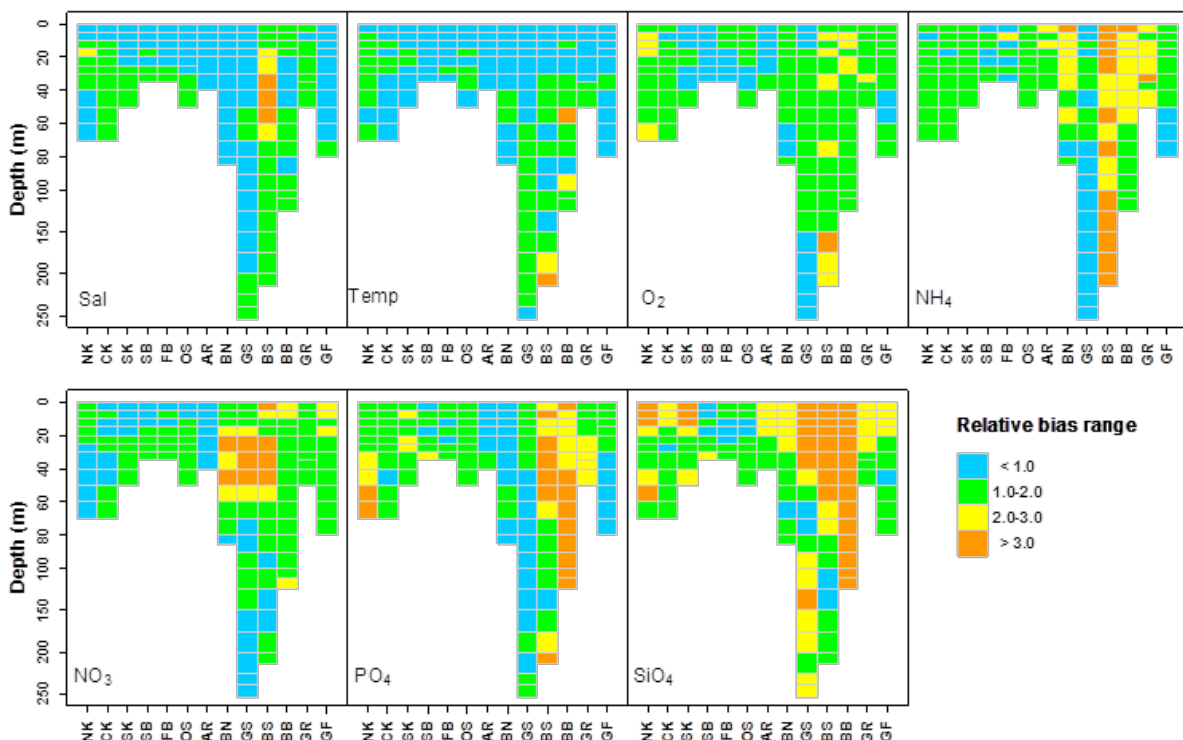

Fig. 13. Spatial distribution of the relative bias between simulated and observed dynamics of BALTSEM variables. Comparisons are made for *Sal* – salinity, *Temp* – water temperature, and concentrations of O_2 – oxygen, NH_4 – ammonium, NO_3 – nitrate, PO_4 – phosphate, SiO_4 – silicate. For abbreviated basin names see Fig. 1

According to Fig. 13, BALTSEM provides a good description of temperature, salinity and oxygen concentrations in all basins. In the deeper part of the Gotland Sea, the model underestimates water temperatures during the 1996-2003 stagnation period, when simulated water temperatures are up to 2 K colder than observed. Deviations also occur in the Bothnian Sea, where waters above the halocline are in the model fresher by about 0.2 – 0.4 PSU. The

model also has difficulties in simulating the temporal dynamics of inflows from the Baltic Proper into the Bothnian Sea. Simulated deep water salinities decline almost continuously during the entire hindcast period, while in the data a decline between the mid-1970s and 1990s was followed by shorter undulations until the significant increase in 2003-2004. Simulated deep water oxygen concentrations are overestimated by about $1 - 2$ mL L^{-1}, especially towards the end of hindcast.

Although BALTSEM mostly simulates nitrate and phosphate concentrations within $1.0 - 2.0$ standard deviations of the monthly data, nitrate underutilization during the vegetative season (cf. Fig. 5) is especially pronounced in the Baltic Proper and the Bothnian Sea. The higher relative biases of nutrient dynamics found in the surface layers of the gulfs are due to the same BALTSEM deficiencies as depicted by Taylor's diagrams (cf. Fig. 6) and discussed above. Particularly, the simulated phosphate concentrations were intentionally overestimated in the entire water column of the Bothnian Bay.

Generally, the reliability of bias in surface ammonium concentrations is difficult to evaluate since low ammonia concentrations are measured in the field with a large uncertainty. The high relative bias of ammonium concentration in the water column of the Bothnian Sea is caused by elevated concentrations (up to 3 mmol N-NH4 m^{-3} in the deep layers) measured here in the well oxidized environments, whereas in the BALTSEM simulation all regenerated ammonium is quickly nitrified in such conditions.

Since silica does not limit primary production in the Baltic Sea and would primarily affect only the species composition of the phytoplankton spring bloom, less attention has been given to tuning silica fluxes in the model. The relative bias for silicate is largest in the Gotland Sea and Bothnian Sea, where simulated silicate concentrations are overestimated in the surface layer and underestimated in bottom waters, and in the Bothnian Bay, where the concentration is overestimated throughout the entire water column.

As already was mentioned in Section 2.3.2, the relative bias values in Fig. 13 cannot be compared to the cost function values presented by Eilola *et al.* (2011a, see Figs. 12-13 and Table 5 there). However, evaluation of cost functions computed strictly according to Eilola (2011a) shows that the latest calibration of BALTSEM resulted in a minor improvement of the global average of the cost function from 0.69 to 0.66, mostly because of improved simulation of phosphate in the Bothnia Bay, which reduced average cost function for phosphate from 1.61 down to 1.06.

