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Model set-up at COCOA study sites

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Summary

COCOA will investigate physical, biogeochemical and biological processes in a combined and coordinated fashion to improve the understanding of the interaction of these processes on the removal of nutrients along the land-sea interface. The results from the project will be used to estimate nutrient retention capacity in the coastal zone of the entire Baltic Sea coast. An ensemble of biogeochemical models will be used in combination with field studies at seven different coastal study sites around the Baltic Sea. The present report is a deliverable of COCOA work package 5 (WP5). Within the objective of WP5 process understanding and process descriptions will be improved in state-of-the-art biogeochemical models of the Baltic Sea coastal zone. This report presents brief information about the models available for the COCOA project and defines the needed input to the models that will be set-up at several learning sites. The aim is to perform ensemble modelling at several sites, using at least two different models at each site. A pilot study to estimate nutrient retention capacity in the Stockholm Archipelago with the existing Swedish model system is ongoing and first results are presented and the concept of nutrient retention is briefly discussed.

The existing models for different learning sites presented in the report are;

1) The Swedish model system SCM (Öre river estuary and the Stockholm archipelago)
   - A multi-box-model approach
2) The Danish model system FLEXSEM (Roskilde fjord)
   - A combined box-model and 3-D model approach
3) The Finnish model system ESIM-BFMSI (Tvärminne Archipelago)
   - A 1D box-model approach
4) The Polish model system M3D UG/ProDeMo (Puck Bay)
   - A 3-D model approach. Operational model.
5) The Lithuanian model system SYFEM/AQUABC (Curonian Lagoon)
   - A combined box-model and 3-D model approach
6) The Swedish open Baltic model system RCO-SCOBI (for the open Baltic Sea and the Gulf of Gdansk/Vistula).
   - A 3-D model approach

In addition a biogeochemical model (Boudreau, 1996) for the Gulf of Finland (Russian State Hydrometeorological University model) is used to study the quantitative effect of Marenzelleria on the Gulf of Finland ecosystem.

Process studies at selected sites will be performed with a reactive transport model developed at Utrecht University. Focus will be on the role of iron and phosphorus cycling. Process studies with the Danish model system will support the development of new parameterizations of nutrient fluxes taking benthic habitat into account. The new parameterizations of the nutrient fluxes will in addition also be implemented into SCM and the models will be used to estimate nutrient fluxes, retention times and the filter capacity of the coastal zones.

The *In Kind* contributions from previously (in the literature) well described open Baltic Sea models RCO-SCOBI, BALTSEM, ERGOM and SPBEM that will be used for the description of open sea conditions are also briefly mentioned in the report with references to the relevant literature.

Keywords: Coastal zone, Eutrophication, Biogeochemistry, Nutrient retention, Numerical modeling

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1. Introduction

Cocoa (Nutrient COcktails in the COAstal zone of the Baltic Sea)

Recently it has been suggested (Duarte et al. 2009; Kemp et al. 2009; Carstensen et al. 2011) that coastal ecosystems may behave in a non-linear manner. Potentially they may display regime shifts with alternative stable states such that an undesirable ecological status can be maintained by internal feed-back processes acting on the system (Fig. 1). In particular, reductions in nutrient removal processes mediated by plants (McGlathery et al. 2007) and fauna (Norkko et al. 2012) are believed to support a regime with low nutrient removal and large nutrient releases from the sediments back to the water column, whereas seagrasses and burrowing macrofauna enhance the permanent burial of nutrients and organic matter (Fourqurean et al. 2012; McGlathery et al. 2012; Norkko et al. 2012). Thus, it is important to understand and quantify how nutrient and carbon cycling is modulated by various biological components and how these processes affect the entire coastal ecosystem.

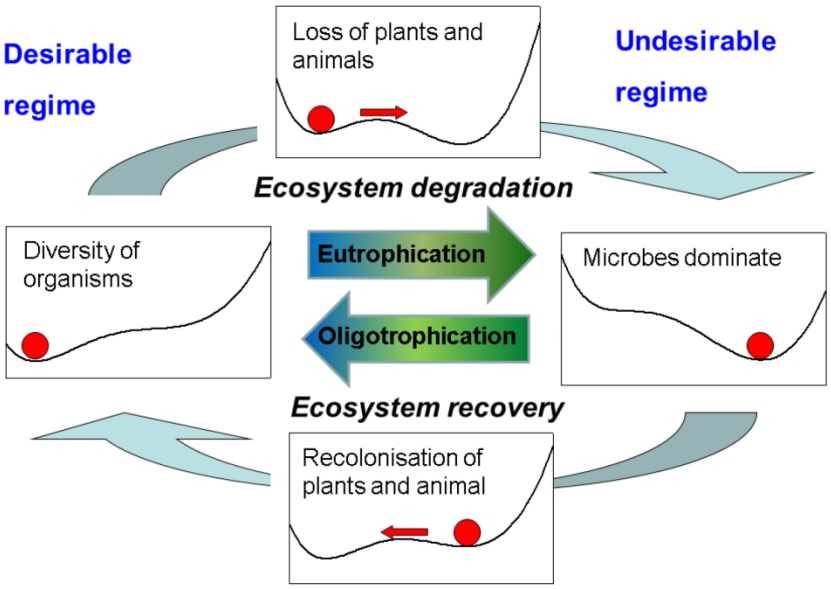


Figure 1. Regime shifts between alternative stable states.

COCOA will investigate physical, biogeochemical and biological processes in a combined and coordinated fashion to improve the understanding of the interaction of these processes on the removal of nutrients along the land-sea interface. An ensemble of biogeochemical models will be used in combination with field studies at different coastal study sites around the Baltic Sea to identify major pathways of nutrients and organic material in various coastal ecosystems, like for instance river-dominated estuaries, lagoons, archipelagos and embayments with restricted water exchange. Nutrients and organic matter are transformed and retained along the land-sea continuum, and COCOA will quantify how physical and chemical conditions as well as the biological components of the coastal zone affect the biogeochemical processes. Improved estimates of the nutrient retention capacity will be obtained by using models to integrate the processes across the ecosystem. These results will be scaled up to the entire Baltic Sea coastal zone by developing a catalogue of coastal ecosystems with

hydromorphological, physical, chemical and biological information and projecting the results from the dynamical models to the entire coastal zone.

The overall aim of COCOA is to:

- *Understand the changing nutrient (**C/N/P/Si**) cocktail across the land-sea continuum.*
- *Quantify processes that transform and accumulate nutrients.*
- *Estimate nutrient retention across coastal ecosystems.*
- *Investigate potential feed-back processes sustaining alternative stable states.*
- *Analyze how these process rates may have changed over time.*
- *Evaluate consequences of altered nutrient pathways on ecosystem services.*
- *Identify possible management responses for present and future projections.*

The present report is a deliverable of COCOA work package 5 (WP5) and aim to describe the planned model set-up at the COCOA study sites. The objective of WP5 is to improve process understanding and process descriptions in state-of-the-art biogeochemical models of the Baltic Sea coastal zone and to quantify carbon and nutrient fluxes between land, coastal zone and open sea as well as between water and sediments. Simulations with the improved model descriptions will also reveal if regime shifts are possible within the realistic range of parameters. Particularly, it is important to parameterize the effects of benthic primary producers and fauna as modulators of nutrient and organic matter fluxes. The models should also be able to simulate Water Framework Directive (WFD) indicators (some or selected Biological Quality Elements) for the assessment of ecological status and linking the changes in the biogeochemical fluxes of nutrients with changes in ecological status. Boundary conditions for nutrients and organic matter for the different coastal ecosystems will be derived from existing physical-biogeochemical models for the open Baltic Sea (BALTSEM and RCO-SCOBI). The latter is a high-resolution 3D model and therefore provides more realistic representation of the conditions near specific coastal areas than the basin-scale BALTSEM. From previous BONUS+ project ECOSUPPORT (http://www.baltex-research.eu/ecosupport/index.html), simulations of both high-quality hind casts (1970-2006) and climate/nutrient load scenarios (1960-2100) are available from both models.

2. Methods

A list of the partners of the COCOA consortium and the corresponding abbreviations used in the document;

AU, Aarhus University, *Denmark*

LU, Lund University, *Sweden*

AAU, Åbo Academi University, *Finland*

SU, Stockholm University, *Sweden*

SYKE, Finnish Environment Institute, *Finland*

UG, University of Gdansk, *Poland*

ZIN, Zoological Institute RAS, *Russia*

SMHI, Swedish Meteorological & Hydrological Institute, *Sweden*

HU, Helsinki University, *Finland*

CORP, Coastal Research and Planning Institute, *Lithuania*

UU, Utrecht University, *The Netherlands*

DTU, Technical University of Denmark, *Denmark*

GU, University of Gothenburg, *Sweden*

IOW, Leibniz-Institute for Baltic Sea Research Warnemünde, *Germany*

2.1 Description of study sites

COCOA will carry out sampling during high and low outflow conditions in coastal ecosystems influenced by large fluvial inputs (off the Vistula River and the Öre River near Umeå) to assess ranges of fluxes, and more frequent sampling in coastal systems receiving variable inputs of nutrients and organic matter (Tvärminne archipelago, Puck Bay, Roskilde Fjord, and the Curonian Lagoon).

The following models (described in the following sections) have an existing set up at the COCOA learning sites (Fig. 2):

- Roskilde fjord: FLEXSEM
- Curonian Lagoon: SHYFEM/AQUABC
- Vistula River Estuary: RCO-SCOBI (*and ERGOM. In kind.*)
- Öre River Estuary: SCM
- Puck Bay: M3D UG/ProDeMo (*operational model*)
- Stockholm Archipelago: SCM
- Tvärminne Archipelago: BFM

WP5 will improve process descriptions in state-of-the-art coastal zone models (SCM, FLEXSEM) and analyze model simulations in detail at the 7 learning sites and more generally for additional coastal systems, where the models have already been calibrated.

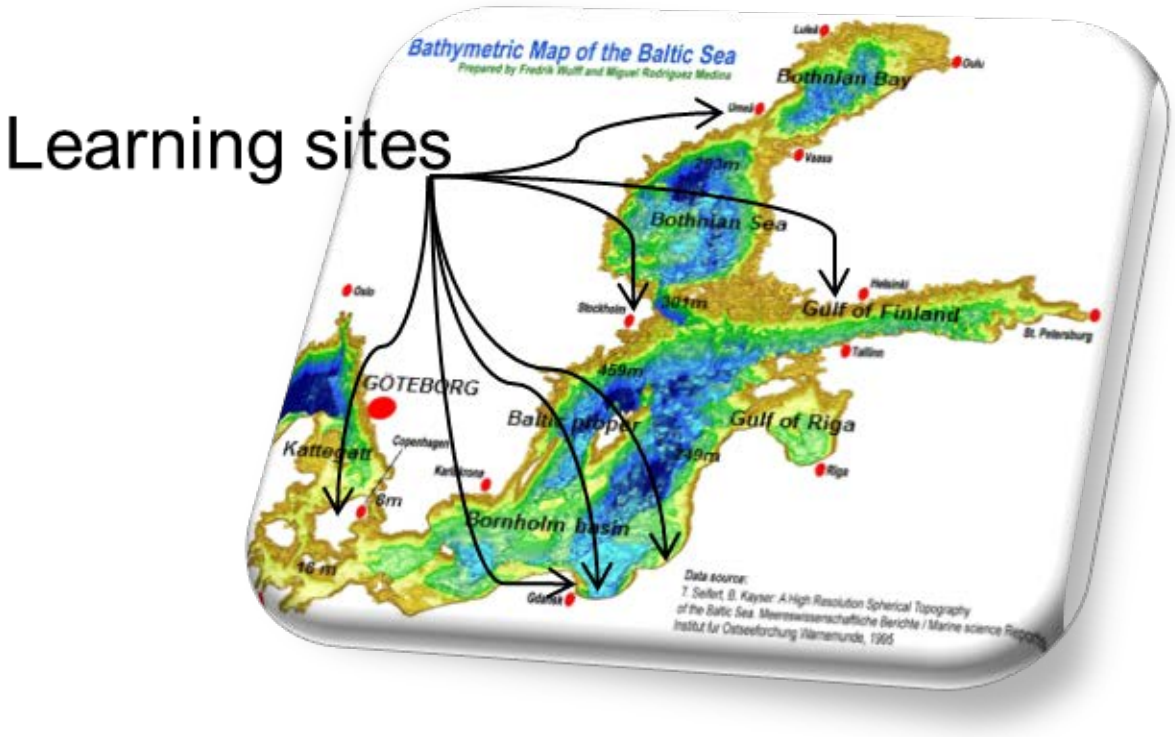


Figure 2. A map pointing out the positions of the learning sites. The bathymetric map was originally prepared by F. Wulff and M. Rodrigues Medina at the Baltic Nest Institute.

2.2 Ensemble modeling

The aim is to perform ensemble modelling at several sites, using at least two different models at each site. The best available, local data sets will be used to force and set-up the models. The data sets will be made available in a common format to be distributed to all models in the ensemble. The following models are potentially available for the modeling at the different learning sites and additional regional areas:

1) (*Oder: additional high-resolution ERGOM model. In kind.*)

2) BFM sites in addition to Tvärminne Archipelago: SYKE will specify the sites later.

3) SCM sites in addition to the Swedish coast: Roskilde fjord, Curonian Lagoon, Puck Bay, Tvärminne Archipelago. SMHI will investigate whether the SCM can be set-up at new sites that are not included in the existing SCM system.

4) FLEXSEM sites in addition to Roskilde fjord: Puck Bay: AU will investigate whether FLEXSEM can be set-up.

5) Baltic Sea model, Gulf of Finland model (*additional high-resolution* SPBEM *model, Vladimir Ryabchenko, St. Petersburg. In kind.*).

6) Russian State Hydrometeorological University (RSHU) model. Biogeochemical model (Boudreau, 1996) for the Gulf of Finland to study the quantitative effect of Marenzelleria on the Gulf of Finland ecosystem

2.3 Experimental set-up and planned new model development

WP5 will improve process descriptions and analyze model simulations in detail at the 7 learning sites and more generally for additional coastal systems, where the models have already been calibrated. Simulations with the improved model descriptions will also reveal if regime shifts are possible within the realistic range of parameters.

Process studies will be performed to support the development of new parameterizations of nutrient fluxes. Model studies at selected sites were new observations are gathered (preliminary Oder and Öre estuaries) will be performed by SU with the reactive transport model developed at Utrecht University (e.g., Reed et al., 2011). Focus will be on the role of iron and phosphorus cycling. FLEXSEM will in addition be used to develop parameterizations of benthic fluxes taking benthic habitat into account. These parameterizations will be implemented into SCM. SCM and the other models will be used to estimate nutrient fluxes, retention times and the filter capacity of the coastal zone. The carbon cycle is included within BALTSEM, FLEXSEM and BFM models.

Process studies at the learning sites. WP5 will extend current process-based model functions by incorporating benthic components for the transformations and retentions via microbes, benthic primary producers and fauna. The added value of the coupled pelagic-benthic model, inducing a more variable process stoichiometry for the sediments, will be assessed through estimates of C sequestration, P release and N transformations.

Improved process description of sediment-water fluxes. For phosphorus, WP5 will specifically focus on the role of iron oxide input from rivers and the composition and functional biodiversity of benthic invertebrate communities. Also the impact of the presence

of invasive bioengineering species such as Marenzelleria in modulating sediment phosphorus retention will be assessed. For nitrogen, WP5 will focus on identifying conditions promoting nitrogen removal over recycling. For carbon, the recycling and burial of allochthonous versus autochthonous organic matter is of specific interest.

Improved benthic habitat modelling. WP5 will develop a module to describe the spatial distribution, biomass and activity of benthos in shallow estuaries. The module will be implemented in a coupled benthic-pelagic 3D coastal model and used to study the role of benthos in the cycling of nutrients and their contribution to ecosystem productivity.

Estimating the retention of nutrients for a variety of coastal systems. Using an ensemble of improved models nutrient fluxes, retention times and the filter capacity of the coastal zone will be estimated. For this task simulations of the entire western Baltic Sea coast during the period 1979-2012 will be performed and analyzed.

2.4 Future scenarios

Assessing nutrient reduction scenarios. Scenarios of nutrient load reductions with changing climate will be computed for the learning sites and the associated consequences for status indicators will be evaluated (WP7). Given target values for these indicators maximum allowable nutrient inputs will be calculated. Thresholds of non-linear responses to nutrient inputs, if possible with the model configurations from WP5, will be quantified and used to define safe operating spaces for coastal ecosystem management. The applicability of the models from WP5 as a more general management tool will be assessed.

2.5 The concept of nutrient retention

The balance between nutrient loads to a coastal area and the export of nutrients to the open sea is determined by the nutrient retention, i.e. the fraction of the loads that are removed or stored within the coastal area. The net effect of nutrients on the water quality of an area can be studied by the simple method of subtracting the output of nutrients from the input (Almroth-Rosell et al., 2014; Johnston, 1991; Karlsson et al., 2010).

Different retention processes are of different magnitudes and irreversibility, e.g. plant uptake and litter decomposition provide short- to long-term retention of nutrients, which depends on release rates, translocations, and the longevity of the plants (Johnston, 1991). Processes like permanent burial and denitrification are irreversible retention, while sedimentation of organic matter can be classified as temporal retention.

The calculation of the permanent nutrient retention is somewhat delicate since it depends on the time period of consideration. There may be drastic temporal changes in the external loads while the changes in total pools in the water and sediment may be relatively slow depending on the residence time of the system. Also the variability of the phosphorus pools in the water may be large due to varying oxygen conditions and exchanges with the sediment. Leaking sediments may therefore continue to add nutrients to the system and mask the actual long-term nutrient retention in the area. Hence, it might be difficult to obtain accurate numbers just by judging from one single year and using information solely from the water column. In order to obtain a representative figure of the sink efficiency, the calculation should preferably be performed during a period of equilibrium or cover a longer period accounting for the impact of natural seasonal and inter-annual variability.

2.6 The present set-up of coastal zone model systems

2.6.1 The Swedish model system

SMHI has developed a model system called the Swedish Coastal zone Model (SCM) for water quality calculations on land, in lakes and rivers and in the coastal zone waters around Sweden (Sahlberg, 2009). The SCM calculates the state of the water bodies along the entire Swedish coast which is divided according to the Swedish water districts into 8 different areas (Fig. 3). The names and the number of sub-basin in each area are; the Bothnian Bay 113 sub-basins, the Bothnian Sea 85 sub-basins, the northern Baltic Sea 167 sub-basins, the Östergötland coast 47 sub-basins, the Småland coast 55 sub-basins, the Gotland coast 21 sub-basins, the Skåne-Blekinge coast 52 subbasins, and finally the West coast has 113 sub-basins.

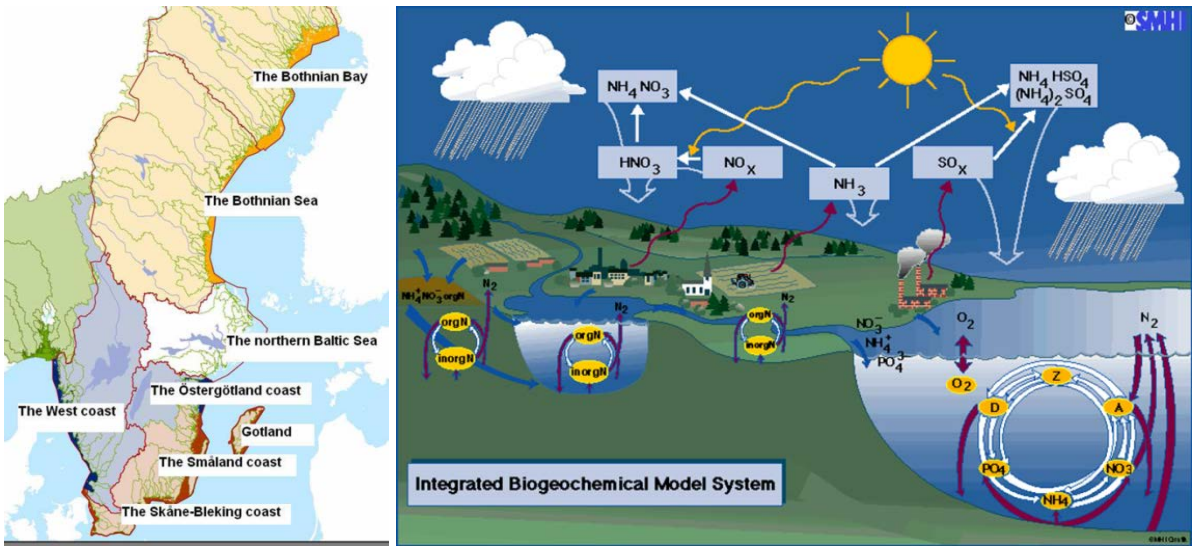


Figure 3. The Swedish coast is divided according to the Swedish water districts into 8 different areas (left) where the SCM (right) is applied.

