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The Predominant Processes Controlling Vertical Nutrient and Suspended Matter Fluxes across Domains - Using the New MOSSCO System from Coastal Sea Sediments up to the Atmosphere

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ABSTRACT: The dynamics of nutrient cycles and suspended matter in coastal seas result from an interplay of processes in a number of earth system domains, such as atmosphere/weather, waves, pelagic and benthic ecosystem, and sea sediment. An integrated approach for a coupled model study is essential to obtain a holistic understanding of key processes in the coastal system, such as erosion and sedimentation, atmospheric deposition, and denitrification. Diverse scientific groups have successfully developed models to describe the dynamics of these key processes. However, exchange of tested, numerical codes and non-invasive, efficient coupling of existing modules is barely practised. The model coupling initiative MOSSCO (MOdular System for Shelves and COasts) provides new software infrastructure to manage modular, multi-way domain coupling of existing high-performance, numerical model codes. While making use of the model coupling framework ESMF, existing models are included through a thin wrapper layer of domain components. Biogeochemical processes get included into the ESMF components through a driver infrastructure for the established framework FABM (Framework for Aquatic Biogeochemical Models). We present examples of coupling state-of-the-art models for hydrodynamics, the pelagic ecosystem, surface waves, weather, benthic geoecology, sea bed composition and early diagenesis in typical coastal sea applications. The interface between water column and sea sediments is predominantly controlling the tidal and seasonal variations of suspended matter concentrations. Additionally, the exchange fluxes at the sea bed interface decouple the simulated nutrient cycles as found in measurements at stations in the southern North Sea. Integrated modelling, using a modular, multi-way coupling scheme across domains as exemplified here, is shown to be a promising avenue to obtain realistic simulations of coastal systems.

Keywords: Model coupling, Coastal system, Nutrient fluxes, Suspended matter

1 INTRODUCTION

The realistic hindcast of water quality and nutrient budgets requires a model system with consistent description of a variety of local processes as well as an effective computational methods to handle these multi-domain and multi-process systems. Demands to coupled modelling approaches are high, especially for coastal systems, where the waterbody is shallow and its quality is highly affected by boundary conditions at the sea floor and the sea surface. These Demands call for integration of physical, chemical and biological processes both between and within domains, and thus for a coupling strategy that goes beyond the either or of domain coupling and process coupling. This is the goal of the MOSSCO infrastructure, which takes a hybrid approach of domain and process coupling relying on ESMF and FABM as major (but not exclusive) coupling technologies. Coupling between domains is a common strategy in coastal modelling. Warner et al. (2010) presented the modular COAWST system and showed that coupling of hydrodynamics, atmospheric simulation and simulation of surface waves improves simulations of suspended particulate matter (SPM) in coastal seas. For a North Sea application Puls et al. (2011) found that erosion in shallow waters shows high lateral variability in influences by waves or currents. In ecosystem modelling, the light climate, as determined by SPM dynamics, plays an important role to simulate the start and strength of phytoplankton blooms (Tian et al. (2009,2011)). Vice versa, the ecosystem might feed back into the energy budget of the sea by changing reflectivity of the sea surface (Sonntag and Hense (2011)). Coupling within domains, which mostly refers to coupling between processes in models requires high modularity of the model implementation. This approach is taken by the Highly Structured Modular Earth Submodel System (MESSy, Jöckel et al. 2005) to describe the coupling of processes within a domain at very high process modularity; this allows for a fine-grained coupling and efficient data flow between processes. In MESSy, which is currently operational in the atmospheric domain and the used submodels, however, had to be written, or rewritten, to meet the specific infrastructure enforced by MESSy. For aquatic modelling of oceans, estuaries, or lakes, the FABM framework (Bruggemann and Bolding (2014)) provides a model library of biogeochemical models, where submodels are implemented as state variables and its trends of evolution in a discretisation-unaware 0d framework. The submodels provide a standard set of interfaces and an extensive run time configured meta-data structure to be used by a numerical host model. In the present study, we want to focus on nutrient dynamics, which follows a typical seasonal cycle in the southern North Sea. Phytoplankton takes up the dissolved nutrients in spring and keeps nutrient concentrations low through balanced growth in summer as shows by Loebl et al. (2007) for shallow waters and Wiltshire et al. (2006) at the more offshore island of Helgoland. In late autumn, nutrients remineralisation of particulate organic material effectively recovers the winter values. Additionally, river input and wet deposition through rain modulates the availability of nutrients (van Beusekom et al. (2009)). The sea sediments contribute to the nutrient budgets by remineralisation of pelagically produced material under suboxic and anoxic conditions in the sea floor. Decoupling of the nitrate and phosphate cycle in summer is observed (Loebl et al. (2007)) and can be handled in models by coupling the water quality model to a diagenesis model (Grunewald et al (2010)). The approach in the present study is to use existing models that potentially contribute tho the coastal nutrient budget and couple these in a modular fashion with the new MOSSCO system. In this paper, we describe the MOSSCO system as used for 1d-vertical simulations of nutrient and SPM fluxes. Results of the coupled multi-annual simulation are shown and discussed in terms of dominating processes.

