Dear Editor,

Please find herewith our revised manuscript “Nutrient transport in the Baltic Sea – results from a 30-year physical-biogeochemical reanalysis” for Biogeosciences.

We remain at your disposal for any further enquiries.

Interactive comment on “Nutrient cycling in the Baltic Sea – results from a 30-year physical-biogeochemical reanalysis” by Ye Liu et al.

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We thank Dr. Savchuk for your very good comments. We have followed all the comments from you and carefully made the improvement in our revision.

The study deals with application of data assimilation approach to reconstruction of long-term dynamics of 3D nutrient fields as a base for analysis of nutrient transport processes in the Baltic Sea. Both the approach and obtained results are significantly novel in methodological and geographical senses to deserve publishing in “Biogeosciences”. However, scientific and presentation qualities should be substantially improved by the major revision of the manuscript along the lines suggested below.

1. General comments and suggestions

1.1 Objectives and applicability. The assimilation of whatever available data is fully justified for an improvement of short-term forecasting of hydrophysical fields aiming at the search-and-rescue operations, propagation and expansion of catastrophic spills as well as management of the maritime activity. However, its applicability for long-term hindcasts of biogeochemical phenomena and properties requires careful consideration and clear explanation of the purposes/objectives of the assimilation (why and what for). Such considerations and explanations should already be given in the Introduction section, with particular attention to the limitations, especially non-conservativeness of the approach (what can and cannot be done).

Response: We have specified the aims of data assimilation in the introduction more clearly. The data assimilation meets the gap between observations and numerical modeling in this study. We aim to reproducing the ocean biogeochemical state with the help of information from both observations and a coupled physical-biogeochemical model. The results of the reanalysis can be used to estimate the water quality and ecological state with high spatial and temporal resolution in regions and during periods when no measurements are available. Regional and local model studies may use the data as initial and boundary conditions. Further, nutrient transports across selected cross-sections or between vertical layers might be calculated with high resolution and accuracy taking the complete dynamics of primitive equation models into account. This information cannot be obtained from neither observations alone or from model results without data assimilation because the latter might have large biases in both space and time. We assess the nutrient budgets of the water column and sediments, as well as of the nutrient exchanges between subbasins and between the coastal zone and the open sea. As a reanalysis can never be dynamical consistent and does not preserve mass, momentum and energy (see our response to 1.2), the calculated budgets are compared to the results of other studies to evaluate our results meant as consistency check. Hereby, we follow studies of other regions applying data assimilation for a biogeochemical reanalysis on long-term scale.

For example, Teruzzi et al. 2014. Journal of Geophysical Research, 119, 1–18.

Ciavatta, S., et al. 2016, J. Geophys. Res. Oceans , 121 , 1824–1845.

Fontana, C., et al.,2013, Ocean Sci., 9, 37-56.

In the introduction section we further clarify the already listed limitations of data assimilation with respect to estimating nutrient budgets and we rewrite the objectives of this study.

1.2 Artificial non-conservation. Biogeochemical variables are non-conservative by definition, while the entire models of biogeochemical cycles are usually designed as conservative, i.e. explicitly accounting for all the external and internal sources and sinks of the matter. In such models (including the implemented RCO-SCOBI system), the dynamics of simulated nutrient fields is determined by continuous, mutually adjusted interaction of physical transport and biogeochemical transformation processes. If these 4D fields (x, y, z, t) are not absolutely identical to the corresponding fields reconstructed from observations, then an every act of "correction" of simulated towards reconstructed fields during assimilation procedure would create in the model fictitious 3D sinks and sources of the matter not generated by either transport or transformation processes. These fictitious fluxes of nutrients are then included into biogeochemical cycles, thus making the model erroneously non-conservative. Evidently, the studies of eutrophication and biological productivity in general are particularly vulnerable for these effects of data assimilation. As can be deduced, for instance, from Figs. 3-5, such effects are quite substantial.

On the other hand, with a certain confidence in simulated transport agents (water currents and mixing) supported, e.g. by the plausible dynamics of "conservative" salinity (e.g. as in Liu et al. 2013), the "corrected" fields of nutrients could be used for improving simulation of nutrient transport processes. Here, again, the discussion on how such improvement would affect simulation of transformation processes and, in turn, would be affected by them could significantly augment the scientific value of the paper. Also, the questions arises – could not the same results regarding transport processes been achieved just with the "observed" nutrient fields used for assimilation, without running and "jerking/correcting" the biogeochemical model.

In any case, the artificial non-conservativeness should be explicitly acknowledged and explained, its effects evaluated, presented, and discussed, in addition to- and, perhaps, together with analysis of biases by means of RMSD. The estimates of non-conservation and its spatial and temporal dynamics must be computed from a difference between model fields before and after acts of assimilation, starting from the initial conditions.Then the knowledge of needed "correction" can also be used in pinpointing possible deficiencies in the biogeochemical parameterizations.

Response: In the long-term simulation, the new initial condition for an assimilation cycle differs from the ending ocean state of the last cycle when at that time observations are available. In this sense, the data assimilation introduces sources and sinks of the nutrient cycles by interrupting the model simulation and adjusting the initial condition. However, we provide the "optimal" initial condition with data assimilation for the RCO-SCOBI for every simulation cycle. It means we don't change the equations of the RCO-SCOBI and just integrate currents and concentrations. The simulation process is conservative during the simulation between two assimilation occasions.

We agree with Dr. Savchuk that the data assimilation affects conservation properties for the long simulation as a whole. Although the reanalysis is conserved during every "independent" simulation cycle, the adjustment of data assimilation implicitly creates unknown complementary sources or sinks to the biogeochemical model. The magnitude of these adjustments depends on the bias between model and observations. The artificial sources/sinks are directly related to the model biases. Figure 3 shows that the model has large biases during the beginning of the simulation. However, data assimilation has corrected the mismatch between model state and observation to an "optimal" level during an initial adjustment period. After the adjustment period, the mismatch between model and observation becomes small and the successive adjustment due to data assimilation also becomes small (Liu et al. 2014). Further, the adjustment of data assimilation is related to the spatial-temporal coverage of observations. Here we assimilated only observed profiles into the model.

The advantage of the data assimilation is that model variables at any station are very likely more accurate than the model output without data assimilation. For instance, time series of profiles or transports across vertical sections have very likely a smaller bias compared to observations than the corresponding model results without data assimilation. Compared to available observations the information from the model is higher resolved and homogeneous in space and time. Of course, it is difficult to evaluate the quality of model results at high resolution because independent observational data sets are usually missing. An exceptional effort to utilize independent data was done by Liu et al. (2014) showing that the statement about the added value of data assimilation is true for the available, independent cruise data at high resolution. However, one can not expect that budgets calculated from the summation of fluxes from model results with data assimilation are more accurate because usually small artificial sources and sinks from the data assimilation are becoming as important as physically motivated sources and sinks when sums of fluxes are compared. Hence, we calculated budgets with the aim to evaluate the reanalysis data and to estimate the magnitude of artificial sources and sinks by comparing our results with other studies using only observations. We are aware that it is impossible to claim that our budgets are more accurate than those budgets that are derived from observations only despite the higher temporal and spatial resolution in model outputs. Hence, the advantage of the reanalysis is that measurements are extrapolated in space and time based upon physical principles of the model. However, the disadvantage is that the reanalysis data does not obey conservation principles. We will discuss advantages and disadvantages of the reanalysis in more detail in the revised version of the manuscript. We add a paragraph to discuss the limit of data assimilation for reanalysis and the artificial non-conservation.

1.3 Plausibility of the RCO-SCOBI model. The RCO-SCOBI model has been extensively used for forecasts (aka projections) of possible changes in the Baltic Sea biogeochemistry under different scenarios of driving forces, practically by the same authors. Therefore, the scientific value of the paper could be significantly increased by the discussion and speculations on how the model's deficiencies in simulation of transport flows and transformation fluxes, which are revealed due to the data assimilation, for instance, in the form of RMSD, could affect the predictions. Good starting point could be a statement at line 387.

Response: RCO-SCOBI has been widely used for the Baltic Sea and the model was carefully evaluated using various observational data sets. As any other model RCO-SCOBI had to be calibrated because many processes including sources and sinks of nutrients are not detailed enough known. Hence, an "optimal" parameterization of unresolved processes is one of the requirements for the predictive capacity of the model. Further requirements to calculate correct transports and transformation processes in addition to optimized model equations are high-quality atmospheric and riverine forcing data, and high-quality initial and lateral boundary conditions.

We discussed already in the present version of the manuscript why FREE has so large biases compared to the results by Liu et al (2014, Tellus A) and compared to biogeochemical observations. Most of the large differences are caused by imperfect initial conditions, which can be seen from the temporal evolution of the RMSD (Figure 3).

For projections of future climate and for nutrient load abatement scenarios the reanalysis has a very high scientific value as reference data set for the historical period of the climate simulations. The evaluation of the regionalized climate (the statistics of mesoscale variability, e.g. the mean state) during the historical period can be done much more accurate based upon the reanalysis data than with sparse observational data. For instance, it is very difficult to calculate the climatological mean state just from observations that are casted only during the ice-free season of the year. Using a reanalysis as reference data for historical climate is a common method in regional climate studies of the atmosphere. Here we provide a corresponding data set for the ocean to evaluate simulated present-day climate. We add a paragraph to the discussion to highlight the value of reanalysis data sets for climate studies.

1.4. Description and explanation of Methods. All the methods implemented in the manuscript must be described in more detail and, considering an intended expansion of the paper's coverage from the "hydrophysical" audience over the "Bio-Geo-Chemical" one, in somewhat more popular style. Assimilation procedure. In addition to references to (Liu et al. 2013, 2014), several details, especially those important for magnitude and distribution of 4D fictitious fluxes, must be repeated and explicitly explained in this paper as well. The explanations should include, for instance, such details as: a) verbal description of procedure for reconstruction of "observed" fields used further in assimilation and in calculation of RMSD in FREE and REAN experiments, b) spatially and temporally varying uncertainties of such fields determined by the scarcity and sparsity of observations, c) frequency of the assimilation acts and its possible effects on the difference between model and observation used in calculation of RSMD (Liu et al., 2014), and whatever else would be necessary for further presentation and discussion of issues from Comment 1.2 above. Without such clarifications, three sentences at lines 170-173 look as isolated abracadabra and might seem almost useless.

Nutrient transports, trends, and budgets. The exact definitions of all the nutrient transports, trends, and budgets measures and characteristics together with algorithms of their calculation, including derived units, should be clearly presented already in Methods. This will clarify possible confusions with the usage and interpretation of the terms vs. phenomena, commented in details below, in Section 2.

Response: We detail and rewrite the text in the method's description according to your comments. See the sections 4 "Methodology and Experimental Setup".

2. Specific comments and suggestions.

2.1 "Cycling" in the title and similar statements to that effect elsewhere Accordingly to comments 1.1-2 above, the non-conservative model cannot be used for comprehensive studies of nutrient CYCLING. Hence, the title should be modified – consider, please, something like "Nutrient TRANSPORTS in the Baltic :::" instead. Correspondingly, the usage of "cycling" and similar statements and expressions about transformation processes should be carefully revaluated throughout the entire text, for instance, at lines 80, 189, 310, 306-307, 362-363, 466, and throughout the entire Section 5.6,

Response: Following your suggestions, we change the text and use nutrient transports instead of nutrient cycles.

2.2 Calculation of RMSD. Line 194 – What is the meaning of "overall" and "monthly mean" in "the overall monthly mean RMSDs" and how they were calculated – for how many fields per month? covering the entire Baltic? cell by cell for interpolated "observational" fields or only for cells with the real observations?

Response: We add the following Equation to specify the calculation process of RMSD in the revised manuscript.

The overall monthly mean RMSD is calculated by the following formula:

$$RMSD = \frac{1}{N_j}\sum_{j=1}^{N_j}\sqrt{\frac{1}{N_t}\sum_{i=1}^{N_t}(\varepsilon_t^i)^2}$$

where N_t is the number of the observations at assimilation time t and N_j are the number of days observed in one month for one field for entire Baltic Sea. $\varepsilon_t^i = x_{sim}^i(t) - x_{obs}^i(t)$ represents the model-observation difference at the time t at the i^{th} observation position. x_{sim} and x_{obs} are the modeled and observed field. We calculated ε_t at only the observation position at the time t, which is calculated by mapping the corresponding model field to the observation space.

2.3 Nutrient transports. Explain and clarify, please, involved terms and interpretations – What does "net" (which is usually used with the word "exchange" and represents a difference between inputs/imports and outputs/exports) mean at lines 17, 259-260, 277, 300, 338, 356, 360, and 492; – Why some characteristics related to single grid cells or a grid "column" are called "net", has it something to do with the difference between in- and out- transport flows or/and is it meant to account for local changes due to transformations, causing difference between inflows to the cell (column) and outflows from it? For instance, at line 694 – How exactly the vertical averages and vertical integrals (e.g. line 259) have been computed? Why ANNUAL average is expressed in ton/ km/MONTH (Fig. 7, lines 694-697)? Would vertical averages multiplied by the depth of grid point be equal to vertical integrals? What is the point presenting/contrasting/comparing (e.g. in Fig. 7) vertically averaged transport for the locations with, for instance, 200 and 20 m depths? – Definitions and explanations for calculations of nutrient sources and sinks from integral transports would be helpful in understanding and interpretation of Section 5.6. Some consideration and discussion on how much the sinks and sources could depend on which transformation processes and how much they would be determined by fictitious fluxes might be useful too. Also, check the consistency of term's usage both in the text and, especially in legend to Figs. 8 and 9 (annual average IMPORT (transports?); again ANNUAL is expressed on per MONTH basis.

Response: We add the following equation to explain the calculation process of the nutrient transports in every grid 'column' or 'cell'. Net transports (VA_{Trans}) are vertically integrated at every grid point at every time step of the integration according to:

$$VA_{Trans} = \sum_{k=1}^{N} C_k u_k \Delta z_k ,$$

where $C_k, u_k, \Delta z_k$ and N are the field (DIP/DIN) concentrations, the current velocity vector, vertical dimensions of a grid cell and the number of wet grid cells in the water column, respectively.

Here the net transports express the difference between inflow and outflow transports. Both "net" and "exchange" are common usage in the description of transport. Just like you mention here the "net" denotes the difference between inputs/imports and outputs/exports. We define "net" in the method part of the revised manuscript.

For example. Eilola et al . Ambio., 41, 574–585, 2012. Treguier et al.,Ocean Sci., 10, 243–255, 2014.

The "net" usages also denote the horizontal local transport change at every grid position.

We correct the legends usage and change the "Monthly average" figures to "ANNUAL average" figures. The calculated process referred to the above Equation.

The Figure 6 shows the annual mean net DIP/DIN transport at every horizontal model grid. The value at every grid in Figure 6 is the sum of annual mean net DIP/DIN transport of total water 'column'. From that we address the description of the nutrient exchanges between sub-basins and between the coastal zone and the open sea. It gives us a hint to detect the intensity and direction of the nutrient transport in the Baltic Sea.