The coastal zone model

The SCM couples the 1-dimensional physical model PROBE (Program for Boundary Layers in the Environment; Svensson, 1998), to the biogeochemical model SCOBI (The Swedish Coastal and Ocean Biogeochemical model; Marmefelt et al., 1999; Eilola et al., 2009). In order to include horizontal variations in a larger region the area is divided into several dynamically interconnected sub-basins (Fig. 4). The sub-basins are identical to the defined national water bodies according to the Water Framework Directive (WFD). Each sub-basin is described by the hypsographical curve and may exchange water and properties with other sub-basins through connecting sounds. The geometry of each sound is extracted from digital sea charts and the cross sectional area and the maximum depths are then manually compared and verified against ordinary sea charts.

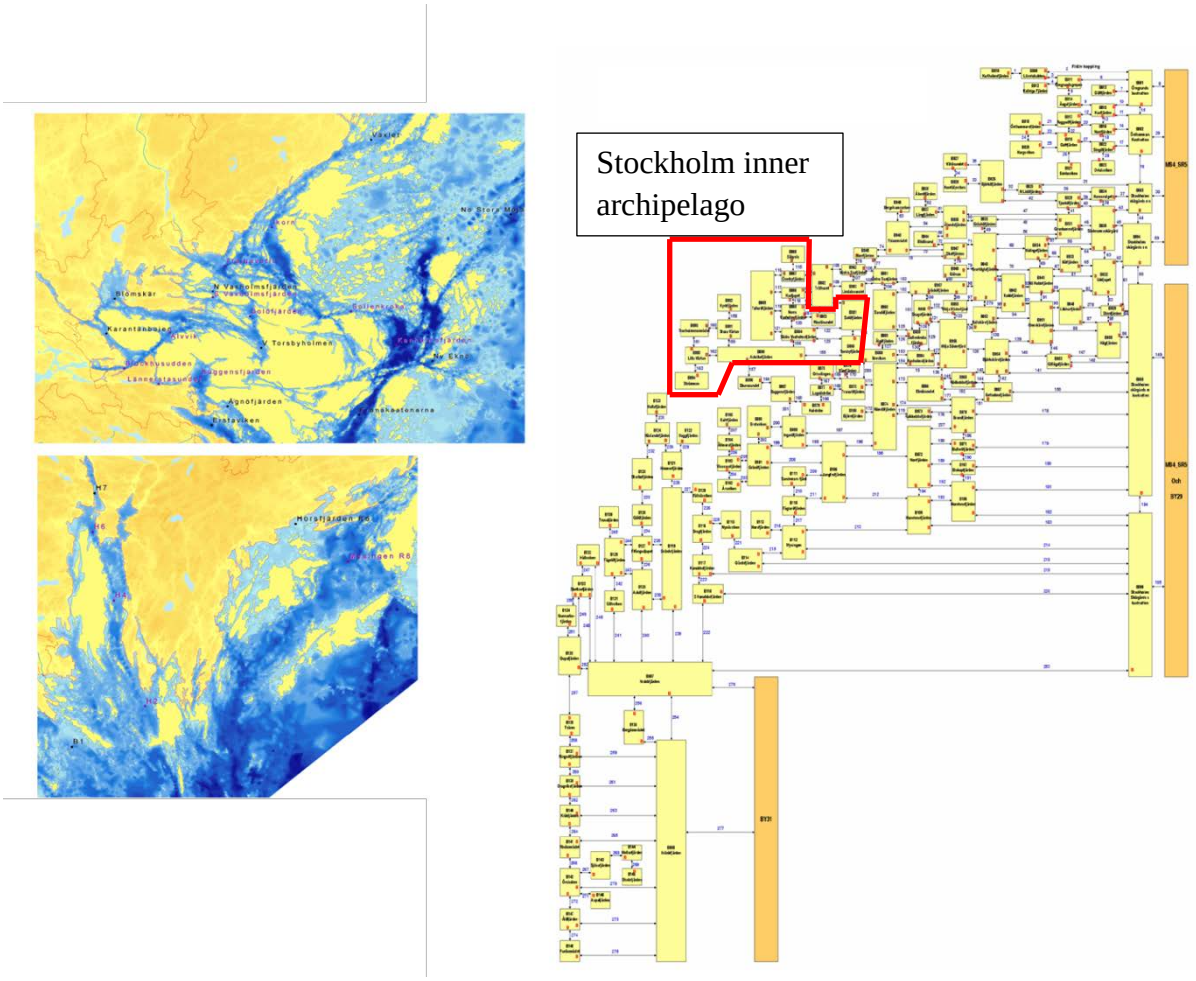


Figure 4.The Stockholm archipelago in the northern Baltic Sea area with the division into several sub-basins shown to the right. The Stockholm inner archipelago is encircled by the red lines.

In the SCM the water exchange between two sub-basins inside the coastal zone or between a coastal zone sub-basin and the outer sea is described in two different ways. First, the water exchange between two sub-basins within the coastal zone is controlled by the sum of the barotropic and baroclinic pressure gradients. The net flow over the connecting sound will be the same as the river discharge from land in order to preserve the volume continuity. Inflowing water to a sub-basin is interleaved into its density level without any entrainment. Heavy surface water in one sub-basin may thus reach the bottom level in the other subbasin. The barotropic part is excluded from the calculation which means that no externally forced sea level variation exists in the model. Several tests with the SCM have shown that on the longer time scales (months) it is the baroclinic part that dominates the water exchange between different sub-basins. The reason for excluding the barotropic part is the possibility to use a longer time step when calculating the horizontal water exchange. This significantly reduces the calculation time. Second, the water exchange over the boundary between the coastal zone and the open sea is assumed to be in geostrophic balance because normally this boundary is open with a width greater the internal Rossby radius.

The physical model

The PROBE model calculates the horizontal velocities, temperature and salinity profiles. The surface mixing is calculated by a *k-ε* turbulence model and the bottom mixing is a parameterization based on the stability in the bottom water. Light transmission as well as ice formation growth and decay are also included in the model. Probe has a high vertical resolution with a vertical grid cell size of 0.5m in the top 4m. The grid cell size then increases as the depth increases. In the depth interval 4 -70m the cell size is 1.0m, from 70 – 100m it is 2m, from 100-250m it is 5m and if the depth is larger than 250m the grid cell size is 10m. The general differential equation of the PROBE solver is formally written as

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x_i} u_i \phi = \frac{\partial}{\partial z}\left(\Gamma_\phi \frac{\partial \phi}{\partial z} \right) + S_\phi$$

Here ϕ is the dependent variable, *t* time, *z* vertical coordinate, *x* horizontal coordinate, *u* horizontal velocity, Γ_ϕ vertical exchange coefficient, and S_ϕ source and sink terms. Vertical advection (and moving surface) is included accounting for vertical transport in a sub-basin due to inland river outflows. The sources and sinks determined by the ecosystem model are added to S_ϕ. Vertical advection and diffusion are excluded for the solution of benthic biogeochemical processes.

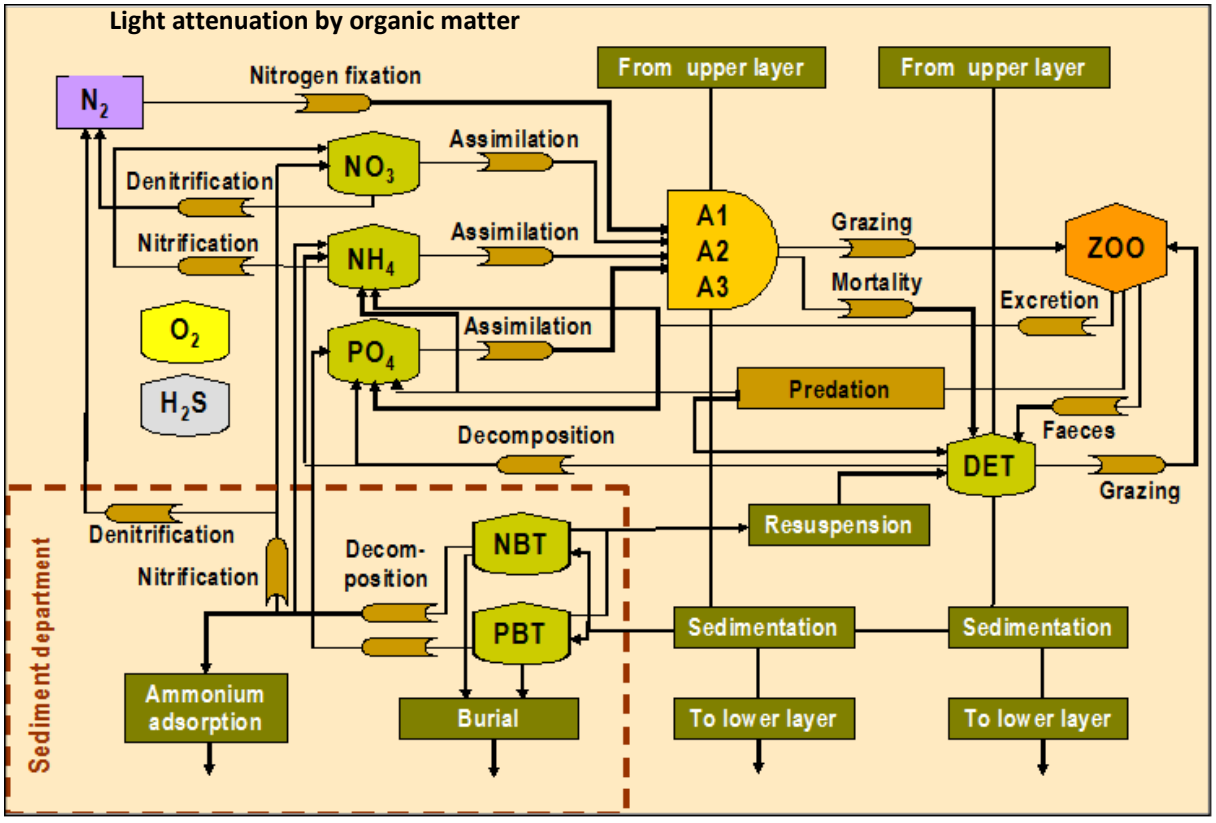


Figure 5. Components of the SCOBI model. The process descriptions of oxygen and hydrogen sulfide are simplified for clarity.

The biogeochemical model

The SCOBI model (Fig. 5) describes the dynamics of nitrate, ammonium, phosphate, phytoplankton, zooplankton, detritus, and oxygen. Hydrogen sulfide concentrations are

represented by “negative oxygen” equivalents (1 ml H_2S l^{-1} = −2 ml O_2 l^{-1}) (Fonselius and Valderrama, 2003). Phytoplankton consists of three algal groups representing diatoms, flagellates and others, and cyanobacteria (corresponding to large, small and nitrogen fixing cells). Processes like assimilation, remineralisation, nitrogen fixation, nitrification, denitrification, grazing, mortality, excretion, sedimentation and burial are considered. The production of phytoplankton assimilates carbon (C), nitrogen (N) and phosphorus (P) according to the Redfield molar ratio (C:N:P=106:16:1) and the biomass is represented by chlorophyll (Chl) according to a constant carbon to chlorophyll ratio C:Chl=50. The carbon cycle is, however, not explicitly modelled. The molar ratio of a complete oxidation of the remineralised nutrients is O_2:P=138:1. The sediment processes include oxygen dependent nutrient remineralization and denitrification as well as burial of nutrients. Burial of nitrogen and phosphorus in the sediment and denitrification are the permanent nutrient sinks in the model. Light attenuation depends on background attenuation due to water and humic substances and a variable attenuation caused by the organic matter (phytoplankton and detritus) handled by the SCOBI model. Sediment resuspension is not active in the present set-up of the SCM. For further details of the SCOBI model the reader is referred to Eilola et al. (2009, 2011) and Almroth-Rosell et al. (2011).

Forcing from land, atmosphere and the open sea boundary

The SCM model system is forced by weather, atmospheric deposition of nutrients, the conditions in the sea outside the archipelago, and nutrient and fresh water loads from land.

To get reliable model results in the coastal zone area it is important to know the physical and biochemical conditions in the open sea. Observations alone are inadequate for this task because the temporal resolution is too low (monthly) and the information is incomplete (e.g. lacking information on zooplankton, phytoplankton and detritus). To solve this problem the PROBE-Baltic model (Omstedt & Axell, 2003) is coupled to the SCOBI model used in the SCM and applied to the Baltic Sea and the West coast in thirteen sub-basins. In order to obtain coastal representative results, the PROBE-Baltic model is assimilated to observations at selected measuring stations in the sea close to the coastal zone boundary. The model results for the period 1990-2013 are stored on data files with a time resolution of one day, and used as the open sea boundary conditions to the coastal zone model.

The land derived forcing is divided in two types; river discharge of water and nutrients given by the S-HYPE model (Lindström et al., 2010) and point sources representing sewage plants and industries. River loads enter the modelled archipelago in the surface cell, while the point sources are assigned to the cell most resembling the actual depth of the discharge. The weather forcing consists of solar radiation, air temperature, wind, relative humidity, cloudiness and atmospheric deposition of nutrients. The solar irradiation and all the irradiation and heat fluxes across the water-air interface are calculated by the PROBE model. The weather variables are taken from a gridded database at the SMHI, using meteorological synoptic monitoring data, and the deposition of nitrogen species (NHX and NOX) is calculated from the MATCH model (Robertsson and Lagner, 1999). For the deposition of phosphate, a literature value of 0.5 kg m^{-2} $month^{-1}$ is used (Areskoug, 1993).

Required input to SCM

The following time series of forcing and other information is required for the set-up of the CSM.

1. Meteorological data. File name B001_VADER.DAT. The model uses: air temperature (^oC), u-and v-wind velocity (m/s) , relative humidity(0-1) and total cloud cover(0-1). These data should be stored on a file every third hour The following example shows one day of data:

DATUM-TIME	TEMP	UVIND	VVIND	MOLN	RELFUKT
1990010100	-0.05	-0.51	-0.11	1	0.8

2. Discharge from land. File name B001_QNP.DAT. The discharge from land is daily values:
Q = Water flux (m^3/s)
TOTN = Total nitrogen (mg/m^3)
NO3 = Nitrate (mg/m^3)
NH4 = Ammonium (mg/m^3)
TOTP = Total phosphorus (mg/m^3)
PO4 = phosphate (mg/m^3)

DATE	Q(M3/S)	TOTN	NO3	NH4	TOTP	PO4	(mg/m3)
19900101	0.272	1243.832	264.2875	13.90987	18.86338	9.916122	

3. Point sources. File name B001_PKT.DAT. This example contains 2 point sources.

QDEPTH = Outlet depth in meters below the surface. Q in m^3/s and the nutrients in mg/m^3.

	Point source 1							Point source 2						
DATE	QDEPTH	Q	TOTN	NH4	NO3	TOTP	PO4	QDEPTH	Q	TOTN	NH4	NO3	TOTP	PO4
19900101	5	0.2	110.35	9.932	89.384	1.427	0.713	5	0.2	781.805	70.362	633.262	89.897	44.949

4. Atmospheric nitrogen deposition. File name B001_MATCH.DAT . Monthly values.
MN = row number
NOX = nitrate (mg/m^2 * month)
NHX = Ammonium (mg/m^2 * month)

YEARMM	MN	NOX	NHX
199001	1	18.689	18.674

5. Outer Sea boundary condition. This file is generated by another model. In this example the number 84 is the number of vertical layers in one profile. There is one new profile every day. Notice the depth-axis starts at the bottom. All nutrient concentrations are in $mmol/m^3$ (se nr 6. below)

84												
Date	Depth	temp	salt	orgn	orgp	zoo	phy	det	nh4	no3	po4	oxy
1990-01-02	85.500	4.304	6.801	16.628	0.295	0.103	0.486	2.087	0.295	3.930	0.508	8.526

6. The initial condition. This is described by an initial file called B001_INIT.DAT. This file describes the hypsographic curve, the vertical resolution and all variables. A short description follows:

Start date Number of vertical levels in this file
Start water level Surface area
Z = Distance from bottom (m)
FU = set zero (m/s)
FV = set zero (m/s)
FH = heat content (joule/m^3)
FT = temperature
FS = salinity
FK = kinetic energy, set 1.E-10
FE = dissipation of kin.energy, set 1.E-10
DZ = set zero
DZC = thickness of each grid cell (m)
RECDZ = set zero
ZBOU = set zero
FZO = zoo plankton (mg C/m^3)
FPH = phyto plankton (mg chl/m^3)
FDE = detritus (mg C/m^3)
FNB = nitrogen bentos (mmol/m^3)
FNH = ammonium (mmol/m^3)
FNO = nitrate (mmol/m^3)
FPB = phosphorus bentos (mmol/m^3)
FPO = phosphate (mmol/m^3)
FOX = oxygen (ml/l)
DON = organic nitrogen (mmol/m^3)
DOP = organic phosphorus (mmol/m^3)

7. The basin characteristics. Each sub-basin is described by the hypsographical curve (Area vs. Depth).

DEPTH (m)	AREA (km**2)
0	2412.9800
1	2373.9475

8. The sound characteristics. The geometry of each sound is extracted from digital sea charts and the cross sectional area and the maximum depths are then manually compared and verified against ordinary sea charts.

MAXDEPTH (m)	AREA (m**2)	Shape of the sound (Triangular=1 or rectangular=0)
45	12412.00	1

2.6.2 The Danish model system

Aarhus University, Denmark, has developed FLEXSEM (Fig. 6), a fast and flexible modelling tool for water quality calculations specifically targeted towards scientific and management challenges of the complex biogeochemical processes in coastal zone ecosystems (Larsen et al., 2013).

FLEXSEM offers a wide range of computational grids from simple box model domains to high-resolution unstructured meshes with thousands of polygons with different shapes and sizes. The computational mesh can be set up to be 0, 1, 2 or 3D. An unstructured mesh has the advantage of geometric flexibility to accurately reproduce the complex coastline characteristic for most estuaries and other types of coastal areas. In addition, the possibility of local grid refinements might be an important factor to improve model predictions in areas where flow dynamics are controlled by strongly varying bathymetry and/or coastlines. FLEXSEM has been used to calculate water quality in a number of Danish estuaries and is currently being tested also in open water environments.

The physical model

FLEXSEM employs a time-dependent, combined box-model and 3-D model approach to calculate water transport and mixing. Water mass exchange in the physical module is realized in the form of volume fluxes between the mesh cells, formulated as an exchange volume per time unit scaled by the time step of the model. Fluxes between mesh cells are automatically calculated from the computational mesh geometry. The water exchange and numerical discretization are described as:

Vertical exchange: A surface exchange volume $V_{Qs} = \frac{C_D \rho_{air} u^2}{f \rho_0} V$ is used to represent the wind induced vertical mixing, where V is the cell volume (m^3), $\tau = c_D \rho_{air} u^2$ is the wind stress (N m^2), c_D = wind-drag coefficient, ρ_{air} = 1.2 kg m^{-3}, u = wind speed (m s^{-1}), f = Coriolis parameter (s^{-1}) = 2* 7.29·10^{-5}sin (latitude), ρ_0 = reference sea water density = 1027 kg m^{-3}.

This exchange volume is scaled in depth by $e^{(-\frac{id}{ad})}$ where *id* is the depth of the interface between the cells and *ad* is the attenuation depth. I.e . the vertical mixing between two cells depends on the depth of the cell interface and the wind speed. The updated concentration C_{new} of all state variables takes the time-dependent form:

$$C_{new,l} = \frac{C_{org,l}\left(V - V_{Qa} - V_{Qb}\right) + C_{org,l+1} V_{Qa} + C_{org,l-1} V_{Qb}}{V}$$

where *l* is the layer index, V_{Qa} the exchange volume from the cell above, V_{Qb} the exchange volume from the cell below and V the volume of the cell. For the surface layer V_{Qa}=0 and for the bottom layer V_{Qb}= 0. Time indices *new* and *org* refer to the current and previous time step respectively.

Horizontal exchange: The exchange between elements is done horizontally, i.e. across the sigma layers. Each cell can exchange volumes, i.e. any state variable, with any number of adjacent cells, because a 2D element can have many adjacent elements (the element is a polygon), and each 3D cell can overlap with many adjacent cells in the vertical. At each time step the concentration in each cell is calculated by

$$C_{new} = \frac{C_{org}\left(V - \sum_{i=0}^{i=n} V_{Qi}\right) + \sum_{i=0}^{i=n} C_{org,i} V_{Qi}}{V}$$

where V is the volume of the cell, n is the number of horizontal adjacent cells and $V_{Qi} = hmc*dt$ is the exchange volume between the current cell and the i'th adjacent cell, where hmc is the horizontal mixing coefficient and dt the length of the timestep. The length of the timestep is limited only by the size of the cells and the horizontal mixing coefficient. Optionally the horizontal mixing can be set to depend on wind speed: $hmc = hmc + whmc\ u^2$, where u is wind speed and $hmcw$ the wind horizontal mixing coefficient. Furthermore the horizontal mixing can also be set to depend on wind direction

$$hmc = \frac{hmc\ [1 + \cos(wd - mmd)]}{2}$$

where wd is the wind direction and mmd is the maximum mixing direction.

Stratification is created by adding fresh water (river runoff) in the surface layer and by penetration of denser salt water from the open oceanic boundaries through horizontal mixing. Stratification is eroded by wind induced vertical mixing.