3.2.2 Dynamics of pelagic and sediment nutrient pools

Considering eutrophication development as a consequence of positive imbalance between nutrient inputs and sinks that results in accumulation of the internal bioavailable nutrient pools, the comparability of long-term dynamics of basin-wide pools and biogeochemical fluxes estimated from both simulations and observations is an important indicator of the model's performance. According to its formulation and set-up, BALTSEM describes the dynamics of only bioavailable nutrients, comprising inorganic compounds and labile fraction

of organic nutrients. Especially important is the distinction between total amount and its refractory fraction in the nitrogen loads and internal pools, a significant part of which consists of dissolved humic substances, rather resistant to mineralization and, thus, almost excluded from biological cycling and hardly playing any role in eutrophication. For instance, Vähätalo and Zepp (2005) found that over 72% of dissolved organic nitrogen was recalcitrant to biological mineralization. According to our unpublished estimates, refractory fraction in the Baltic Proper and Bothnian Sea constitutes 60-70% of total nitrogen and its concentration is rather invariable in space and time. On the other hand, almost all the phosphorus compounds are eventually biodegradable (*e.g.* Stepanauskas *et al.*, 2002; Nausch and Nausch, 2006; Ekholm *et al.*, 2009) and contribution of the refractory fraction to the total phosphorus is assumed to be insignificant. Therefore, in the following evaluation we compare simulated pools to the pools of DIN and TP, estimated from observations (Table 5). Also, while considering the different indices of model-data comparability, one should bear in mind that deterministic simulated pools are computed by true integration of simulated concentrations over basin domains, whereas estimates of annual pools reconstructed with DAS from measurements are subject to several sources of unknown and varying uncertainty (see, *e.g.* Savchuk 2010).

Table 5 Comparison of annual nutrient pools, simulated and estimated from the data

Basin	BB	BS	BP	GF	GR	DS	KT	Total
Ratio between long-term (1970-2006) averages of simulated and observed pools								
DIN/DIN	0.99	1.20	0.80	1.07	1.19	0.52	0.98	0.91
N_{bio}/DIN	1.03	1.38	0.98	1.39	1.47	0.87	1.36	1.10
P_{bio}/TP	0.57	0.92	0.90	0.96	0.84	0.50	0.94	0.89
Coefficient of linear correlation								
DIN/DIN	0.57	0.73	0.54	0.34	0.24	0.05	0.12	0.66
N_{bio}/DIN	0.59	0.73	0.59	0.40	0.26	0.21	0.13	0.69
P_{bio}/TP	0.32	0.69	0.53	0.46	0.51	0.27	0.36	0.61
Relative bias built on annual values								
DIN/DIN	0.64	0.76	1.04	0.83	1.27	1.65	0.79	0.66
N_{bio}/DIN	0.61	1.21	0.74	1.09	1.53	0.83	1.42	0.60
P_{bio}/TP	1.98	0.62	0.98	0.69	1.28	2.80	1.67	1.03
Theil's inequality index								
DIN/DIN	0.091	0.135	0.157	0.188	0.249	0.359	0.145	0.090
N_{bio}/DIN	0.090	0.182	0.099	0.223	0.279	0.168	0.194	0.081
P_{bio}/TP	0.265	0.074	0.083	0.115	0.137	0.428	0.155	0.084

Note: comparisons are made between pools of simulated and observed DIN (DIN/DIN), simulated bioavailable nitrogen and observed DIN (N_{bio}/DIN), and simulated bioavailable phosphorus and observed total phosphorus (P_{bio}/TP)

As can be expected from a choice of variables to compare, simulated DIN and bioavailable nitrogen pools are generally slightly smaller and larger, respectively, than observed DIN pool. Simulated bioavailable phosphorus pool is always smaller than observed TP pool. However, for the entire Baltic Sea the differences are in the order of 10%, which can be regarded as a minor deviation considering both the uncertainties of pools' reconstruction

from observations with DAS and BALTSEM deficiencies, already indicated in previous Sections and highlighted here by different quantitative measures of the model performance.

As indicated by a combination of different indices, the large-scale nutrient dynamics is most reasonably described in the Baltic Proper and Bothnian Sea, the two largest basins with long nutrient residence times implying significant inertia. Less satisfactory BALTSEM performance seems to be in the Gulf of Riga and, especially in the Entrance area with its well-flushed small basins, where even the applicability of annual averaging can be questioned because of the short residence times, significantly shorter than a year.