Definitions and explanations of sources and sinks have been given in the text of Section 5.5(also see our response to 2.6). Further, we give how transport is calculated in every grid cell or 'column' (see Equation in the reply to 2.4).

We change the legend usage in the Figures and now they use the consistent description.

2.4 Nutrient budgets. Explain, please, how the budgets were computed: – How nutrient in- and outflows (as product of velocity and concentration) been obtained from integrals of continuous computations for period 1970-1999 or from averaging of monthly or annual integrals? – How have annual sink/sources been calculated? Have the transformation processes (sediment-water exchanges, burial, nitrogen fixation, denitrification) been accounted for? – How trends in Table 1 been estimated? What does P sources in the KT, GF, and BB (sic!) as well as N source in GF mean? – How the total amounts (pools) of nutrients were calculated, by averaging of which fields, integrated with which frequency?

Response: The calculations of nutrient budgets are better explained in the revised version. The nutrient flow for the budgets is calculated by the similar method to the above shown integral equation at the selected borders of Baltic sub-basins. We obtain the annual average nutrient flow from integrals of continuous computations for period 1970-1999.

In the nutrient budgets the P and N external sources are computed from the combined supplies from land and atmosphere. Nitrogen fixation is not included in the external supplies. The sediment sinks are calculated from the difference between the net deposition of nutrients to the sediments and the release of nutrients from the sediments.

The model includes all these transformation processes (sediment-water exchanges, burial, nitrogen fixation, denitrification). The results have taken these processes into account. (refer to Eilola et al, J. Mar. Syst., 75, 163–184, 2009 and Almroth-Rosell et al, Journal of Marine Systems, 144, 127–141, 2015.)

The potential impact from artificial sources or sinks due to data assimilation is of course also included in the results. Because of the unknown impact from this “process” it is better to avoid detailed discussions especially about the changes in the nutrient pools. The trends in Table 1 are calculated from the differences between the nutrient inputs and nutrient exports seen in Figures 9 and 10.

The total amounts (pools) of nutrients were calculated as the sum of the inorganic and organic bioavailable nutrients in the water.

The total amount of nutrients for every sub-basin is calculated from the integral of nutrient concentrations from phytoplankton, zooplankton, detritus and dissolved nutrient times the volume of the sub-basin according to:

$$Total = \sum_{i}^{N_i} \sum_{j}^{N_j} \sum_{k}^{N_k} C_{i,j,k} \Delta x_{i,j} \Delta y_{i,j} \Delta z_k$$

where $C, \Delta x, \Delta y$ and Δz are the field concentrations (including nutrients from phytoplankton, zooplankton, detritus and dissolved nutrient), the horizontal and vertical dimensions of a grid cell, respectively. N_i, N_j and N_k are the number of grid in horizontal and vertical direction for every sub-basin, respectively.

These explanations are necessary but not sufficient for understanding how 30-year average annual “tendencies” (trends? deviations?) agree with pools? Most illustrative are P sources. In BB, 0.8 Kt P/yr *30 yrs=24 Kt P comparing to the pool of 5.9 Kt P; in GF, 5.9 Kt P/yr *30 yrs=177 Kt P comparing to the pool of 29.9 Kt P. Where has such hefty P excess gone, accumulated in the sediments? Evidently, the changes of nutrient pools in sediments must be included into consideration as well regardless of how plausible they are.

Response: We redefine the borders of the sub-basins (Fig. 1) and recalculate the total nutrient budget based on the new borders. Meanwhile we correct the mistake caused by the unit transform. The results are regarded reliable and reasonable. For example, the net phosphorus tendency for the Gulf of Finland is 24.3-22.5+8.6-6.7 = 3.7 Kton/yr. Further, in the Bothnian Bay, the net nitrogen tendency is zero. Comparison with the results of Savchuk (2005, 2007) based on Knudsen approach, the difference is mainly caused by the external supply from atmosphere and land. But phosphorus tendency in Gulf of Riga still a net loss of 0.5 Kton/yr. The difference between our result and Savchuk (2005) is due to different internal removal. Our results and Savchuk (2005, 2007) are treating different periods, the loads in the 1970s and the 1980s were larger indeed compared the loads in 1990s.

– Legend to Figs. 10 and 11 says: ”External nutrient inputs are separated into terrestrial and atmospheric sources. Terrestrial loads are reduced by phosphorus retentions for the coastal zones.” However, external inputs are presented with single numbers. Is it a sum of terrestrial and atmospheric loads, then the word is “combined”? What is the coastal P retention, how it was estimated and which values were prescribed? Was N inputs treated in a similar way?

Response: the value of external inputs is a sum of the supply from atmosphere and land. We change the text in these figures description. We remove the text “Terrestrial loads are reduced by phosphorus retentions for the coastal zones” since our model has consider these process during the model calculating nutrient flux.

Similar explanations and considerations, starting from algorithm of calculation should be given also to horizontally integrated flows at transects (Fig.12, lines 349-378) with special attention paid to explanation of the purpose of their analysis in a view of complex picture of water circulation and nutrient transports in Fig. 7. Considerations about possible contributions of transformation vs. fictitious processes would be appropriate in Section 5.7 or in discussion of presented results as well.

Response: we have given the answer for these comments. Please refer to the reply to 1.2 and 2.3.

2.5 Secchi depth (see also comment for lines 185-186 below). The water transparency seasonal variations and long-term trends depend on too many factors that either are not included in the model (e.g. CDOM and SPM distribution and variation) or are determined by complicated feedbacks from transformation processes (e.g. primary production and sedimentation of decomposing organic matter) to be used as unequivocal indicator of improved simulation of the nutrient fields. In result, the related analysis (lines 250-253) looks weak and unconvincing, for instance, the decrease of inorganic nutrients should cause the decreased primary production and how realistic is that? Or is it a correct effect by the wrong reason? Therefore, I would recommend deleting consideration of Secchi depth from the paper entirely. However, if the authors will chose to retain these considerations then a few words about how Secchi depth is estimated in the model (what it does and does not account for) would be useful for readers.

Response: we follow the suggestion by the reviewer and delete this section about the Secchi depth in the revised manuscript.

2.6 Presentation of pelagic and sediments pools. As it appears from Comments 2.4 and lines 380-388 in Discussion, presentation of pelagic and sediment nutrient pools could help to untangle several issues in interpretation of results

Response: As mentioned earlier, the potential impact from artificial sources or sinks due to data assimilation is of course also included in the results. Because of the unknown impact from this "process" it is better to avoid detailed discussions especially about the changes in the nutrient pools.

3. Minor things, technical corrections and language cosmetics.

In the revised version, we have several major changes in the text that may affect the interpretation of the detailed suggestions given by the reviewer. We seriously consider and take into consideration all minor comments from the reviewer also in the reworking of the text.

Lines: 3 – I guess, it is Eilola not Eolila;

Response: we correct it in revised manuscript.

11-12 – What is "improvement in ::: concentrations"? Consider, please, something like "improved simulation/reproduction/imitation of concentrations" or similar;

Response: We change it to "…improvement in the simulation of both oxygen and nutrient concentrations"

33-34 – Perhaps, not as much "living conditions" as redox dependent biogeochemical processes; here the reference to (Conley et al., 2009) or/and (Savchuk, 2010) would be appropriate in addition to- or instead of (Fu, 2013)

Response: We change this sentence to "MBIs can significantly affect the biogeochemical processes in the deep basins because of the inflow of large volumes of saline and oxygen-rich water into the Baltic Sea (e.g. Conley et al. 2009; Savchuk, 2010)."

50-54 – poor choice of words: " ::: of BIOLOGICAL formulations (either empirical or mechanistic) to UPDATE biogeochemical concentrations" that sounds as (physical) oceanographers' slang; why only "biological", what is "update" and "simulation accuracy", why "In reality..", "applicability" to what purposes? Please, reformulate more carefully;

Response: To clarify, now we delete "In general, coupled physical-biogeochemical models use a variety of biological formulations (either empirical or mechanistic) to update biogeochemical concentrations. As a result, the model formulation and the reliability of their parameterizations play a key role in determining the simulation accuracy of biogeochemical processes. In reality these processes governing the interactions between biogeochemical compartments vary in space and time (Losa et al., 2004; Doney, 1999)." in the revised version.

92 – "The reanalysis is mainly based on ::: " Consider, please, replacing something like with "The success of reanalysis ::: " or "The confidence in reanalysis is based on (or stems from) ::: " or similar;

Response: We delete this sentence in the revised manuscript.

94-96 – neither ICES nor SHARK "are monitoring" the Baltic Sea, both just maintain databases with monitoring results, correct appropriately;

Response: We change it to "For example, the International Council for the Exploration of the Sea (ICES) (http://www.ices.dk) and the Swedish Oceanographic Data Centre (SHARK) (http://sharkweb.smhi.se) are collecting the observations with the aim to monitor the Baltic Sea. Furthermore, the Baltic Sea Operational Oceanographic System (BOOS) (http://www.boos.org/) is providing near real-time observations." and we move them to the observation description section.

104 – in that context a reference to Gustafsson et al. (2012) would be more appropriate in addition to- or instead of Savchuk et al. (2008);

Response: We delete the corresponding paragraph text in revision.

110-111 – is " ::: a better assessment of HISTORICAL changes in the nutrient budgets of the water column and (OS – especially) sediments ::: " , true and legitimate aim of this study? Where are historical changes then?

Response: we change description of the aim of this study. Please see the reply to 1.1.

119 – unusual usage of "sea surface heights", replace, please, with "sea level (variations)";

Response: we replace the "sea surface heights" by "sea level elevation"

148 vs. 165 – is it SHARK only or SHARK and BED together? If the later, then there are much more observations in BED, for instance, for the Gulf of Riga;

Response: Yes, data from SHARK are assimilated into RCO-SCOBI. But data from both SHARK and BED are used for validation. We correct it in revised manuscript.

178-180 vs. 81-82 – repetition, delete, perhaps, from Introduction;

Response: we delete the "However, in Liu et al. (2014), only a shorter assimilation experiment for a 10-year period is presented, and so far the stability of the assimilation scheme in multi-decadal simulations has not been shown." in introduction section.

182 – instead of "we focus ::: on nutrient budgets and transports ::: ", perhaps, "we ::: on nutrient transports and budgets derived from them ::: " would better reflect both the focus and importance of results;

Response: we accept your comments and change it to "we focus mainly on nutrient transports derived from the reanalysis." in the revised manuscript.

185-186 – consider simplification as " ::: long- term trends in eutrophication as indicated by Secchi depth (Section 5.4)", because if the water transparency can be used as indicator of the eutrophication as the entire phenomenon, it seems too far-fetched to use it for evaluation of the "excess of nutrients in the water column".

Response: we delete this sentence: "and long-term trends in eutrophication (excess of nutrients in the water column) as indicated by Secchi depth (Section 5.4)".

198-199 – what does " ::: positive impact on the model simulation" mean, improved model-data comparability, or model-data resemblance or similar? Is it unexpected?

Response: the positive impact means reanalysis results closer data relative to FREE, which reduce the uncertainty (bias) of model simulation. We have clarified it in revision.

216 – perhaps, " ::: how data assimilation makes simulated nutrient dynamics in the Baltic proper look more realistic" would be more correct introduction to Fig. 4?

Response: we change it according to your comment.

266 – concentrations should be HIGHER not GREATER.

Response: We change the word "greater" to "higher".

268 – Why AMPLITUDES, most common meaning is as the measure of range, fluctuation, difference between maximum and minimum, i.e. large amplitude could mean small NET transports. Maybe, MAGNITUDE?

Response: We change the word "amplitude" to "magnitude". Thanks for your kind comment.

285 – maybe, "contrast" would be better word than "contradiction"?

Response: We change the word "contradiction" to "contrast".

306 – What "uptake and deposition of DIP", by which process (es)?

Response: We change this sentence by "This result might be explained by local processes causing the phytoplankton uptake and sediment deposition of DIP.".

310 – "taken up" or retained?

Response: it should be "retained" and we correct it in revision.

311-313 – needs better, clearer explanation.

Response: The phosphorus sink may also be partly caused by oxygen dependent water–sediment fluxes that bind DIP to ironbound phosphorus in oxic sediments (Almroth et al., 2015). This effect is not included in the Eilola et al. (2012), but might potentially be accounted for by the adjusted DIP transports in REANA. The results of REANA indicate that there is an additional sink but the relative importance of different processes causing this sink (data assimilation or sediment processes) is, however, not possible to evaluate from the reanalysis data set.

315 – Which "vertical exchange", in the water column or along the bottom, how estimated?

Response: the "vertical exchange profile" description is related to the internal nutrient sink/source at different water depth (Figure 8). But for clarification, we delete "vertical" in the revised manuscript.

380-388 vs. 177-178 – Has not initialization somewhat adjusted the fields? In any way, these considerations once more call for presentation of sediments' pools.

Response: Both REANA and FREE take the start initial condition from the same earlier run. However, to REANA, we firstly use the data assimilation method to "optimize" the initial condition and then forward the integration. FREE forward the integration based on the non-"optimal" the initial condition.

428-432 – There is a confusion and misinterpretation about P loads that should be corrected. Possible underestimation of P load was guessed by Savchuk and Wulff (2007) only for the Gulf of Riga. In all other basins, HELCOM data on unfiltered samples were used and GF load of 7 Kt P/yr used by Savchuk and Wulff (2007) are actually very close to the latest compilation by Knuuttila et al. (JMS, 2016). However, the loads in the 1970s and especially, the 1980s were larger indeed.

Response: we clarify it by delete this sentence: "However, their total phosphorus load, for example to the Gulf of Finland, is underestimated because the particulate phosphorus fraction is neglected (Savchuk et al., 2012)."

454 – Isn't location of halocline and, correspondingly, different volumes of hypoxia prone layers a rather important explanation?

Response: Yes, we also think it is good explanation of model biases. We add it into revised manuscript.

484 – Is it denitrification and not PP? Why?

Response: Thank you for the comment. The high productivity in the shallow areas effectively transfers DIN to OrgN. The denitrification act on larger scales and decrease the exports of nitrogen from coastal areas to the deeper areas. The potential impact from artificial sources or sinks due to data assimilation is also included in the results. The discussion in the manuscript will be revised accordingly.

Interactive comment on “Nutrient cycling in the Baltic Sea – results from a 30-year physical-biogeochemical reanalysis” By Ye Liu et al.

Anonymous Referee #2

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We thank you for your most helpful and thoughtful comments in the evaluation of our manuscript.

