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МОДЕЛИРОВАНИЕ РАСТВОРЕННОГО ОРГАНИЧЕСКОГО ВЕЩЕСТВА В ФИНСКОМ ЗАЛИВЕ

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Цель работы — усовершенствование Санкт-Петербургской модели эвтрофикции Балтийского моря (SPBEM) за счет включения уравнений неконсервативной примеси для растворенного органического азота и фосфора в двух формах — легкоокисляемой и стойкой. Численные эксперименты по тестированию усовершенствованной версии модели было выполнено для Финского залива для периода 2009—2014 гг. Начальные и граничные условия для численных экспериментов были получены на основе данных натурных наблюдений. Сравнение результатов моделирования с данными наблюдений показало хорошее совпадение пространственно-временной изменчивости гидрофизических и биогеохимических характеристик, в том числе почти идеальное соответствие между моделируемой и наблюдаемой динамикой органических форм азота и фосфора. Важнейшим отличием между рассчитанными и наблюдаемыми характеристиками является завышенное содержание неорганического азота и фосфора, что может быть вызвано неточностями в задании начальных и граничных условий, а также в используемых параметризациях потоков минерализации. Более тонкая настройка SPBEM-2 требует более тщательного анализа чувствительности.

Ключевые слова: растворенное органическое вещество, модель SPBEM, Финский залив.

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MODELLING DISSOLVED ORGANIC NUTRIENTS IN THE GULF OF FINLAND

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St.-Petersburg model of eutrophication (SPBEM) has been modified for improving description of organic matter as a part of the nutrient biogeochemical cycles. The dynamics of labile and refractory fractions of dissolved organic nitrogen and phosphorus are now described with four additional equations. The modification was tested at the Gulf of Finland in a numerical experiment made with plausible initial and actual boundary conditions for the years 2009—2014. Comparison of simulation with the available field observations indicates quite reasonable reproducibility of seasonal and inter-annual variations of spatial distribution of hydrophysical and biogeochemical characteristics, including almost a perfect match between simulated and observed dynamic of organic nutrients. The most important distinction from natural prototypes is the overestimated total amounts of inorganic nitrogen and phosphorus, which can be caused by the deficiencies in the prescription of initial and boundary conditions as well as in the current parameterizations of pathways and rates of mineralization fluxes. The finer tuning of SPBEM-2 requires more extensive sensitivity analysis.

Key words: dissolved organic matter, SPBEM model, Gulf of Finland.

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Introduction. From a large scale long-term perspective, the changes in trophic state of the Gulf of Finland ecosystem as a whole are driven by nutrient inputs (comprising both the external inputs from land and atmosphere and the exchange with the Baltic Proper), which impact is modified by internal transports and transformations of nutrients. From a regional perspective, the spatial dynamics and peculiarities of eutrophication are determined by a complex interplay between geographical distribution of the local nutrient inputs and the biogeochemical fluxes within and between the pelagic, coastal and bottom ecosystems. Despite the ongoing reductions of total external inputs, which in the Gulf of Finland decreased between 2000 and 2014 from 124×10^3 to 112×10^3 tonnes Total Nitrogen (TN) yr^{-1} and from 9.3×10^3 to 4.4×10^3 tonnes Total Phosphorus (TP) yr^{-1} [1], these annual inputs are still somewhat higher than Maximum Allowable Inputs (MAI) agreed in the Baltic Sea Action Plan as 102×10^3 tonnes TN yr^{-1} and 3.6×10^3 tonnes TP yr^{-1}, respectively [2]. Similarly to the other Baltic Sea marine basins, the total pools of nutrients in the Gulf of Finland in 2000—2016 stay from year to year remarkably stable: 341 ± 22 and 29 ± 3 thousand tonnes TN and TP, respectively [3]. Being presented as the basin-wide long-term average concentrations, 358 mg N m^{-3} of total nitrogen consisted of 85 mg N m^{-3} and 273 mg N m^{-3} of dissolved inorganic and total organic nitrogen, respectively, with 25 % of the latter being estimated as labile fraction. Similarly, 37 mg P m^{-3} of TP consisted of 26 mg P m^{-3} of DIP and 11 mg P m^{-3} of total organic phosphorus comprising 64 % of labile fraction.

On the other hand, these MAI values have been estimated with the help of mathematical model BALTSEM [4] that at the time had been formulated as describing biogeochemical cycles of only bioavailable fractions of organic compounds of nitrogen and phosphorus, which were assumed being entirely contained only in particulate form. Regarding both the external nutrient inputs delivering significant amounts of Dissolved Organic Matter (DOM) [5] and the importance of DOM in internal ecosystem interactions [6, 7], these formulations necessitate two kinds of parametrizations based on rather uncertain assumptions. The coefficients of bioavailability are poorly constrained for such geographically diverse terrestrial inputs as a river and diffuse runoff draining contrasting watersheds as well as direct point sources with a differing degree of wastewater treatment. Lumping together dissolved and particulate organic forms into the model variable "detritus" that cannot be directly compared to measurements and requires artificial adjustments of its dispersion, sedimentation, and resuspension. Such formulations with their inherent uncertainties are met in most of the Baltic Sea ecosystem models [8—12]. In result, the external loads of bioavailable nutrients to the Baltic Sea, prescribed both in hindcast and forecast simulations, nominally from the above papers, range between models up to 50 % for nitrogen and almost three-fold for phosphorus. Further propagation of such uncertainties into simulation of internal biogeochemical processes has not even been evaluated.

As this kind of assumptions quantitatively affects the management of nutrient inputs, one of the major intentions of BSAP, the uncertainties in prescription of land loads in scenario simulations have to be somehow reduced before the foreseen re-evaluation of MAI. Therefore, the major goal of the present study is to modify the St. Petersburg Eutrophication Model (SPBEM) [12] by explicit description of both dissolved and particulate forms of organic nutrients, while presenting their differing susceptibility (lability) to processes of OM destruction through the separate model variables. The modifications are then tested in simulation of the modern ecosystem dynamics of the Gulf of Finland.