2 METHODS

In the present simulations, we utilise the MOSSCO system (Modular System for Shelfs and Coasts) as currently under development in a coastal project network (Wirtz et al. 2012). which is a software architecture, that maintains exchangeability among modules (compartments) in various levels through standard interfaces. This software architecture utilizes the Earth System Modeling Framework (ESMF) to couple processes between earth compartments and the Framework for Aquatic Biogeochemical Models (FABM) to set up communication among different processes within each compartment. MOSSCO couples several physical, chemical and biological processes across and with domains.

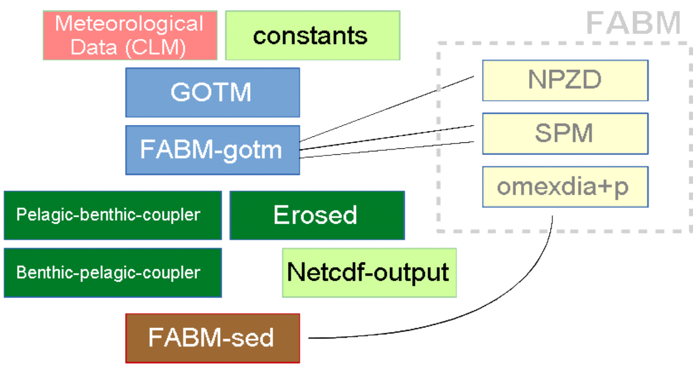

Figure 1. The schematic setup of MOSSCO components for the coupled simulations. The coloured boxes represent ESMF components that exchange fields with standard names.

The MOSSCO system makes use of the FABM framework to describe the local pelagic dynamics of suspended particulate matter (SPM) and the diagenetic processes in the porous sediment. FABM provides a library, that holds models, each containing state variables with its local zero-dimensional rate of change, its vertical movement and local light extinction. Non-local processes of pelagic dynamics on a numerical grid, such as mixing, advection and boundary fluxes of FABM's state variables, are handled by the gridded 1d pelagic ecosystem component (FABM-gotm) and the gridded 1d sediment component (FABM-sed), that act as FABM drivers. The state variables in FABM have a meta data structure including properties to be used in the numerical driver component. The MOSSCO system provides an integrated infrastructure to communicate data arrays and meta data between components, such as EROSED and the pelagic ecosystem as well as between MOSSCO components and FABM's variables and process descriptions. In the present setup, the SPM state variables in FABM have defined essential properties such as density and equivalent spherical diameter, which are communicated in MOSSCO together with the data, a standard name and unit description in ESMF fields.

The station of Helgoland is located offshore the south-eastern coast of the North Sea (see Fig. 2). The mean water depth closely around the location of Helgoland varies between 10 m and 40 m, such that a, effective depth of 25 m is used in the setup. Tidal currents are affected by the M2 and S2 tide, such that a spring-neap cycle is a characteristic feature. Current velocities do not exceed 100 cm/s. The water column is resolved by 12 vertical layers, that vary in heights with the tidal surface elevation. Wind stress, radiation and heat fluxes at the sea surface are calculated based on meteorological data from simulation with the COSMO-CLM model for the years 2002 to 2005.

Figure 2. The location of station Helgoland (7.89°E, 54.19°N) in the North Sea.

Due to the distance of the station from the coast, lateral, coastal SPM transport is a secondary effect. The SPM dynamics is expected to be controlled mainly by vertical exchange processes, such as turbulent mixing, erosion, settlement of SPM and sedimentation. However, the nutrient dynamics might be influenced by the discharge of rivers into the German Bight, which could be parameterised in the 1d approach by diffuse nutrient fluxes into the water column.