General comments

this manuscript the authors use a numerical model in combination with data assimilation to estimate nutrient fluxes within the Baltic Sea. They show that the data assimilation scheme greatly improves the results in terms of spatiotemporal concentrations fields. Without data assimilation the model have significant bias in both the annual cycle of the surface layers as well as spatial distribution of nutrient levels, but as shown, the assimilation procedure eliminate significantly of these systematic biases in a very impressive way. I am unfortunately not at all familiar with data assimilation methods. I tried to get a quick grip on what and how it is done by reading the method description in not only this manuscript, but also previous papers by the authors. Unfortunately, my background knowledge is too small to really understand even the basics of how it is done. Therefore, I hope that another reviewer is able to penetrate the technicalities of the method and judge its applicability. I can only see the end result and that the assimilated model results really do resemble the reality at the scales presented. I think given that the end results are useful for a wider community and focus on the discussion is not on the technical aspects, it would be useful if the authors include a brief paragraph describing in words how observations and model are merged in the assimilation procedure. Liu et al presents a solid reanalysis of 4 dimensional nutrient fields in the Baltic Sea. The nice correspondence with observations indicate that resulting data set is probably the best available data set and should provide useful for many purposes. Further that present interesting spatial budgets on both fine and basin-wide scales. One can, of course, question our knowledge of the certainty of the detailed source/sink calculations, but anyway the results are interesting and could definitely be considered best available. Given the journal one could have wished for deeper analysis of the results in terms of biogeochemical processes. Because of my limited understanding of the methodology I cannot really advice on how far such analysis could go, but now there is very little analysis on whether the spatial fields of sources and sinks may be due to or how they are connected to various processes. Although discussion is rather weak, I think the results are interesting enough, both in terms of the apparently excellent data quality the method results in as well as the Baltic Sea specific results on nutrient fluxes that I recommend publication.

Response: We detail and rewrite the text in the method’s description according to your comments. See the sections 4 “Methodology and Experimental Setup”, which describes how the observations and model are merged in the assimilation procedure.

In general, by relatively small effort, the manuscript text can be improved and I provide some, hopefully helpful, comments below to most sections.

Specific comments

Section 5.1 It is not surprising that the authors find some significant RMSD for e.g. ammonia in the 1970s. There are substantial temporal trends in data quality and consistent high-quality data is generally achieved only after international inter calibration became standard in the first half of the 1990s. I also believe that ammonia is one of the parameters with largest errors in the 1970s, while phosphate and nitrate was more reliable.

I do not understand “stability” of the assimilation, but that is surely due to my ignorance of the methodology.

Response: Thanks for specifying the quality of the ammonia observation.

Here we mean the assimilation results give a reliable estimation of the ocean state during the whole period. EnOI relies on the selected ensemble sample to estimate the background error covariance of model. The poor sample ensemble can cause the failure of the analysis. With the evolution of simulation, the performance of the data assimilation is different. The success of data assimilation at one time can't guarantee continued success of data assimilation at another time. Therefore, the "reliable" of a data assimilation system is key to the successful reanalysis. The RMSDs in Figure 3 denoted our estimation with EnOI is successful during the whole simulation period, which proved that our data assimilation system is valid and "reliable". To clarify, we instead "stability" by "reliable" in revised manuscript.

Section 5.2 The improvement in capturing the seasonal cycle is impressive. When I study figure 4 in Liu et al (2014) referred to in the text, it seems however, that the improvement is not due to the improved halocline only, but really due to the assimilation of chemical variables. In that figure DIN and DIP seem to be worse when only S and T is assimilated. I am not exactly sure how much interpretation on processes that can be done comparing different assimilated runs, but it seems that when assimilating only S and T, the model fails in using the additional In nutrients mixed up. However, I agree that a prerequisite for a deep spring bloom is a deep halocline.

Response: As shown by Liu et al. (2014), adjusting the physical condition for biogeochemical model doesn't guarantee the better biogeochemical simulation

Requirements to calculate correct simulation in additional to optimized model equations are high-quality atmospheric and riverine forcing data, and high-quality initial and lateral boundary conditions. As any other model, RCO-SCOBI had to be calibrated because many processes including sources and sinks of nutrients are not detailed enough known. Hence, an "optimal" parameterization of unresolved processes is one of the requirements for the predictive capacity of the model. The "optimal" physical forcing field is one of conditions to guarantee the correct the biogeochemical simulation. Assimilating only S/T will possibly break the balance of physical-biogeochemical condition, which provides the "optimal" initial condition for the circulation model and maybe degrade the usage of the former "optimal" parameterization for biogeochemical model. As a result, the physical-biogeochemical simulation using only T/S assimilation is done with "non-optimal" initial condition. Therefore, both physical and biogeochemical observations are necessary to be assimilated into the model to produce the "optimal" initial condition for a coupled physical-biogeochemical model simulation.

Section 5.3 Also here the improvements are impressive and the spatial variations in winter nutrient concentrations are well captured. This really gives credibility to use these results in flux calculations.

Response: thanks for your comments!

Section 5.4 Secchi depth is a complex variable including strong dependence also on coloured organic matter. It is evident that a higher Secchi depth is obtained using the assimilation, but calculating Secchi depth in the Baltic Sea from modeled algae biomass is not really well constrained so one could argue that by recalculating Secchi using somewhat different attenuation from CDOM could also give a fit to observations with the model without assimilation. Since temporal variation is not captured (which may be due to other causes than biomass), there is no way of knowing which calculation is actually the best and thus applicability of Secchi depth for validation is not very promising. Therefore I suggest that you can remove this section and the associated

Response: Following your advice we delete this content from the revised manuscript.

Section 5.5 I am not really sure what these horizontal fluxes tell us!

Response: The aims of presenting mean horizontal nutrient currents in the Baltic Sea is helpful to address the description of the nutrient exchanges between sub-basins and between the coastal zone and the open sea in manuscript. The nutrient transport in Baltic Sea is differing from other regions because of its physical and biological condition (e.g. the shallow mean water depth, much river runoff, the weak tide, the much source/sink). The horizontal distribution of the nutrient transport gives the hint to detect the intensity and direction of the nutrient transport.

Section 5.6 Does the assimilation as such affect conservation or constitute a part of the source/sink? Baring in mind my limited understanding of the methodology, I am wondering whether by having an underlying model simulation with error, corrected by the assimilation scheme the total source/sinks may give some erroneous results? However, I guess if you just integrate currents times concentrations, there should not be any problem. These results are quite interesting, although a bit challenging to understand. Perhaps it would be somewhat easier to explain if Total P (N) and DIP (DIN) were used instead of Org P (N). The totals would then give the net source/sink of the nutrient and the inorganic show the "gross" source/sink due to net turnover. It would be easier to read if the comparison with Eilola 2012, was postponed to the discussion. Now, I think the main results from this study is unnecessary difficult to follow, because of the frequent comparison with the previous paper.

Response: In the long-term simulation, the new initial condition for an assimilation cycle differs from the ending ocean state of the last cycle when at that time observations are available. In this sense, the data assimilation introduces sources and sinks of the nutrient cycles by interrupting the model simulation and adjusting the initial condition. However, we provide the "optimal" initial condition with data assimilation for the RCO-SCOBI for every simulation cycle. It means we don't change the equations of the RCO-SCOBI and just integrate currents and concentrations. The simulation process is conservative during the simulation between two assimilation occasions.

We agree that the data assimilation affects conservation properties for the long simulation as a whole. Although the reanalysis is conserved during every "independent" simulation cycle, the adjustment of data assimilation implicitly creates unknown complementary sources or sinks to the biogeochemical model. The magnitude of these adjustments depends on the bias between model and observations. The artificial sources/sinks are directly related to the model biases. Figure 3 shows that the model has large biases during the beginning of the simulation. However, data assimilation has corrected the mismatch between model state and observation to an "optimal" level during an initial adjustment period. After the adjustment period, the mismatch between model and observation becomes small and the successive adjustment due to data assimilation also becomes small (Liu et al. 2014). Further, the adjustment of data assimilation is related to the spatial-temporal coverage of observations. Here we assimilated only observed profiles into the model.

We want to keep the discussion of internal dynamics of inorganic and organic nutrient. As mentioned earlier, the potential impact from artificial sources or sinks due to data assimilation is included in the reanalysis results. Because of the unknown impact from this "process" it is better to avoid detailed discussions about the net sources and sinks.

We move the comparison with Eilola et al. (2012) to the discussion section.

Section 5.7 To my knowledge, the model used does only include bio available nutrients. This is fine but should be clearly stated to avoid confusion. Especially for nitrogen, there is a significant net flux through the system of refractory N that is not captured here. I further assume that the budgets are made summing inorganic and organic nutrients, but adding a sentence about that makes it easier for the reader to follow. I am confused by the fact that the budgets in figs 10-11 does not add up. A small net could be attributed to changes in water column storage, but looking for example at phosphorus in Gulf of Finland the net is 8.6+54.7-50.7-6.7 = 12.6 -6.7 = 5.9 kton/yr. This is far too much to be storage change. I thought that it could be that only a part of the load was used, but looking at Gulf of Riga there is a net loss of 1.4 kton/yr. Is it a consequence of the data assimilation? In that case, how should this residual be interpreted? In any case it should be clarified and shown in figures 10-11. That gross fluxes are different between approaches are not surprising since it will depend on time-resolution as the authors point out. Oscillating flows due to various processes cause a dispersive transport that to some extent is resolved by the 3D model, but it is not given that the net effect is correct if the processes that regulate the dispersive transport such as e.g., mixing and frontal movements are appropriately modeled. Without really detailed observations of currents and concentrations one have to resort the validation of the dispersive transport to the net effect on e.g. salinity in the basin. Thus, in some sense, the estimate of net transport by a full 3D model may not be that different from the assumptions behind those of using the diagnostic Knudsen approach, i.e. a strong correlation between salinity and the constituent of interest. Having said that, the level of detail is of coarse massively different and the possibilities to make temporal and spatial analyses also greater.

Validation currents and circulation patterns are very difficult and I do not demand that, but it could have been nice with a discussion on how confident we can be in the results of nutrient circulation and source/sink spatial variations in light of how the data assimilation improves circulation. A starting point could be the consequences of that a clear majority of the hydrochemical data has been collected at single locations usually quite central in the basins and not along the stretches of strong circulation. A naive issue that I personally wondering about is whether assimilation of point wise observations may induce spurious circulation patterns?

Response: Thanks for your comments. Yes, the budgets are made summing inorganic and organic bio-available nutrients. We add text for clarifying the total nutrient in this section in revised manuscript.

The budget calculation is recalculated with new borders. Meanwhile we corrected the mistake caused by the unit transform. The results are regarded reliable and reasonable. For example, the net phosphorus tendency for the Gulf of Finland is 24.3-22.5+8.6-6.7 = 3.7 Kton/yr. Further, in the Bothnian Bay, the net nitrogen tendency is zero. Comparison with the results of Savchuk (2005, 2007) based on Knudsen approach, the difference is mainly caused by the external supply from atmosphere and land. But phosphorus tendency in Gulf of Riga still a net loss of 0.5 Kton/yr. The difference between our result and Savchuk (2005) is due to different internal removal. Our results and Savchuk (2005, 2007) are treating different periods, the loads in the 1970s and the 1980s were larger indeed compared the loads in 1990s.

In the Baltic Sea, wind forcing and topography are the main factors that affect the variability of the circulation in the shallow region where stratification is weak and the surface circulation may affect the sea floor. Our reanalysis changes salinity and temperature of seawater but it does not change the horizontal circulation explicitly since the equations of RCO-SCBI have not been changed. Further, we change the stratification in the Baltic Sea which will affect the vertical circulation in our assimilation experiment (Liu et al. 2013). Fu et al. (2011) has validated the improvement of sea level in assimilating temperature and salinity observations with EnOI method. In this study, the forcing isn’t changed and assimilated physical state variables include the sea level, temperature and salinity. We consider the impact of barotropic and baroclinic balance during the assimilation. Besides, Wenzel et al. (2001) proved that, when sea level is assimilated in the circulation model in addition to temperature and salinity to adjust the small-scale variability, the large-scale circulation will not be degraded. We estimated the assimilation increment according to optimal statistics of the water column in every grid point. The water mass is mainly controlled by the temperature and salinity. We estimated the “optimal” characteristics (temperature and salinity) of water mass in our reanalysis. The “optimal” characteristics will produce the “optimal” hydrological dynamic balance based on the model dynamic equations. As a result, we don't degrade the estimation of horizontal transport

M. Wenzel et al. (2001) Progress in Oceanography 48 73–119.

It is difficult to evaluate the quality of model results at high resolution because independent observational data sets are usually missing. An exceptional effort to utilize independent data was done by Liu et al. (2014) showing that the statement about the added value of data assimilation is true for the available, independent cruise data at high resolution. However, one can not expect that budgets calculated from the summation of fluxes from model results with data assimilation are more accurate because usually small artificial sources and sinks from the data assimilation are becoming as important as physically motivated sources and sinks when sums of fluxes are compared. Hence, we calculated budgets with the aim to evaluate the reanalysis data and to estimate the magnitude of artificial sources and sinks by comparing our results with other studies using only observations. We are aware that it is impossible to claim that our budgets are more accurate than those budgets that are derived from observations only despite the higher temporal and spatial resolution in model outputs.

I would argue that the sub-basin boundaries in the model of Gustafsson etc also (2012) is not arbitrary chosen. As far as possible sub-basin boundaries of this model is chosen according to dynamical constraints such as sills or fronts that can be parametrizised. A discussion of the implications of the high-resolution sink/source fields for our understanding of major processes would have been quite interesting. What does the spatial distribution of e.g. net sedimentation or denitrification imply? What are the pathways for organic matter? I am not sure how far you can take this given methodological limitations, but it could be nice here with a few things and not only referring to other model simulations.

Response: We clarify the boundaries description in Gustafsson et al. (2012). The importance of regional variations of sources and sinks for nutrients on the calculation of transports between sub-basins seem to be significant and need to be furthers studied. The nutrient cycling inside the sub-basins include many complicated process like the sediment, internal exchange of nutrient and denitrification and decomposition. Given the uncertainty caused by data assimilation in the present study we must however save the detailed studies of these issues to future work where the artificial impact of data assimilation on sources and sinks will be traced and quantified during the run.

Nutrient transport in the Baltic Sea - results from a 30-year physical-biogeochemical reanalysis

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Abstract. Long-term oxygen and nutrient transports in the Baltic Sea are reconstructed using the Swedish Coastal and Ocean Biogeochemical model (SCOBI) coupled to the Rossby Centre Ocean model (RCO). Two simulations with and without data assimilation covering the period 1970–1999 are carried out. Here, the "weakly coupled" scheme with the Ensemble Optimal Interpolation (EnOI) method is adopted to assimilate observed profiles in the reanalysis system. The reanalysis shows considerable improvement in the simulation of both oxygen and nutrient concentrations relative to the free run. Further, the results suggest that the assimilation of biogeochemical observations has a significant effect on the simulation of the oxygen dependent dynamics of biogeochemical cycles. From the reanalysis, nutrient transports between sub-basins, between the coastal zone and the open sea, and across latitudinal and longitudinal cross sections, are calculated. Further, bottom areas of nutrient import or export are examined. Our results emphasize the important role of the Baltic proper for the entire Baltic Sea, with large net exports of nutrients into the surrounding sub-basins (except the phosphorus transport into the Gulf of Riga and the nitrogen transports into the Gulf of Riga and Danish Straits). In agreement with previous studies, we found that the Bothnian Sea imports large amounts of phosphorus from the Baltic proper that are buried in this sub-basin. For the calculation of sub-basin budgets, it is crucial where the lateral borders of the sub-basins are located, because net transports may change sign with the location of the border.