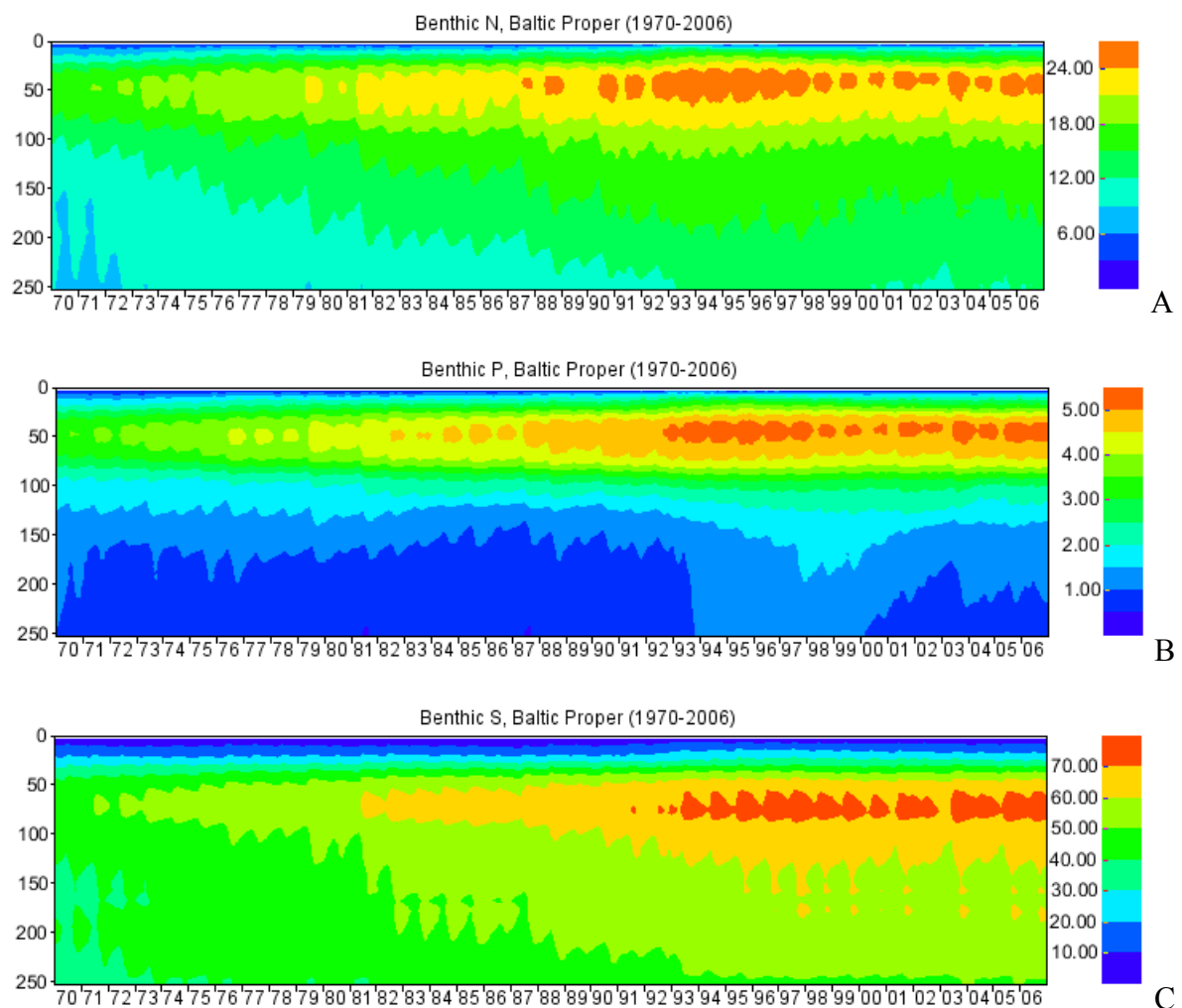Long-term dynamics of sediment nutrients are also exemplified for the Gotland Sea (Fig. 14).

Fig. 14 Simulated dynamics of benthic nitrogen (A, g N m^{-2}), phosphorus (B, g P m^{-2}), and silica (C, g Si m^{-2}) in the Gotland Sea

As has already been shown and validated with available observations by Savchuk and Wulff (1996; 2001), the vertical distribution of areal concentrations with its intermediate maximum is different from a more common perception of "accumulation-with-depth", which is based on presentation of nutrient concentration in g/g units resulting in the higher values found in muddy, mostly deep water sediments that actually on 95-99% consist of water and, thus,

contain rather low nutrient pools. In BALTSEM, the shape of simulated vertical distribution is determined by an imbalance between nutrient inputs to the sediments due to sinking of particles (phytoplankton and detritus) vs. nutrient sediment sinks due to burial and redox dependent biogeochemical processes. For example, due to a faster sinking of diatoms and their remnants the silica maximum in the Gotland Sea sediments is situated at about 75 m depths, that is deeper than nitrogen and phosphorus maxima at about 50 m. Larger amplitude of temporal variation of sediment phosphorus in the deepest layers compared to the variations of nitrogen and silica is generated by redox alterations that augment retention of phosphate in the oxic conditions and its release in anoxia.

Amplitude of seasonal variations of simulated sediment nutrient concentrations exceeds 10% only at very shallow bottoms (less than 5-10 m water depth), which actually contain very little nutrients. The amplitudes are much smaller than inter-basin differences created by the gradients of productivity, water temperature, and dissolved oxygen concentrations (Fig. 15). Correspondingly, the sediments are depleted of phosphorus in the often anoxic deeps of the Gotland Sea and enriched with phosphorus in the well oxygenated Bothnian Bay due to the high retention capacity.
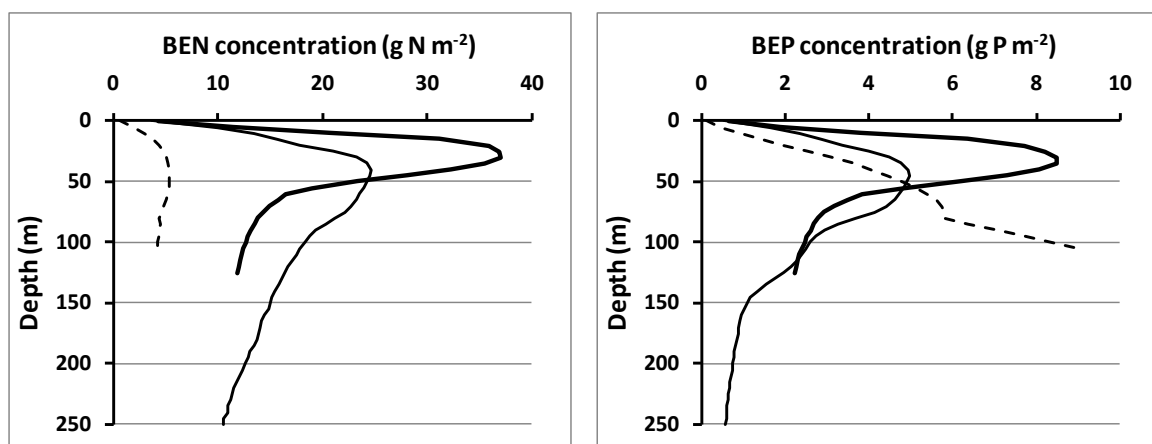

Fig. 15 Distribution of simulated sediment nitrogen (left) and phosphorus (right) along the bottom slopes in the Central Kattegat (thick curve), Gotland Sea (thin curve), and Bothnian Bay (dashed curve).