We use the GOTM model (Umlauf and Burchard (2005)) in the water column. GOTM is a one-dimensional hydrodynamical model using Boussinesq approximation to resolve physical quantities of the water state. The water density varies with temperature due to meteorological forcing. A k-epsilon turbulence model resolves turbulent exchange coefficients, that are internally coupled to temperature stratification and current profiles. The current velocities are forced by analytical tidal pressure gradients. Salinity is taken as constant in the present setup.

The pelagic ecosystem component uses an NPZD-type ecosystem model and two instances of the SPM model in FABM (Bruggemann and Bolding (2014)) to represent a heavy and a light fraction of SPM. The parameter configuration is given in table 1. Turbulent mixing and vertical advection of SPM and the ecosystem compartments are calculated by the GOTM routines as used for the water physics.

Table 1. parameter configuration of SPM model classes.

parameter	fraction	value	unit
Sinking velocity	1	0.0005	m/s
	2	0.001	m/s
density	1	2650	kg/m³
	2	2650	kg/m³
Mean diameter	1	20	µm
	2	100	µm

The biogeochemical NPZD-type model from Buchard et. al (2006) has a phytoplankton, zooplankton, detritus and dissolved nutrients compartments, each measured in mole concentration of nitrogen. Initial conditions for the dissolved nutrients are set to 25 mmol-N/m³ as observed at the station of Helgoland (Wiltshire et al. (2010)).

In the sea sediment, the diagenesis model OMEXDIA (Soetaert et al. (1996)) is used with an added phosphorus cycle, represented by phosphorus in detritus and dissolved phosphate. OMEXDIA uses a labile and refractive fraction of particulate organic matter (POM) measured as mole concentration of carbon. Each POM class has a fixed nitrogen to carbon ration, such that exchange with the pelagic detritus maps fluxes of the detritus nitrogen to the two POM classes in a mass conservative distribution. The diagenesis model is implemented in the FABM framework and is utilised by the MOSSCO sediment component. The state variables in the sediment are measured in mass per volume pore water and are identified from the FABM state variable properties as either particulate or dissolved quantities. Bioturbation in the sediment mixes the particulate fractions and is increasing with sediment temperature, whereas diffusion in the pore water mixes the dissolved quantities. The porosity of the sediment is a temporally constant vertical profile with a surface porosity of 0.7 and linearly decreasing with depth to 0.6 for 16 cm below the sediment surface. The sediment component discretises the sediment column by an exponentially increasing grid spacing with grid heights of 3 mm at the sediment surface up to 11.4 mm for 16 cm below the sediment surface. Exchange with the water column is diffusive for the dissolved quantities, whereas the particulate organic matter from the water column is sedimented into the sea bed by a fraction of 20% of the downward sinking flux to emulate a fluffy layer of POM near the sediment surface. The sea sediment temperature is taken to be the same as the bottom water temperature, as simulated by the GOTM model. Given the recurring winter nutrient conditions in Wiltshire et al. (2010), the loss of nitrogen through denitrification is recovered by lateral nutrient fluxes and rain. These fluxes are not resolved in the 1d model such that a constant flux of 100 mM-N/m²/y is used to balance the nutrient budget. Modeling sediment flux at the sea bed is achieved using an abridged version of Delft3D. This model is capable of modeling the vertical flux of cohesive, non-cohesive and a mixture of both sediment types. The non-cohesive sediment flux is calculated based on the method of vanRijn (1984) for waves and currents. The cohesive sediment flux is computed using Pardenaides equation including the effect of rough and smooth bed on the bed shear stress using the method of Soulsby and Clarke (2005). The model constitutes an extra earth system component as an interface layer. For the current simulation 30% cohesive and 70% non-cohesive sediment mixture were applied.

3 RESULTS

The coupled model system simulates the years 2002-2006 at the station Helgoland in the southern North Sea. The sediment component initialises with a spinup simulation under constant boundary conditions for a period of 5 years, when vertical profiles of the sediment state are balanced and sudden release of nutrients due to initialisation is prohibited. Diagnostics of the coupling are saved into NetCDF (Network Common Data Format) format by an output infrastructure component in the coupled system. Figure 3 shows a compilation of results as vertically aligned with the coupled system.

The results of the coupled simulation show a prevailing seasonal cycle in the model states. Dissolved nutrients (referred as dissolved inorganic nitrogen DIN in the Figure 3) are taken up by phytoplankton, which fills the pool of particulate organic nitrogen (PON in Figure 3) with the spring bloom. The organic, particulate matter sinks slowly into the sediments, where its remineralisation by bacteria enhances denitrification, which shows a peak in late summer. At the end of a year, nutrient concentration are high in the sediment and diffuse back into the water column up to winter values of 20-25 mmol-N/m³.