Although the overall transport patterns resemble the results of previous studies, our calculated estimates differ in detail considerably.

Keywords: reanalysis; data assimilation; numerical modelling; Baltic Sea; biogeochemical transports; nutrient budgets

1 Introduction

The water exchange between the Baltic Sea and the North Sea is restricted by the narrows and sills in the Danish transition zone (Fig. 1). The hydrography of the Baltic Sea also depends on freshwater from rivers, which causes large salinity gradients between the surface layer and the saltier bottom layer, and between the northern sub-basins and the entrance area (e.g. Meier and Kauker, 2003). The low-saline outflowing surface water is separated from high-saline inflowing bottom water by a transition layer, the halocline. The bottom water in the deep sub-basins is ventilated mainly by so-called Major Baltic Inflows (MBIs) (Matthäus and Franck, 1992; Fischer and Matthäus, 1996). MBIs can significantly affect biogeochemical processes in the deep basins because of the inflow of large volumes of saline and oxygen-rich water into the Baltic Sea (e.g. Conley et al. 2009; Savchuk, 2010). In the Baltic Sea, the density stratification and long water residence time hamper the ventilation of deep waters. As a result, oxygen deficiency is a common feature. Additionally, nutrient loads from agriculture and other human activities of the large population in the catchment area increased nutrient concentrations in the water column. Actually, eutrophication has become a large environmental problem in the Baltic Sea in recent decades (e.g. Boesch et al., 2008; Pawlak et al., 2009; Wulff et al., 2001; Andersen et al., 2015). Therefore, accurate estimates of the ecological state and nutrient and water exchange between sub-basins and between the coastal zone and the open sea are of particular importance in managing the marine environment system.

On one hand, the estimation of biogeochemical processes, ecological state and nutrient exchange may rely on coupled marine ecosystem-circulation models (e.g. Neumann et al., 2002; Eilola et al., 2009; 2011; Almroth-Rosell et al., 2011; 2015; Maar et al., 2011; Daewel and Schrum, 2013). However, addressing biogeochemical cycles is a challenging task due to the complexity of the system. Obviously, there are large uncertainties in marine ecological simulations (e.g. Eilola et al., 2011). In contrast to the modelling of the physics of the atmosphere or ocean, where a basic description of the motion is provided by conservation equations, there is no basic set of equations that describe the marine ecosystem. Many biogeochemical processes are still poorly known and their uncertainties are difficult to quantify accurately. These potential sources of errors limit the applicability of the models both in forecasting and reanalysis. Further, imperfect initial conditions and model forcing also cause biases in the simulation results.

On the other hand, estimating nutrient budgets and transports between sub-basins may directly rely on observations and basin integrated budget models (Savchuk, 2005). The estimation accuracy depends on the spatial and temporal coverage of the measurements and the locations of borders between sub-basins. Although the data coverage in the Baltic Sea has gradually increased over time, the lack of observations still makes it difficult to estimate reliable biogeochemical cycles. Today, the availability of satellite sensor data like ocean color data from the OCTS (Ocean Color and Temperature Sensor) and from the SeaWiFS (Sea-Viewing Wide Field-of-View Sensor) has provided the best spatial coverage of measurements. However, these sensors only give an estimate of a few biogeochemical parameters at the surface of the marine ecosystem, and not the state of the entire marine ecosystem in the water column. Continuous observations of the deep ocean are only possible with in situ sensors, which have been deployed at only a limited number of stations (Claustre et al., 2010).

Given the coverage of observations and model deficiencies, we decided to perform a reanalysis based upon a high-resolution, coupled physical-biogeochemical model to estimate the physical and biogeochemical state of the Baltic Sea. For this purpose, data assimilation continuously updates the model variables at the locations of the observations and in their neighborhood. Integration in time of the prognostic model equations allows the spread of the information from the observations within the model domain.

The assimilation of data into coupled physical-biogeochemical models is confronted by various theoretical and practical challenges. For example, the response of the three-dimensional biogeochemical model to external forcing caused by the physical model is highly non-linear. Further, it is difficult to use the biological observational information to reduce biases in the simulation of ocean physics which has an impact on modeled biogeochemistry (Beal et al., 2010). Presently, the use of data assimilation to complement ecosystem modeling efforts has gained widespread attention (e.g. Hoteit et al., 2003; Allen et al., 2003; Natvik and Evensen, 2003; Hoteit et al., 2005; Triantafyllou et al., 2007; While et al., 2012; Triantafyllou et al., 2013). A comprehensive review of biological data assimilation experiments can be found in Gregg et al. (2009).

In the Baltic Sea, the biogeochemical data assimilation has started to become a research focus. For example, Liu et al. (2014) used the Ensemble Optimal Interpolation (EnOI) method to improve the multi-annual, high-resolution modelling of biogeochemical dynamics in the Baltic Sea. Fu (2016) analyzed the response of a coupled physical-biogeochemical model to the improved hydrodynamics in the Baltic Sea. Recently, several data assimilation studies have focused on the historical reanalysis of salinity and temperature in the Baltic Sea (e.g. Fu et al., 2012; Liu et al., 2013; 2014). Reanalysis has helped enormously in making the historical record of observed ocean parameters more homogeneous and useful for many purposes. For instance, ocean reanalysis data have been applied in research on ocean climate variability as well as on the variability of biochemistry and ecosystems (e.g. Bengtsson et al., 2004; Carton et al., 2005; Friedrichs et al., 2006). Ocean reanalysis can also be used for the validation of a wide range of model results (e.g. Fontana et al., 2013). For instance, the ocean mean state and circulation can be calculated from reanalysis results to evaluate regional climate ocean models (e.g. Meier et al., 2012). Moreover, reanalysis in the ocean is beneficial to the identification and correction of deficiencies in the observational records, as well as filling the gaps in observations. Regional and local model studies may use reanalysis results as initial and boundary conditions.

The present paper focuses on the assimilation of profiles of temperature, salinity, nutrients and oxygen in the Baltic Sea following Liu et al. (2014). We aim to reproducing the ocean biogeochemical state with the help of information from both observations and a coupled physical-biogeochemical model for the period 1970-1999. Since 1970 the data coverage in the Baltic Sea is satisfactory. The results of the reanalysis are supposed to be used to estimate the water quality and ecological state with high spatial and temporal resolution in regions and during periods when no measurements are available. Further, nutrient transports across selected cross-sections or between vertical layers are calculated with high resolution and accuracy taking the complete dynamics of primitive equation models into account. This information can't be obtained from neither observations alone or from model results without data assimilation because the latter might have large biases in both space and time. We assess the nutrient budgets of the water column and sediments, as well as of the nutrient exchanges between sub-basins and between the coastal zone and the open sea. As a reanalysis can never be dynamical consistent and does not preserve mass, momentum and energy, the calculated budgets are compared to the results of other studies to evaluate our results meant as consistency check. Hereby, we follow studies of other regions applying data assimilation for a biogeochemical reanalysis on long-term scale (Fontana et al., 2013; Teruzzi et al., 2014; Ciavetta et al., 2016).

This paper is organized as follows. The physical and biogeochemical models are described in Section 2. Then the observational data set and the method of the reanalysis are introduced in Section 3 and 4, respectively. The experiment results, including comparisons with observations, are presented in Section 5. Finally, in Section 6 and 7, discussion and conclusions finalize the paper.

2 Models

The RCO (Rossby Centre Ocean) model is a Bryan–Cox–Semtner primitive equation circulation model with a free surface (Killworth et al., 1991). Its open boundary conditions are implemented in the northern Kattegat, based on prescribed sea level elevation at the lateral boundary (Stevens, 1991). An Orlanski radiation condition (Orlanski, 1976) is used to address the case of outflow, and the temperature and salinity variables are nudged toward climatologically annual mean profiles to deal with inflows (Meier et al., 2003). A Hibler-type dynamic–thermodynamic sea ice model (Hibler, 1979) with elastic–viscous–plastic rheology (Hunke and Dukowicz, 1997) and a two-equation turbulence closure scheme of the k–ε type with flux boundary conditions (Meier, 2001) have been embedded into RCO. The deep-water mixing is assumed inversely proportional to the Brunt–Väisälä frequency, with the proportionality factor based on dissipation measurements in the Eastern Gotland Basin (Lass et al., 2003). In its present version, RCO is used with a horizontal resolution of 2 nautical miles (3.7 km) and 83 vertical levels, with layer thicknesses of 3 m. RCO allows direct communication between bottom boxes of the step-like topography (Beckmann and Döscher, 1997). A flux-corrected, monotonicity-preserving transport (FCT) scheme is applied in RCO (Gerdes et al., 1991). RCO has no explicit horizontal diffusion. For further details of the model setup, the reader is referred to Meier et al. (2003) and Meier (2007).

The biogeochemical model called SCOBI (Swedish Coastal and Ocean Biogeochemical model) has been developed to study the biogeochemical nutrient cycling in the Baltic Sea (Marmefelt et al., 1999; Eilola et al., 2009; Almroth-Rosell et al., 2011; 2015). This model handles biological and ecological processes in the sea as well as sediment nutrient dynamics. SCOBI is coupled to RCO (e.g. Eilola et al., 2012; 2013; 2014). With the help of a simplified wave model, resuspension of organic matter is calculated from the wave and current-induced shear stresses (Almroth-Rosell et al., 2011). SCOBI has a constant carbon (C) to chlorophyll (Chl) ratio C:Chl = 50 (mg C (mg Chl)$^{-1}$), and the production of phytoplankton assimilates carbon (C), nitrogen (N) and phosphorus

(P) according to the Redfield molar ratio (C:N:P = 106:16:1) (Eilola et al., 2009). The molar ratio of a complete oxidation of the remineralized nutrients is O_2:C = 138. For further details of the SCOBI model, the reader is referred to Eilola et al. (2009, 2011) and Almroth-Rosell et al. (2011).

RCO-SCOBI is forced by atmospheric forcing data calculated from regionalized ERA-40 data using the regional Rossby Centre Atmosphere (RCA) model (Samuelsson et al., 2011). The horizontal resolution of RCA is 25 km. A bias correction method following Meier et al. (2011) is applied to the wind speed. Monthly mean river runoff observations (Bergström and Carlsson, 1994) are used for the hydrological forcing. Monthly nutrient loads are calculated from historical data (Savchuk et al., 2012).

3 The Dataset

The Baltic coastal shelf observation systems have been largely improved by the joint efforts of the countries surrounding the Baltic Sea. For example, the International Council for the Exploration of the Sea (ICES) (http://www.ices.dk) and the Swedish Oceanographic Data Centre (SHARK) (http://sharkweb.smhi.se) are collecting the observations with the aim to monitor the Baltic Sea. Furthermore, the Baltic Sea Operational Oceanographic System (BOOS) (http://www.boos.org/) is providing near real-time observations and the publicly available database BED (Baltic Environmental Database, http://nest.su.se/bed) of the Baltic Nest Institute (BNI) (http://www.balticnest.org) store physical and environmental data from BNI partner institutes (see http://nest.su.se/bed/hydro_chem.shtml). As a result, a comprehensive data set is collected for the Baltic Sea region. The assimilated observations in this study comprise both physical (temperature and salinity) and biogeochemical variables (oxygen, nitrate, phosphate and ammonium) from the SHARK database. Before assimilation, the data were quality controlled. These controls include checks of location and duplication, and examination of differences between forecasts and observations. A profile was eliminated from the assimilation procedure when the station was located on land defined by the RCO bathymetry. We also removed observations when the difference between model forecasting field and observations exceeds the given standard maximum deviation (for example 4.0 mL L^{-1} for oxygen concentration). We used an average of the observations in the same layer when there was more than one observation per layer. These observations cover almost the whole Baltic Sea including Kattegat and the Danish Straits. Figure 2 shows the number of biogeochemical observation profiles in different sub-basins, and the temporal distribution of these biogeochemical observations. The number of observations is inhomogeneous in both temporal and spatial distribution over the period from 1970 to 1999. There are relatively more observations in the Baltic proper than in other sub-basins. In the Gulf of Riga, a minimum number of observation profiles (30 for oxygen, 30 for phosphate, 28 for nitrate and 28 for ammonium) is found. Obviously, the number of observations during the period of 1988-1994 is higher than that during other periods. Further, there are generally less observations from 1981-1983 than during other periods. The maximum number of observation profiles occurred in 1991 for oxygen (1,844), phosphate (1,728) and nitrate (1,758). However, the number of ammonium observation profiles has a maximum value of 1,222 in 1992. Moreover, the number of the oxygen and ammonium observations is largest and smallest, respectively, compared to the other variables. These observations from SHARK and BED are used to validate the model and assimilation results.

4 Methodology and Experimental Setup

Here we briefly describe the configuration of the data assimilation system of this study. We focus on the state estimation via EnOI. The distribution of stochastic errors are assumed to be Gaussian and non-biased. EnOI estimates an 'optimal' oceanic state at a given time using observations, the numerical model and assumptions on their respective bias distribution. The relationship between them can be expressed as following:

$$\psi^a = \psi^f + \mathbf{K}(d - H\psi^f) \quad (1),$$

$$\mathbf{K} = \mathbf{P}^f H^{\mathrm{T}} (H\mathbf{P}^f H^{\mathrm{T}} + (N-1)\mathbf{R})^{-1} \quad (2).$$

Where d is the vector of observations and ψ is the model state vector which includes the sea level anomaly, temperature, salinity, oxygen, phosphate, ammonium and nitrate. $\mathbf{K}$ is the Kalman gain matrix and H is the observation operator that maps the model state onto the observation space. $d - H\psi^f$ is the innovation which is calculated in the observation space. $\mathbf{R}$ is the observation error covariance. The superscripts a and f denote the analysis and forecast, respectively. N is the number of the ensemble samples. EnOI computes the Background Error Covariance (BEC) matrix by the centered state ensemble $\mathbf{A}'$ (i.e. $\mathbf{A}' = \mathbf{A} - \overline{\mathbf{A}}$), as follows:

$$\mathbf{P} = \frac{\alpha}{N-1} \mathbf{A}'(\mathbf{A}')^{\mathrm{T}} \quad (3).$$

Here the subscript T denotes the transpose of a matrix and the scaling factor $\alpha \in (0,1]$ is introduced to tune the variance of the model ensemble perturbations to a realistic level in order to capture the variability of model parameters like temperature and dissolved oxygen, which is dominated by misplacement of mesoscale features, and which varies in location and intensity seasonally. Therefore, we hypothesize that the background errors are proportional to the model variability on intra-seasonal time scales. A total of 100 model samples by "running selection" are adopted to obtain a quasi-stationary background error covariance (BEC). The "selection" is in one and a half month period before and after the calendar date of the assimilation time from the period 1964–1968 (Liu et al., 2013). Hence, from every year during the selected period 1964–1968 20 snapshots have been selected. An adaptive scaling factor was calculated to adapt to the instantaneous forecast error variance before each local analysis (Liu et al., 2013; 2014). Further, localization is used to remove unrealistic long-range correlation with a quasi-Gaussian function and a uniform horizontal correlation scale of 70 km. As a result, the quality of fields obtained by data assimilation is determined by the coverage and quality of observations (She et al., 2007). Moreover, the assimilation frequency or window is another factor to affect the assimilation fields. They are directly related to how many observations are entering the assimilation cycling and how often the model initial condition is adjusted by data assimilation (Liu et al., 2013). Here, we select an assimilation window of three days and the assimilation frequency is once every seven days in the reanalysis experiment. It means that all the observations in three days before and after the assimilation time are selected to yield the "new" initial condition for the following simulation during the current assimilation cycle.