Salinity and temperature are treated as conservative parameters. Salinity is modified by freshwater sources. The surface layer is set to the atmospheric temperature. The salinity and temperature at the oceanic boundary can be prescribed and are mixed as any other parameter.

Tidal mixing is not explicitly included in the model. The model is calibrated to implicitly represent the effects of horizontal tidal mixing as part of the combined wind and tidally driven exchange rate at the oceanic boundary.

The Roskilde Fjord model was setup using a high-resolution unstructured mesh with 452 elements and 6 vertical sigma layers, yielding a total of 2712 computational cells.

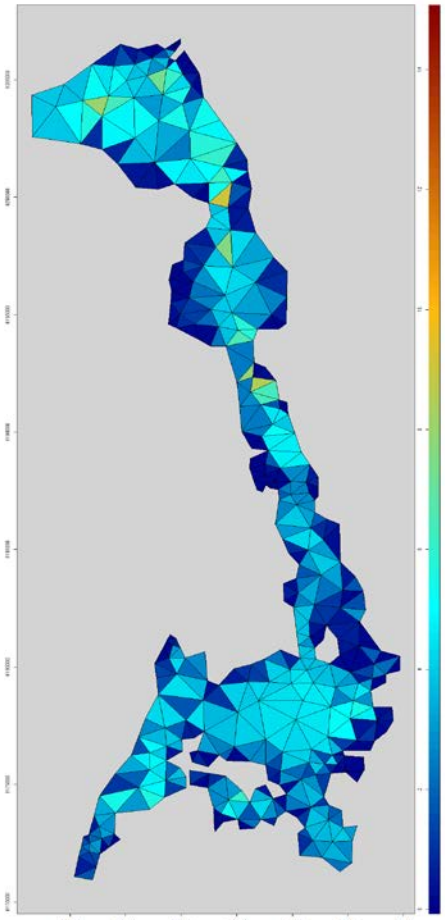


Figure 6. Computational grid of the FLEXSEM model setup of Roskilde fjord.

The biogeochemical model

The applied ecological model is based on the microplankton-detritus model (MPD model) developed for the North Sea (Tett, 1998) and modified in order to provide a more adequate description of the major bio-geochemical processes in estuarine systems. The modified MPD model describes the cycling of C, N and P through microplankton and detrital compartments and includes the dynamic coupling of pelagic and benthic biogeochemical processes (Fig. 7). The parameterizations of the C, N and P biogeochemical cycles are described in Tett (1998), Maar et al. (2009) and Timmermann et al. (2010). Briefly, nutrients enter the model estuary as NH_4, NO_3, PO_4, particulate organic bound nutrients and as PO_4 adsorbed to mineral particles. Forcing functions for nutrient loadings is calculated from TN and TP measurements and by using a distribution pattern measured in Horsens fjord (S. Markager unpublished results). For TN, the applied distribution pattern is: 0.2, 0.61 and 0.19 for NH_4, NO_3 and detritus-N, respectively. For TP, the applied distribution pattern is: 0.12, 0.71 and 0.17 for PO_4, adsorbed-P and detritus-P, respectively. The uptake of dissolved inorganic nutrients by phytoplankton is described by Michaelis - Menten kinetics and is dependent on the internal nutrient-to-carbon ratio which allows N- and P-excretion (negative uptake) if the internal quotas exceed a maximum as well as luxury uptake and internal storage of phosphorous. Microplankton growth rate is calculated on the basis of the cell quota threshold limitation theory (Droop et

al., 1982) as the minimum growth rate predicted from light, nitrogen or phosphorous. Chl *a* concentrations is derived from the internal N concentrations by using a conversion factor of 2.0 mg chl *a* mmol-N^{-1}.

Modified Ivlev formulations are used to describe ingestion of phytoplankton by zooplankton and mortality of zooplankton due to predation by pelagic predators. Detritus is produced by zooplankton assuming an assimilation efficiency of 80%. Remineralization of detritus and the associated release of inorganic nutrients (ammonia and phosphate) are dependent on the "lability" of the detritus. In the applied parameterization the N to C ratio in the detritus is used as a proxy for lability assuming that the more aged detritus with lower N to C ratio is less labile. Sedimenting phytoplankton and detritus is burrowed into the sediment where it is gradually mineralized to PO_4 and NH_4. The mineralization of detritus and production of inorganic nutrients is described by the same functions as for the water column. The inorganic nutrients may then diffuse to the overlying water. The fate of pore water PO_4 is redox dependent. Under oxidized conditions PO_4 is retained in the sediment by adsorbtion to Fe or Mn and released when the sediment becomes reduced. An oxygen concentration of 100 mmol m^{-3} in the bottom water is used as a threshold value determining the redox condition of the top layer in the sediment.

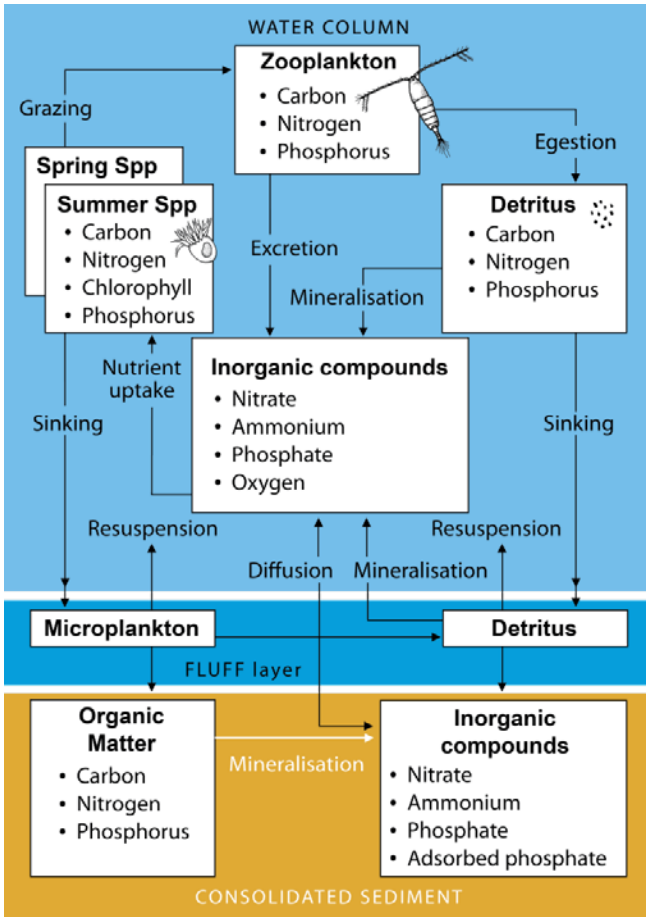


Figure 7. The biogeochemical module used in FLEXSEM. The module describes benthic and pelagic cycling of cycling of C, N and P.

Forcing from land, atmosphere and the open sea boundary

The model is forced with hourly meteorological fields of 2 m air temperature, 10 m wind speed and direction, cloud cover and relative humidity at a nearby point source provided by an operational atmospheric model (Brandt et al., 2001).

Open Sea boundary conditions for the hydrodynamic and ecological state variables are based on data provided from the Danish monitoring program (Conley et al., 2002). Open boundary conditions of temperature, salinity, nutrients (PO_4, NO_3+NO_2, NH_4) and Chl *a* are based on measurements from station FRB75 located in the northern part of the model domain at the border between Roskilde fjord and Isefjorden. These parameters are measured approximately once a week and linearly interpolated over time and in the vertical in order to provide proper boundary conditions. The horizontally uniform boundary conditions were updated once a day.

Boundary conditions representing daily riverine input of water and nutrients (TN and TP) are derived from a combination of measurements and model estimations (Andersen et al., 2005; Kronvang et al., 2008). Loads of total nitrogen (TN) and phosphorus (TP) is then distributed into the relevant pools using a distribution pattern measured in Horsens estuary in 2001 (Markager et al. submitted). For TN the applied distribution pattern is: 0.2: 0.61: 0.19 for NH_4, NO_3 and detritus-N, respectively. For TP the applied distribution pattern is: 0.12: 0.71: 0.17 for PO_4, adsorbed-P and detritus-P, respectively.

River loads are added to the surface cells in the part of the model domain that resembles the actual locations of the streams.

Required input to FLEXSEM

The following information on grid, time series of forcing and other information is required for the set-up of the FLEXSEM. FLEXSEM supports multiple inputs formats. For time series data, the most convenient format is tab separated values – see example below.

datetime	wSpeed	wDir	gloRad	airTemp	precip
2005-01-01 00:00:00	5.86	333.06	0	6.7	0.000e+00
2005-01-01 01:00:00	6.04	327.64	0	6.9	0.000e+00
2005-01-01 02:00:00	6.28	322.15	0	7	0.000e+00

1. Mesh construction

The information necessary to construct the modelling grid consists of coastline and bathymetry data, horizontal and vertical l resolution. Also the modelling time period needs to be specified.

2. Meteorological data. The model uses: air temperature (^oC), wind speed and direction, incoming radiation and precipitation.

3. Discharge from land.
Q = Water flux (m^3/s)
NO3 = Nitrate ($mmol/m^3$)
NH4 = Ammonium ($mmol/m^3$)
PO4 = phosphate ($mmol/m^3$)
DetritusN=Particulate organic Nitrogen
DetritusP= Particulate organic phosphorus

4. Open Sea boundary condition.

Salt = salinity (PSU)
Temp =temperature (deg. C)
O2 = Oxygen (mg/l)
NO3 = Nitrate (mmol/m^3)
NH4 = Ammonium (mmol/m^3)
PO4 = phosphate (mmol/m^3)
B = Plankton Carbon (mmol/m^3)
P = Plankton phosphorous (mmol/m^3)
N = Plankton nitrogen (mmol/m^3)
C = Detritus carbon (mmol/m^3)
DetritusN=Particulate organic Nitrogen
DetritusP= Particulate organic phosphorus

5. The initial condition. Initial conditions can be prescribed as constants of 3D fields for all variables.

2.6.3 The Finnish model system

The Finnish model system is based on the Biogeochemical Flux Model (BFM) community model (Vichi et al. 2007) described at the homepage *(http://bfm-community.eu/)*. The BFM in sea ice (BFMSI) is described by Tedesco and Vichi (2010) and the BFMSI coupled to the sea ice model ESIM2 is described by Tedesco et al. (2010).

The Biogeochemical Flux Model

The BFM is a numerical model (Fig. 8), which describes the dynamics of major biogeochemical processes occurring in marine systems. Presently BFM considers the cycles of nitrogen, phosphorus, silica, carbon, and oxygen in the water dissolved phase, as well as in the plankton, detritus, and benthic compartments. Plankton dynamics are parameterized by considering a number of plankton functional groups, each representing a class of taxa. BFM plankton functional groups are subdivided in producers (phytoplankton), consumers (zooplankton), and decomposers (bacteria). These broad functional classifications are further partitioned into functional subgroups to create a planktonic food web (e.g. diatoms, picophytoplankton, microzooplankton, etc.). The BFM code can be easily coupled to standard hydrodynamics codes, allowing for explicit description of the dynamics of biogeochemical properties in a spatially heterogeneous system. Presently BFM has been successfully coupled to the Princeton Ocean Model (POM), the Ocean Parallelise' (OPA), and Nucleus for European Modelling of the Ocean (NEMO) and applied at the global ocean, regional, subregional and local space scales. When coupled with the hydrodynamics BFM can be used as a short term forecasting model or as a climate simulation model. From a mathematical point of view, the BFM is a set of ordinary differential equations describing the time rate of change of a number of biogeochemically active tracers. The BFM structure is flexible and modular, so that the number, type and properties of the functional groups can be easily modified and different model configurations can be used to focus on different aspects. The code is written in the FORTRAN90 language.

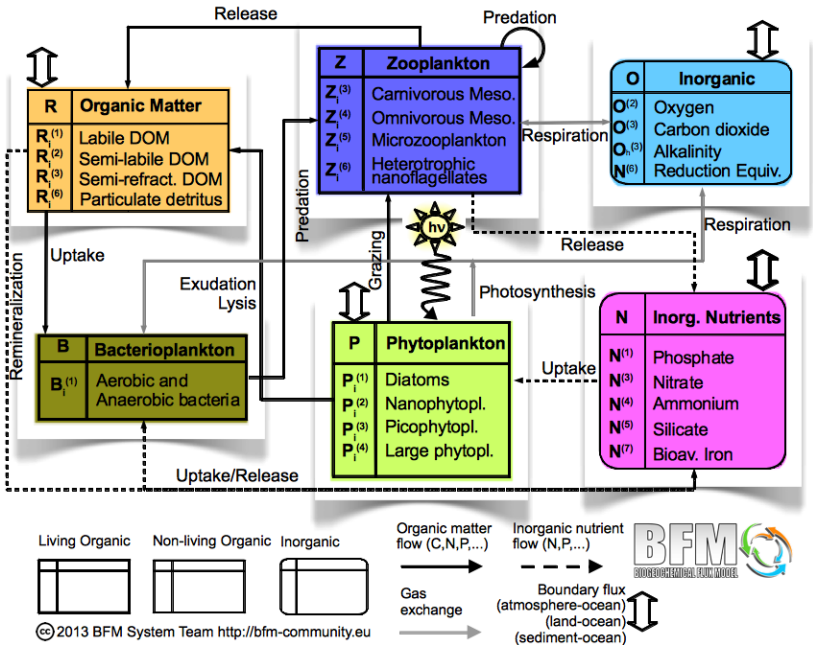


Figure. 8. The Biogeochemical Flux Model as presented on the BFM community homepage http://bfm-community.eu/model-description-1.

ESIM-BFMSI1D Baltic Configurations

New Baltic configurations of the BFM have been developed and are ready for testing in 0D---1D---3D applications. The configurations are:

1) pelagic only: COMPILATION + RUNNING BALTIC TEST CASE READY
2) pelagic + sea ice : COMPILATION + RUNNING BALTIC TEST CASE READY
3) pelagic + benthic: COMPILATION COMPLETED + RUNNING TEST CASE UNDER DEVELOPMENT
4) pelagic + benthic + sea ice: COMPILATION COMPLETED + RUNNING TEST CASE UNDER DEVELOPMENT

The PELAGIC model

-=-=-=

Z5 : Microzooplankton
Z6 : Heterotrophic Nanoflagellates (HNAN)
-=-=-=

State Variable(s) for Sea ice Fauna
group SeaiceZoo[cnp] (SZO) : mg C/m2 : mmol N/m2 : mmol P/m2
X1 : Sea ice fauna
-=-=-=

group BenthicAmmonium[n] (BNA) :mmol N/m2
K4 : Ammonium in oxic layer
K14 : Ammonium in denitrification layer
K24 : Ammonium in anoxic layer

K6r : Reduction equivalents in oxic layer : mmolS--/m2
K16r : Reduction equivalents in denitrification layer : mmolS--/m2
K26r : Reduction equivalents in anoxic layer : mmolS--/m2

K3n : Nitrate in sediments : mmol N/m2
K5s : Silicate in sediments : mmol Si/m2
G2o : Benthic O2 : mmol O2/m2
G4n : N2 sink for benthic system. :mmol N/m2

D1m : Oxygen penetration depth :m
D2m : Denitrification depth :m
D6m : Penetration Depth organic C :m
D7m : Penetration Depth organic N :m
D8m : Penetration Depth organic P :m
D9m : Penetration Depth organic Si :m

Input data to the ESIM2-BFMSI models.

1. Meteorological data. File name input_intepolation.m. ESIM2 (sea ice thermodynamic model) uses :

- air temperature (deg K),
- u-and v-wind velocity (m/s) ,
- specific humidity at the surface (0-1),
- specific humidity at 2 m height (0-1),
- precipitation rate (kg/m2/s),
- downward shortwave radiation ()
- and total cloud cover (0-1).
- These data can be taken form any meteorological source. NCEP and ECMWF 6-h reanalysis have been largely used and interpolated:
  - Linearly on the specific location of the simulation (Grads script)
  - Linearly from 6 h to generally 1.5 h time steps, but any other time steps is possible

An example of the script for one input (cloudiness)

```
load /Users/LETI/Linux-work/ESIM/ESIM2/ESIM_for_Users/NCEP/Cl.txt
%(total cloud cover in percentage)

x=1:4:4368; %%% to be set up by user
xi=1:1:4368; %%% to be set up by user

Cl=Cl';
Cl=interp1(x,Cl,xi,'linear');
Cl=Cl'/100; %%% convert cloudiness from percentage to fraction
Cl(4366:4368)=[];
```

And an example of one forcing file (Cl.txt)

```
1.00000e+02
9.90472e+01
9.84846e+01
8.68935e+01
7.51955e+01
8.89343e+01
3.04050e+01
1.80193e+01
3.73629e+01
3.34344e+01
1.38031e+01
2.29101e+00
3.94806e+01
```

2. Discharge from land. Can be implemented in src/BFM/SeaIce/SeaicetoPelCoup.F90

3. Point sources. Can be implemented in routine /src/standalone/event_data.F90

4. Atmospheric deposition. Implemented for any compound of interest in routine src/BFM/SeaIce/SeaicetoPelCoup.F90

5. Outer Sea boundary condition. Not applicable

The initial conditions

This is described in the file main model script ESIM2XX.m for the sea ice thermodynamic model ESIM2. Below an example when the run starts with open water (no sea ice):

```
Tmix(1)=274.00;                % Initial mixed layer temperature
T0(1)=Tmix(1);                 % Initial surface temperature
Ts(1)=Tfr;                     % Initial snow temperature
Tsi(1)=Tfr;                    % Initial snow ice temperature
Ti(1)=Tfr;                     % Initial sea ice temperature
hi(1)=ZERO;                    % Initial sea ice thickness
hs(1)=ZERO;                    % Initial snow thickness
hmi(1)=ZERO;                   % Initial snow ice/superimposed ice thickness
hmi_new(1)=0.0;
hs_prec_bucket(1)=0.0;         % Initial snow thickness in the bucket model
hs_prec(1)=0.0;                % Initial snow precipitation
ki(1)=1.90;                    % Initial sea ice thermal conductivity
ks(1)=0.25;                    % Initial snow thermal conductivity
cpi(1)=2200.0;                 % Initial sea ice heat capacity
ros(1)=250;                    % Initial snow density
ros_new(1)=150;                % Initial new snow density
Vbr_ice(1)=0.0;                % Initial brines volume
Sbr_ice(1)=0.0;                % Initial brines salinity
Sice(1)=0.0;                   % Initial sea ice bulk salinity
Tice(1)=Tfr-273.15;            % Initial sea ice temperature
```

```
Vbr_i(1)=0.0;                % Initial internal brines volume
Sbr_i(1)=0.0;                % Initial internal brines salinity
Si(1)=0.0;                   % Initial internal sea ice bulk salinit
ro_sice_bott(1)=0.917;       % Initial sea ice bulk density at the bottom
ro_sice_surf(1)=0.900;       % Initial sea ice bulk density at the surface
ks_snow(1)=25.0;             % Initial mean of snow extiction coefficient
kmi_av(1)=-3.3*Cl(1)+21.05;  % Initial mean of snow ice/superimposed ice extiction
coefficient
ksi_10_av(1)=-6.6*Cl(1)+17.1; % Initial mean of sea ice extiction coefficient (10 cm
layer)
ksi_av(1)=-0.1*Cl(1)+1.6;    % Initial mean of sea ice extiction coefficient
alpha(1)=0.15;               % Initial albedo value
ki_ice_bott(1)=2.0;          % Initial sea ice thermal conductivity at the bottom
Sw(1)=32.0;                  % Seawater salinity
```

For BFM, the initial conditions are given for the pelagic model only (no need for the sea ice model) in the running environment:/run/STANDALONE.XX/BFM_General.nml. Below an example of setting some initial conditions:

```
&bfm_init_nml
   N1p0     =  0.05     (PO4)
   N3n0     =  7.0      (NO2+NO3)
   N4n0     =  1.0      (NH4)
   N5s0     =  8.0      (SiO4)
   O2o0     =  300.0    (O2)
   O3c0     =  27060.00  (CO2)
   P1c0     =  1.0     (diatoms, carbon content)
   P2c0     =  1.0      (flagellates, carbon content)
   P3c0     =  1.0      (picophytoplankton, carbon content)
   P4c0     =  1.0      (large phytoplankton-dinoflagellates, carbon content)
   Z3c0     =  1.0      (omnivorous mesozooplankton, carbon content)
   Z4c0     =  1.0      (herbivorous mesozooplankton, carbon content)
   Z5c0     =  1.0      (microzooplankton, carbon content)
   Z6c0     =  1.0      (heterotrophic nanoflagellates, carbon content)
   B1c0     =  1.0      (aerobic and anaerobic bacteria, carbon content)
   R1c0     =  1.0      (DOC)
   R6c0     =  1.0      (POC)
```

More details on BFM and BFMSI nomenclature, parameters and variables can be taken from the website: http://www.bfm-community.eu

2.6.4 The Russian model system

There are some complex physico-chemical processes that occur in the sediments, such as sedimentation, adsorption, oxidation and reduction, burial, release, bioturbation and bioirrigation. These processes determine the fluxes of matter at the water-sediments interface and, obviously, should be included in the diagenetic model of temporal variability of biogeochemical characteristics in the pore waters and bottom sediments.