A comparison of simulated nutrient sediment content to estimates derived from measurements is far from straightforward and is highly uncertain because of very patchy distributions (*e.g.* Winterhalter, 2001; Hille, 2005). Besides, there are almost no evaluations enveloping the entire basins, for instance, for the Kattegat and Danish Straits such generalized estimates are lacking. Even comparison between the basin-wide integral pools compiled in Table 6 requires an additional interpretation. Although the benthic variables BEN and BEP are vaguely described as occupying the active surface layer of sediments, the mathematical formulations do not involve an exact specification of its thickness, which in reality is determined by many factors and has uneven distribution as well. Because the total

Table 6 Simulated and estimated from measurements pools of nitrogen and phosphorus in the Baltic Sea sediments (10^3 tonnes N and P)

Basin	BB	BS	BP	GF	GR	DS	KT
BEN	146	684	4205	704	478	519	505
TN	246	543	2441	374	178		
BEN/TN	*0.6*	*1.3*	*1.7*	*1.9*	*2.7*		
BEP	124	136	740	151	103	105	102
TP	151	316	691	160	99		
BEP/TP	*0.8*	*0.4*	*1.1*	*0.9*	*1.0*		

Note: BEN and BEP – long-term averages (1970-2006) of simulated integral pools of bioavailable nitrogen and phosphorus, respectively, in the surface "active" sediment layer of undefined thickness; TN and TP – basin-wide integral pools of total nitrogen and phosphorus, respectively, estimated for the uppermost centimeter of sediments from a comprehensive compilation by Carman and Cederwall (2001)

nitrogen content of the sediments consists mostly of organic nitrogen (*e.g.* Carman *et al.*, 1996; Carman and Rahm, 1997), assumed eventually bioavailable, the ratio BEN:TN implies that typical thickness of homogeneous surface layer is around 2 cm, at least, southwards of the Gulf of Bothnia. For the sake of consistency, the same layer thickness must be pertinent to BEP as well. However, the bioavailable fraction of total sediment phosphorus is significantly smaller, comparing to nitrogen. Within different definitions and methods of fractionation, the mobile fraction of P in surface sediments, comprising organic P, loosely sorbed P, and iron-bound P, varies in the range of 50 – 80 % (*e.g.* Carman and Jonsson, 1991; Jensen *et al.*, 1995; Carman *et al.*, 1996; Carman and Rahm, 1997; Lehtoranta, 2003; Mort *et al.*, 2010). Factoring this fraction in the ratio BEP:TP would result in values closer to the same 2 cm. Therefore, we consider simulated total pools of about 7-8 million tonnes of nitrogen and 1.4-1.6 million tonnes of phosphorus a plausible estimate of the bioavailable nutrient stocks residing in the Baltic Sea sediments nowadays (Fig. 16 below). Unfortunately, the available information about silica occurrence in the sediments of different basins is too sparse and less reliable for similar integral estimates (but see *e.g.* Conley *et al.*, 2008).

As was already demonstrated in the long-term hindcast of the Baltic Sea trophic state (Gustafsson *et al.*, 2012), nutrients had been accumulating in the sediments until leveling off since the mid-1990s (Fig. 16), that is with a few years delay after beginning of a general reduction of the external nutrient loads in the 1980s (cf. Fig. 3 above). Temporal evolution of sediment nutrients in this report differs from the dynamics presented by Eilola *et al.* (2011a), where we prescribed initial pools as almost double of the ones used here (Fig. 17). These larger initial sediment pools generated then a spin-up adjustment to initial pelagic pools estimated from observations (see Sect. 2.2.1) and, thus, considered more reliable and kept identical in both simulations. However, even after initial spin-up a significant difference between these two simulations remains until the end of numerical experiments, thus implying that feedbacks from the relatively enriched sediments were augmented enough to keep the entire system at a higher trophic state necessary for maintaining similar pace of sediment accumulation.
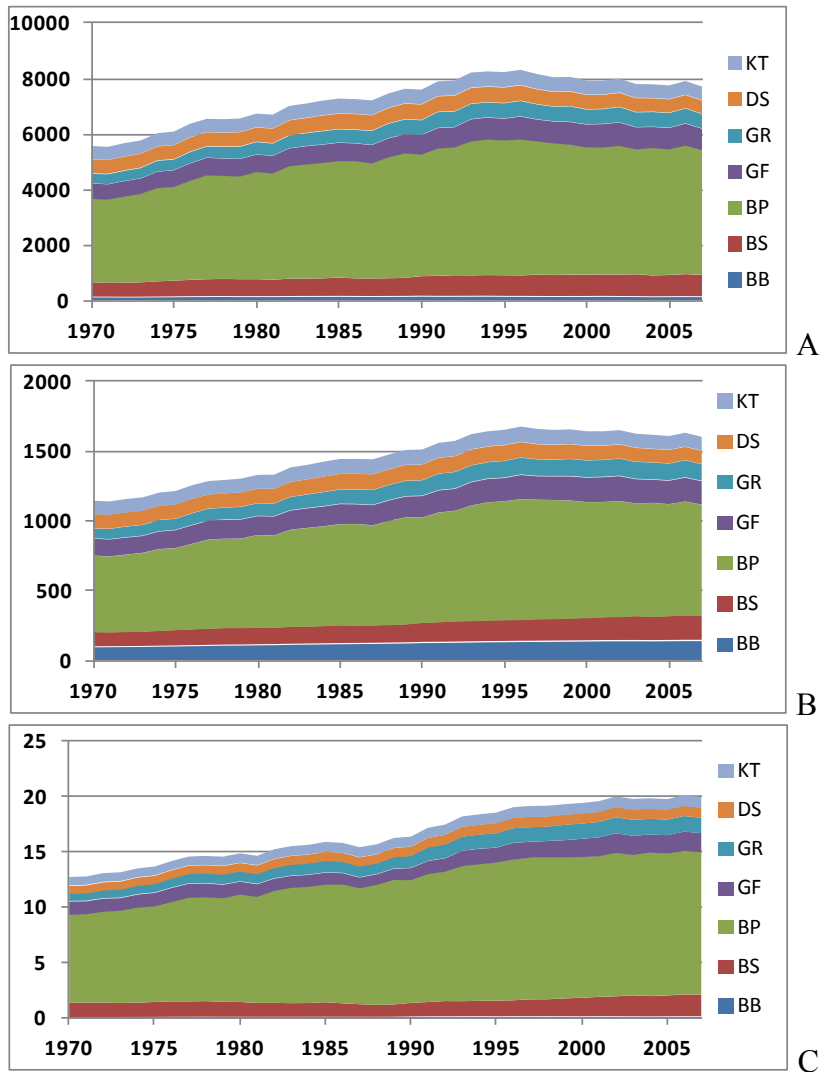
Fig. 16 Long-term dynamics of simulated nitrogen (A, 10^3 tonnes), phosphorus (B, 10^3 tonnes) and silica (C, 10^9 tonnes) pools in the Baltic Sea major basins. For abbreviated basin names see Fig. 1
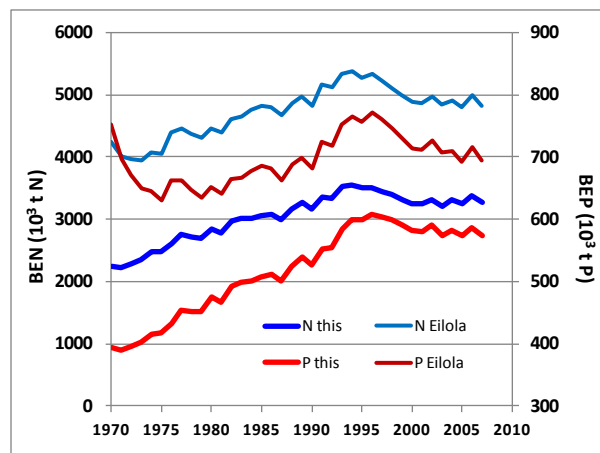