Based on the above configuration, two experiments from January 1970 to December 1999 have been carried out. One experiment is a simulation without data assimilation (FREE). The other simulation is constrained by observations using the "weakly coupled" assimilation scheme based upon the EnOI method following Liu et al. (2014) which was briefly described before (REANA). Both simulations, FREE and REANA, are initialized for January 1970. The initial conditions are taken from an earlier run with RCO-SCOBI. The observation error in REANA is defined according to Liu et al. (2014). However, in Liu et al. (2014), only a shorter assimilation experiment for a 10-year period is presented, and so far the reliability of the assimilation scheme in multi-decadal simulations has not been shown. Following Liu et al. (2014), our REANA experiment assimilated both physical and biogeochemical observations. In this study, we focus mainly on nutrient transports derived from the reanalysis.

To assess the results with (REANA) and without (FREE) data assimilation, the overall monthly mean RMSDs (root mean square differences) of oxygen, nitrate, phosphate and ammonium were calculated relative to observations during the whole integration period. The overall monthly mean RMSD is calculated by the following formula:

$$RMSD = \frac{1}{N_j}\sum_{j=1}^{N_j}\sqrt{\frac{1}{N_t}\sum_{i=1}^{N_t}(\varepsilon_t^i)^2} \qquad (4),$$

where N_t is the number of the observations at assimilation time t and N_j is the number of days observed in one month for one field for entire Baltic Sea. $\varepsilon_t^i = x_{sim}^i(t) - x_{obs}^i(t)$ represents the difference between model result (x_{sim}) and observation (x_{obs}) at time t and at the i^{th} observation location. We calculated ε_t at only the observation location at the time t, which is calculated by mapping the model field onto the observation space. Here it should be noted that the RMSDs were calculated before the time of assimilation analysis, and the corresponding observations were not yet assimilated into RCO-SCOBI (Liu et al., 2014).

Based on the reanalyzed simulation, the annual mean net DIN and DIP transports, as well as DIP persistency are also calculated. Net transports (VA_{Trans}) are vertically integrated at every grid point at every time step of the integration according to:

$$VA_{Trans} = \sum_{k=1}^{N} C_k u_k \Delta z_k \qquad (5),$$

where $C_k, u_k, \Delta z_k$ and N are the field concentrations of DIN, DIP and organic phosphorus (OrgP), the current velocity vector, vertical dimensions of a grid cell and the number of wet grid cells in the water column, respectively. From the net transport vector field both magnitude and streamlines are calculated.

The total nutrient budgets are calculated from the sum of inorganic and organic bioavailable nutrients. The combined nutrient supplies from land and from the atmosphere have been taken into account. Nitrogen fixation is not included in the external supplies. The nutrient fluxes caused by sediment-water exchanges are also calculated. The sediment sinks (burial) are calculated from the difference between the net deposition of nutrients to the sediments and the release of nutrients from the sediments. The nutrient flows for the total budgets are integrated along the selected borders of sub-basins using Equation 5. Annual nutrient flows are averaged for the period

1970-1999. The total amount of nutrients for every sub-basin is calculated from the integral of nutrient concentrations from phytoplankton, zooplankton, detritus and dissolved nutrient times the volume of the sub-basin according to:

$$Total = \sum_{i}^{N_i}\sum_{j}^{N_j}\sum_{k}^{N_k} C_{i,j,k}\Delta x_{i,j}\Delta y_{i,j}\Delta z_k \quad (6),$$

where $C, \Delta x, \Delta y$ and Δz are the field concentrations (including nutrients from phytoplankton, zooplankton, detritus and dissolved nutrient), the horizontal and vertical dimensions of a grid cell, respectively. N_i, N_j and N_k are the number of grid in horizontal and vertical direction for every sub-basin, respectively. Further, the tendencies in Table 1 are calculated from the differences between nutrient inputs and exports of all sub-basins.

5 Results

In the following sub-sections, we evaluate the impact of data assimilation on the long-term evolution of biases (Section 5.1), and on vertical (Section 5.2) and horizontal (Section 5.3) distributions of nutrient concentrations. For the evaluation of time series of simulated oxygen, nitrate, phosphate and ammonium concentrations, the reader is referred to Liu et al. (2014, their Figs. 6 and 7). After the evaluation of the assimilation method, we focus on the analysis of nutrient transports in the Baltic Sea based upon our reanalysis data that we consider to be the best available data set for such an analysis. In particular, we analyze the horizontal circulation of nutrients (Section 5.4), the horizontal distribution of nutrient sources and sinks, the nutrient exchange between the coastal zone and the open sea (Section 5.5), and the nutrient budgets of sub-basins (Section 5.6).

5.1 Temporal evolution of biases

The data assimilation has significantly positive impact on bias reduction of the model simulation. Generally, the RMSDs of oxygen and nutrient concentrations in REANA are smaller than that of FREE. However, the improvements of these four variables simulation have different variation characteristics caused by the assimilating of biogeochemical observations. The RMSD of oxygen is mostly greater and smaller than 1.0 mL L^{-1}

for FREE and REANA, respectively. The mean RMSD of oxygen during this period has been reduced by 59% (from 1.43 to 0.59 mL L^{-1}). Similar improved simulation also appears in nitrate and phosphate concentrations. The RMSDs of nitrate and phosphate in REANA were reduced by 46% (from 2.04 to 1.11 mmol m^{-3}) and 78% (from 1.05 to 0.23 mmol m^{-3}) relative to that in FREE, respectively. Furthermore, the variability of RMSD of phosphate in FREE is large during the first 10 years, and decreases afterwards with time. However, the data assimilation cannot always improve the model results (Liu et al., 2014). For instance, although the overall RMSD of ammonium is reduced by 45% (from 1.15 to 0.63 mmol m^{-3}), the ammonium concentrations in REANA become worse relative to those in FREE during some months. An example appears in February 1975 when the RMSD of the ammonium concentrations in REANA (3.07 mmol m^{-3}) is greater than that in FREE (2.75 mmol m^{-3}). These results are similar to the findings by Liu et al. (2014). However, here we show that the 30-year-long assimilation is reliable, and that the RMSD of phosphate concentrations decreases even further with data assimilation continuing after 10 years.

5.2 The seasonal cycle of nutrients

The long-term average seasonal cycles of temperature and inorganic nutrients at monitoring station BY15 at Gotland Deep (for the location, see Fig. 1) give a hint of how data assimilation makes simulated nutrient dynamics in the Baltic proper more realistic (Fig. 4). The surface layer temperature and stratification show rapid increase in April to May, with concurrent rapid decrease of nutrient concentrations due to primary production down to 50-60 m depths. The cooling and increased vertical mixing in autumn and winter reduce temperatures and bring nutrients from the deeper layers into the surface layers. RCO-SCOBI captures these variations. However, compared to BED, the model has obvious biases, such as from late winter to early spring temperature stratification in FREE around the 30-50m depth, higher concentration of nutrients at the 50-60m depth, stronger vertical stratification of nutrient concentrations and less decrease of nutrients in the summer, especially below the thermocline, as well as also in the surface layers for phosphate. One reason for the biases is the vertical displacement of the halocline that is too shallow in RCO (e.g. Fig. 4 in Liu et al., 2014). The causes for the model bias in nutrient depletion below the summer thermocline are not known, but possible reasons are discussed by Eilola et al. (2011). The reanalysis has significantly reduced all these biases and provides an improved model description of vertical transports of nutrients in the layers above the halocline.

5.3 Spatial variations of late winter nutrient concentrations

The average March concentrations of dissolved inorganic phosphorus (DIP) and nitrogen (DIN) in the upper layers (0-10m), as well as their ratio (DIN:DIP), were calculated (Fig. 5). In BED the highest concentration of DIP occurs in the Gulf of Riga and the Gulf of Finland. Relatively high concentrations of DIP are found in the entire Gotland Basin. The DIP concentrations in the Bothnian Sea and Bothnian Bay are obviously lower than in other regions. Generally, the DIP in FREE has been largely overestimated in all regions relative to BED, especially in the Gotland Basin and Bornholm Basin. In BED, low DIP concentrations appear at the eastern coast of the Eastern Gotland Basin. In FREE, this spatial feature of DIP concentrations is not found. Further, in BED high concentrations of DIN occur in coastal waters close to the river mouths of the major rivers in the southern Baltic proper. DIN concentrations in the Gulf of Finland and in the Gulf of Riga are also high, and cover large areas of these gulfs. Unlike the BED data, the DIN in FREE has high concentrations also in the entire southern and eastern coastal zones of the Baltic proper. As a result, FREE shows a gradient in DIN concentrations between the coastal zone and the open sea in the entire southern Baltic proper. -The DIN and DIP patterns result in high and low DIN:DIP ratios in the Bothnian Bay and Baltic proper, respectively. The highest DIN:DIP ratios are found in the Bothnian Bay in BED and in the Gulf of Riga in FREE. RCO-SCOBI has captured this large-scale pattern, but there are substantial regional differences. By the constraints of the observation information, REANA has improved the spatial distributions of DIN and DIP significantly. In particular, DIP concentrations in REANA are much closer to observations.

5.4 Mean horizontal circulation of nutrients

Nutrient transport directly affects the biogeochemical cycles and the eutrophication of the Baltic Sea. The persistency of the net transports (Fig. 6) is defined, for instance, by Eilola et al. (2012). One should note that the results by Eilola et al. (2012) are based upon 30-year averages for the control period 1978-2007 of a downscaled climate scenario from a global circulation model. Similar calculations of transports and sources and sinks will therefore be briefly presented in the present study, since the hindcast period is better represented when the model is forced by the assimilated atmospheric (ERA–40) and Baltic Sea data (REANA). DIP has the largest transports in the central parts of the Baltic proper, with high persistency because the volume transports are generally larger in deeper rather than in shallower areas. In the Bornholm Basin and the eastern parts of the central Baltic proper, cyclonic circulation patterns are found. In the western parts of the central Baltic proper, southward transports prevail. Relatively large magnitudes of transports of DIP are also found in the northwestern Gotland Basin, in the southern Bornholm Basin, and through the Slupsk Channel connecting Bornholm Basin and Gotland Basin. Similar transport patterns are also found for DIN, OrgP and OrgN (not shown). In contrast to Eilola et al. (2012), DIN, DIP, OrgP and OrgN transports and their persistency are obviously stronger, although the overall patterns are similar. For example, in Eilola et al. (2012, their Fig. 1), large DIN transports appear in the southern Baltic proper and the Bornholm Basin. Similar differences are also found in both DIP and OrgP transports.

5.5 Internal nutrient sources and sinks

The horizontal distributions of areas with internal sources and sinks of phosphorus and nitrogen are illustrated in Fig. 7. A net inflow (inflow ≥ outflow) of nutrients to an area is defined as a sink (import) and counted as positive, while net outflow (inflow ≤ outflow) is defined as a source (export) and counted as negative (Eilola et al., 2012). Source areas of DIP generally coincide with sink areas of OrgP, and vice versa. This is also partly true for DIN and OrgN, but the sink for DIN has a large contribution from denitrification that transfers DIN to dissolved N_2. The difference between phosphorus and nitrogen sources and sinks is oxygen dependent, because the removal of N is enhanced at lower oxygen concentrations, while the sediment phosphorus sink is weakened (e.g., Savchuk, 2010). Sediments may even temporarily become a source under anoxic conditions, when older mineral-bound P can be released to the overlying water. Source areas of DIN are mainly found in the Gulf of Riga, and the deeper parts of the Arkona Basin and Bornholm Basin. The largest DIP sources occur in the eastern parts of the Gotland Basin as well as in the deepest parts of the Bornholm Basin and Arkona Basin, whereas the largest sink of OrgP occurs in the central Baltic proper. The main sources of DIP are generally found in regions where water depth is greater than 70 m (in other words below the permanent halocline in the Baltic proper), while the main sources of OrgP (and OrgN) are found in the productive coastal areas shallower than about 30–40 m (see also Fig. 8). Indeed, DIP export is largest in areas with a water depth between 70 and 100 m, and decreases towards greater water depths (Fig. 8).

According to the accumulated import of nutrients (Fig. 8), the magnitude of the DIP export is larger than that of the DIP import. This indicates that not all of the supply of phosphorus from land and atmosphere is retained within the Baltic proper. For DIN, however, we may notice only a very small net export from the Baltic proper to adjacent sub-basins, while for OrgP and OrgN, imports and exports are almost balanced (Fig. 8). The nitrogen and phosphorus supply from land is implemented in sea areas with a bottom depth usually of 6 m. This is where the river mouths are located in the model.

There is a large import of DIP to areas with a depth range between 40–70 m (Fig. 8). This import does not show a counter-part in the export of OrgP in Fig. 8. This result might be explained by local processes causing the phytoplankton uptake and sediment deposition of DIP. There is an import of DIN to these areas that together with nitrogen fixation and sediment–water fluxes of DIN may support local production of organic matter. The phosphorus sink may be partly caused by oxygen dependent water–sediment fluxes that bind DIP to ironbound phosphorus in oxic sediments (Almroth-Rosell et al., 2015). This effect is not included in Eilola et al. (2012)-, but might potentially be accounted for by the adjusted DIP transports in REANA. The results of REANA indicate that there is an additional sink but the relative importance of different processes causing this sink (data assimilation or sediment processes) is, however, not possible to evaluate from the present reanalysis data set.

A partly opposite exchange profile is found for OrgP (Fig. 8). Coastal areas with a water depth of up to 40 m are exporting organic phosphorus, whereas deeper areas import OrgP. Production in the coastal zone of the Baltic proper and sedimentation in the open sea is almost balanced.

The largest export of DIN occurs due to rivers in the very shallow coastal zone. The magnitude of DIN imports and exports in areas with greater water depths are much smaller. Obviously, DIN supplied from land is already consumed in the coastal zone (Voss et al., 2005; Almroth-Rosell et al., 2011) and, consequently, only a minor fraction of the nitrogen supplied to the shallow area can continuously reach regions deeper than 100 m (Eilola et al., 2012; Radtke et al., 2012).

5.6 Nutrient budgets of sub-basins

The Baltic Sea is divided into seven sub-basins according to the selected sections, which form the borders of the sub-basins (Fig. 1). We calculate total nutrient budgets for each of the sub-basins from the reanalysis (Fig. 9 and 10). The largest annual external phosphorus load occurs in the Baltic proper and amounts to 34.2 kton yr^{-1} (Fig.