Model and data

Modification of SPBEM-2 model. A new version SPBEM-2 is a three-dimensional coupled eco-hydrodynamic model with a modular structure. The modern hydrodynamic module is based on the ocean circulation model of the Massachusetts Institute of Technology general circulation model (MITgcm) in the hydrostatic approximation [13, 14]. In the present version, the coefficients of horizontal turbulent exchange of momentum, heat, and salt are assumed constant. The vertical turbulent exchange is parametrized by the TKE closure scheme [15]. Modelling of sea ice dynamics in MITgcm is based on a model with viscous-plastic rheology [16], subsequently modernized and generalized in [17]. The flow velocity components at the open liquid boundary are calculated from a modified Stevens scheme [18], that is the barotropic velocity component is calculated using the sea level observations at the boundary.

The biogeochemical module describing biogeochemical cycles of nitrogen, phosphorus, and silicon in the water column and bottom sediments is based on the BALTSEM model [19, 20], which was expanded by equations and parametrizations representing the dynamics of labile and refractory fractions of dissolved organic nutrients (fig. 1). The formulations of this expansion are largely borrowed from the "carbon version"

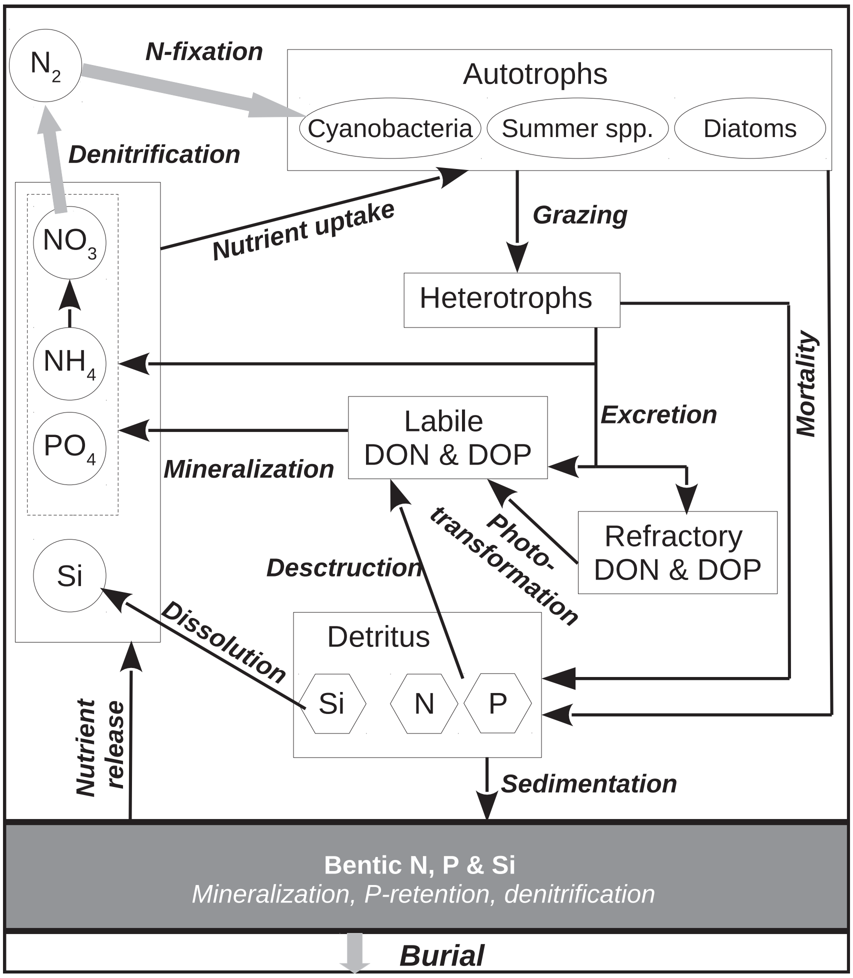


Fig. 1. Simplified description of model variables and nutrient fluxes.

Рис. 1. Схема взаимодействия переменных модели и потоков вещества.

of BALTSEM [21]. As before [12], the pelagic subsystem is presented by biomasses of zooplankton, three functional groups of phytoplankton (diatoms, flagellates, cyanobacteria), concentrations of detritus nitrogen, phosphorus, and silica, inorganic ammonium and oxidized nitrogen, phosphates, silicates, and dissolved oxygen. According to the Baltic tradition, hydrogen sulfide is considered as negative oxygen: 1 mL of H_2S L^{-1} = –2 mL O_2 L^{-1} [22]. Benthic sub-model describes dynamics of three variables representing total amounts of bioavailable fractions of nitrogen, phosphorus, and silica in the upper “active” layer of bottom sediments. In the present modification, the dynamics of labile and refractory fractions of dissolved organic nitrogen and phosphorus in pelagic sub-model are described with additional four equations. In contrast to earlier formulations, the products of detritus decomposition are not directed into inorganic nutrient variables but enter the labile dissolved organic variables that are then mineralized further. The specific rates of decomposition and mineralization are temperature dependent. The refractory fraction transforms into the labile one solely due to the process of photo-transformation, which specific rate depends on the underwater light distribution. Parametrization of zooplankton excretion is also changed. Products of catabolism are now distributed between not only inorganic nutrients (ammonium and phosphate) but also are a source of labile and refractory fractions of dissolved organic nutrients.

Data. To prescribe the initial and boundary conditions, as well as to compare simulations with field observations, we used the international database compiled within the international project The Year of the Gulf of Finland 2014 [23]. This database contains most of the field measurements made by Estonia, Finland and Russia during 1999—2014. Continuous time series of sea level variations at several locations (see fig. 2) have been borrowed from the Copernicus Marine Environment Monitoring Service (http://marine.copernicus.eu).