The simulated lithogenic suspended matter also shows a seasonal cycle of more turbid surface water in winter and more clear surface water in summer. The onset of the phytoplankton spring bloom is determined by light availability and thus is directly influenced by the SPM concentration in the water column. With the onset of warming of the water column, the vertical, turbulent mixing is partially suppressed, such that less SPM is mixed into the upper water column and radiation can penetrate deeper into the water column. The erosion/sedimentation module resolved SPM fluxes on the tidal scale coupled to the transport of Spm in the water column. The results of the tidal dynamics can be found in Nasermoaddeli et al. (2014).

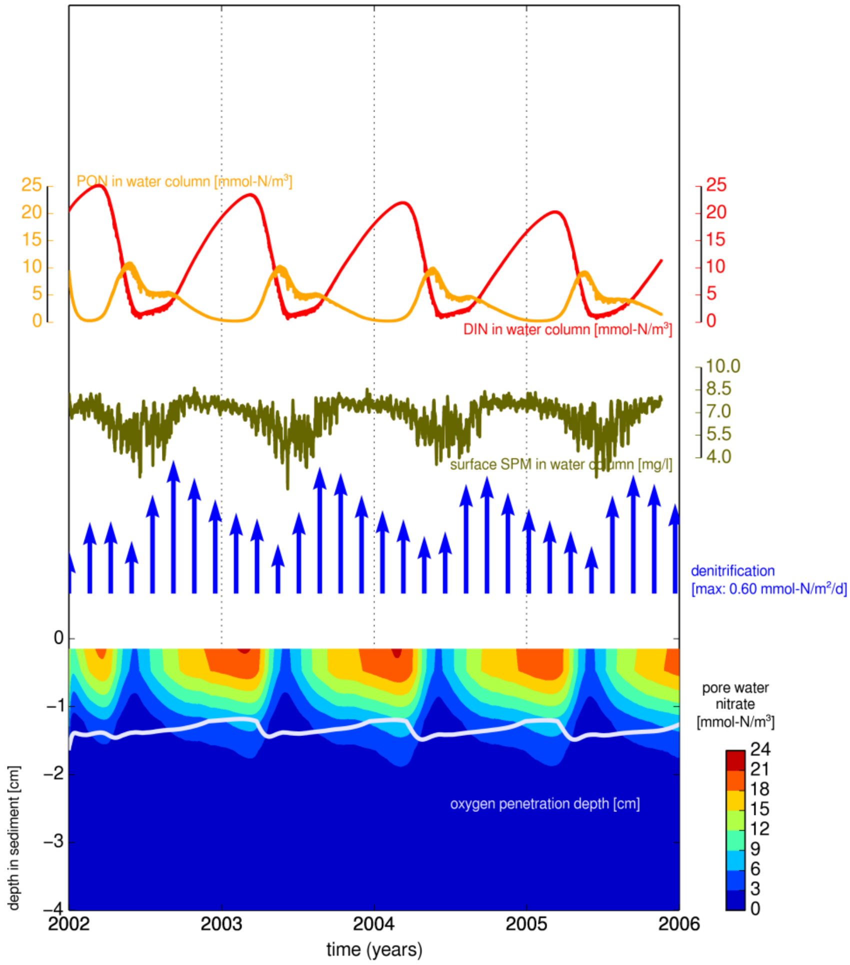

Figure 3. The results of the fully coupled 1d system at Helgoland. The SPM, PON, and DIN concentrations are given for the center of the water column, denitrification fluxes are integrated over the sediment depth and the while line in the lower panel shows the oxygen penetration depth, at which the oxygen concentrations are below 0.1 mmol-O2 /m³.