Formulation of diagenetic model and its adaptation to the conditions of the Eastern part of the Gulf of Finland

In the Boudreau diagenetic model (Boudreau, 1996) bioirrigation factor is represented by nonlocal exchange term that depends on the geometrical parameters of the worm's burrows. For understanding the impact of macrozoobenthos on the chemical composition of the pore water Aller submodel is used (Aller, 2001). Many benthic fauna inhabit quasi-vertical burrow structures that are regularly flushed with overlying waters. In the so-called «Aller tube model», worm burrows are explicitly represented by means of vertical tubes within cylinders of sediment (Aller, 2001). The direct aim of this experiment was to identify the effects of the size and number of pores on the process of bioirrigation.

Community of polychaetes can be represented by an array of cylinders, whose diameter depends on population density. Therefore, the nonlocal exchange term employed by our model can be directly related to biogenic structures, specifically *Marenzelleria* burrows.

Adopting this approach, the intensity of pore water exchange with the overlying water is defined by a nonlocal bioirrigation coefficient α (year^{-1}), which is solute-specific due to different reaction geometries and molecular diffusion coefficients. Oxidation of dissolved iron and manganese occurs very rapidly and therefore as for these compounds is set to zero (Meile et al., 2005). For all other solutes, α is determined using the relationship (Norkko et al., 2011):

$$\alpha = \gamma * D_s, \quad (1.1)$$

where D_s (cm^2 year^{-1}) – molecular diffusion coefficient;

γ (cm^{-2}) – empirically derived parameter, called bioirrigation factor, it is a function of worm's population (ind. cm^{-2}) and the radius of their burrows (Norkko et al., 2011).

In laboratory experiments with *Marenzelleria* (Quintana et al., 2007) it was found that on density of worms populations of 2550 ind. m^{-2} bioirrigation factor γ is equal to 0.53 cm^{-2}. Then, knowing these two parameters, it is possible to obtain the burrow radius (equation 1.2) (Sandnes *et al*., 2000):

$$\gamma = \frac{r}{\left(\frac{1}{\pi N} - r^2\right)\left(\frac{1}{2\sqrt{\pi N}} - \frac{3r}{2}\right)} \quad (1.2)$$

Using the relation above and the values of the *Marenzelleria spp*. population, obtained by measurements in the sea, bioirrigation coefficient α can be calculated for different values of the population.

In application of diagenetic model (Boudreau, 1996) 2 stations were selected: with high abundance of *Marenzelleria spp*. (station 2UGMS) and low (20F). Factors of bioirrigation γ and bioirrigation coefficients α were calculated for each of these stations. The results of the calculations are given in the table 1.1.

Table 1.1 Parameters and characteristics, used in the diagenetic model

Station	N, ind. m^{-2}	r, m	γ, cm^{-2} (equation 1.2)	D_s, cm^2 $year^{-1}$	α, $year^{-1}$ ($\gamma * D_b$)
20F	240	0.00183	0.01	358	3.202
2UGMS	3912		1.33	364	483

D_s, (cm^2 $year^{-1}$) – molecular diffusion coefficient for O_2*

Note that this table contains not all the parameters and characteristics used in the model, the list of input data is significant.

Molecular diffusion coefficient of oxygen depends on the temperature, salinity and pressure at monitoring stations and is calculated inside the diagenetic model.

Biodiffusion coefficient is specified as a Gaussian decrease according to the equation:

$$D_b^0 = D_0 * e^{-\frac{x^2}{2\sigma^2}} \quad , \tag{1.3}$$

where D_0 (cm^2 $year^{-1}$) – diffusion coefficient on the sediment-water interface;
x (cm) – depth;
σ (cm) – depth of effective mixing.

Running the model, it was found that the rate constants for oxidation reactions of various substances and elements described by the model do not affect the final result of the simulation, i.e. the model is not sensitive to them. This allows using in the model rate constants, found in the literature.

However, some of the model parameters have a significant influence on the simulation result. Thus, the variation of Monod constants for oxygen, nitrates and sulfates, as well as phosphates and ammonia adsorption constant are important. Thus, these constants should be determined by identifying the model parameters, i.e. on the basis of better aligning their values with the data of field observations.

The following boundary conditions are specified in the model. For organic matter G boundary conditions at x=0 are specified as flux F_G

$$-\varphi_s D_b^0 \frac{\partial G}{\partial x} + \varphi_s w^0 G^0 = F_G \tag{1.4}$$

where φ_s – solid volume fraction (1-φ);
D_b^0 (cm^2 $year^{-1}$) – biodiffusion coefficient on the sediment-water interface;

w^0 (cm $year^{-1}$) – burial velocity of solids on the sediment-water interface;
G^0 (%) – organic matter concentration on the sediment-water interface;
x (cm) – sediments depth for the calculation.

Boundary conditions for the solute at x=0: their transfer across the sediment-water interface is regulated by mass transfer in a diffusive boundary layer (Boudreau and Guinasso, 1981):

$$-\varphi D_i' \frac{\partial C_i}{\partial x}\Big|_{x=0} = \frac{D_i^0}{\delta}(C_{iw} - C_i(0)) \quad (1.5)$$

where D_i' (cm^2 $year^{-1}$) – effective diffusion coefficient;
D_i^0 (cm^2 $year^{-1}$) – molecular diffusion coefficient for i solute;
δ (cm) – diffusion sublayer thickness;
C_{iw} (mmol l^{-1}) – concentration of i solute in the well-mixed overlying waters;
$C_i(0)$ (mmol l^{-1}) – concentration of i solute on the water-sediments interface.

For all solutes, the bottom conditions at x = L can be either that the gradients (diffusive fluxes) disappear:

$$\frac{\partial C_i}{\partial x} = 0 \quad (1.6)$$

2.6.5 The Polish model system

The Gulf of Gdańsk model (Vistula plume and Puck Bay)

The ecohydrodynamic model was developed at the Institute of Oceanography Gdansk University (IOUG). It contains two essential parts - hydrodynamic the M3D_UG (Fig. 9) and ecosystem part – the ProDeMo (Fig. 10). The model works as pre-operational one at the southern Baltic area and the Gulf of Gdansk. The 48 hours forecasts deliver the surface current fields, the temperature and salinity sea water. Moreover, the model forecasting fields of the following nutrients: nitrates, ammonia, phosphates, silicates, total nitrogen and total phosphorus, dissolved oxygen and phytoplankton biomass. The model and its validation are described in detail at the website http://model.ocean.univ.gda.pl/indexeng.html.

Puck Bay is situated in the western part of the Gulf of Gdańsk and is partly separated from deeper region by the Hel Peninsula. Puck Bay is divided into the inner Puck Lagoon and the outer Puck Bay by the Seagull Shallow.

Puck Lagoon is a shallow (mean 3.1 m) water basin. The waters exchange between the Puck Lagoon and the Outer Puck Bay is limited. Water salinity in the basin is rather stable during a year (around 7.3).

Outer Puck Bay is the deeper part of the Puck Bay with mean depth of 21 m (max. 54 m) and bottom with steep slope. The residence time depending on depth and takes from 7 to 30 days. The hydrological conditions depends on inflows of marine and terrestrial waters. There are seasonal vertical water salinity and temperature stratification. Surface water salinity in the basin is around 7.7 (Kruk – Dowgiałło & Szaniawska 2008).

In the Puck Bay whole range of sediment types could be found (inner part – sands, peat, mud and in outer part– sands, silts, silty sandy sediments, muds). Total organic carbon varied from 0.1 to around 8 % (Uścinowicz 2011). Sandy sediment in the coastal area is covered by vascular plants: *Zostera marina, Zanichelia palustris, Potamogeton* spp. and algae: *Chara* spp., *Cladophora* spp., *Enteromorpha* spp. and *Ectocarpacea*. Benthic fauna communities are composed of less than 40 taxa. The sandy sediment of the inner part of the Puck Bay is dominated by *Cerastoderma glaucum* and *Hydrobia* spp., whereas outer part is dominated by: *Macoma balthica*, *Hediste diversicolor*, *Marenzelleria* spp. (Janas & Kendzierska 2014). Puck Bay is a eutrophicated water region under the antropogenic pressure.

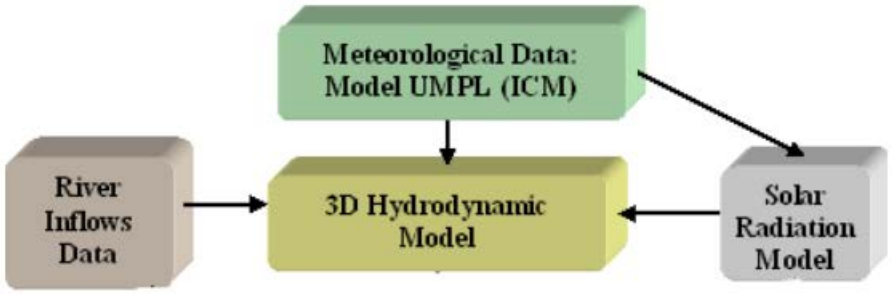


Figure 9. Scheme of the the hydrodynamic model M3D_UG (source of the figure http://model.ocean.univ.gda.pl/indexeng.html)

The ProDeMo model includes 18 state variables, which can be divided into several functional groups: phytoplankton, zooplankton, nutrients, detritus, dissolved oxygen and nitrogen, phosphorus and silicon compounds in sediment (Fig. 10) (Kowalewski et al. 2003, Kannen et al. 2004)

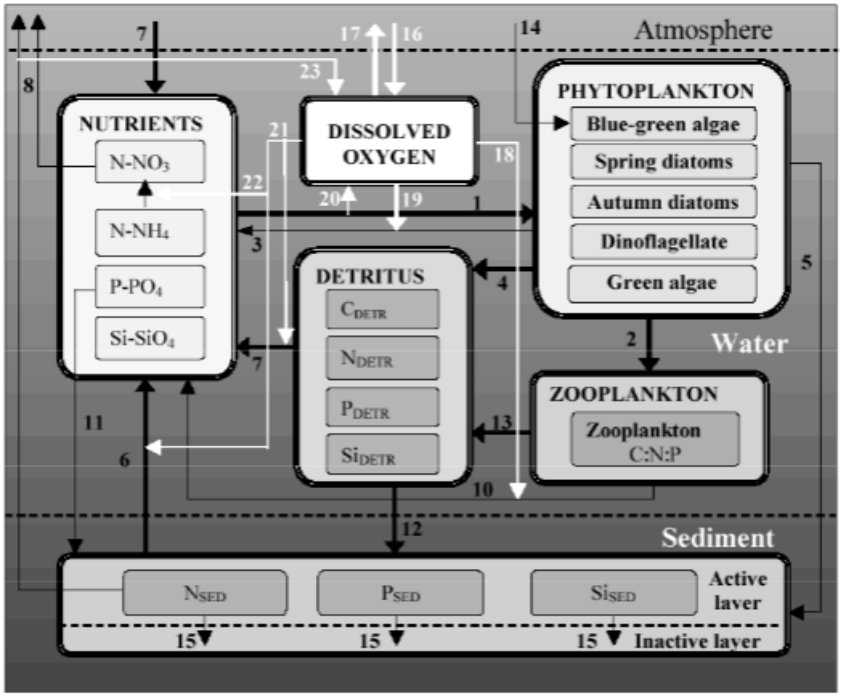


Figure 10. Scheme of the ProDeMo Model. Processes included in the ProDeMo: 1) nutrient uptake by phytoplankton, 2) phytoplankton grazing by zooplankton, 3) phytoplankton

respiration, 4) phytoplankton decay, 5) sedimentation, 6) nutrients release from sediment, 7) atmospheric deposition, 8) denitrification, 9) mineralization, 10) zooplankton respiration, 11) sedimentation of phosphorus adsorbed on particles, 12) detritus sedimentation, 13) zooplankton decay, 14) nitrogen fixation, 15) nutrient deposition. Processes influenced the dissolved oxygen: 16) reaeration, 17) flux to atmosphere due to the over saturated conditions, 18) zooplankton respire ation, 19) phytoplankton respiration, 20) assimilation, 21) mineralization, 22) nitrification, 23) denitrification (Kowalewski et al. 2003) (source of the figure Kannen et al. 2004).

Using the M3D_UG and ProDeMo it is possible to compute data in different formats e.g. maps or vector data. Various options are available at the web page of the SatBaltic Project after registration (http://satbaltyk.iopan.gda.pl/?lng=eng).

Some monitoring data are available in ICES database. Biological and chemical data for validation models could be found in small research data base at Gdańsk University.

2.6.6 The Lithuanian model system

Curonian lagoon is the largest lagoon in Europe receiving most of the riverine discharge from Nemunas River (98% of the total freshwater runoff ~ 23 km3/year) that enters the lagoon in its central area, dividing the water body into two different parts (Jurevičius, 1959). Curonian lagoon and the coastal Baltic see according to the WFD fall into the definition of the transitional coastal waters. The conditions in the Curonian lagoon is highly eutrophic and productive water body also effectively decide the water quality in the neighboring Baltic Sea north of Klaipeda because of the significant freshwater runoff and dominating water currents. Phytoplankton remains the most important autochthonous organic matter producer both in Baltic Sea and in the Curonian lagoon Not surprisingly the phytoplankton seasonal dynamics is highly related to the seasonal changes in the water quality. The spring bloom, mostly formed of diatoms is not so critical to the water quality because of lower temperatures. However, the summer cyanobacteria bloom is often of higher intensity (up to 20 mgChlA/l) and often cases a number of water quality problems inside the lagoon (hypoxia, fish kills, cyanotoxins) as well as transported to coastal zone creates sanitary problems at the popular resorts along the Lithuanian coast (Razinkovas et al., 2008).

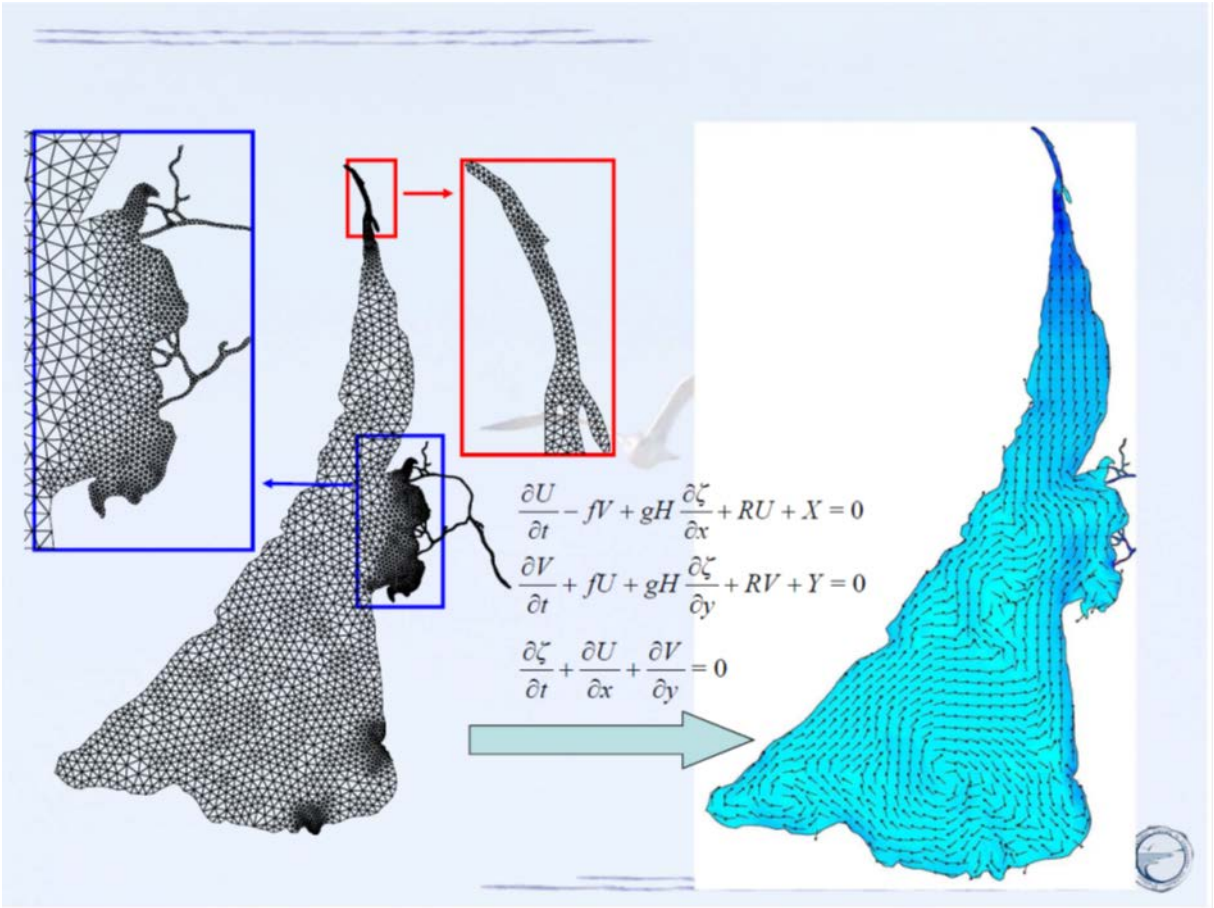


Figure 11a. The circulation model of the Curonian lagoon.

SHYFEM-AQUABC

In the Curonian lagoon we use the hydrodynamic model SHYFEM - a finite element model developed at the CNR-ISMAR of Venice and successfully applied to many coastal

environments (Umgiesser, 1997; Zemlys et al, 2013) was applied. The model is freely available on the SHYFEM web page: http://www.ismar.cnr.it/shyfem. Detailed description of model hydrodynamic and transport equations is given in Zemlys et al (2013).

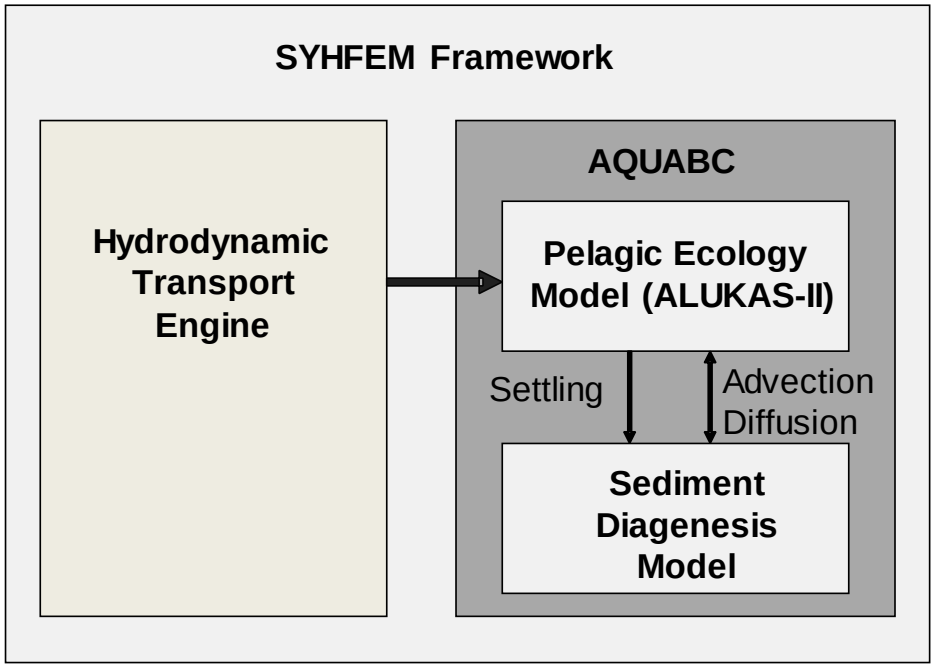


Figure 11b. General framework of SHYFEM-AQUABC model.

Besides the hydrodynamic equations, SHYFEM has an internal solver for advection-diffusion equation, so that modelling the transport of any dissolved substance is possible. The transport equation is solved for each node reactor (control volume) that is made from neighboring elements (triangles) (Fig. 11a).

Ecological model

The ecological model AQUABC (Fig. 11b) was developed initially as a model focusing on pelagic ecological processes, later incorporated the bottom sediment model, which is currently under development. The linkage between the water column and sediment model is ensured by coupling the state variables in pelagic ecology and bottom sediments sub-models where the transport processes in the bottom sediments model make the two way transfer of nutrients and organic matter possible. Since there are no primary producers in the bottom sediment model, phytoplankton carbon is immediately converted to the POC in the benthic zone representing dead organic matter.

Pelagic Ecology Model

The pelagic ecology submodel (Fig. 11c) called ALUKAS-II (Advanced Level nUtrient Kinetics for Aquatic ecoSystems), is a fully featured eutrophication analysis model with nutrient cycles, primary production, organic matter mineralization and a simplified

zooplankton sub-model. ALUKAS-II supersedes ALUKAS, which was developed by Ertürk (2008) and applied to Curonian Lagoon by Ertürk et al (2008) and Razinkovas et al (2008).