9). In addition, in the Baltic proper the largest annual phosphorus sink of 21.7 kton yr^{-1} is also found. The tendencies of phosphorus in the various sub-basins differ. Whereas during the period 1970–1999 the phosphorus content in the Gulf of Finland, Baltic proper, Kattegat and Bothnian Bay increased, we found decreasing content in the Gulf of Riga, Bothnian Sea and Danish Straits (Table 1). Largest export and import of phosphorus between sub-basins are found for the exchange between the Baltic proper and the Gulf of Finland, which amount to 24.3 and 22.5 kton yr^{-1}, respectively. However, the largest net exchange appears between the Baltic proper and Bothnian Sea. It is also found that the Baltic proper exports more phosphorus to neighboring sub-basins than it imports, except for the Gulf of Riga. The annual net phosphorus exported from the Baltic proper into the Danish Straits, the Bothnian Sea, the Gulf of Finland and Gulf of Riga amounts to 1.7, 3.6, 1.8, and -0.6 kton yr^{-1}, respectively. The exchange of phosphorus between the Baltic proper and the Gulf of Riga is smallest relative to the other three neighboring sub-basins. Further, we found that the net transport, import and export of phosphorus into the Bothnian Bay are smallest relative to the other sub-basins.

Nitrogen transports between Baltic Sea sub-basins are different compared to phosphorus transports (Fig. 10). For example, the Baltic proper has larger nitrogen sinks than external sources. Further, the nitrogen content decreased in the Baltic proper and increased in the Gulf of Riga during the period from 1970–1999, respectively. In Bothnian Bay, the difference between external supply and internal sink of nitrogen is equal to the net transport into the Bothnian Bay. The large burial of nitrogen in the Bothnian Bay is noteworthy. We also found relatively large net transports of nitrogen from the Gulf of Riga into the Baltic proper. This is mainly explained by the relatively high nitrate concentrations in the Gulf of Riga relative to other sub-basins.

To further analyze the variability of the budget of the reanalyzed nutrients, Fig. 11 provides the cross sectional, integrated nutrient flows in the different sub-basins. Here the eastward and northward net transports are, by definition, positive. Obviously, the integrated nutrient flows vary significantly in space according to the nutrient loads from land. The inflows and outflows also vary depending on the depth of the water column and nutrient concentrations that influence the vertically integrated mass fluxes. In general, the magnitude of nutrient transports declines along transect A from south to north. For instance, the largest annual northward flow of nitrogen in the Baltic proper reaches 392 kton yr^{-1}, while it is only 133 and 87 kton yr^{-1} for the Bothnian Sea and Bothnian Bay, respectively.

In the Baltic proper, inflow and outflow as well as the net northward flow of phosphorus increase from the south until a section along 56.8^{o} N; they then remain about constant until a section along 58.7^{o} N, and thereafter decrease rapidly further to the north. This indicates that major sources are located in the south where the large rivers pour their loads into the Baltic Sea, while the major net sinks are mainly found in the northern parts of the Baltic proper. The behavior of net northward flow of nitrogen is different. Nitrogen transports decrease constantly with increasing latitude because the major sink (i.e. denitrification) works differently for nitrogen than for phosphorus, which is retained mainly by burial in the sediments. The net northward flow decreases at the latitude of the Gulf of Finland where phosphorus (and nitrogen) is transported towards the Gulf, as seen in transect C.

In the Arkona and Bornholm basins, nitrogen and phosphorus transports increase from the west to the east. Due to the nitrogen load from the Oder River, the inflow of nitrogen increases significantly at the border between the Arkona and Bornholm basins, whereas the outflow does not show any discontinuity. As a result, the net flow of nitrogen shows an accelerated increase. The situation for phosphorus in the Arkona and Bornholm basins is different compared to the nitrogen transports because in- and outflow, as well as the net flow, change direction. The phosphorus loads from the Oder River turn the outflow in the western parts into an inflow of phosphorus in the eastern parts.

In the Gulf of Finland, in– and outflows generally decline from the west to east. In the entrance of the Gulf of Finland, the net inflows of nutrients are almost zero. The largest net flow (westward) of nutrients appear at the inner end of the Gulf of Finland, where the large river Neva enter the Gulf, with a magnitude of 33 kton yr^{-1} for nitrogen and 2.6 kton yr $^{-1}$ for phosphorus, respectively. The net flows of both phosphorus and nitrogen change their directions in the Gulf of Finland and for nitrogen this change take place closer to the Baltic proper entrance than for phosphorus. These results indicate that the large supply of nutrients from the Neva River are accumulated or removed within the Gulf of Finland.

6 **Discussion**

6.1 Biases of FREE

RCO-SCOBI has been widely used for the Baltic Sea and the model was carefully evaluated using various observational data sets. As any other model, RCO-SCOBI had to be calibrated because many processes including sources and sinks of nutrients are not detailed enough known. Hence, an “optimal” parameterization of unresolved processes is one of the requirements for the predictive capacity of the model. Further requirements to calculate correct transports and transformation processes in addition to optimized model equations are high-quality atmospheric and riverine forcing data, and high-quality initial and lateral boundary conditions.

Most of the large biases in FREE are caused by imperfect initial conditions. The reason is that the nutrient pools in the sediments have not been spun up appropriately. As a consequence, phosphate concentrations in FREE are higher than observed concentrations at all depths. The biases in surface phosphate concentrations between model results and observations can influence the seasonal primary production. In REANA, however, from the beginning of the experiment, the biases are already significantly reduced and remain relatively small during the integration compared to FREE. The biases of phosphate reduce with time both in the FREE and REANA runs. Hence, this indicates a need of new initial conditions of the sediments.

6.2 Non-conservation in REANA

In the long-term simulation, the new initial condition for an assimilation cycle differs from the ending ocean state of the last cycle when at that time observations are available. In this sense, the data assimilation introduces sources and sinks of the nutrient cycles by interrupting the model simulation and adjusting the initial conditions. The magnitudes of these artificial sources and sinks are directly related to the biases between model results and observations. Figure 3 shows that the model has large biases during the beginning of the simulation. However, data assimilation has corrected the mismatch between model state and observation to an “optimal” level during an initial adjustment period. After the adjustment period, the mismatch between model and observation becomes small and the successive adjustment due to data assimilation also becomes small. Further, the adjustment of data assimilation is related to the spatial-temporal coverage of observations. Here we assimilated only observed profiles into the model.

After every assimilation cycle, the simulation continues with “optimal” initial conditions based upon conservation principles. As the equations of RCO-SCBI have not been changed, masses of all constituents of the model are conserved at least during the simulation between two assimilation occasions.

6.3 Advantages of data assimilation

The advantage of the data assimilation is that model variables at any station are very likely more accurate than the model output without data assimilation. For instance, time series of profiles or transports across vertical sections have very likely a smaller bias compared to observations than the corresponding model results without data assimilation. Compared to available observations the information from the model is higher resolved and homogeneous in space and time. Of course, it is difficult to evaluate the quality of model results at high resolution because independent observational data sets are usually missing. An exceptional effort to utilize independent data was done by Liu et al. (2014) showing that the statement about the added value of data assimilation is true for the available, independent cruise data at high resolution.

The results of the reanalysis can be used to estimate the water quality and ecological state with high spatial and temporal resolution in regions and during periods when no measurements are available. Regional and local model studies may use the data as initial and boundary conditions. For projections of future climate and for nutrient load abatement scenario simulations the reanalysis has a very high scientific value as reference data set for the historical period of the climate simulations. The evaluation of the regionalized climate (the statistics of mesoscale variability, e.g. the mean state) during the historical period can be done much more accurate based upon the reanalysis data than with sparse observational data. For instance, it is very difficult to calculate the climatological mean state just from observations that are casted only during the ice-free season of the year. Using a reanalysis as reference data for historical climate is a common method in regional climate studies of the atmosphere. Here we provide a corresponding data set for the ocean to evaluate simulated present-day climate.

Further, nutrient transports across selected cross-sections or between vertical layers are calculated from the reanalysis with high resolution and improved accuracy. However, one cannot expect that budgets calculated from the summation of fluxes from model results with data assimilation are more accurate because usually small artificial sources and sinks from the data assimilation are becoming as important as physically motivated sources and sinks when sums of fluxes are compared. Hence, we calculated budgets with the aim to evaluate the reanalysis data and to estimate the magnitude of artificial sources and sinks by comparing our results with other studies using only observations. It is impossible to claim that our budgets are more accurate than those budgets that are derived from observations only, despite the higher temporal and spatial resolution in model outputs. Hence, the advantage of the reanalysis is that measurements are extrapolated in space and time based upon physical principles of the model. However, the disadvantage is that the reanalysis data does not obey conservation principles as discussed above.

6.4 Comparison with other assimilation methods

Fu (2013) estimated the volume and salt transports during the 2003 MBI with 3DVAR in the Baltic Sea. In the present study, we estimate the impact of the data assimilation based on the EnOI method on the net volume and nutrient transports as well as calculate budgets for major sub-basins of the Baltic Sea. The volume transports obtained with different assimilation methods may be different. The sea level in Fu (2013) is kept constant in the assimilation process, while sea level in this study is varying accordingly during the assimilation of temperature and salinity based upon the statistical covariances. The variability of sea level may enhance the barotropic flow, which is one of the reasons for the differences in net volume transport in the two simulations. However, transports within the sub-basin are also indirectly affected by the interaction of baroclinicity and topography.

6.5 Comparison with other studies on nutrient_budgets

In contrast to Eilola et al. (2012), in this study areas with DIN export are also found at the southern and eastern coasts as well as at some small local regions in the inner parts of the Baltic proper (Fig. 7). In REANA, the magnitudes of DIP imports and exports are larger than in Eilola at al. (2012), and there is pronounced import of DIP in the western part of the Eastern Gotland Basin below 100 m (Fig. 7) that is not as significant in Eilola et al. (2012). This, and the larger variability of DIN imports and exports, indicates that there is a higher degree of small-scale localized transport and production patterns that are not captured by Eilola et al. (2012). Main sinks of DIN are found in the deeper areas, but significant sinks are also seen in shallow areas and water depths of about 60m. As the assimilation of salinity observations result in a deeper halocline (Liu et al., 2014), the bottom water in a depth range of 40–70 m contains higher oxygen concentrations than in the simulation without data assimilation. Hence, in the REANA simulation of this study, more phosphorus is retained by the sediments in the depth range of 40–70 m than in the simulation by Eilola et al. (2012). The present results show, however, an export contribution from DIN sources in deeper areas (e.g. 60–90 m depths) that may have been caused by reduced denitrification efficiency of oxidized sediments in the REANA simulation compared to Eilola et al. (2012).

The in- and outflows of phosphorus between the sub-basins, except the Gulf of Riga and Gulf of Finland, simulated in REANA are smaller than the results by Wulff and Stigebrandt (1989), Savchuk (2005) and Savchuk and Wulff (2007). However, the net transports of phosphorus are similar between our results and these earlier studies in all sub-basins. Moreover, the nitrogen budgets are much lower than the results of earlier studies, especially in the Baltic proper. It should be kept in mind that the above mentioned studies estimated the nutrient budgets from mass balance models together with inter-basin transport calculations based upon Knudsen's formulae to calculate nutrient budgets of the Baltic Sea (see, e.g. Savchuk, 2005). Obviously, there are limitations in calculations of previous studies. Despite overall uncertainties that also limit the reliability of our results, like incomplete understanding of selected biogeochemical processes (e.g. nitrogen fixation), lacking information of sediment parameters, and under-sampled observations in space and time, our approach has the advantage of using both high-resolution modeling and all available observations made over a 30-year period. Our model results consider the complete set of primitive equations in high-resolution, taking into account not only the volume and salt conservation of sub-basins according to Knudsen's formulae, but also the wind-driven circulation between and within sub-basins. Hence, we have, for the first time, the potential to quantify spatial transport patterns with high~~er~~ confidence even within sub-basins, as in the exchange of nutrients between the coastal zone and the open sea.

Eutrophication of the Baltic Sea is directly affected by the long-term evolution of external nutrient supply that has three components (waterborne land loads, direct point sources at the coasts, and atmospheric depositions) which are associated with the biogeochemical dynamics of the Baltic Sea. In our study, we used the reconstructed external nutrient input data by Savchuk et al. (2012). Nutrient budgets (Figs. 9 and 10) of sub-basins are time-averaged and represent in our study the overall results of the period 1970–1999. The phosphorus loads vary in different periods, for example, the phosphorus loads in the 1980s are larger relative to the 1990s (see Savchuk et al., 2012). Therefore, the phosphorus supply into the Gulf of Finland is greater in our study compared to Savchuk and Wulff (2007). The greater phosphorus supply changes the phosphorus content and phosphorus concentration in the Gulf of Finland. This is one reason why phosphorus transports between the Gulf of Finland and the Baltic proper in our study are greater than the transports calculated by Savchuk (2005) and Savchuk and Wulff (2007).

Since our study covers a different time period compared to the studies by Wulff and Stigebrandt (1989), Savchuk (2005) and Savchuk and Wulff (2007) nutrient concentrations and related budgets differ in time and space. Hence, it is not surprising that other studies show deviating results. For example, during the period 1970–1999, HELCOM (2013) showed that the total phosphorus (TP) concentration generally decreased in the Bothnian Bay and has increased in the Gulf of Riga. However, these changes in TP concentrations were not monotonous. For example, the TP concentration obviously increased during the period 1970–1976 in the Bothnian Bay. While in the Bothnian Sea, TP concentration increased during the period 1970–1983 and decreased during the period 1990–1999. Similarly, changes in total nitrogen (TN) concentration differed during different periods.

Gustafsson et al. (2012) used a process-oriented model that resolves the Baltic Sea spatially in 13 dynamically interconnected and horizontally integrated sub-basins with high vertical resolution to reconstruct the temporal evolution of eutrophication for 1850–2006. Savchuk (2005) and Savchuk and Wulff (2007) applied mass balance models as mentioned above to calculate nutrient budgets of the Baltic Sea. The results of all these models depend on the locations of the sub-basin borders which are chosen as far as possible according to dynamical constraints such as sills or fronts that are parameterized to obtain estimates of the water exchanges. Using a high-resolution circulation model, we showed that nutrient flows within the sub-basins may vary considerably (Fig. 11). For instance, we found east- and westward net transports of nitrogen between the Baltic proper and Gulf of Finland depending on border locations at 23.2° and 24.0 ° E, respectively. The importance of regional variations of sources and sinks for nutrients on the calculation of transports between sub basins therefore seem to be significant and need to be furthers studied. Given the uncertainty caused by data assimilation in the present study we must however save the detailed studies of these issues to future work where the artificial impact of data assimilation on sources and sinks will be traced and quantified during the run.

7 Summary and Conclusion

For the first time, a multi-decadal, high-resolution reanalysis of physical (temperature and salinity) and biogeochemical variables (oxygen, nitrate, phosphate and ammonium) for the Baltic Sea was presented. The reanalysis covers the period 1970–1999. A "weakly coupled" assimilation scheme using the EnOI method was used to assimilate all available physical and biogeochemical observations into a high-resolution circulation model of the Baltic Sea.