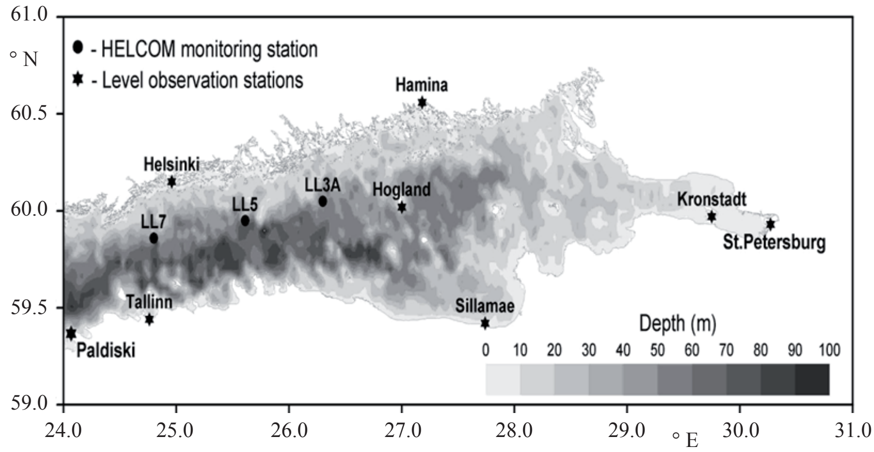


Fig. 2. Model domain with positions of oceanographic stations and sea level observations.

Рис. 2. Область моделирования с обозначением океанографических станций и пунктов наблюдения за уровнем моря.

Model-data comparison. Model-data comparison was performed primarily on observations made in close vicinity, within 5—10 nautical miles (NM), to positions of the international monitoring stations LL3A, LL5, and LL7. As observations in the Eastern Gulf of Finland (east of Hogland Island) have been made less regularly, especially at the fixed monitoring stations, comparison in the surface layer was made with all the available surface measurements. Calculations of the annually averaged total nutrient pools were made with the Data Assimilation System [24, 25] from all the data available within the geographical coordinates of the model domain.

Considering rather rugged bottom topography of the Gulf of Finland, the simulated values for every single comparison were selected from the three-dimensional grid as close to measured values as possible, both in space and in time. In addition to visual comparison of simulated curves with measurements, the model skill is also estimated by a cost function [26, 10]. A dimensionless cost function (CF) is the absolute value of a difference between averages of measured and simulated variables, which is related to the standard deviation of observed variable. Thus, it shows how large are the systematic model-data differences comparing to the natural variations. Usually, the simulation is considered good, when CF do not exceed 1, acceptable - with CF found between 1 and 2, and poor, if CF exceeds 2. The availability of continuous time-series of sea level observations permitted calculation of two more rigorous metrics of the model skill, the mean-absolute-error (MAE) and root-mean-square-error (RME).

Model setup and forcing. Simulation domain covers the Gulf of Finland from the easternmost Neva Bay to the open liquid boundary at 24.08°E (fig. 2). The horizontal resolution of the spherical grid is 2' by latitude and 4' by longitude, which approximately corresponds to 2 NM along both meridian and parallel. The vertical resolution is 3 m from surface to bottom in the z-coordinate grid.

The initial distributions of temperature, salinity, and biogeochemical variables were constructed by interpolation of field observations, made during winter months of 2002—2012, into grid cells. Concentrations of dissolved organic nitrogen (DON) and phosphorus (DOP) were calculated as a difference between concentrations of total nutrients and their inorganic fractions, assuming contribution of particulate fraction negligible in the winter time. Low and homogeneously distributed values were prescribed for biomasses of plankton variables and detritus concentrations. The sea level height and components of the current velocity were set equal to zero. Initial distributions of benthic variables were prescribed by projecting onto the three-dimensional bottom topography the values of identical variables picked up from the final horizontally homogeneous vertical distributions simulated with BALTSEM model for 1970—2006 [20].

The time-series of variables at the open boundary, resolving both seasonal and inter-annual variations, were reconstructed from the Gulf of Finland Year 2014 database [23] by first aggregating into a single vertical profile all the observations made in a strip between 23° and 24.7°E and averaging them within consecutive 15-day windows. Next, the step-wise averaged time-series were interpolated into continuous time-series of the requested temporal resolution. In such a way, the boundary conditions were prescribed for temperature, salinity, inorganic and dissolved organic nitrogen and phosphorus, and silicate. For zooplankton, phytoplankton, and detritus nutrients the values at the open boundary were prescribed equal to values obtained from the simulation.

The hourly sea level values at the boundary were taken from the observational data at Paldiski station (fig. 2). The atmospheric pressure fields, wind velocity components, temperature, humidity, precipitation, and short-wave and long-wave incoming radiation were prescribed from the ERA-Interim reanalysis fields (https://www.ecmwf.int). The average monthly values of river runoff and nutrient land loads were taken from the Baltic Environmental Database at the Stockholm University [27] and the latest load compilation by HELCOM [28].

This test simulation was run for 2009—2014 using numerical values of parameters borrowed from [29] without any calibration.

Results and Discussion. SPBEM-2 describes a complex interplay between external nutrient inputs and internal transports and transformations with a help of advection-diffusion equations for non-conservative substances. A rich experience in implementation of such a tool, both our personal and published by others show that the necessary condition for a plausible simulation of marine ecosystem dynamics is a realistic simulation of transports driven by the water dynamics. Rates of most biogeochemical processes are also dependent on the water temperature and salinity. Therefore, we start the model-data comparison with simulated hydrophysical characteristics.