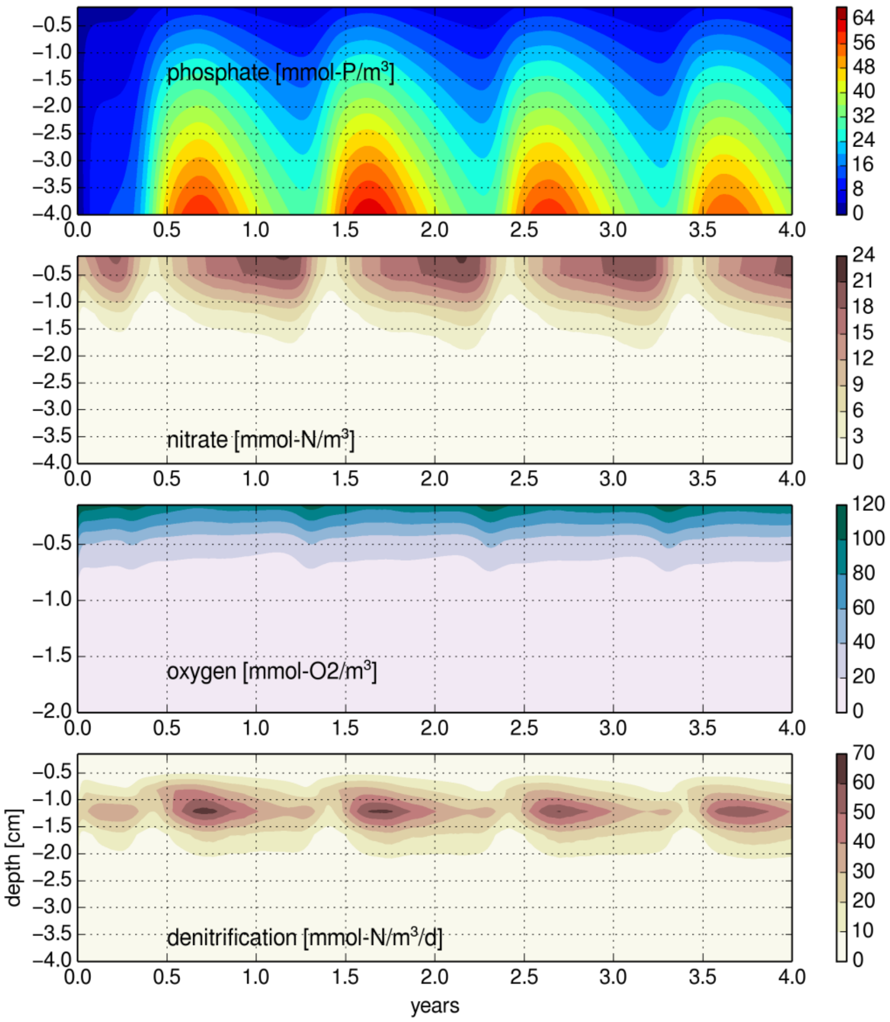

Figure 4. The vertical profiles of phosphate, nitrate, oxygen and the denitrification rate over time. The vertical axis always shows depth below the sediment surface.

Results of the sediment model in the coupled context also show seasonal variation in the emerging of strong vertical gradients. The lower panel shows the vertically resolved denitrification rate, that shows its maximum values in the suboxic part of the water column at about 12 mm below the sediment surface. In the upper panel of Figure 4, the phosphate profiles show a minimum in spring, which is enforced by phosphate adsorption under oxic conditions, when remineralisation is reduced due to lacking fresh material and temperature, and oxygen penetrates deeper into the sediments. The sediment profiles show decoupling of nitrate and phosphate dynamics, since phosphate shows its peak in autumn, whereas nitrate concentrations are highest in late winter. Nitrification in the sediments is enhanced by the availability of dissolved oxygen, which coincides with the nitrate maximum. At the same time, the pelagic concentrations of nitrate are comparable to the pore water concentrations, such that the flux of nitrate out of the sediment in the coupled system is low (compare with Figure 5). Additionally, denitrification reduces the available nitrate in the second half of the year. Therefore, the dissolved nitrogen concentrations are levelled relatively low compared to the available dissolved phosphorus.