Both assimilated and independent observations collected from different databases were used to evaluate the reanalysis results (REANA). Based on the model–data comparison presented in this study, we found that the model results without data assimilation (FREE) exhibit significant biases in both oxygen and nutrients. The reasons for these biases are not totally understood yet, although it is speculated that the main reasons might be related to the imperfect initial conditions, limitations of model parameterizations, the inaccurate halocline position and correspondingly the hypoxic volume (Liu et al. 2014). Based on the calculation of the overall RMSD of oxygen and nutrient concentrations between model results and not-yet-assimilated observations, the results in REANA are considerably better than those in FREE. The total RMSD of the oxygen, nitrate, phosphate and ammonium is reduced respectively by 0.84 mL L^{-1}, 0.99 mmol m^{-3}, 0.88 mmol m^{-3}, 0.52 mmol m^{-3}. This means that the overall qualities of simulated oxygen, nitrate, phosphate, and ammonium concentrations are improved by 59, 46, 78 and 45%, respectively. These results demonstrate the strength of the applied assimilation scheme.

The observation information entering the model affects the oxygen dependent dynamics of biogeochemical transports significantly due to both improved simulation of physical (e.g. vertical stratification) and biogeochemical parameters (e.g. nutrient concentrations). As examples, we presented improved results of mean seasonal cycles of nutrients, the spatial surface distributions of DIN, DIP and DIN:DIP of the entire Baltic Sea. Based on the reanalysis simulation, we analyzed nutrient transports in the Baltic Sea. We found that vertically integrated nutrient transports follow the general horizontal water circulation, and vary spatially to a large extent. In particular, large nutrient transports were found in the Eastern Gotland Basin, in the Bornholm Basin, in the Slupsk Channel and in the north-western Gotland Basin. The persistence of nutrient transports is greater in the eastern and southern than in the northern and western Baltic Sea.

The horizontal distributions of sources and sinks of inorganic and organic nutrients show large spatial variations and may be partly explained by (1) the external supply of nutrients from land, (2) the topographically controlled horizontal nutrient exchange between sub-basins and between the coastal zone and the open sea, and (3) vertical stratification that determines redox conditions at the sea floor. The latter is important for the sediment-water fluxes of nutrients, and consequently for burial of nutrients in the sediments. The reanalysis results suggest that in the Baltic proper, in most areas with a water depth less than the depth of the permanent halocline at about 70–80 m, DIP is imported and transformed either to OrgP, or buried in the sediments in water depths greater than the wave-induced zone at 40–70 m. Whether the latter is an artefact of the assimilation method or a real sink is unclear. On the other hand, in areas with greater water depth, DIP is exported (e.g.

released from the sediments under anoxic conditions). Overall, the Baltic proper exports DIP to neighboring sub-basins.

Nitrogen transports are very different compared to phosphorus transports. The shallow coastal zone with water depths less than 10 m plays an outstanding role for DIN, because within it, large exports occur due to supplies from land. The high productivity in the shallow areas effectively transfers DIN to OrgN and denitrification decreases the exports of nitrogen from coastal areas to the deeper areas. Most of the exported DIN is removed in shallow waters while at greater depths imports and exports of DIN are much smaller, indicating the important role of the coastal zone for nitrogen removal.

Detailed nitrogen and phosphorus budgets suggest that nutrient transports in the various sub-basins are controlled by different processes and show different response to external loads and internal sources and sinks. In particular, the Baltic proper is the sub-basin with the largest nutrient exchanges with its surrounding sub-basins. The Baltic proper exports phosphorus to all sub-basins except the Gulf of Riga. Similarly, the Baltic proper also exports nitrogen to all sub-basins except to the Gulf of Riga and Danish Straits. In this sub-basin, also the largest internal sink of all sub-basins was found. Noteworthy is the relatively large net export of phosphorus from the Baltic proper into the Bothnian Sea, where the second largest sink for both phosphorus and nitrogen was found. This finding is in agreement with previous studies. For the budgets of the sub-basins, it is important where the borders of the sub-basins are located, because net transports may change sign with the location of the border. For instance, in the entrance of the Gulf of Finland, the net phosphorus transport from the Baltic proper is directed eastward, but changes direction at about 26ºE. Further to the east, the net phosphorus transport is directed westward.

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Table 1. The 30-year mean tendencies of total phosphorus and nitrogen in Baltic sub-basins. Names of the sub-basins are the Kattegat (KT), Danish Straits (DS), the Baltic proper (BP), the Gulf of Riga (GR), the Gulf of Finland (GF), the Bothnian Sea (BS), and the Bothnian Bay (BB).

kton yr^{-1}	KT	DS	BP	GR	GF	BS	BB
ΔP	2.7	-2.2	6	-0.5	3.7	-3.5	0.6
ΔN	30	-33	-115	7	16	-39	0

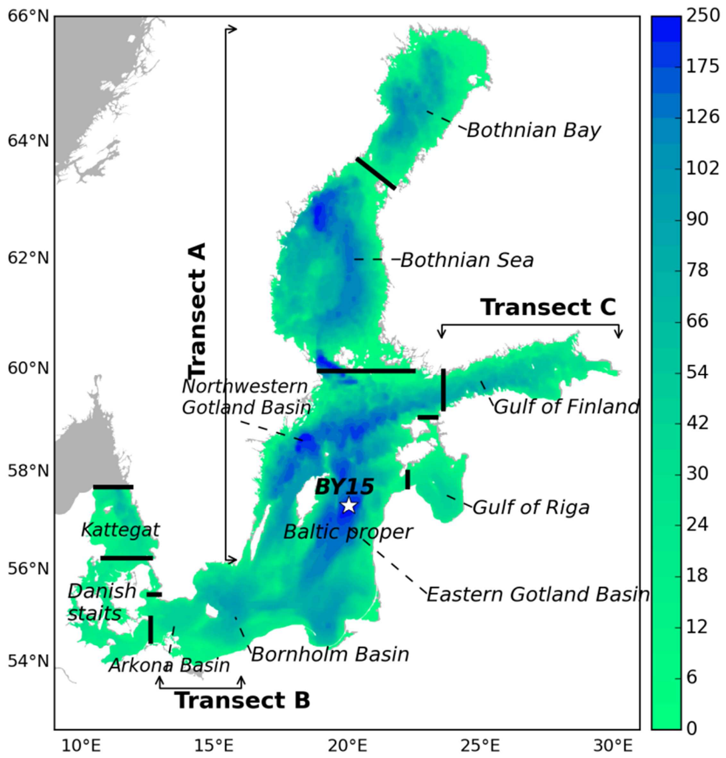

Figure 1. The bathymetry of the model (depth in m). The border locations of sub-basins of the Baltic Sea used in this study are shown by the black lines, and the BY15 station is shown by the white star.

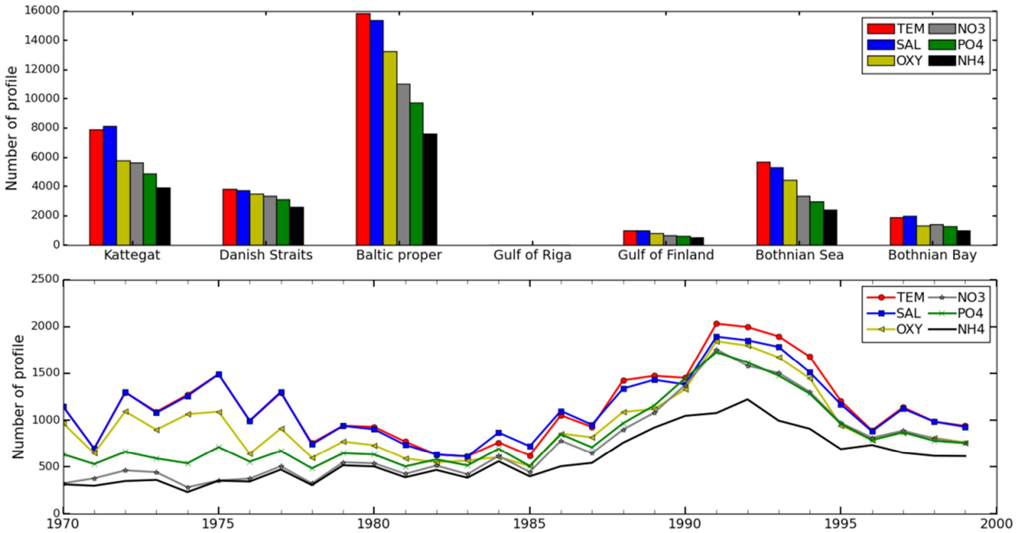

Figure 2. Number of observed profiles in different sub-basins (upper panel) and annual number of profiles from 1970-1999 (bottom panel).

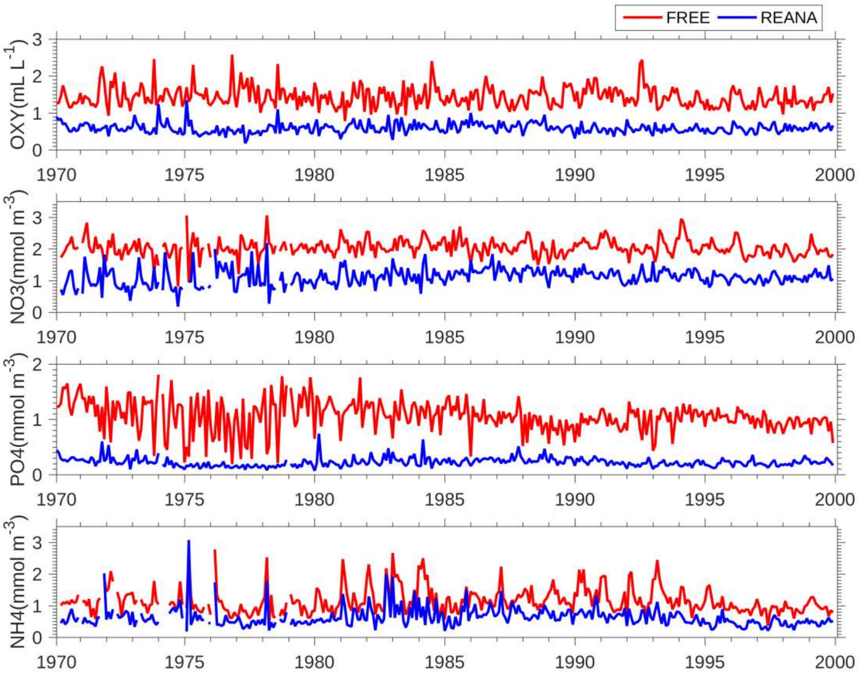

Figure 3. Monthly mean root mean square deviation (RMSD) between model results and observations for oxygen, nitrate, phosphate and ammonium in FREE (red) and REANA (blue).

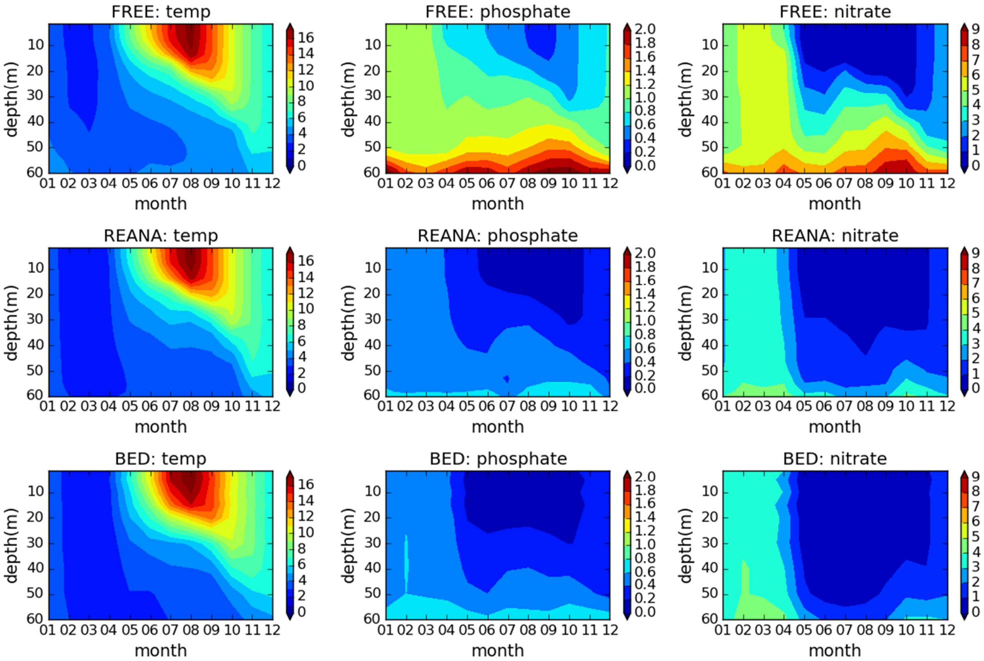

Figure 4. The seasonal cycle of monthly average (1970–1999) temperature (°C), phosphate concentration (mmol m^{-3}), and nitrate concentration (mmol m^{-3}) at BY15 for FREE (row 1), REANA (row 2), and BED data (row 3), respectively.

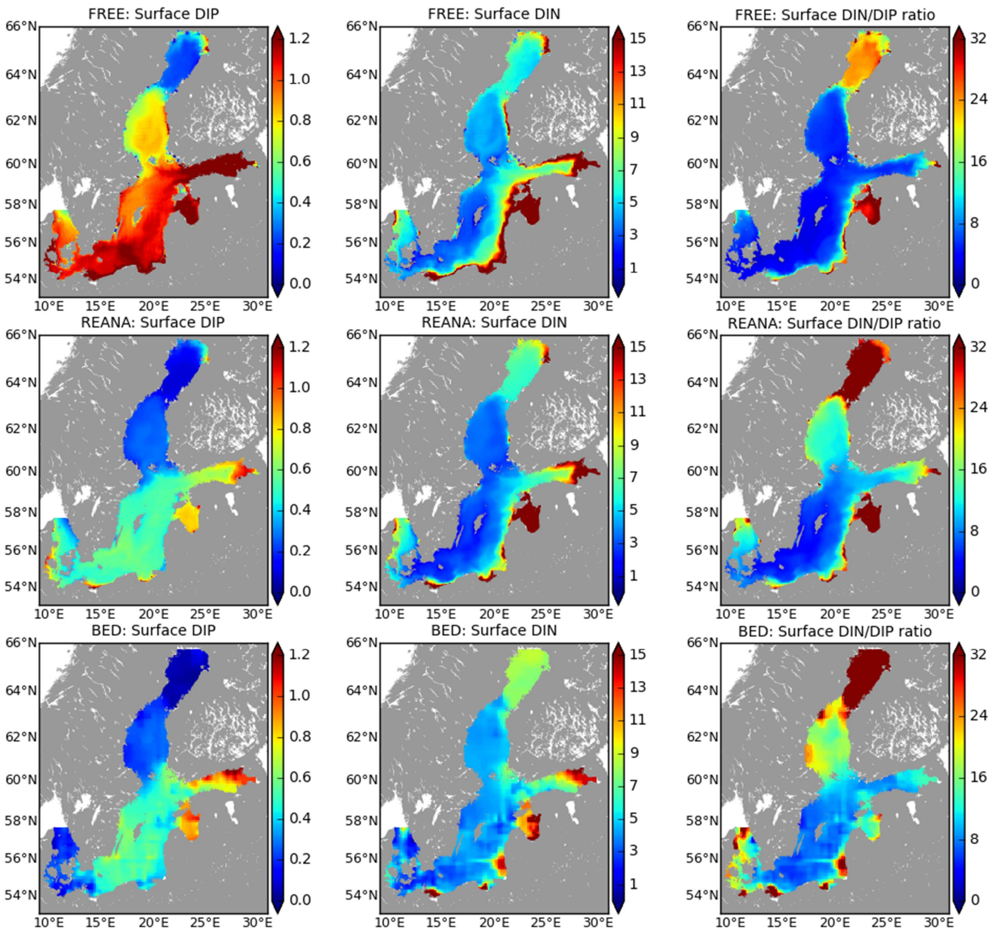

Figure 5. Monthly (March) mean (1970–1999) surface layer (0–10 m) concentrations of DIP (mmol m^{-3}) (left), DIN (mmol m^{-3}) (middle), and the corresponding DIN to DIP ratio (right). Results from FREE, REANA and BED are shown from above in rows 1, 2 and 3, respectively.