Sea level variations caused by the real volume displacements are considered a reliable integral indicator of water movements. As shown by a good comparability between several statistics often implemented for evaluation of the model skill (table 1), the overall reproducibility of the water advection with the adapted version of MIT model can be considered quite satisfactory. The details of spatial and temporal comparability of simulated water temperature and salinity to the observed ones can be estimated visually and are quantified by cost functions CFs (fig. 3, *a*, *b*). Judging by the graphs and CFs, simulation of the water temperature can be considered as a very good, with CF values being generally lower than 0.3, although the summer maximum are somewhat underestimated (fig. 3, *a*). In result, the overall means of sea surface temperature (SST) obtained by selecting simulated values most close in space and time to available measurements differ by almost 2 °C (table 2). Nevertheless, as indicated by correlation coefficient of 0.97, both seasonal and interannual patterns are captured pretty well, at least, in the surface layer. The simulated sea water salinity looks also underestimated, comparing to observations (fig. 3, *b*). On average, the discrepancy in the surface layer is about 0.5 ‰. Considering hydrographic variables alone, it is difficult to evaluate to a what degree these discrepancies are caused by an imperfect simulation of the vertical mixing comparing to uncertainties in the prescription of such boundary conditions as components of the freshwater balance and incoming sun radiation. The contribution of uncertainties at the open boundary is even less clear. As was shown by a careful analysis of the long-term observations, the finer details of the water- and mass exchange through the Gulf of Finland boundary at the shorter time scales are rather variable both horizontally and vertically [30].

Table 1

Statistics of simulated and observed sea level variations (cm) in the Gulf of Finland. Position of stations is shown in fig. 2

Статистика рассчитанных и наблюдаемых изменений уровня моря (см) в Финском заливе. Положение станций показано на рис. 2

Station	Correlation coefficient	Standard deviation		Mean absolute error	Root mean square error
		Data	Model		
Hamina	0.97	0.24	0.23	0.041	0.054
Helsinki	0.98	0.22	0.22	0.037	0.047
Hogland	0.95	0.24	0.24	0.058	0.078
Kronstadt	0.97	0.26	0.25	0.049	0.068
Sillamae	0.94	0.23	0.24	0.070	0.084
St. Petersburg	0.95	0.25	0.26	0.059	0.082
Tallinn	0.97	0.22	0.22	0.040	0.056