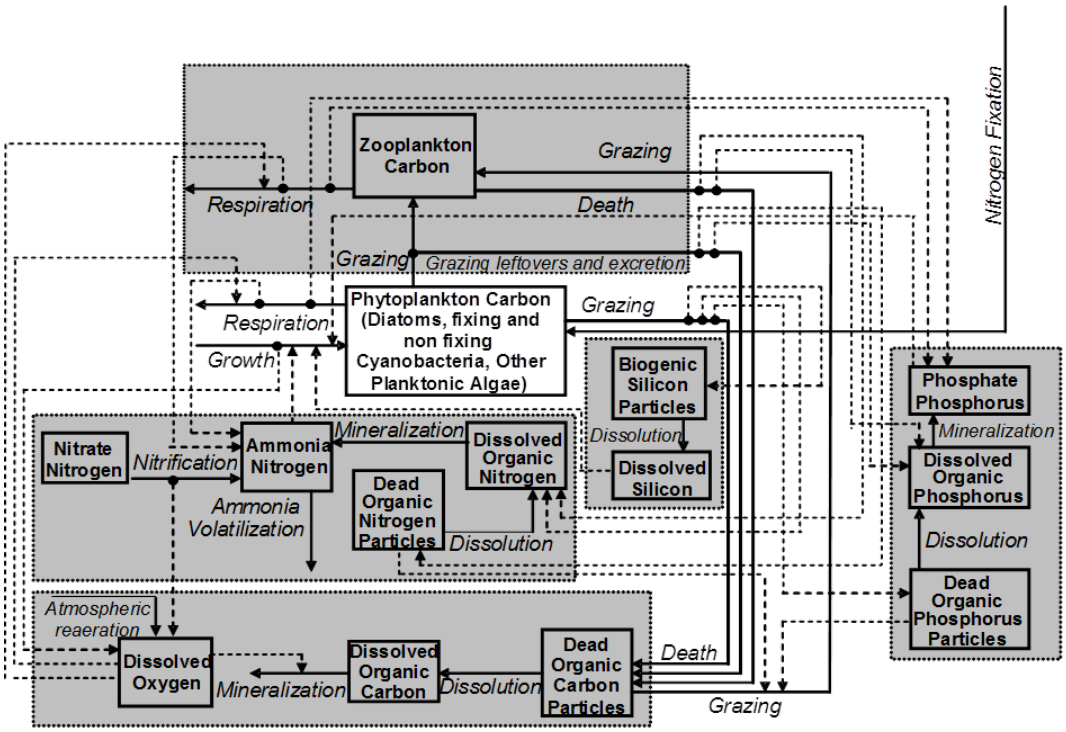


Figure 11c. Conceptual diagram of pelagic model ALUKAS-II.

Benthic diagenesis model

The bottom sediment submodel is a one dimensional model that considers the vertical transport and biogeochemical transformation processes of organic matter nutrients in the benthic zone. General scheme representing state variables used in the benthic compartment is presented in Fig. 11d.

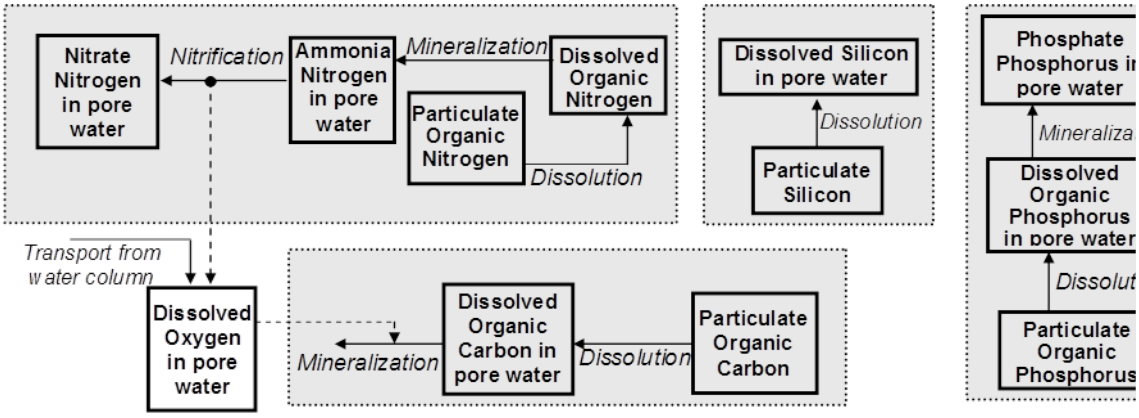


Fig 11d. Generalized scheme of the AQUABC bottom sediment submodel

2.6.7 The Swedish Open water model system for the Gulf of Gdansk/Vistula

Open sea conditions for nutrients and organic matter for the Gulf of Gdansk off the outlet of the Vistula River will be derived from an existing high-resolution physical-biogeochemical model for the open Baltic Sea (RCO-SCOBI).

The coupled model system is based on the Swedish Coastal and Ocean Biogeochemical model (SCOBI) (Eilola et al., 2009) and the Rossby Centre Ocean circulation model (RCO) (Meier et al., 2003; Meier, 2007). The SCOBI model is basically the same as described before for the SCM model system. The open sea version, however, also include current stress and wind wave driven resuspension of the sediments with the help of a simplified wave model (Almroth-Rosell et al., 2011). The model domain of RCO-SCOBI model covers the Baltic Sea with open boundaries in the northern Kattegat. Boundary conditions are based on Stevens (1991) with prescribed sea surface heights. In case of inflow temperature and salinity variables are nudged towards observed climatological mean profiles. In case of outflow an Orlanski radiation condition is utilized (Orlanski, 1976). In RCO a flux corrected transport scheme (Gerdes et al., 1991), a bottom boundary layer model (Beckmann and Döscher, 1997), a two-equation turbulence closure scheme of the k-ε type (Meier, 2001) and a Hible-type (Hibler, 1979), multi-category sea ice model (Mårtensson et al., 2012) with elastic-viscous-plastic rheology (Hunke and Dukowicz, 1997) are implemented. The horizontal grid resolution amounts to 2 nautical miles or 3.7 km which is regarded as eddy-permitting. 83 vertical levels with layer thickness of 3 m are used. Atmospheric forcing data for the period 1970-1979 are calculated from regionalized ERA-40 data using a regional atmosphere model with a horizontal grid resolution of 25 km (Samuelsson et al., 2011). For the wind speed a bias correction method following Meier et al. (2011) is applied. The hydrological forcing is based upon monthly mean river runoff observations (Bergström and Carlsson, 1994). Monthly nutrient loads from rivers and point sources and of atmospheric nitrogen deposition are calculated from historical data (Savchuk et al 2012). Initial conditions for January 1970 are taken from an earlier run with RCO-SCOBI.

For further details of the RCO configuration the reader is referred to Meier et al. (1999, 2003) and Meier (2007). For further details of the SCOBI model the reader is referred to Eilola et al. (2009, 2011) and Almroth-Rosell et al. (2011).

2.6.8 The Open water model systems

Open sea conditions for nutrients and organic matter are described by the models RCO-SCOBI (described in Section 2.6.7), The BAltic sea Long-Term large-Scale Eutrophication Model (BALTSEM) (Gustafsson, 2000, 2003; Savchuk, 2002), the Ecological Regional Ocean Model (ERGOM) (Neumann et al., 2002; Neumann and Schernewski, 2008), and the St. Petersburg Baltic Eutrophication Model (SPBEM) (Neelov et al., 2003; Myrberg et al., 2010; Savchuk, 2002).

The models are structurally different in that ERGOM, SPBEM and RCO–SCOBI are three-dimensional (3D) circulation models with uniform high horizontal resolution while BALTSEM resolves the Baltic Sea spatially in 13 dynamically interconnected and horizontally integrated sub-basins with high vertical resolution. Further information and results from the models may be found e.g. in Eilola et al. (2011) (for BALTSEM, ERGOM, RCO) and Skogen et al. (2014) (for SPBEM and RCO-SCOBI).

3. Preliminary results

3.1 SCM model results

Example from the Stockholm inner archipelago

The SCM calculates the mean vertical profiles in 173 basins, connected by 317 straits, representing northern Baltic Proper, including the Stockholm archipelago (Fig. 4). The model evaluates water quality in the water bodies of the Water Framework Directive. As such, it is part of the vattenwebb online tool (http://vattenweb.smhi.se/) provided by the SMHI (http://www.smhi.se/tema/vattenforvaltning). The model is available for calculations of the physical and biogeochemical state along the whole Swedish coast, but in this case study we have only used a sub-set of the model area. The overall validation of the model results in the Stockholm archipelago is presented by Sahlberg et al. (2008). The investigation of nutrient retention in the inner parts of the Stockholm archipelago (see encircled area in Fig. 4) has started as part of the COCOA project.

The nutrients, N and P to the inner Stockholm archipelago (Fig. 4) are supplied by rivers, point sources and atmosphere (Fig. 12). Biogeochemical processes, such as assimilation of nutrients by phytoplankton and sinking of detritus to the sediment surface, contributes to temporary retention of N and P. These processes lead to variations in the benthic and pelagic nutrients pools (Fig. 13), while burial of the nutrients and (for N) denitrification processes contributes to permanent retention. The total retention would then be the sum of permanent and temporary retention (Fig. 14).

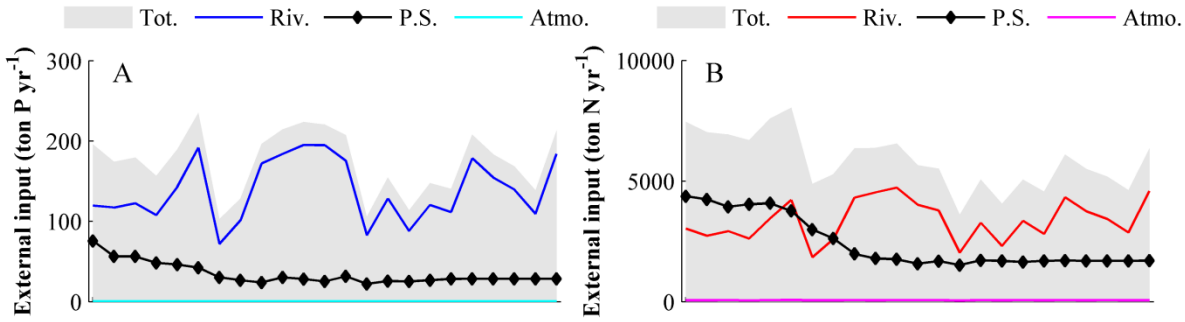


Figure 12. Annual external supplies of phosphorous (ton P yr^{-1}) and nitrogen (ton N yr^{-1}) with rivers (Riv.), point sources (P.S.) and atmospheric deposition (Atmo.) for the inner Stockholm archipelago.

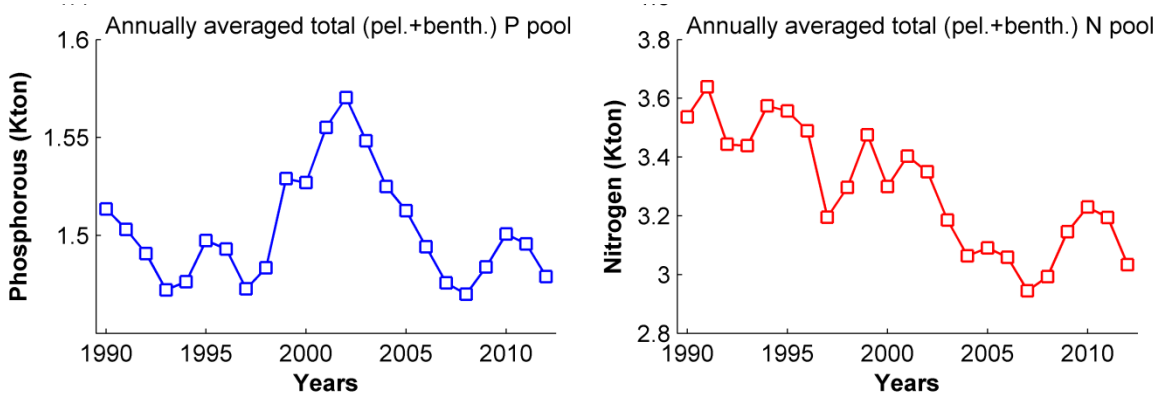


Figure 13. Annual mean of the pelagic+benthic pools of phosphorous (Kton P) and nitrogen (Kton N) in the inner Stockholm archipelago.

These results indicate a modelled mean retention of about 31 ton P and 850 ton N annually, corresponding to about 20% and 19 % of the nutrient input, respectively, in the inner Stockholm archipelago. The variation of the retention capacity during the simulation period is however rather variable as is seen in Fig. 14.

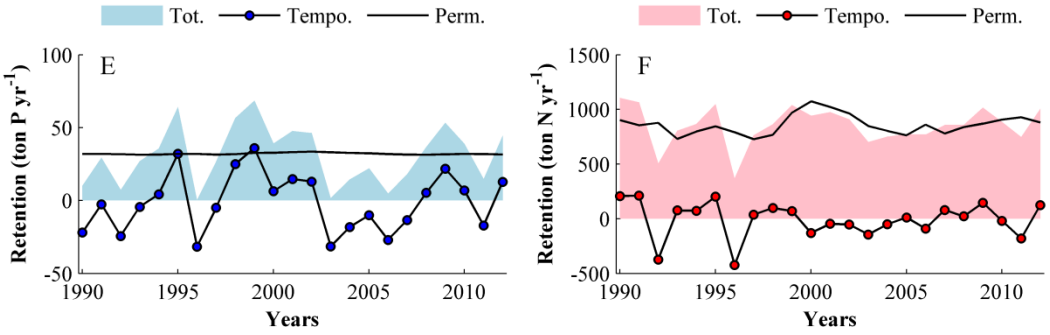


Figure 14. Annual total (Tot.), temporary (Tempo.) and permanent (Perm.) retention of phosphorous (ton P yr^{-1}) and nitrogen (tonN yr^{-1}) in the inner Stockholm archipelago.

3.2 ESIM2-BFMSI model results

BALTIC PELAGIC TEST CASE
Baltic test case located at Tvärminne, Finland (60N, 23E)
Standalone mode
Mixed Layer Depth 15 m
Time step of the model 864 s (14.4 min)
Output saved every 100 timesteps (1 day)

Forcing:

- Solar radiation, winds and ice concentrations: daily long term mean (CDC Derived NCEP Reanalysis Products Other Gaussian Grid Data from NCEP website 1980-2010)
- SST, SSS, PO4, NO3, SiO4: 1900-1998 climatological mean from World Ocean Atlas 2013 (WOA2013, NOAA website)

These forcing provides a mean climatological year. Then 10 years runs are prepared with cycled forcing (i.e. the same climatological year repeated 10 times).

Initial (winter) conditions are from WOA:

N1p0	= 0.3
N3n0	= 2.5
N4n0	= 0.5
N5s0	= 11.2
N6r0	= 1.0
O2o0	= 300.0
O3c0	= 27060.00
O3h0	= 2660.0
O4n0	= 200.0
P1c0	= 1.0
P2c0	= 1.0
P3c0	= 1.0
P4c0	= 1.0
Z3c0	= 0.1
Z4c0	= 0.1
Z5c0	= 0.1
Z6c0	= 0.1

However, in order to have the same winter values each repeated winter, the effective initial conditions for N1p = 0.6 and for N3n =12.0. See plots below. The steady state is reached at the 3rd year. This can also be done in a cleaner way by adding an external input of nutrients during winter.

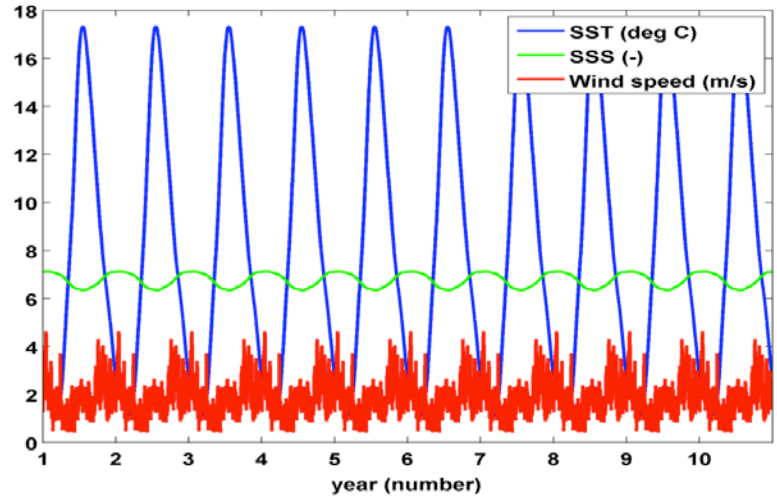


Figure 15. SST, SSS, WIND

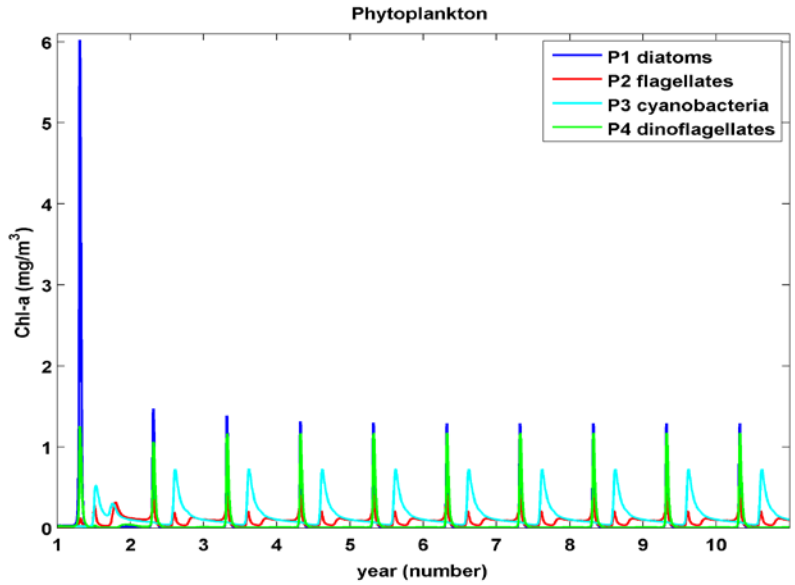


Figure 16. PHYTOPLANKTON DYNAMICS. Note the competition diatoms/dinoflagellates for the spring bloom

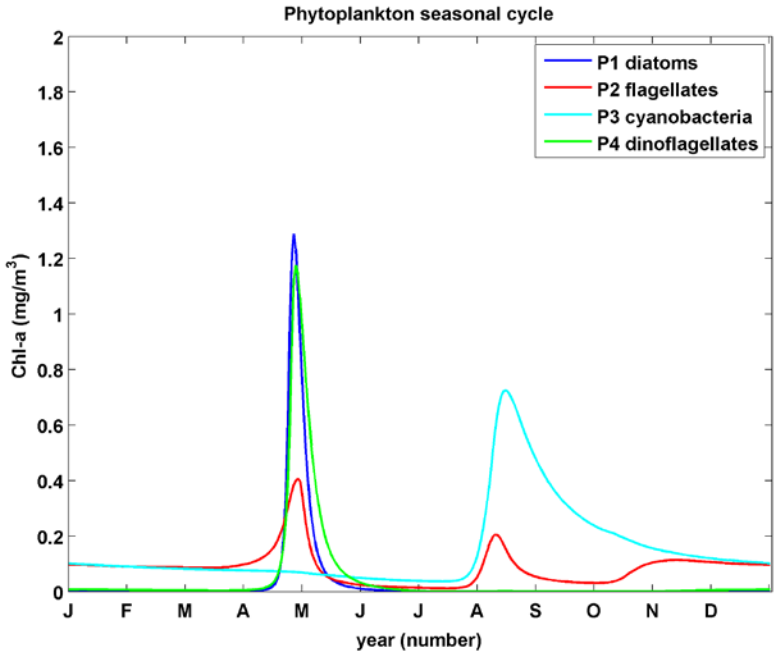


Figure 17. PHYTOPLANKTON SEASONAL CYCLE.