Fig. 17 Nutrient pool dynamics in the Gotland Sea sediments emerged from simulations presented both in this report and by Eilola *et al.* (2011a)

Unfortunately, a judgement about higher plausibility any of these two simulations cannot be supported by the available real-world field data on sediment nutrients. Although recent acceleration of nutrient accumulation is evident from many studies (*e.g.* Jonsson and Carman, 1994; Emeis *et al.*, 2000; Hille, 2005; Conley *et al.*, 2008; Mort *et al.*, 2010), neither temporal resolution of dated cores, nor spatial resolution and accuracy of analysis based on sparse sampling of mosaic distributions are sufficient enough for necessary justification of such a judgement.

3.2.3 Long-term dynamics of integral characteristics

The studies of the Baltic Sea eutrophication, particularly its effects on fishery and responses to nutrient load reductions and climate variations, benefit from analysis of some complex relationships established from observations. For instance, the so-called "cod reproductive volume", defined as comprising waters with salinity over 11 PSU and oxygen concentration higher than 2 mL O_2 L^{-1}, is used in ichthyologic and fishery studies, including development of scenarios (*e.g.* MacKenzie *et al.*, 2000; Niiranen *et al.*, 2012; Tomczak *et al.*, 2012); the hypoxic area and volume, which are defined here as confining the waters containing no more than 2 mL O_2 L^{-1}, are used in studies of redox alterations of biogeochemical cycles (*e.g.* Conley *et al.*, 2002; Vahtera *et al.*, 2007a; Savchuk, 2010). Apparently, BALTSEM capability to realistically simulate such integral characteristics, whose dynamics is determined by a combined interaction of physical and biogeochemical processes, can be considered as an important test of the model performance.
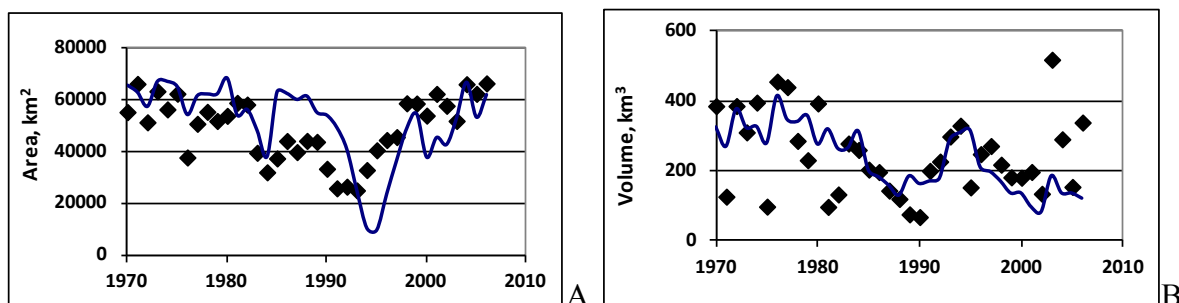

Fig. 18. Variations of hypoxic area (A) and cod reproductive volume (B) in the Baltic Proper simulated with BALTSEM (curve) and computed from three-dimensional annual average fields (symbols) reconstructed with DAS from observations