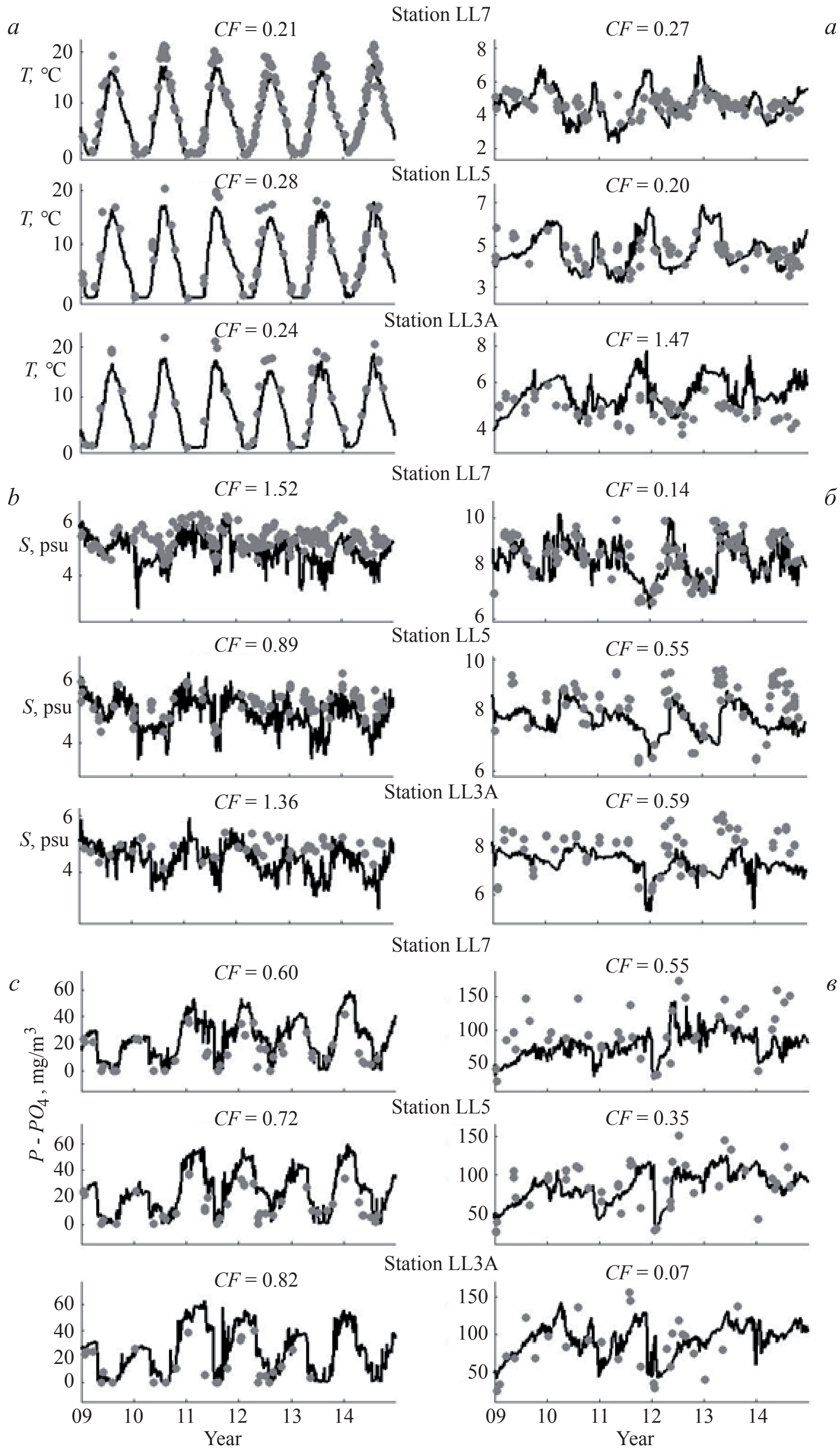
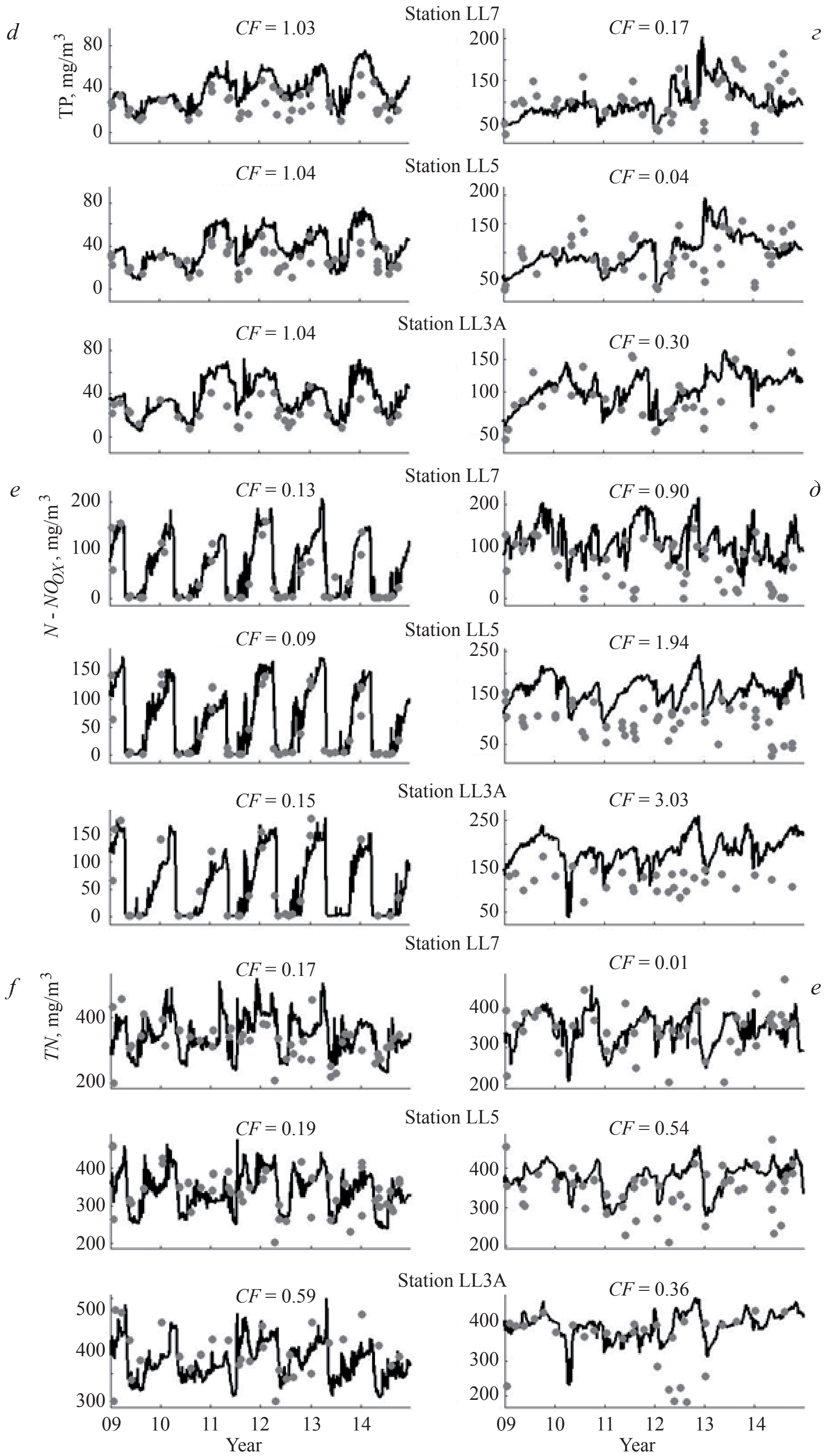


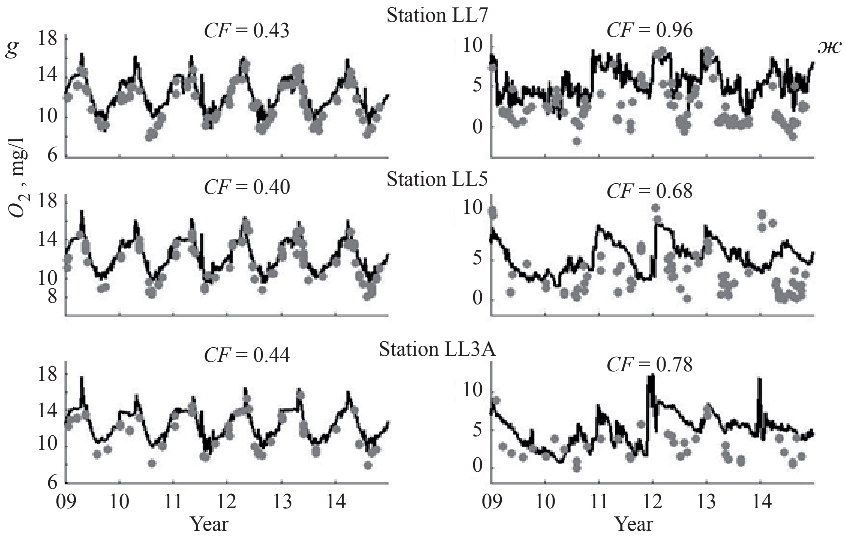
Fig. 3. Model-data comparison for temperature (*a*), salinity (*b*), phosphate (*c*), total phosphorus (*d*), oxidized dissolved inorganic nitrogen (*e*), total nitrogen (*f*), and dissolved oxygen (*g*) at oceanographic stations LL7, LL5, and LL3A. Left and right graphs present surface and bottom layers, respectively.