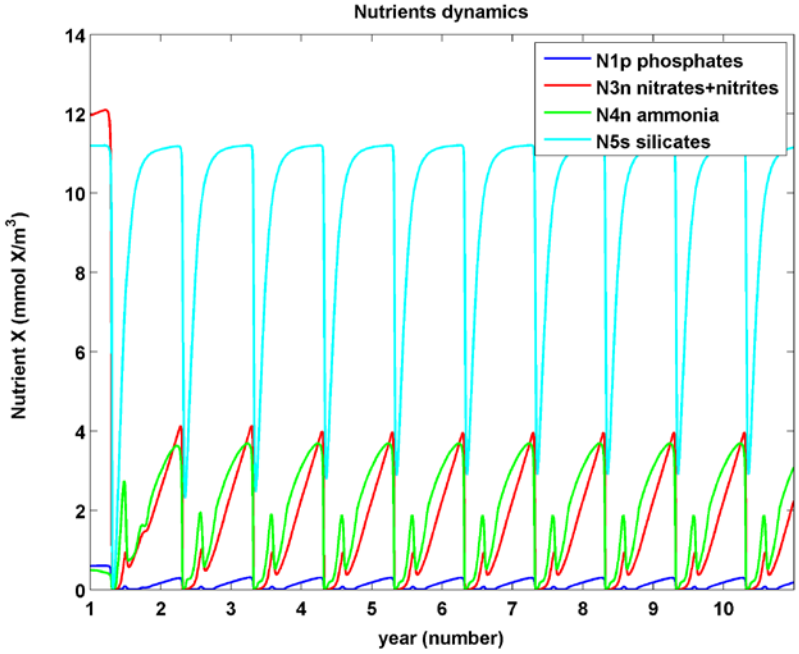


Figure 18. NUTRIENTS DYNAMICS

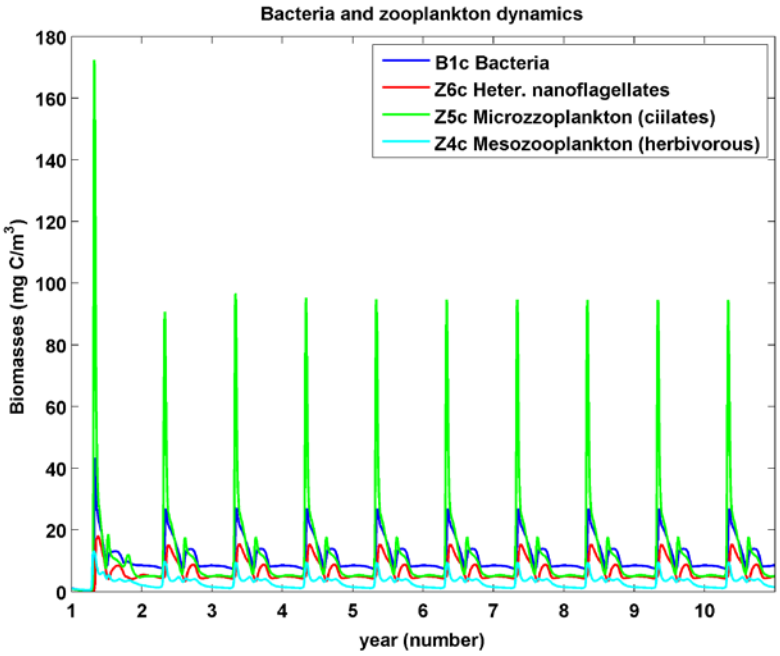


Figure 19. ZOOPLANKTON AND BACTERIA BIOMASSES

BALTIC PELAGIC + SEA ICE TEST CASE

The pelagic model is forced and set up in the same way as in the pelagic only configuration.

The sea ice model simulates the dynamics in the permeable part of sea ice (bottom communities, BAL, see also Tedesco et al., 2010). However, it is not possible to use the same method to keep the winter values of nutrients as interaction with sea ice has major consequences. An external source of nutrients must be added each winter. The routine is already developed for such a task. However, for sake of simplicity, only the first year of simulation is presented year and the model is initialized with the real winter values of nutrients: PO4 0.3 and NO3 2.5 mmol/m3

Sea ice forcing are:

- Ice concentrations and solar radiation are from daily long term mean (CDC Derived NCEP Reanalysis Products Other Gaussian Grid Data from NCEP website 1980-2010)
- Ice and snow thickness, ice temperature and salinity are taken from typical values of the area (e.g Kaartokallio, 2004)
- Brine salinity and volume are derived assuming thermal equilibrium

These forcing provides a mean climatological year. See Tedesco and Vichi, 2014 for more details on how to set up a typical sea ice season.

BALTIC PELAGIC + SEA ICE TEST CASE: Results

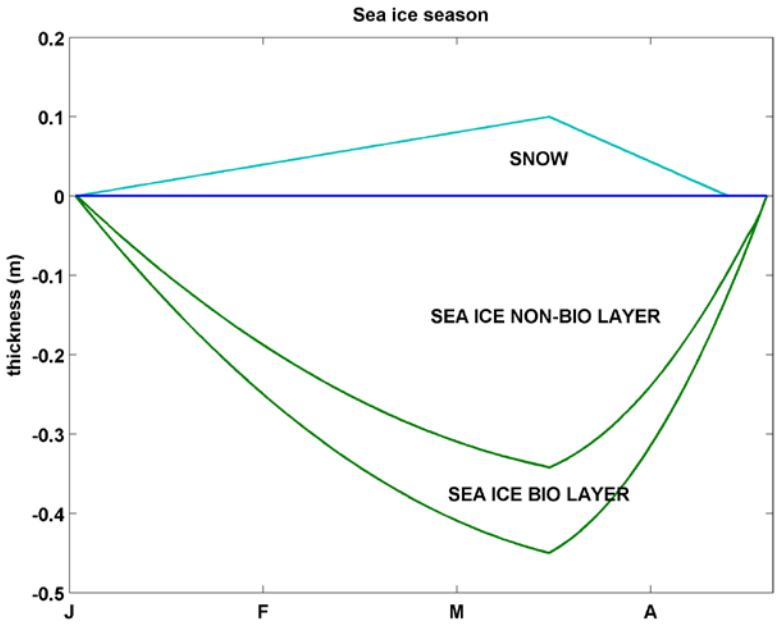


Figure 20. SEA ICE SEASON

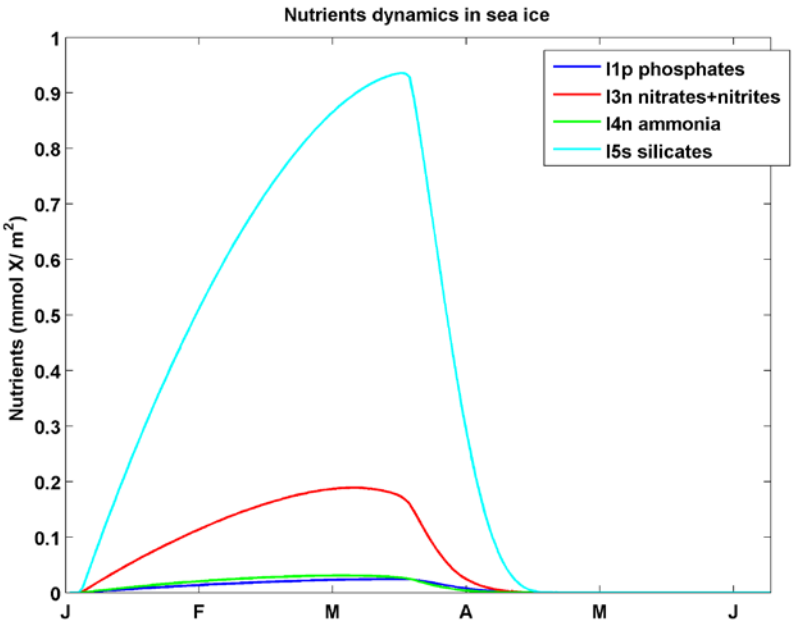


Figure 21. SEA ICE NUTRIENTS. Note the units are mmol/m2.

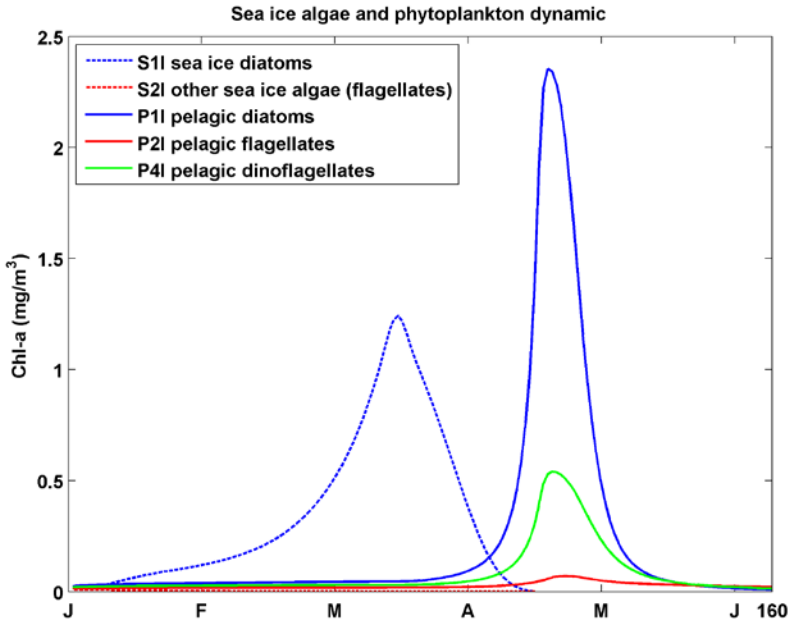


Figure 22. SEA ICE ALGAE/PHYTOPLANKTON DYNAMIC. Note that in this run blooming sea ice algae (diatoms) are assumed to be viable once sea ice melts. This provides a seeding population and modifies the spring bloom with a dominance of diatoms vs dinoflagellates. See Tedesco et al, 2012 for more details on the coupling between sea ice algae and phytoplankton.

NEXT PLANS/DEVELOPMENTS

- Development of a benthic test case that works with pelagic only and with pelagic and sea ice configurations.
- Testing the Baltic standalone configurations with Tvärminne learning site new and old measurements (COCOA)
- Testing the Baltic standalone configurations with Tvärminne mesocosm experiments done in 2012 and 2013 (AKADEMY)
- Implementation of a 1D NEMO-Nordic (3.6)-BFM Baltic new configuration, technically based on the existing 1D NEMO configuration.
- Test of 0D/possibly 1D at other COCOA learning sites
- Tess of the 1D with Aranda cruise data (AKADEMY)

3.3 RSHU model results

Model validation

Scientific research expedition in the Eastern part of the Gulf of Finland was held in September 2013. The stations locations are presented in Fig. 23. Water and sediment samples were taken at 6 stations. In the laboratory the following substances were determined in the pore water: PO_4^{3-}, NO_3^-, NO_2^-, NH_4^+, SO_4^{2-}, total Mn and total Fe; total C_{org}, Mn and Fe – in the sediments. Abundance and biomass of polychaetes of the genus *Marenzelleria* spp. in sediments were also obtained.

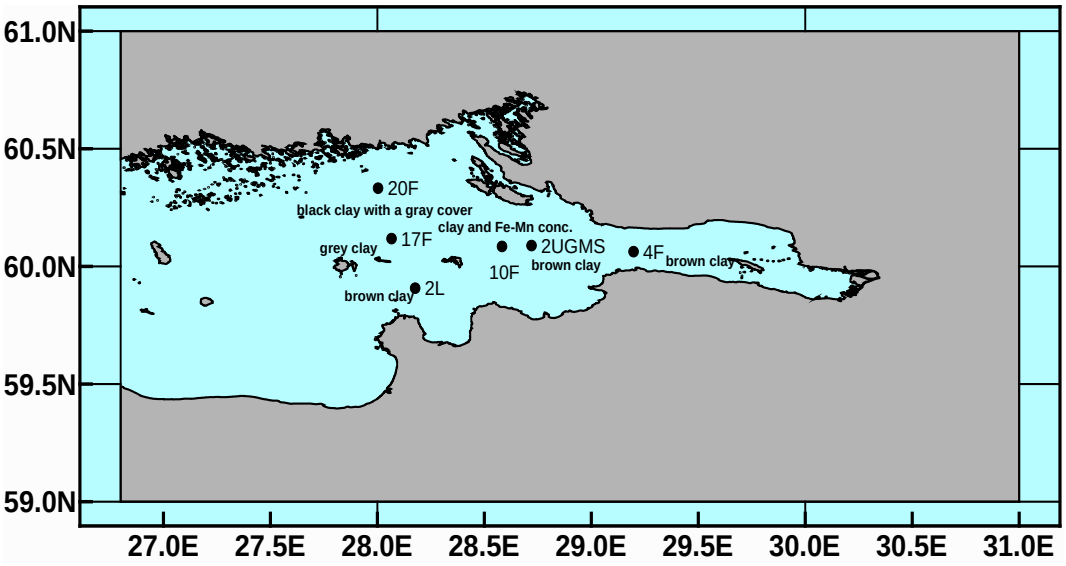


Figure 23. Map of stations in the Eastern part of the Gulf of Finland, where samples of water and sediments were taken in September 2013.

Samples were carried out so that to capture areas of the bottom with high and low polychaetes population.

The collected material was used to analyze the current status of benthic communities, assessment of the polychaete *Marenzelleria* spp. impact on the biogeochemical processes and also for diagenetic model validation.

In general, the oxygen conditions in the Eastern part of the Gulf of Finland in September 2013 can be defined as favorable (Fig. 24).

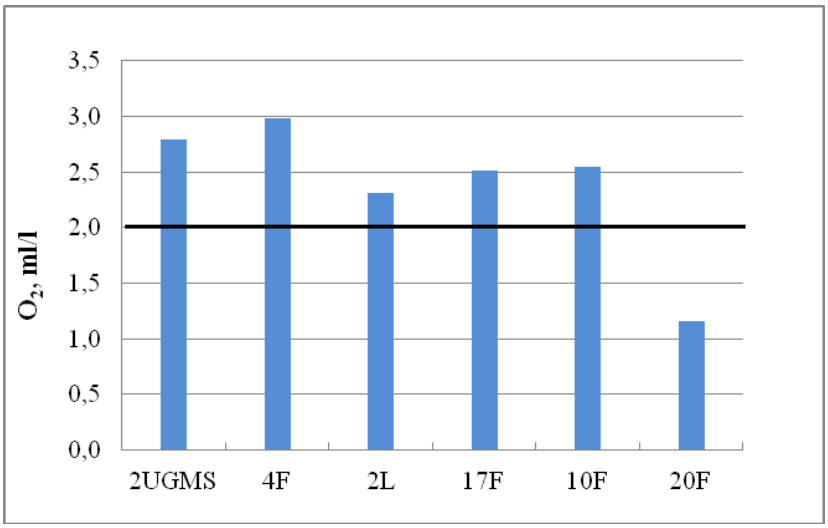


Figure 24. Oxygen content in the near-bottom water layer at the stations of the Eastern part of the Gulf of Finland in September 2013.

At most of the stations oxygen concentration in the near-bottom layer did not fall below 2 ml/l (samples were collected in the water layer 1-2 m from the bottom). The exception was the deep (46 m) station 20F, where oxygen concentration was only 1.16 ml/l. At this station, as well as at 17F station hydrogen sulfide (H_2S) smell was identified when sediments sampling. Comparative analysis of biogeochemical changes in bottom sediments was also held at 2 stations in the Eastern part of the Gulf of Finland – 2UGMS and 20F. 2UGMS is the station with high population of *Marenzelleria* spp. (3912±198 ind. m^{-2}) and 20F station – with low (240±40 ind. m^{-2}). Bioirrigation coefficients for these stations are 483 $year^{-1}$ and 3 $year^{-1}$, respectively.
Figures 25a-25d presents the vertical profiles of phosphate and nitrate concentrations in the pore water of the sediments according to field data and the model running.

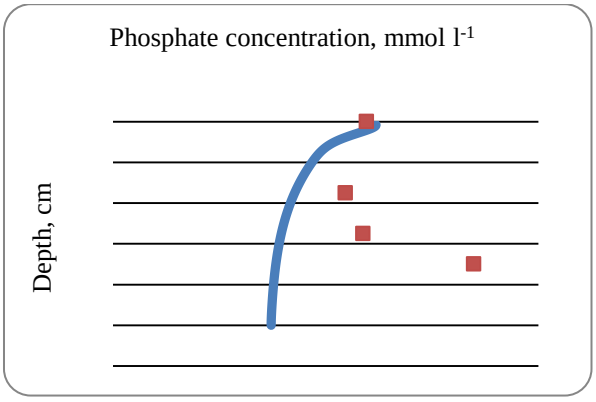


Figure 25a. Vertical profile of phosphate concentration at station 2UGMS.

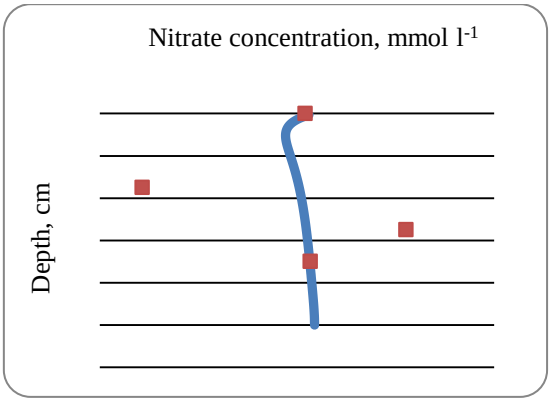


Figure 25b. Vertical profile of nitrate concentration at station 2UGMS.

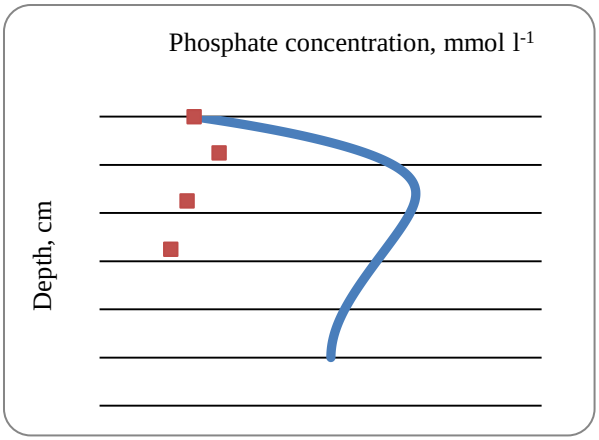


Figure 25c. Vertical profile of phosphate concentration at station 20F.

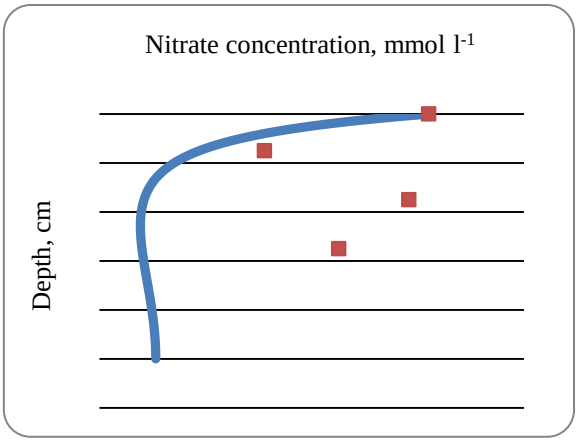


Figure 25d. Vertical profile of nitrate concentration at station 20F.

Field data
Model constrained

Unfortunately, it is not possible to compare quantitatively the field and model data of phosphate and nitrate concentrations. Field methods of taking samples let us to obtain only average concentrations in the layers 0-2 cm, 2-4 cm, etc. But as you can see on those model pictures the main sharp leap is inside or near this interval. Nevertheless, we can consider model results acceptable for further calculations.

Results analysis of numerical experiments with the model

Figures 26a-26f presents the vertical profiles of modelled phosphates and nitrates concentrations in the pore water of the sediments in the investigated stations 2UGMS and 20F in the Eastern part of the Gulf of Finland. Vertical profiles were constructed at time 2 months, 1 year and 5 years. By the time 5 years reactions are considered to be in a steady-state.

It is also known (Conley *et al*., 2009; Savchuk, 2010; Vahtera *et al*., 2007) that under anaerobic conditions some of biochemical processes run with release of molecular nitrogen. Therefore, the improvement of the oxygen conditions of the sediments due to bioirrigation, apparently, should prevent the loss of nitrates from the pore water. We should also take into account excretion of the polychaetes which add N compounds into the pore water. Thus, at the station with higher *Marenzelleria* population (2UGMS) the loss of nitrates will be less. And, as can be seen in figure 26a-26c, the storage of nitrates at station 2UGMS higher than at station 20F.
Relations of the stores of various substances in the pore water of the sediment at 2 stations in the Eastern part of the Gulf of Finland are presented in the table 3.1.
Polychaetes of the genus *Marenzelleria* burrow the sediments much deeper than the native inhabitants of the Baltic Sea, which leads to the intensification of metabolic processes on the sediment-water interface. In particular, bioirrigation of the sediment due to worms activity promotes the penetration of oxygen inside the sediments and formation of a thick oxidized layer, which leads to the increase in the phosphorus burial in the bottom sediments. Figure 26d-26f shows that at the station with higher polychaetes population (2UGMS) phosphate concentration in the profile is considerably lower than at station 20F, which has low abundance of their population.