Considering limitations and discrepancies of simulated salinity and oxygen dynamics discussed above in Sect. 3.2.1, the variations of hypoxic area and cod reproductive volume computed from simulated characteristics compare rather well to those derived from observations (Fig. 18). In quantitative terms, the comparability between estimated from observations and simulated time series are characterized by linear correlation coefficients of 0.5 and 0.45, and by the relative biases of 1.1 and 0.7, respectively.
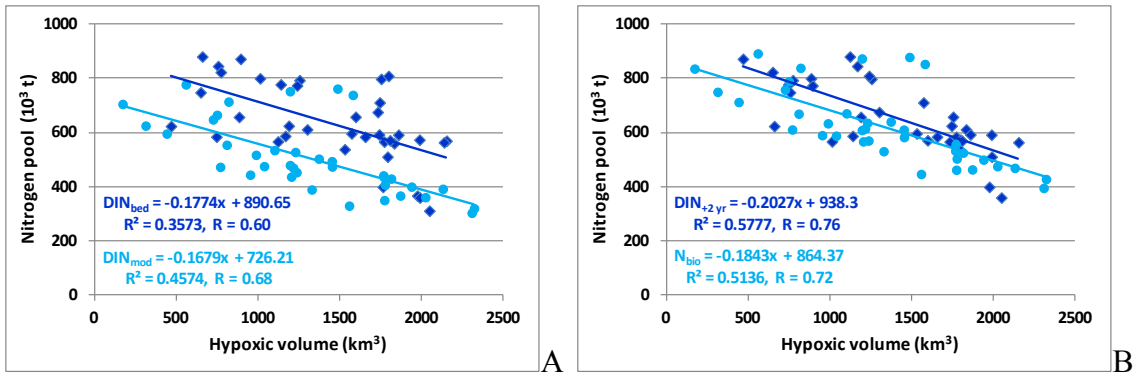
Fig. 19 Hypoxia effects on nitrogen pool in the Baltic Proper. Relationships between annual means of simulated and reconstructed from observations hypoxic volume and DIN pool (A) or reconstructed DIN pool with a 2 year delay and simulated bioavailable nitrogen (B)

The negative relationship between hypoxic volume and DIN pool had been found from the annually averaged three-dimensional fields of oxygen and inorganic nitrogen compounds (Vahtera *et al.*, 2007a; Conley *et al.*, 2009; Savchuk, 2010) and was recently questioned (Heitanen *et al.*, 2012; Jäntti and Hietanen, 2012). Here we compare the empirical relationship with that built on BALTSEM simulation (Fig.19) and conclude that appropriate simulation of expansion and shrinkage of the hypoxic and anoxic zones resulting in correspondent variations of denitrification, from complete shutting down to augmentation, can be considered as an additional justification of BALTSEM validity. Remarkably, both a 2 year delay of DIN time series relatively to hypoxic volume in field data, suggested also in Savchuk (2010), and usage of simulated bioavailable nitrogen N_{bio} instead of simulated DIN considerably increase correlations.
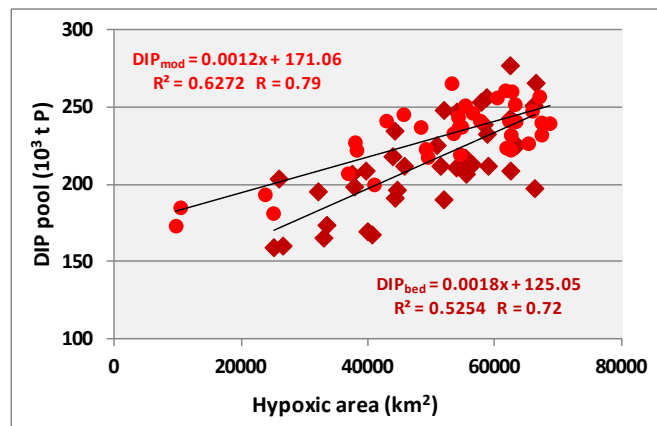
Fig. 20 Hypoxia effect on the deep-water (> 60 m) phosphorus pool in the Baltic Proper. Relationships between annual means simulated (sum of BN and GS pools) and reconstructed from observations for the Baltic Proper hypoxic area and DIP pool

A relationship between changes of hypoxic area and phosphate pool have first been established by Conley *et al.* (2002) and was further expanded by Savchuk (2010), who also found a straightforward and even stronger relationship between hypoxic area and deep-water phosphate pool (Fig. 11b in Savchuk, 2010) similar to those presented in Fig. 20, only for the

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larger area, including also the Gulf of Finland and Gulf of Riga. Importantly, despite the visually substantial underestimation of simulated concentrations in the deepest layers seen in Fig. 12 above, the simulated integral pool is comparable if not even larger than the pool reconstructed from observations.

3.2.4 Long-term dynamics of annual nutrient uptake

Unfortunately, there are no long-term time series for any of biogeochemical fluxes based on measurements and suitable for comparison to BALTSEM simulation. Therefore, here we just demonstrate the dynamics of basin-wise nutrient uptake (Fig. 21) as the major bottom-up connector between abiotic and biotic parts of the ecosystem that to a great degree determines a temporal pattern of other important fluxes (see *e.g.* Figs. 6 and 7 in Gustafsson *et al.*, 2012).
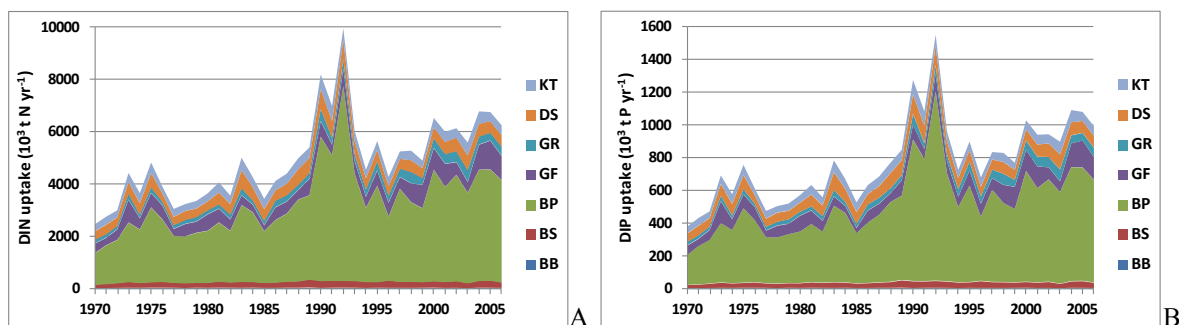

Fig. 21 Simulated dynamics of annual dissolved inorganic nitrogen (A) and phosphorus (B) uptake in the Baltic Sea major basins. Note that nitrogen fixation is not included in DIN uptake but is accounted for in DIP uptake. For abbreviated basin names see Fig. 1