Рис. 3. Сравнение данных наблюдений с результатами моделирования для температуры (*а*), солености (*б*), фосфатов (*в*), общего фосфора (*г*), окисленных форм минерального азота (*д*), общего азота (*е*) и растворенного кислорода (*ж*) на океанографических станциях LL7, LL5 и LL3A. Поверхностный горизонт справа и придонный слева.



Continuation of Fig. 3.

Продолжение рис. 3.



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Продолжение рис. 3.

Apparently, such details can be difficult to reproduce with implemented boundary conditions, where all the dynamics of water exchange have been governed by sea level variations at only one side of the gulf (Paldiski station in fig. 2), while the boundary concentrations were prescribed from monthly values of measurements aggregated from a vast area and averaged into a single vertical profile. Within all these uncertainties, a sustained reproducing of the water dynamics and hydrophysical structure of the Gulf of Finland, including its seasonal variations can be regarded as rather realistic.

Results of the routine monitoring and most of oceanographic surveys are usually reported as measurements of total amounts of nitrogen (TN) and phosphorus (TP) in unfiltered samples as well as its dissolved inorganic fractions. The concentrations of "organic" fractions (TON and TOP) are then found by difference between the totals and inorganic fractions except of the rare cases with specific analysis of organic compounds as such [31, 7, 32]. Correspondingly, we continue comparison with the most available measurements, including also dissolved oxygen as an important indicator of production-destruction processes and regulator of the "vicious" circle [33, 3].

Both visual comparison and simple statistics indicate generally good model-data comparability also for nutrients, including their total amounts, and oxygen (fig. 3, *c*—*g*, table 2). In the surface layer, simulated seasonal dynamics of oxidized nitrogen (NOx) are almost a perfect match to the observed ones, both station-wise with CFs values less than 0.15 (fig. 3, *e*) and over the entire surface area with CF = 0.02 and correlation coefficient of 0.66 (table 2). The simulated seasonal and inter-annual patterns of phosphate look also quite reasonable, albeit simulated concentrations are slightly overestimated, by about 20 %, on average (fig. 3, *c*, table 2). The simulation of dissolved oxygen dynamics in the surface layers, aided by the constraining effect of the air-sea gas exchange is quite realistic as well (fig. 3, *g*). Generally, both in the eastern and western parts the model performed equally reasonable, including reproduction of the latitudinal gradients. To the contrary, being compared to measurements, simulated dynamics of oxygen and nutrients in the near-bottom layer seem somewhat defective: NOx concentration is greatly overestimated (nearly doubled) and almost out of sync, oxygen concentration is also significantly overestimated, while resemblance between simulated and measured concentration of phosphate improves eastward, from underestimation at LL7, to better comparability at LL3A (fig. 3). In our model, oxygen is consumed not only for ammonification and nitrification but also, following [34], for oxidation of such reductants not being explicitly described in the model as, for instance, iron, manganese, and sulfur compounds. As these parameterizations of oxygen consumption had been proven realistic in numerous past simulations [e.g. 12, 20, 21, 29], the overestimation could be generated by occasionally high ventilation of the deep layers, the reasons of which are not clear at the moment but should be analyzed in detail in future studies.

The reasons of these discrepancies are not easy to elucidate as they can be caused both by the inherent biases associated with a pairing of measured to simulated values and by the deficiencies in model formulation

Table 2

Model-data comparison for the entire surface layer during the whole simulated period. *R* is a coefficient of linear correlation; *N* is a total number of compared model-data pairs

Сравнение модели с данными наблюдений для поверхностного слоя в целом в течение всего рассматриваемого периода. *R* — коэффициент линейной корреляции; *N* — общее количество сравниваемых пар модельный результат — данные наблюдений

	Mean		Std		CF	R	Number of pairs
	Model	Observed	Model	Observed	Dimensionless		
Temperature, °C							
GoF	9.27	11.09	6.07	6.84	0.27	0.97	2656
EGoF	9.84	11.96	6.38	7.01	0.33	0.97	817
WGoF	9.02	10.72	5.92	6.74	0.29	0.98	1839
Salinity, g kg^{-1}							
GoF	4.26	4.75	1.57	1.79	0.26	0.92	2656
EGoF	3.06	3.49	1.04	1.23	0.41	0.79	812
WGoF	4.79	5.32	1.48	1.71	0.36	0.92	1844
NO_{2+3}, mg N m^{-3}							
GoF	32	30	57	60	0.02	0.66	2656
EGoF	47.49	46.83	71.34	77.36	0.01	0.60	1101
WGoF	21.16	18.88	41.63	41.57	0.05	0.75	1555
Total N, mg N m^{-3}							
GoF	359	381	77	127	0.17	0.35	1571
EGoF	382	430	84	138	0.58	0.27	819
WGoF	334	328	60	88	0.10	0.27	752
Phosphate, mg P m^{-3}							
GoF	9.0	7.8	11.7	8.2	0.14	0.70	2656
EGoF	8.21	7.89	12.31	9.71	0.03	0.61	1019
WGoF	9.50	7.79	11.33	7.22	0.15	0.81	1637
Total P, mg P m^{-3}							
GoF	31	27	15	12	0.34	0.41	1509
EGoF	29	26	15	13	0.21	0.36	767
WGoF	33	27	15	12	0.37	0.48	742
Oxygen, mg O_2 m^{-3}							
GoF	10.2	9.7	3.8	3.5	0.14	0.92	2656
EGoF	10.5	9.8	3.8	3.5	0.17	0.90	954
WGoF	10.0	9.6	3.8	3.5	0.11	0.94	1702