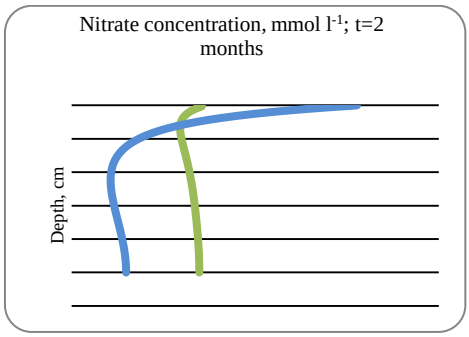


Figure 26a

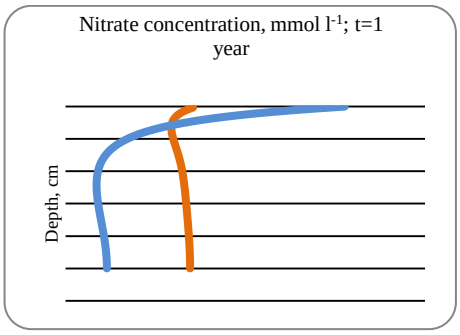


Figure 26b

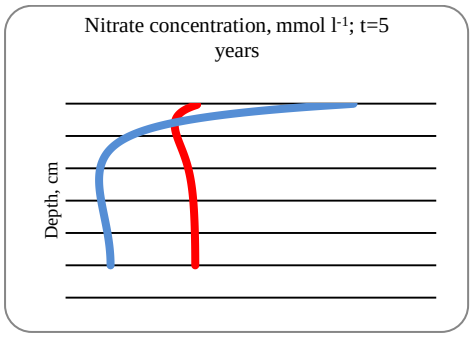


Figure 26c

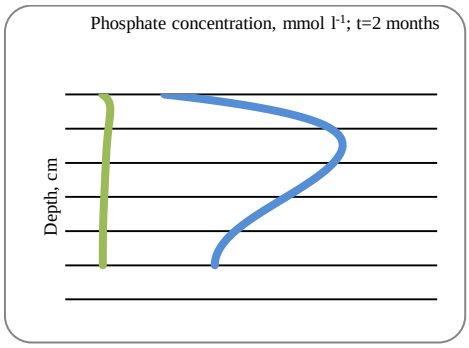


Figure 26d

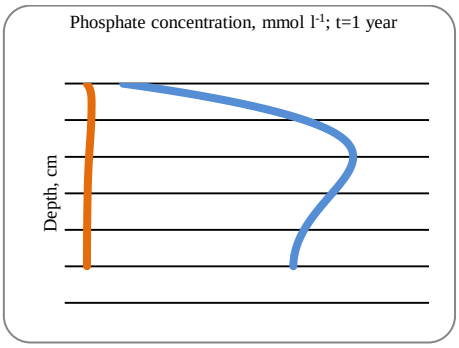


Figure 26e

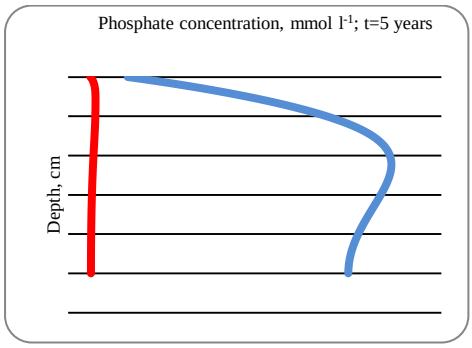


Figure 26f

Figure 26 (a-f). Vertical profiles of nitrates (upper) and phosphates (lower) concentration in the pore water of sediments at stations 2UGMS (green, brown and red lines) and 20F (blue lines) at different times of simulation. From left to right: t= 2 months, 1 year and 5 years, respectively.

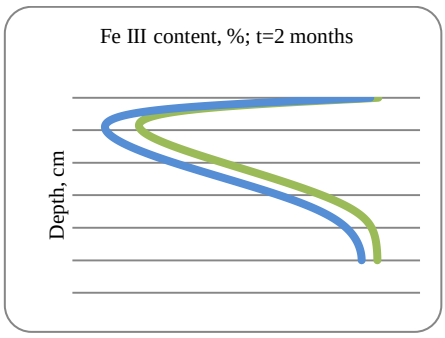


Figure 27a

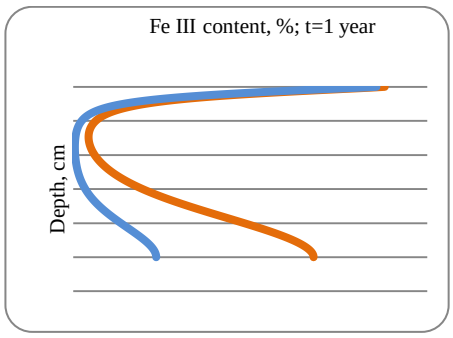


Figure 27b

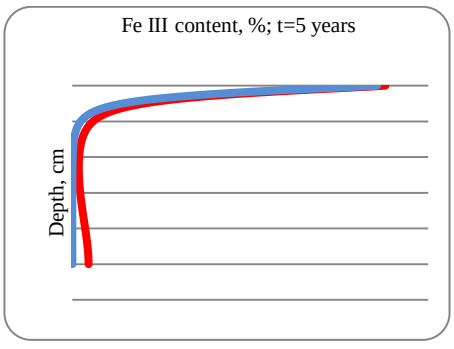


Figure 27c

Figure 27 (a-c). Vertical profiles of Fe^{3+} content in the sediments at stations 2UGMS (green, brown and red lines) and 20F (blue lines) at different times of simulation. From left to right: t= 2 months, 1 year and 5 years, respectively.

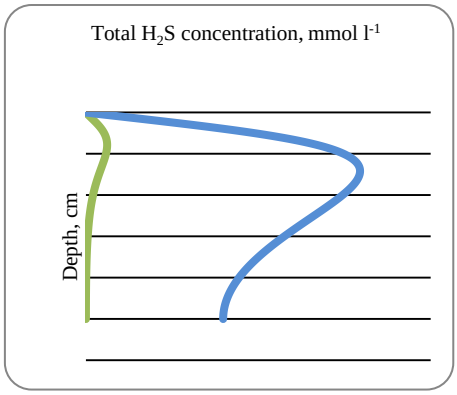


Figure 28a

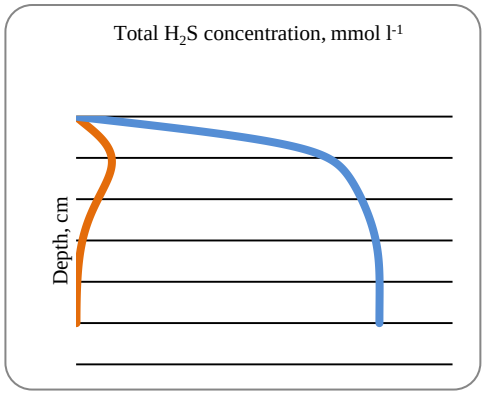


Figure 28b

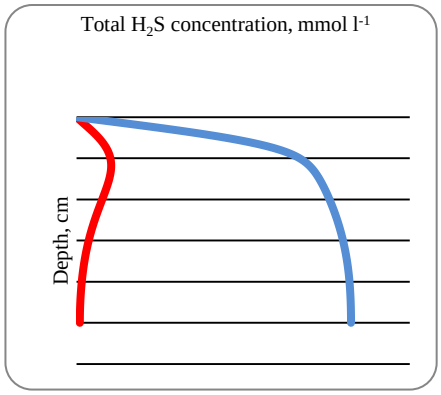


Figure 28c

Figure 28 (a-c) Vertical profiles of hydrogen sulfide concentration in the pore water of the sediments at stations 2UGMS and 20F at different simulation time.

Unfortunately, we don't have field measurements of P content in the sediments, but it can be quantified indirectly through solid Fe^{3+} content in the sediments (assume, that total solid Fe is ferric). As we know Fe-oxyhydroxides (Fe^{3+}) adsorb P (Norkko *et al*., 2011) and, thus, quantity of Fe^{3+} should be in direct correlation with sedimentary phosphorus. In Figure 27a-27c you can see slight difference in Fe^{3+} content between two stations. So, P burial at the station with high *Marenzelleria* spp. abundance in 5 years might be in 1.6 times higher than at the station with its low population (see also table 3.1). It is also of great interest to compare the store of H_2S concentration in the pore water at two stations by the model running (Figure 28a-28c and Table 3.1).

From the table 3.1 it is seen that the phosphates store in the pore water in the layer 0-10 cm at station 20F in 2 months will be 5.3 times greater than the phosphates store at 2UGMS station. The longer simulating time, the larger ratios in phosphate store.
For H_2S store in the pore water for the two stations, the maximum difference observed after 2 months is 28.7 times, and then the ratio in store decreases with increasing simulation time. Similar trends are observed for nitrate store in the pore water of the sediments.
So, results of short-term simulations show that cycles of bio- and abiogenic substances in 1-5 years might begin to function differently, which ultimately can lead to significant alterations in benthic systems.

Table 3.1. The ratio of the store of phosphates, nitrates, Fe^{3+} and hydrogen sulfide in the pore water of the sediments at 2 stations in the Eastern part of the Gulf of Finland on the simulation results for different time.

$\frac{\text{Store of the } PO_4^{3-} \text{ station 20F}}{\text{Store of the } PO_4^{3-} \text{ station 2UGMS}}$			
t = 2 months	t = 1 year	t = 5 years	t = 10 years
5.3	**10.0**	**11.1**	**11.0**
$\frac{\text{Store of the } NO_3^- \text{ station 2UGMS}}{\text{Store of the } NO_3^- \text{ station 20F}}$			
t = 2 months	t = 1 year	t = 5 years	t = 10 years
1.6	**1.7**	**1.7**	**1.7**
$\frac{\text{Store of the } Fe^{3+} \text{ station 2UGMS}}{\text{Store of the } Fe^{3+} \text{ station 20F}}$			
t = 2 months	t = 1 year	t = 5 years	t = 10 years
1.3	**2.4**	**1.6**	**1.5**
$\frac{\text{Store of the } H_2S \text{ station 20F}}{\text{Store of the } H_2S \text{ station 2UGMS}}$			
t = 2 months	t = 1 year	t = 5 years	t = 10 years
28.7	**19.1**	**14.4**	**14.4**

The simulation results revealed significant differences in the store of various environmental compounds, first of all, phosphates in terms of high and low Marenzelleria spp. population. According to the simulation results, in 5 years the phosphates store at the station with higher population of polychaetes can be less in 11 times in comparison with the station with low Marenzelleria spp. population (assuming unchanging number of polychaetes).

3.4 SHYFEM/AQUABC model results

Model validation
Model was validated using seasonal survey data carried out in 2009 in the Curonian lagoon carried out by the CORPI, Klaipeda University and covered all state variables listed below (Table 3.2).
The simulation covered the year 2009, no benthic part of the model was used.

Curonian lagoon case :
The following sampling locations were used for the validation of model results:
Klaipeda (station 1S) (E21.1197,N55.7185)
Nida (station 2N) (E21.0072,N55.2987),
Vente (station 3V) (E21.1917,55.3414),

The water column assumed to be fully mixed
Time step of the model 800 s
Output saved every 2h

Forcing:
Solar radiation, winds, air temperature, relative humidity air pressure, rivers discharge from Lithuanian Hydrometeological Service

Boundary conditions (Baltic boundary):
Hydrodynamics - HIROMB BS01

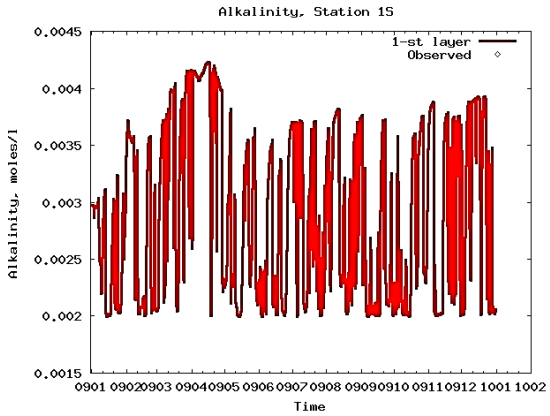
Water quality parameters for the boundary conditions were derived from seasonal (Baltic sea) and monthly (Nemunas river) monitoring data provided by the Marine Reasearch Department of the Lithuania EPA.
.

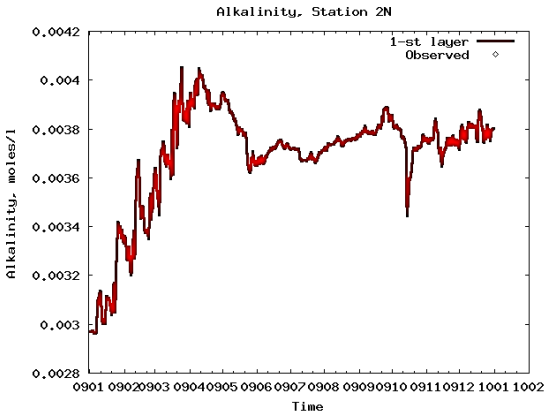
Table 3.2. The list of variables used in the simulations for year 2009 case.

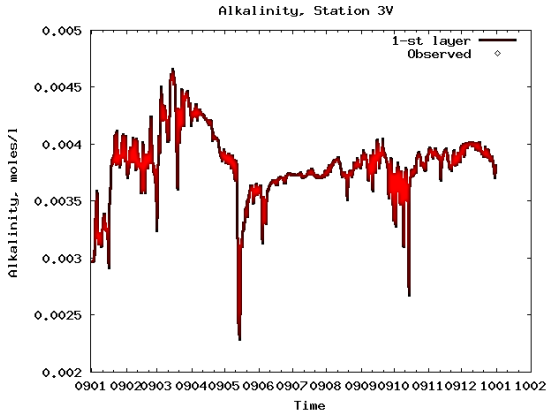
No	**State varaible name**	**Abbreviation**	**Dimentions**	**Comments**
1	AMMONIUM NITROGEN	NH4_N	mgN/l	
2	NITRATE NITROGEN	NO3_N	mgN/l	
3	ORTHOPHOSPHATE PHOSPHORUS	PO4_P	mgP/l	
4	DISSOLVED OXYGEN	DISS_OXYGEN	mgO_2/l	
5	Chemoautotrophic(Nitrification) bacteria carbon	NITR_BAC_C	mgC/l	Switched off
6	Aerobic-anaerobic heterotropic bacteria carbon	AER_HET_BAC_C	mgC/l	Switched off
7	Facultative anaerobic heterotrophic bacteria carbon	DENITR_BAC_C	mgC/l	Switched off
8	DIATOMS CARBON	DIA_C	mgC/l	

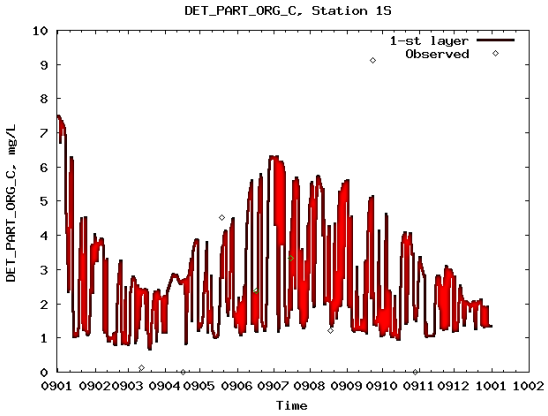
9	ZOOPLANKTON CARBON	ZOO_C	mgC/l	
10	ZOOPLANKTON NITROGEN	ZOO_N	mgC/l	derived variable, switched to constant stoichiometry
11	ZOOPLANKTON PHOSPHORUS	ZOO_P	mgC/l	derived variable, switched to constant stoichiometry
12	DETRITUS PARTICULATE ORG. CARBON	DET_PART_ORG_C	mgC/l	
13	DETRITUS PARTICULATE ORG. NITROGEN	DET_PART_ORG_N	mgN/l	
14	DETRITUS PARTICULATE ORG. PHOSPHORUS	DET_PART_ORG_P	mgP/l	
15	DISSOLVED ORGANIC CARBON	DISS_ORG_C	mgC/l	
16	DISSOLVED ORGANIC NITROGEN	DISS_ORG_N	mgN/l	
17	DISSOLVED ORGANIC PHOSPHORUS	DISS_ORG_P	mgP/l	
18	CYANOBACTERIA CARBON	CYAN_C	mgC/l	
19	OTHER PHYTOPLANKTON CARBON	OPA_C	mgC/l	
20	DISSOLOVED SILICA	DISS_Si	mgSi/l	
21	BIOGENIC SILICA	BIOG_Si	mgSi/l	
22	NITROGEN FIXING CYANOBACTERIA CARBON	FIX_CYN_C	mgC/l	
23	DISSOLVED INORGANIC CARBON	INORG_C	mol/m³	
24	TOTAL ALKALINTY	TOT_ALK	mol/m³	

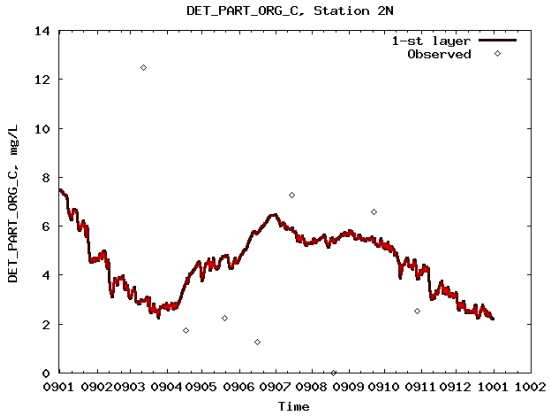
Model was run for the whole year 2009, the model results for selected stated variables plotted against the measured data are presented in the graphs below. Model results are shown by red lines and observations by open diamonds. The model predicted the seasonal dynamics of inorganic nutrients and main autotrophic plankton groups quite well representing two seasonal peaks of chlorophyll A and plankton carbon.