Both these graphs clearly emphasize the dominating contribution of the Baltic Proper in the overall nutrient cycling in the Baltic Sea, albeit the not entirely coinciding temporal patterns indicate some decoupling of other basins' dynamics. However, the most conspicuous feature is the large increase of nutrient uptake in the Baltic Proper during 1989 – 1993, together with nitrogen fixed by cyanobacteria peaking in 1992 with 8 million t N annually that would correspond to the primary production of 214 g C m^{-2} yr^{-1}. In BALTSEM, the reason for this increase is a strong augmentation of nitrogen fixation (Fig. 22) and, consequently the summer nutrient recycling (see also Fig. 10 above and Gustafsson *et al.*, 2012) that, in turn, was propped up by elevated phosphate excess resulted from the long stagnation in the 1980s (cf. Fig. 12 above).
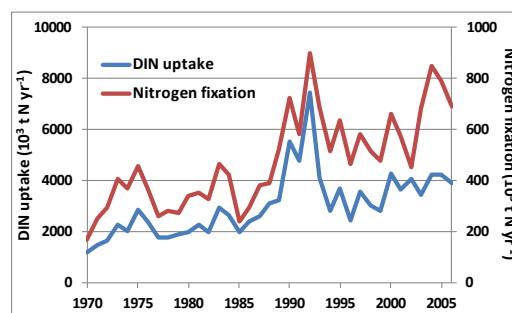

Fig. 22 Simulated dynamics of annual DIN uptake and nitrogen fixation in the Baltic Proper

The different aspects of this strong coupling between nitrogen fixation and primary production as well as their hypoxia mediated interdependence have been studied in the Baltic Sea since long time ago (*e.g.* Savchuk, 1986; Savchuk and Wulff, 1996; 1999; 2001; 2007; Vahtera *et al.*, 2007a; Savchuk 2010; and references therein). Unfortunately, the recent time series of the frequency of cyanobacteria accumulations has a gap over 1985-1997 (Kahru *et al.*, 2007). However, both corrected and uncorrected satellite time series of cyanobacteria accumulations indicated a large increase in the beginning of 1990s compared to the 1980s (Kahru *et al.*, 1994, Kahru, 1997), which correlates to simulated nitrogen fixation with the coefficient r = 0.57.

3.3 Nutrient budgets

The essential presentation of BALTSEM performance are the nutrient budgets combining external inputs, internal interactions, and advective exchange that are integrated here both for the entire Baltic Sea (Fig. 23) and for its major basins (Tables 7 – 10) over 1994 – 2006 time interval as ensured with more reliable estimates of the external nutrient loads (cf. Sect. 2.2.3 and Savchuk *et al.*, 2012).

A

	N fixation	Atm dep	Landload
	607	262	529
		6.2	40

<= to Ska	Uptake		Recycling
135	5693		4405
28	900		654

fr Ska =>	Sinking		Output
122	1992		706
23	264		230

	Burial	Denitrification
	174	1253
	36	

B

	N fixation	Atm dep	Landload
	1.5	0.6	1.3
		0.0	0.1

<= to Ska	Uptake		Recycling
0.3	14		10.6
0.1	2.2		1.6

fr Ska =>	Sinking		Output
0.3	4.8		1.7
0.1	0.6		0.6

	Burial	Denitrification
	0.4	3.0
	0.1	

Fig. 23 Average (1994 – 2006) annual budgets of bioavailable nitrogen (blue) and phosphorus (red) for the entire Baltic Sea, presented in 10^3 tonnes (A) and g m^{-2} (B). See Table 7 below for definitions

In addition to estimates of the primary production based on measurements and compared in Table 2 to simulated values, there are also a few estimates of other fluxes of comparable aggregation and scale.

Several published estimates of the annual nitrogen fixation are related only to the Baltic Proper and cover the range of 180 – 434 10^3 t N yr^{-1} (Larsson *et al.*, 2001; Wasmund *et al.*, 2001b; 2005b) that is fully correspond to simulated fluxes.

The latest estimates of integral sediment denitrification of 426 and 652 10^3 t N yr^{-1} made for the entire Baltic Sea and differing by 50% are based on the same set of measurements performed at 11 sites in various times during summer-autumn 2008 (Deutsch *et al.*, 2010) and differ only due to assumptions implemented for calculations. In BALTSEM simulation, the sediment denitrification removes 1144 ± 23 10^3 t annually. One of the reasons of this two-three fold difference is the implementation by Deutsch *et al.* (2010) of extremely low

Table 7 Simulated annual fluxes (10^3 tonnes) of bioavailable nitrogen in the Baltic Sea basins (mean ± sd, 1994-2006)

	BB	BS	BP	GF	GR	DS	KT
Atm. dep.	9.8 ± 1.6	29 ± 5	152 ± 18	12 ± 1.8	11 ± 1.5	26 ± 3	22 ± 3
Land loads	29 ± 6	35 ± 6	250 ± 57	75 ± 9	50 ± 11	40 ±16	52 ± 12
N_2 fixation	0	17 ± 9	431 ± 106	52 ± 13	31 ± 8	49 ± 9	26 ± 9
Uptake	28 ± 4	238 ± 28	3556 ± 610	697 ± 237	350 ± 62	449 ± 58	373 ± 62
Recycling	9.5 ± 1.3	101 ± 15	2918 ± 661	569 ± 226	251 ± 60	331 ± 61	225 ± 64
Sinking	32 ± 4	172 ± 21	1130 ± 87	195 ± 33	140 ± 16	165 ± 9	158 ± 7
Sed. output	14 ± 0.5	70 ± 2	393 ± 27	71 ± 6	54 ± 2	52 ± 3	158 ± 7
Burial	3.2 ± 0.1	17 ± 0.3	102 ± 3	17 ± 0.5	12 ± 0.2	11 ± 0.6	11 ± 0.5
Denitrific.	16 ± 0.6	85 ± 3	769 ± 60	104 ± 7	74 ± 4	108 ± 5	98 ± 4