and implementation. Regarding comparison with measurements made from discrete water samples, one should recall that the deepest samples were usually taken from several meters above the bottom, whereas the simulated values have always been selected from the bottom grid cells. In the former case, the sampled water could be influenced by the sediments to a different degree, depending on the concentration gradients in the diffusive and viscous sub-layers [22]. In the latter case, the simulated fragments of the pelagic ecosystem are always directly affected by the nutrient exchange with the sediments. Unknown uncertainties originate also from: a) conditions given at the open boundary, b) assumptions made for splitting ”organic” nutrients into different fractions, and c) prescribed initial distributions of benthic variables. As all the models have their own internal dynamics, the three-dimensional sediment fields converted from one-dimensional BALTSEM solution without any biogeochemical adaptation are certainly biased, most likely overestimated, relatively to SPBEM-2 solution. Such preliminary adaptation could be made either by running long spin-up simulations with repeating forcing [35] or starting simulation long before the targeted period [36]. Both approaches require considerable computing resources and were neglected in this study aimed at the general testing of modifications.

Finally, these discrepancies can be partly caused by an appropriate behavior of implemented parameterizations, constituting the "vicious circle", in response to faulty simulation of its links. Accordingly to these parameterizations, the overestimated deep water concentration of oxygen results in reduced denitrification, hence the large amount of NOox is left unremoved and resides in the deep layers (fig. 3, *e*). Regarding the phosphate dynamics, the overestimated deep water oxygen concentration implies a smaller area of anoxic bottoms and higher sediment retention of mineralized phosphate. As can be seen from a detailed comparison of oxygen (fig. 3, *g*) and phosphate (fig. 3, *c*) dynamics in the deep layers (for instance, short-term trends in 2009—2010, maxima-minima in 2012), the redox alterations, similar to demonstrated by the analysis of field measurements [30], realistically affect simulated phosphorus cycle as well, especially westwards. However, as shows an overall comparison between integral nutrients pools (table 3, fig. 4), the simulated total amounts are pretty much overestimated because of overestimated amounts of inorganic nitrogen and phosphorus, most likely due to excessive nutrient content in the initial sediment fields. Most importantly, the integral amounts of organic fractions derived as a difference between total amounts and inorganic fractions, both simulated and observed, match one another very well.

The validity of simulated dynamics of organic nutrients is further confirmed by its close resemblance with results of the goal-oriented analysis of sea surface samples collected by the ship-of-opportunity on repeated cross-sections in the Eastern Gulf of Finland from April till December in 2005 [32]. Matching these results to the average (2009—2014) seasonal dynamics of simulated total organic nitrogen (TON) and phosphorus (TOP) demonstrates a reasonable comparability of their spatial-temporal dynamics (fig. 5, see an insert). The major conspicuous feature is a sharp increase in TON concentration for a few weeks in April—May, caused by the spring bloom of diatoms and especially pronounced in the open Eastern Gulf of Finland (28°E—29°E). There and then, the TON concentrations exceed 500 mg N m^{-3}, both in the model and in the field. Cyanobacteria blooming generates summer maximum of TON over the entire gulf, albeit slightly decreasing westward. In the model this maximum looks more prolonged, over July—September vs. July—August indicated by the infrequent cross-sections, and less pronounced, around 350 mg N m^{-3} in the model vs. up to 450 mg N m^{-3} in surveys. In the winter, TON concentrations are at comparable minimum levels, less than about 250 mg N m^{-3}. Most specific feature of both simulated and observed TOP variations is a significant eastward increase of its concentrations, up to 30—40 mg P m^{-3} in the Neva Bay. According to fig. 5, relative contribution of labile fraction of dissolved organic nitrogen (LDON) is around 25 % in the Neva Bay and decreases westward, less sharply during a summer development of cyanobacteria that, in contrast to fast-sinking diatoms, decompose largely in the surface layers. Following approximately the same pattern, the contribution of labile fraction of dissolved organic phosphorus (LDOP) is higher and decreases westward less sharply, from about 70 % to 40 %. Plausibility of such disaggregation of TON and TOP into fractions is difficult to evaluate because

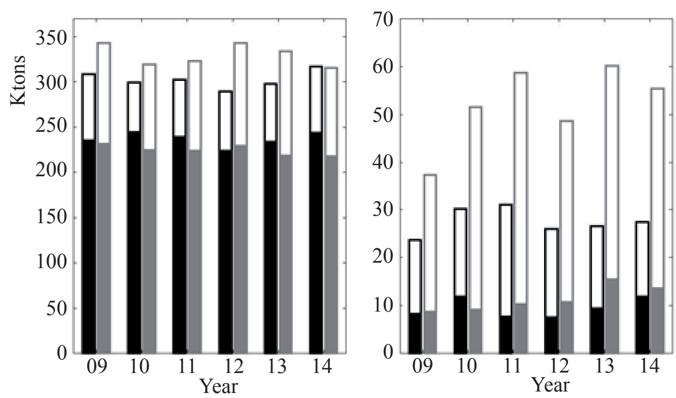

Fig. 4. Inter-annual variations of annually averaged integral pools of simulated (*grey*) and observed (*black*) organic (*filled*) and inorganic (*open*) fractions of nitrogen (*left panel*) and phosphorus (*right panel*).

Рис. 4. Межгодовая изменчивость среднегодового содержания органического (*закрашенная*) и неорганического (*незакрашенная*) азота (*слева*) и фосфора (*справа*) по натурным данным (*черные*) и результатам моделирования (*серые*).