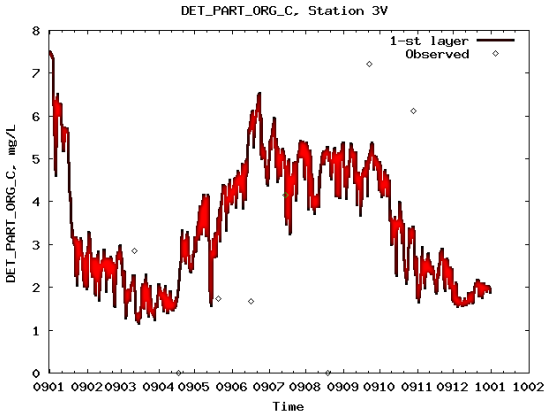

Alkalinity, Station 1S
1-st layer
Observed
Alkalinity, moles/l
Time

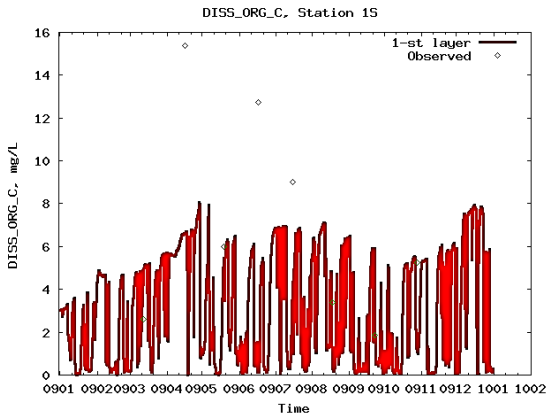

Alkalinity, Station 2N
1-st layer
Observed
Alkalinity, moles/l
Time

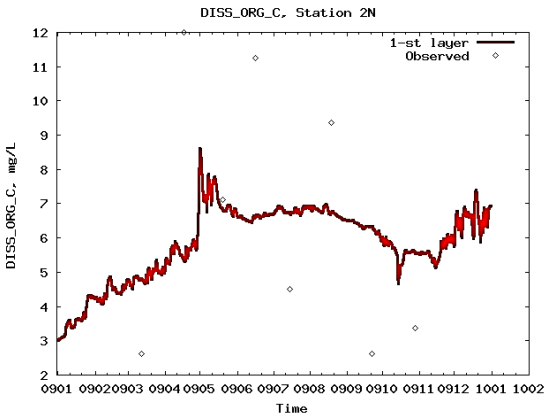

Alkalinity, Station 3V
1-st layer
Observed
Alkalinity, moles/l
Time

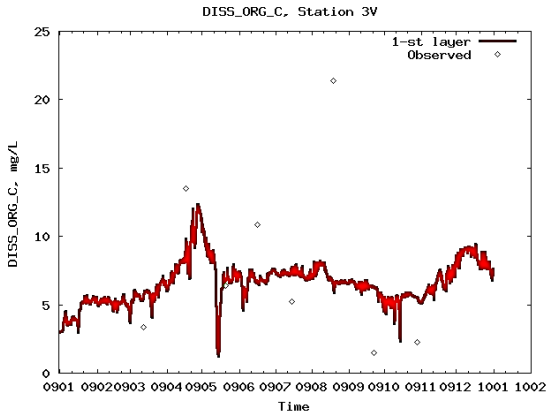

DET_PART_ORG_C, Station 1S
1-st layer
Observed
DET_PART_ORG_C, mg/L
Time

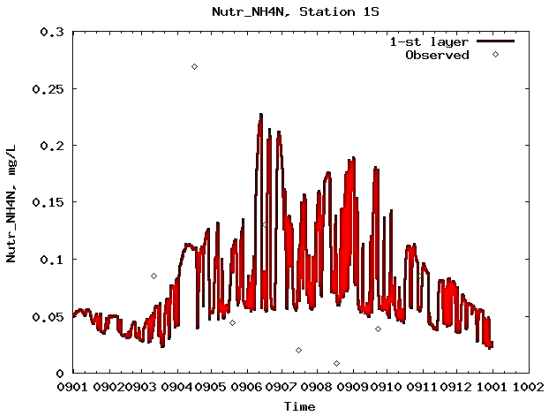

DET_PART_ORG_C, Station 2N
1-st layer
Observed
DET_PART_ORG_C, mg/L
Time

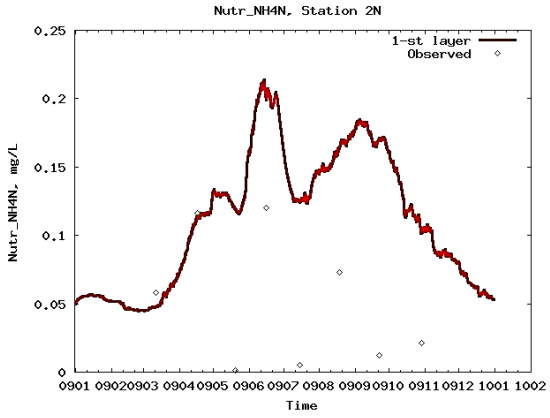

DET_PART_ORG_C, Station 3V
1-st layer
Observed
DET_PART_ORG_C, mg/L
Time

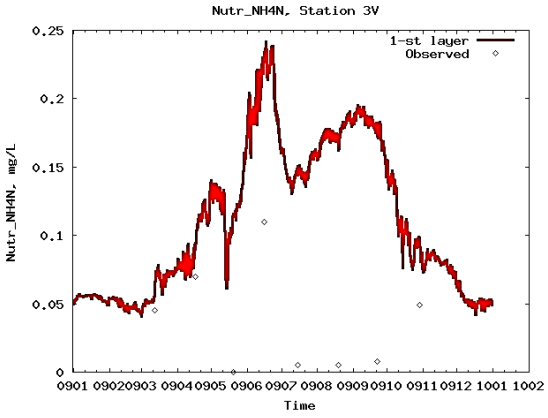

DISS_ORG_C, Station 1S
1-st layer
Observed
DISS_ORG_C, mg/L
Time

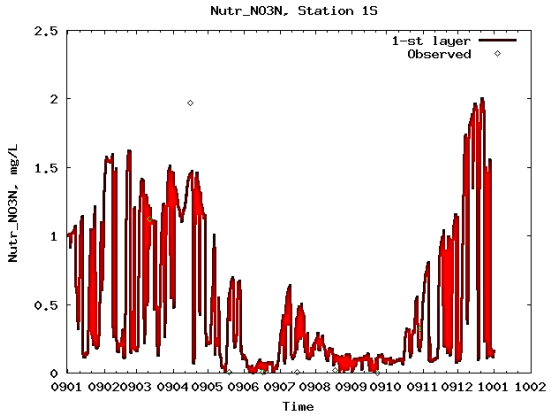

DISS_ORG_C, Station 2N
1-st layer
Observed
DISS_ORG_C, mg/L
Time

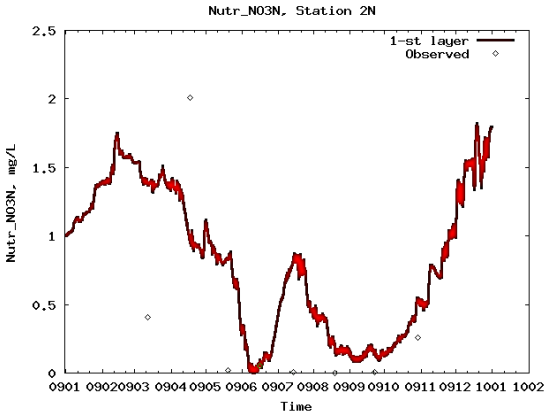

DISS_ORG_C, Station 3V
1-st layer
Observed
DISS_ORG_C, mg/L
Time

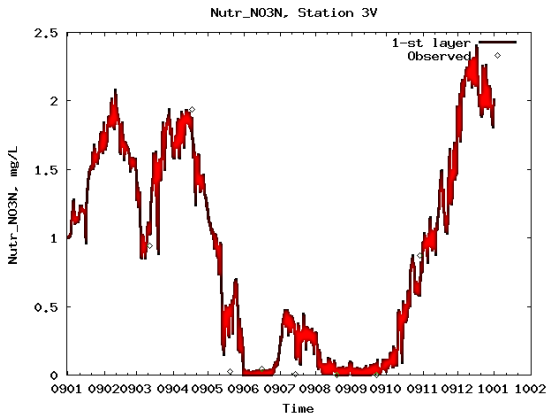

Nutr_NH4N, Station 1S
1-st layer
Observed
Nutr_NH4N, mg/L
Time

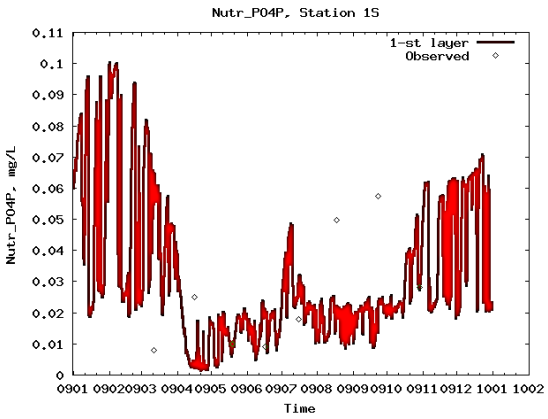

Nutr_NH4N, Station 2N
1-st layer
Observed
Nutr_NH4N, mg/L
Time

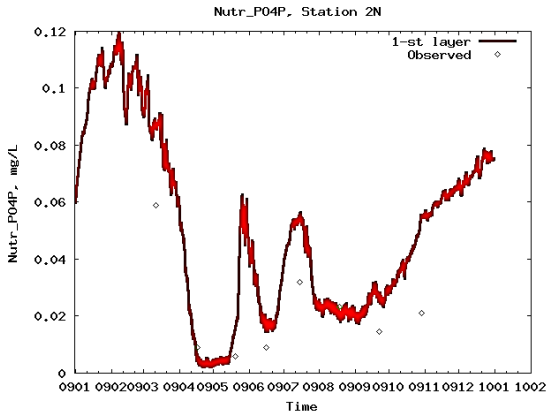

Nutr_NH4N, Station 3V
1-st layer
Observed
Nutr_NH4N, mg/L
Time


Nutr_NO3N, Station 1S
1-st layer
Observed
Nutr_NO3N, mg/L
Time


Nutr_NO3N, Station 2N
1-st layer
Observed
Nutr_NO3N, mg/L
Time


Nutr_NO3N, Station 3V
1-st layer
Observed
Nutr_NO3N, mg/L
Time


Nutr_PO4P, Station 1S
1-st layer
Observed
Nutr_PO4P, mg/L
Time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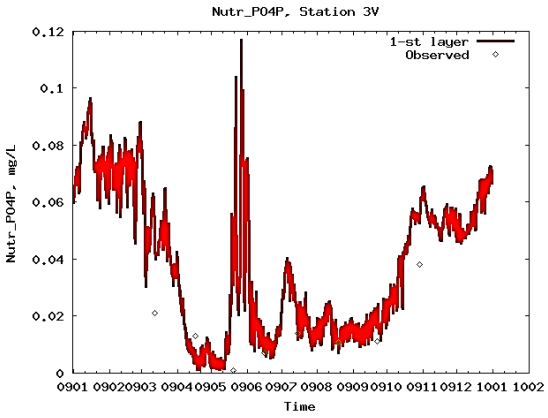
1-st layer
Observed
Nutr_PO4P, mg/L
Time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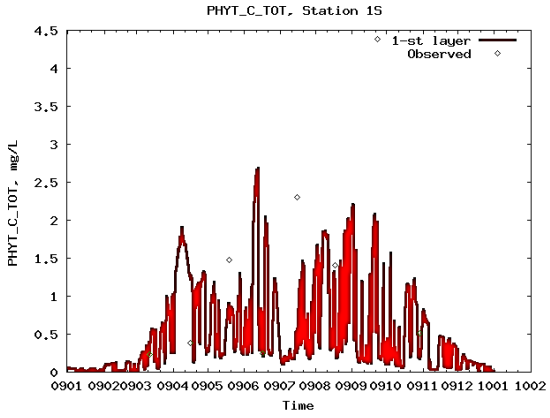
Observed
Nutr_PO4P, mg/L
Time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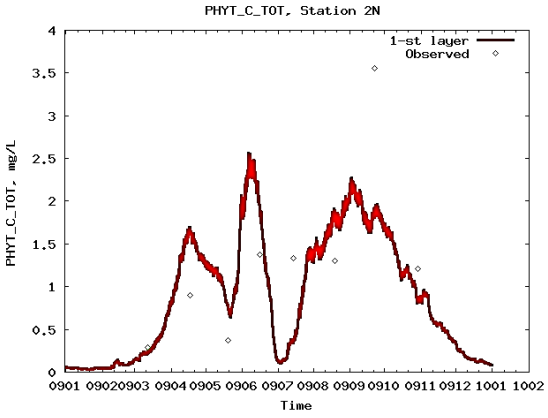
Observed
PHYT_C_TOT, mg/L
Time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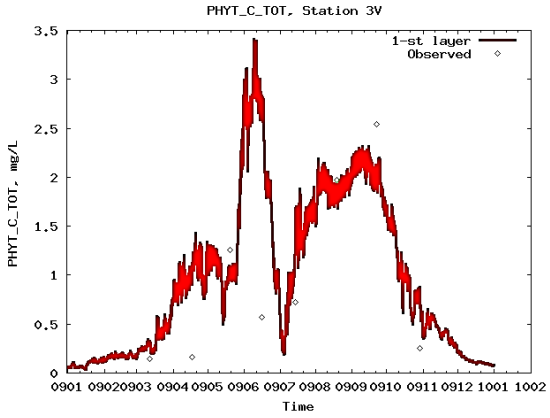
Time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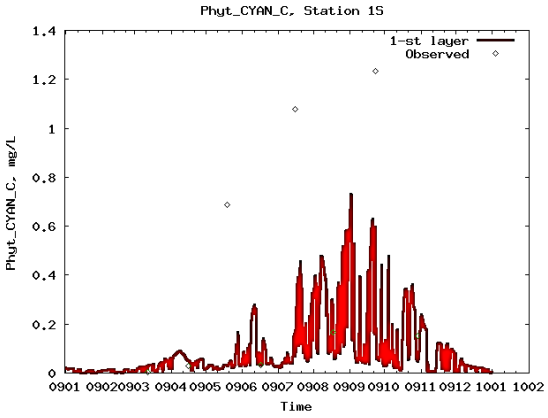
Time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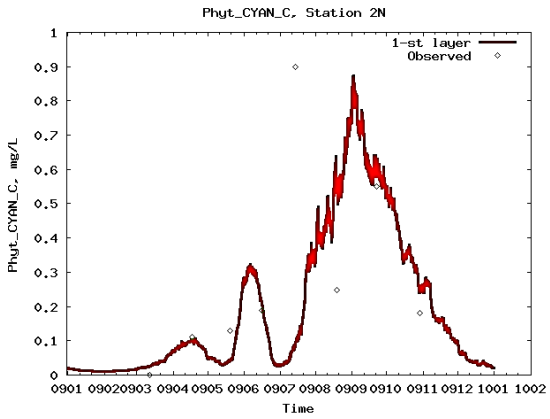
Time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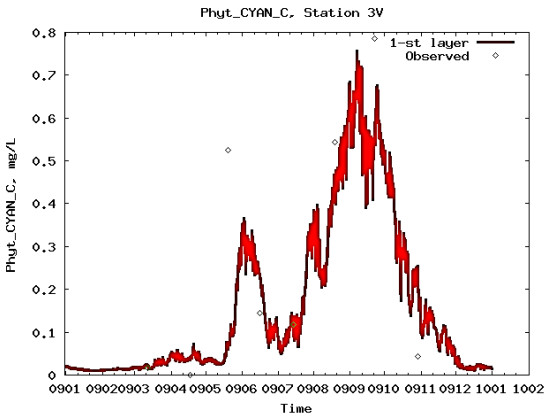
Time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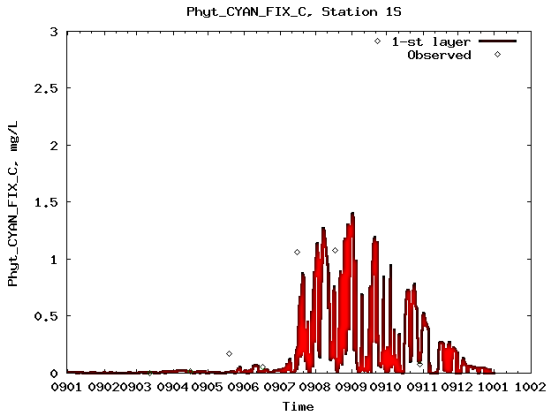
Time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Observed
Phyt_CYAN_FIX_C, mg/L
Time
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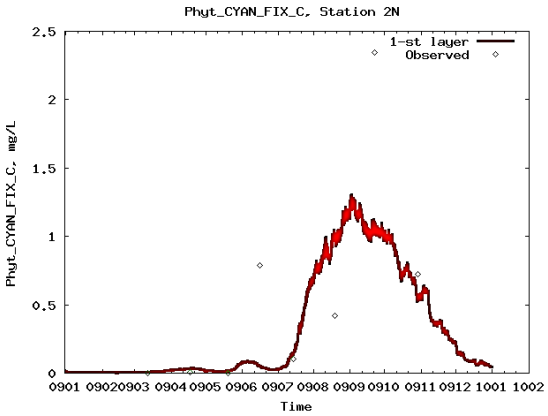
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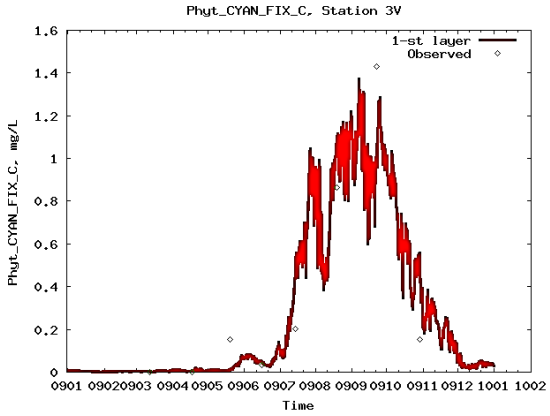
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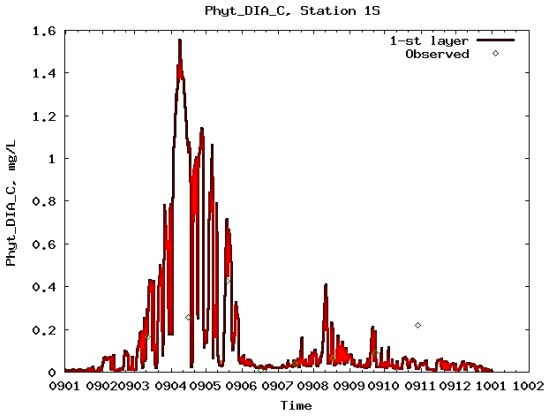
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Time
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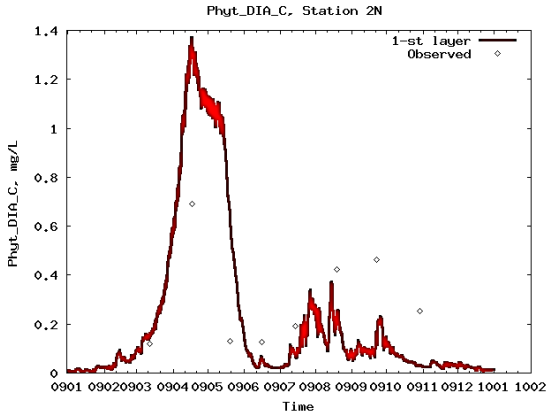
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Time
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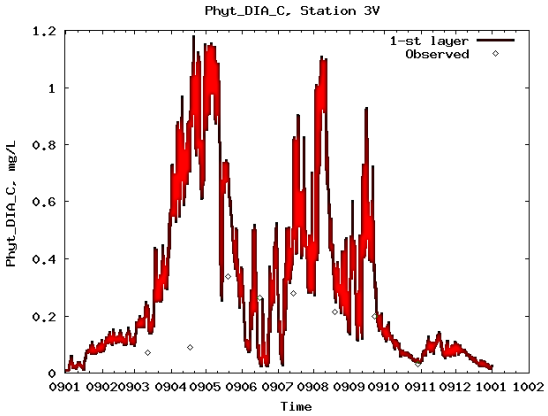
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Observed
Phyt_DIA_C, mg/L
Time
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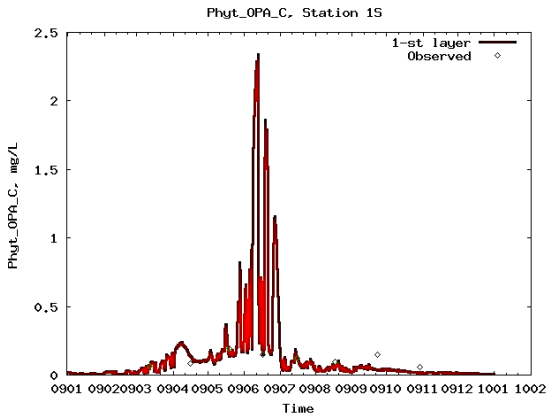
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Observed
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Time
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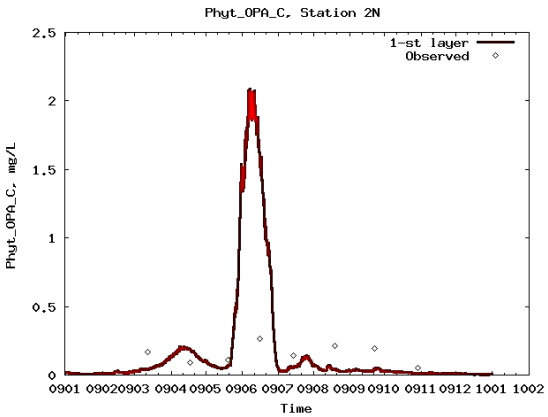
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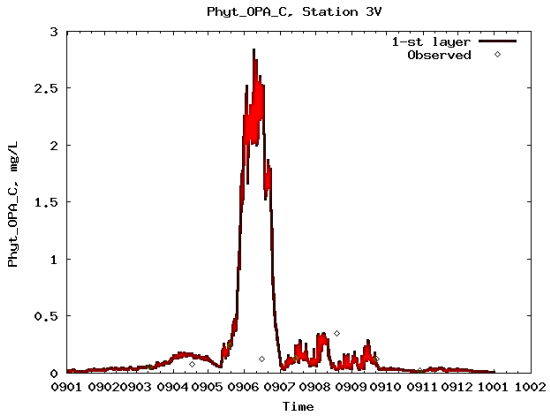
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Time
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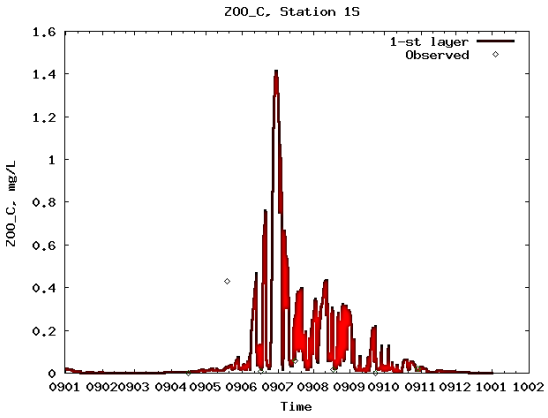
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1-st layer
Observed
ZOO_C, mg/L
Time
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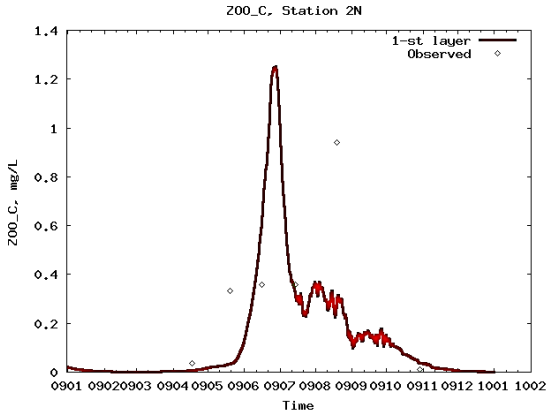
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ZOO_C, mg/L
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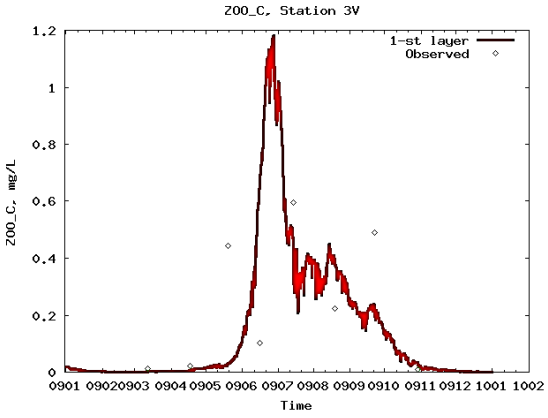
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1-st layer
Observed
ZOO_C, mg/L
Time
0901 09020903 0904 0905 0906 0907 0908 0909 0910 0911 0912 1001 1002

4. Acknowledgement

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