Notes: for abbreviated basin names see Fig. 1; *Atm. dep.* – atmospheric deposition, *Land loads* – sum of river loads and direct sources, *N_2 fixation* – nitrogen fixation by cyanobacteria, *Uptake* – sum of ammonium and nitrate uptake by phytoplankton, *Recycling* – sum of zooplankton excretion and detritus mineralization, *Sinking* – sum of phytoplankton and detritus sedimentation, *Sed. ouput* – release from the sediments into the water column; *Burial* – permanent loss due to sediment burial, *Denitrific.* – sum of pelagic and sediment denitrification

denitrification rates, in the order of 0.3 – 3.0 mg N m^{-2} d^{-1}, for calculation of nitrogen removal over vast shallow areas. These values are one to two orders of magnitude smaller than the median of 21 mg N m^{-2} d^{-1} and average of 31 mg N m^{-2} d^{-1} calculated from a rather impressive data set compiled for the shallow oxic bottoms (Fennel *et al.*, 2009), which also justify our simulated rates (cf. Fig. 9C above). However, estimates of pelagic denitrification of 200 – 300 10^3 t N yr^{-1} (Deutsch *et al.*, 2010), which are a double or triple of simulated 109 ± 75 10^3 t N yr^{-1}, would bring total nitrogen removal by denitrification closer to counteracting external inputs, including nitrogen fixation (cf. Fig. 23).

Table 8 Simulated annual fluxes (10^3 tonnes) of bioavailable phosphorus in the Baltic Sea basins (mean ± sd, 1994-2006)

	BB	BS	BP	GF	GR	DS	KT
Atm. dep.	0.6	1.0	3.0	0.4	0.3	0.3	0.3
Land loads	2.6 ± 0.6	2.4 ± 0.6	19 ± 5	8 ± 1	4 ± 1	1.4 ± 0.5	1.6 ± 0.4
Uptake	4 ± 0.6	36 ± 5	570 ± 99	107 ± 35	55 ± 9	71 ± 9	57 ± 10
Recycling	1.6 ± 0.2	17 ± 2	433 ± 95	84 ± 32	37 ± 8	48 ± 9	33 ± 9
Sinking	4 ± 0.6	22 ± 3	147 ± 11	27 ± 5	20 ± 2	23 ± 1	21 ± 1
Sed. output	0.3 ± 0.0	16 ± 0.6	132 ± 5	23 ± 1	17 ± 0.7	21 ± 1	20 ± 0.7
Burial	3.1 ± 0.0	4 ± 0.2	18 ± 0.5	4 ± 0.1	2.6 ± 0.0	2 ± 0.1	2.3 ± 0.1

Note: for explanations see Table 7

The description of only bioavailable fraction of nutrient cycling in BALTSEM prevents quantitative comparison with other budget estimates made for the total nitrogen and total phosphorus including their refractory fractions (*e.g.* Wulff *et al.*, 2001b, Savchuk, 2005; Savchuk and Wulff, 2007). Qualitatively, the main conclusion following from the major transport and transformation fluxes simulated with BALTSEM remain the same: since the rates of internal biogeochemical processes are one to two orders of magnitude larger than

external inputs and advective fluxes (Fig. 23 and Tables 7 – 10), the trophic status of the entire sea and its basins would respond slowly to any external perturbations either anthropogenic or induced by climatic changes.

Table 9 Simulated annual flows (10^3 tonnes) of bioavailable nitrogen between the major Baltic Sea basins (mean ± sd, 1994-2006)

	BB	BS	BP	GF	GR	DS	KT
BB		25 ± 1					
BS	6 ± 0.70		30 ± 4				
BP		30 ± 3		28 ± 5	5 ± 0.6	62 ± 9	
GF			43 ± 5				
GR			10 ± 2				
DS			47 ± 8				105 ± 17
KT						88 ± 10	

Note: flows are directed from row basin to column basin;   from North Sea: 122 ± 18, to North Sea: 135 ± 19

Table 10 Simulated annual flows (10^3 tonnes) of bioavailable phosphorus between the major Baltic Sea basins (mean ± sd, 1994-2006)

	BB	BS	BP	GF	GR	DS	KT
BB		0.8 ± 0.1					
BS	1.3 ± 0.2		6.4 ± 0.9				
BP		8.9 ± 0.6		8. 6 ± 1.0	1.4 ± 0.2	16 ± 2.3	
GF			12 ± 2				
GR			2.6 ± 0.3				
DS			12 ± 1.5				26 ± 1.8
KT						21 ± 1.5	

Note: flows are directed from row basin to column basin;   from North Sea: 23 ± 2.7, to North Sea: 28 ± 1.7

4 Conclusions

The coupled physical biogeochemical model BALTSEM has been developed as a tool to study the nitrogen, phosphorus, and silica cycles in the Baltic Sea driven by external forcing functions and internal interactions at basin-wide scales. As justified by comparison of hindcast simulations to available data, BALTSEM reproduces both inter-basin spatial gradients and temporal variations at seasonal to long-term scales realistically enough to confidently serve as a tool for studies of the Baltic Sea eutrophication, including scenario simulations. Particularly, the nutrient budgets constructed from the simulated fluxes for the major basins of the Baltic Sea can be used as a common platform to bring together and test a mutual coherence of the available information on concentration and fluxes acquired within different scientific disciplines.

At the same time, in its current state BALTSEM performance suffers a few deficiencies deserving special attention during further development and calibration: a) at a current state of calibration with available forcing functions BALTSEM is not capable yet to reproduce exact timing of events occurred at the concrete time interval of 1970 – 2006; b) realistically

reproduced phosphorus limitation in the Bothnian Bay does not allow to reach in the model the observed depletion of DIN pool and reported levels of the primary production; c) possible underestimation of DIN utilization during the vegetative season in the Gotland Sea may result in some underestimation of the primary production; d) underestimated phosphate concentrations in the anoxic zone of the Baltic Proper compared to observed may indicate at underestimated downward transports of phosphorus.

However, as might be deduced from successful reproduction of the major large-scale features, especially from the realistic dynamics of nutrient pools, these minor deficiencies could hardly significantly affect BALTSEM quantitative responses to external perturbations, including scenario simulations of the nutrient load reductions.

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