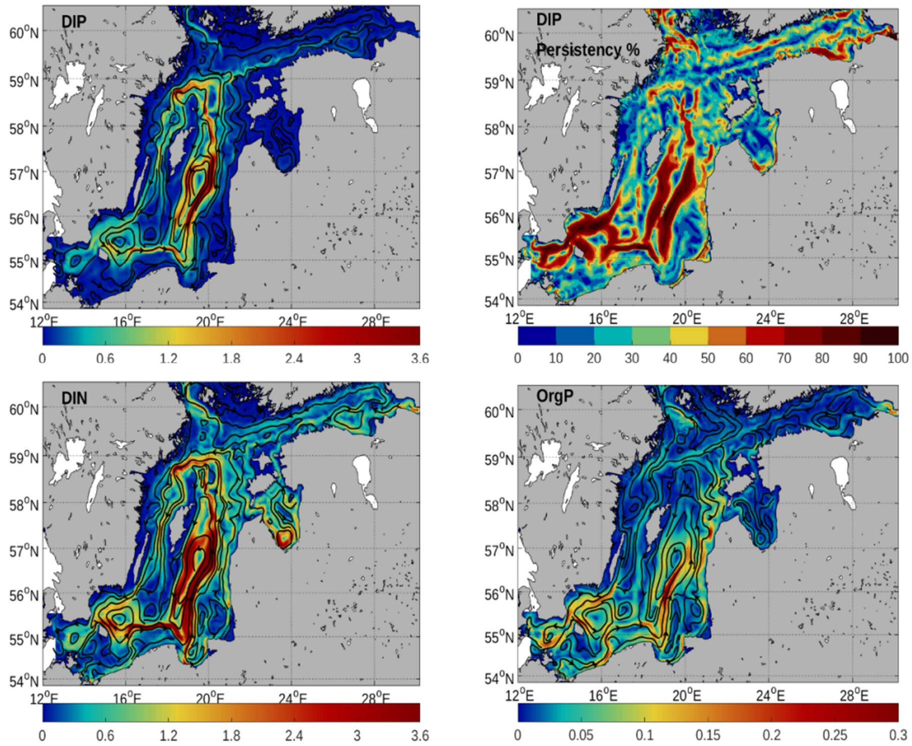

Figure 6. Annual mean DIP transports and the corresponding DIP persistency, DIN and OrgP transports for REANA averaged for the period 1970-1999. The black solid lines with arrows show the streamlines and direction of transports. The magnitude of transports (kton km^{-1} yr^{-1}) and the persistency (%) are shown by the background color. The corresponding values are shown in the colored bars.

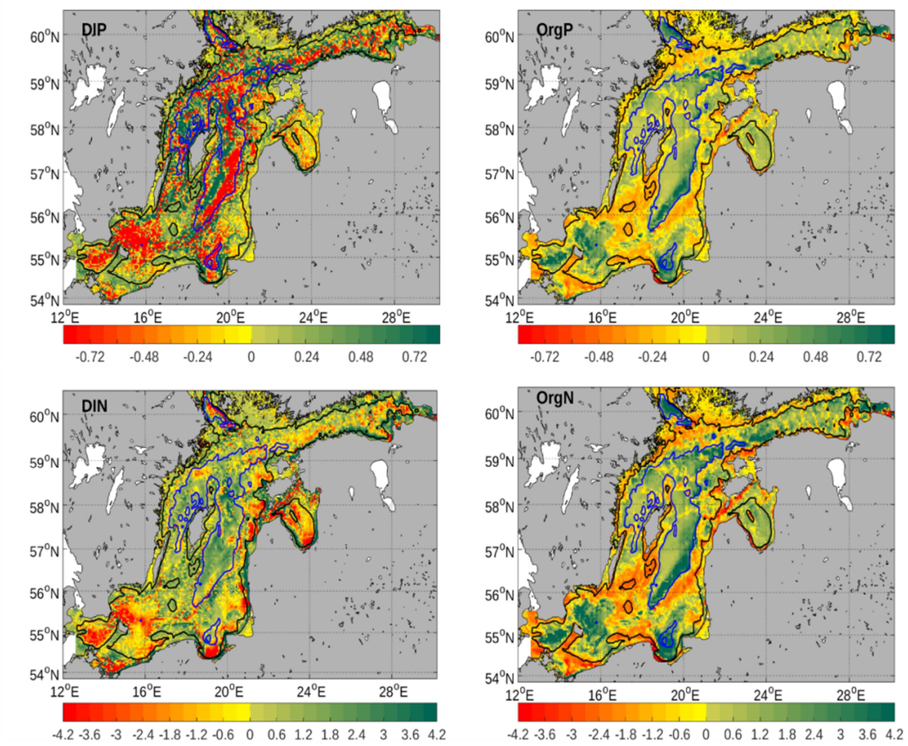

Figure 7. Spatial distributions of annual mean import of DIP, OrgP, DIN and OrgN averaged for the period 1970-1999. The magnitude of import and its corresponding value (kton km^{-2} yr^{-1}) are shown by the background color and color bar, respectively. Green colors denote positive values (import), and yellow to red colors denote negative values (export). The black and blue lines show 30 and 100 m depth contours of the model, respectively.

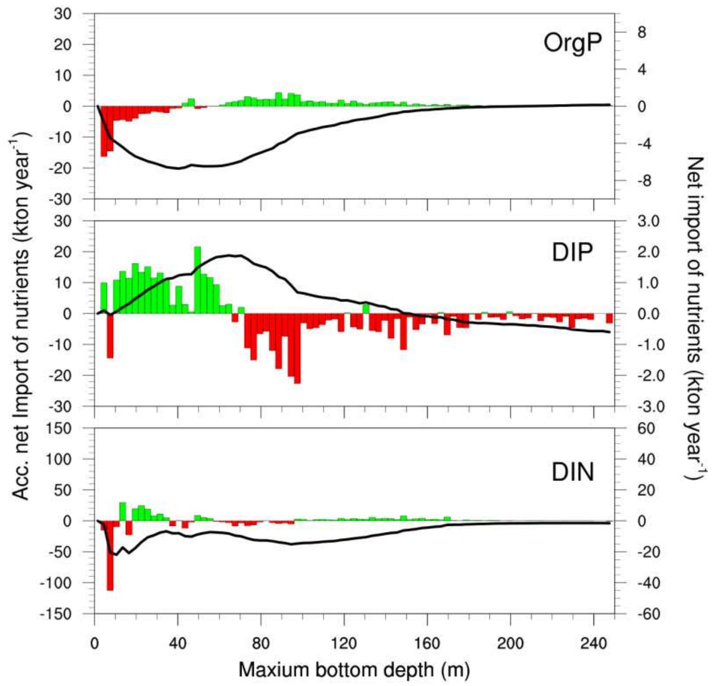

Figure 8. Annual mean, accumulated net imports (black lines) and imports of OrgP, DIP and DIN (color bars) to regions with the same depth in the Baltic proper averaged for the period 1970-1999.

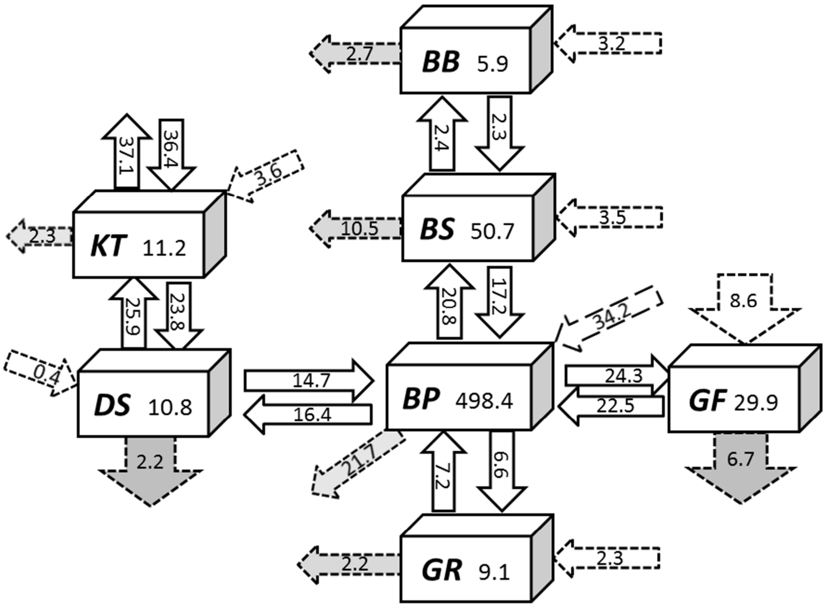

Figure 9. Annual mean total phosphorus budgets of the Baltic Sea averaged for the period 1970–1999. The average total amounts are in kton, and transport flows and sink/source fluxes (external nutrient inputs/burial) are in kton yr^{-1}. External nutrient inputs from atmosphere and land are combined.

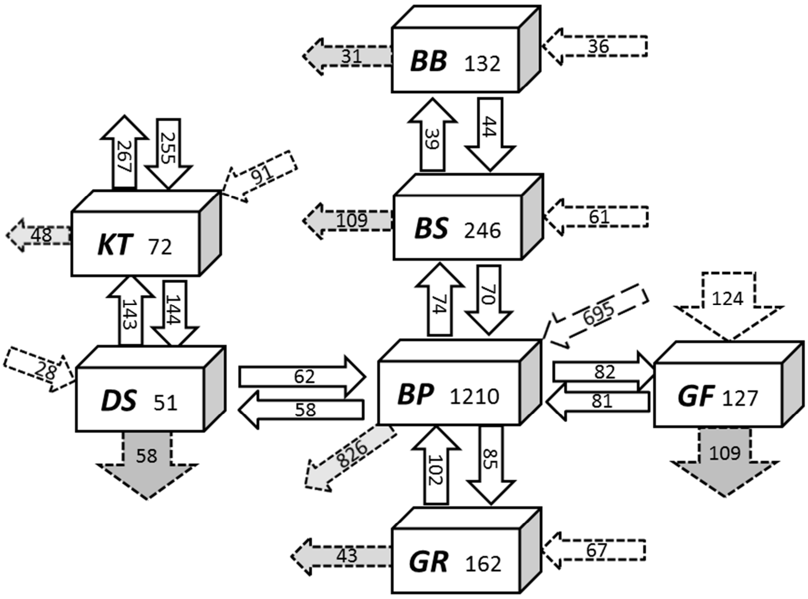

Figure 10. The same as Figure 9, but for nitrogen.

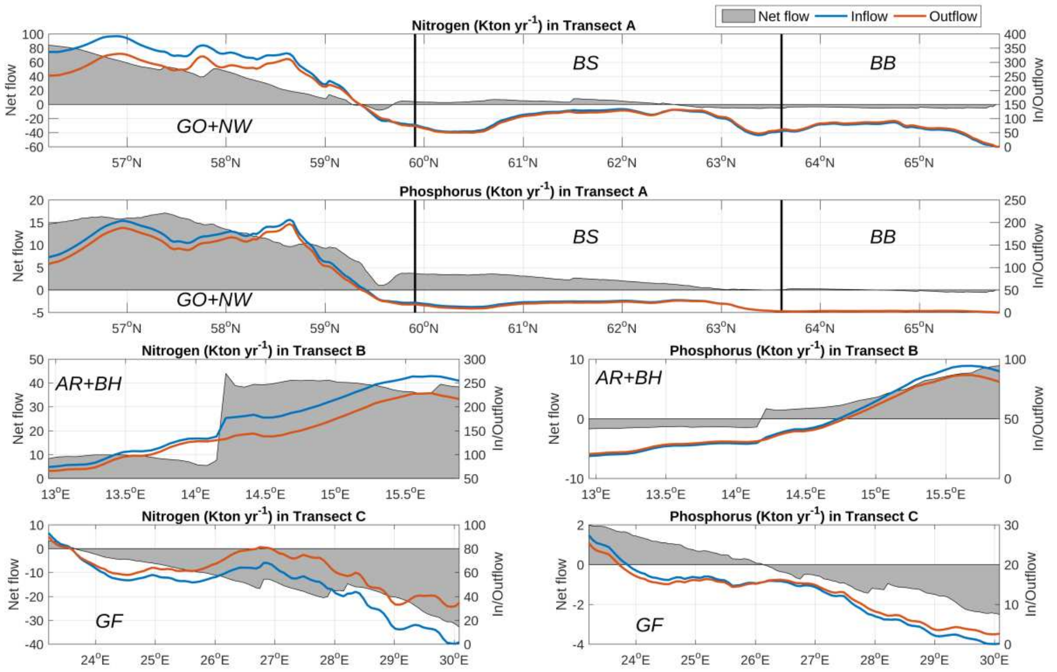

Figure 11. Annual mean fluxes of nitrogen (in kton yr^{-1}) and phosphorus (in kton yr^{-1}) as a function of the cross sections along transects following the latitude and longitude in the Baltic sub-basins. Northward and eastward fluxes are, by definition, positive and called inflows. Southward and westward flows are called outflows. Net flow is the difference between in and outflows. Here, AR, BH, GO, NW, GF, BS, and BB represent the Arkona Sea, Bornholm Sea, Eastern Gotland Basin, Northwestern Gotland Basin, Bothnian Sea and Bothnian Bay, respectively. Transect A summarizes fluxes from the southern Baltic proper to the Bothnian Bay. Transect B describes the Baltic Sea entrance area from the Arkona Basin to the Bornholm Basin, and transect C summarizes fluxes in the Gulf of Finland (see Fig. 1).