The nutrients fluxes in the coupled system are shown in Figure 5 for the last three years of the simulation and explain the seasonality and the temporal decoupling. After the phytoplankton spring bloom, the flux of particulate organic matter peaks in early summer, which accumulates organic matter in the sediments. Subsequently, remineralisation and high concentrations of dissolved nutrients in the sediments force a flux of mainly ammonium and phosphate in late summer, whereas the nitrate flux is delayed due to available oxygen and denitrification. An early increase of phosphate after the spring bloom well before the increase of nitrate is a recurring feature shown for different stations in the southern North Sea (Wiltshire et al. (2006), Loebl et al. (2007)) and can be explained by the N:P ratio of the nutrient fluxes (see Figure 5). In our simulation, the internal N:P ratio of the particulate organic material in the water column is fixed to the Redfield value of 16 (Redfield (1963)). The flux of dissolved nutrients shows significantly lower values due to denitrification. A balances growth of phytoplankton (see Figure 3) in summer is then limited in nitrogen and would remain the excess dissolved phosphate in the water column. Lohse et al (1993) and Deek et al. (2011) report about attempts to measure denitrification in the southern North Sea and provide winter and summer values of the N_2 flux. The vertically integrated denitrification rate in the present coupled simulation varies between 3.5 µM/m²/h in spring and 9.5 µM/m²/h in late summer, which compares well to the measured values of 1.9 to 8.2 µM/m²/h for the German Bight by Lohse et al (1993). Deek et al (2011) measured the N_2 flux in the shallower areas of the German Bight with also comparable values of 2.1 – 3.9 µM/m²/h. The simulated water column of 25 m depth is expected to produce more particulate organic matter as also indicated through the comparison with Lohse et al. (1993). The data comparison justifies the compensating nutrient input of 100 mM-N/m² nitrogen per year.

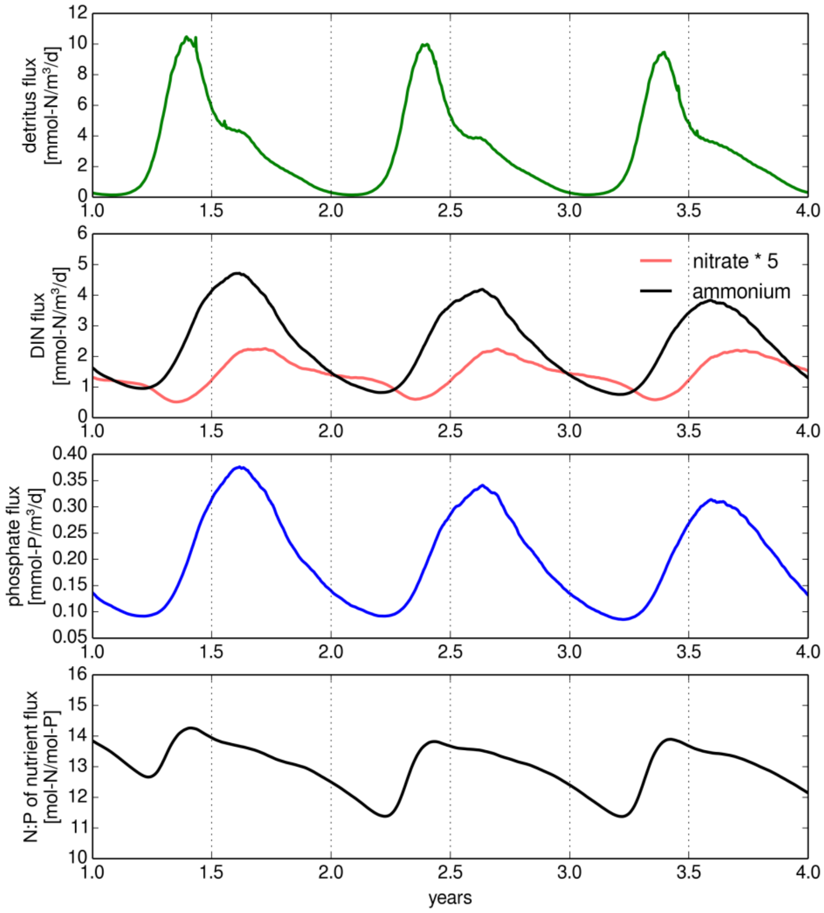

Figure 5. Nutrient fluxes between sediment and water column. The detritus flux is directed into the sediment, whereas the DIN and phosphate flux is directed into the water column. The N:P ratios are well below the Redfield ratio of 16 molN:molP.

4 CONCLUSIONS

The MOSSCO system provides a consistent model coupling framework, in which existing models are wrapped into components and exchanged quantities are exchanged using a standard naming scheme. Ecosystem/water quality models are effectively integrated with the 0d approach of the Framework of Aquatic Biogeochemical Models (FABM) in the pelagic compartment as well as in the porous sea sediment. The simulated SPM dynamics as a result of the pelagic SPM transport and the coupled erosion/sedimentation component provides the light climate for the ecosystem model. Through the coupled model setup, we find, that denitrification and phosphate adsorption provide seasonally varying stoichiometric ratio of the nutrient flux into the water column, which could explain observed decoupling in phosphate and nitrate dynamics. Atmospheric and riverine supply of dissolved nutrients is necessary to close the local nutrient budget.

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