Table 3

Annual statistics of integrated pools of nitrogen and phosphorus fractions (10^3 tonnes), simulated and reconstructed from observations

Годовая статистика интегральных запасов фракций азота и фосфора (10^3 тонн) по результатам моделирования и оценок по данным наблюдений

	DIN		TON		TN		DIP		TOP		TP	
	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod
Mean	65	105	237	225	302	330	18.0	40.6	9.5	11.3	27.5	51.9
Std	6.9	8.3	7.6	4.4	9.6	10.2	2.9	6.2	2.0	2.5	2.9	7.6
CV, %	11	7	3	2	3	3	16	15	21	21	10	14

of almost total absence of relevant measurements. Nevertheless, simulated proportions are similar to a few reported estimates of 25 % and 64 % [3] and 0—41 % and 44—46 % [7], for LDON and LDOP, respectively.

Conclusions. SPBEM has been modified for improving description of organic matter as a part of the nutrient biogeochemical cycles, which is especially important for a realistic prescription of boundary conditions, including scenario simulations of the nutrient load reductions. In modification, the “detritus” variable and related interactions were redefined as representing strictly particulate form of organic matter, while both dissolved organic nitrogen and phosphorus were presented each by its labile and refractory fractions. The modification was tested at the Gulf of Finland in a numerical experiment made with plausible initial and actual boundary conditions for the years 2009—2014.

Within all the uncertainties, inherent to a model-data comparison and generated by the set-up of simulation, the test can be considered as rather successful. Spatial and temporal dynamics of both hydrophysical and biogeochemical variables appear quite realistic, especially assessing the model skill by the comparability of concentrations, as is common in modelling practice. However, comparison between the reconstructed from observations and simulated integral amounts of nutrients, which dynamics are more pertinent to studies and management of eutrophication [3] but has been rarely used in skill assessments, reveals important discrepancies. The total amounts of inorganic nutrients are significantly overestimated in the model, which results in corresponding overestimation of their total amounts. Consequently, there is almost a perfect match between the reconstructed and simulated total amounts of organic nutrients, the latter being a major goal of SPBEM-2 modification.

Revealed discrepancies could be generated by the deficiencies in the prescription of initial and boundary conditions. The sources of such deficiencies should be found and corrected in future calibration and sensitivity experiments with SPBEM-2.

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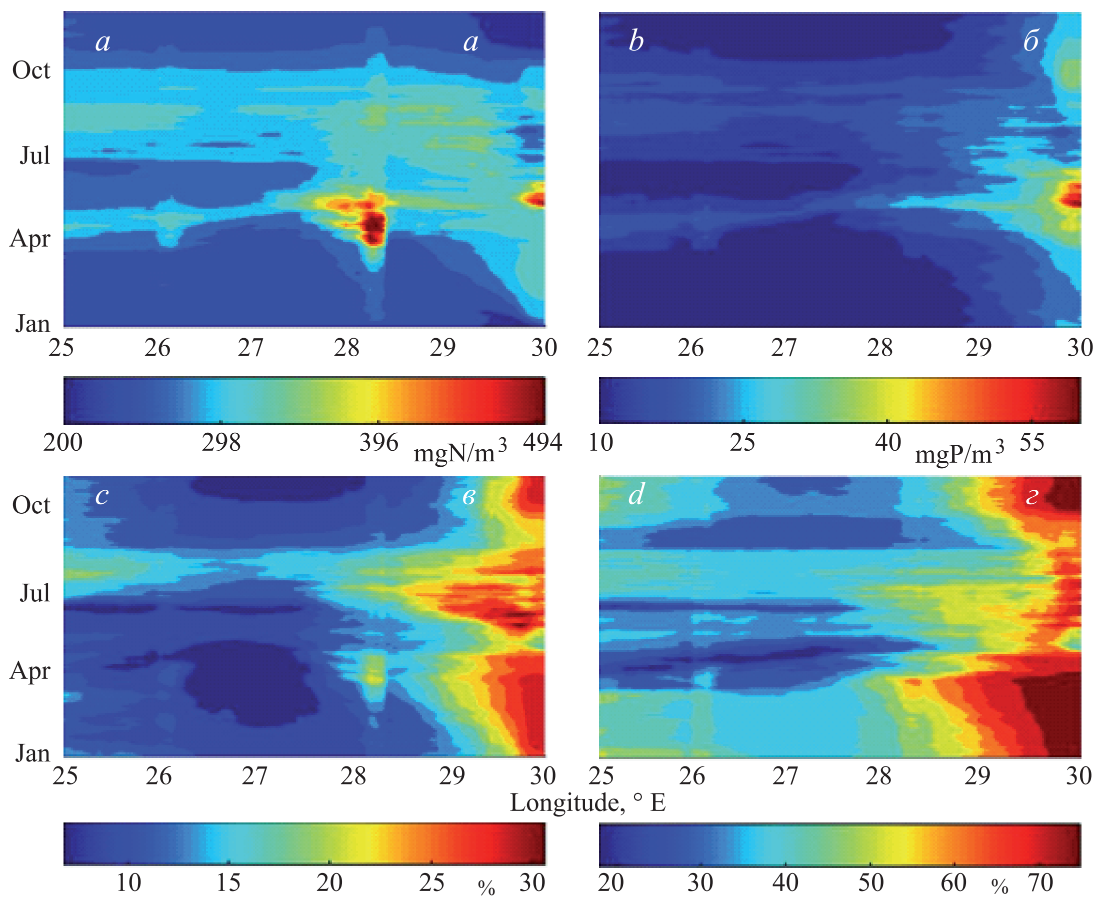

Fig. 5. Simulated seasonal and latitudinal distribution of TON (*a*), TOP (*b*), proportion of LDON in TON (*c*), and proportion of LDOP in TOP (*d*) averaged over 2009—2014.

Рис. 5. Рассчитанные пространственно-временное распределения TON (*а*), TOP (*б*), процентного содержания LDON в TON (*в*) и LDOP в TOP (*г*) осредненные за период с 2009 по 2014 гг.