Mud dynamics in the Ems Estuary

Set-up of primary production model

Deltares

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Title
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Rijkswaterstaat WVL	1205711-000	1205711-000-ZKS-0032	96

Keywords
Water quality model, primary production, estuary, turbidity, Ems-Dollard, Wadden Sea.

Summary
This is the final report on the set-up for the water quality/primary production model. The model will be used to explore measures in the Ems Dollard estuary that aim to reduce turbidity. The current set-up is described, including the incorporation of model inputs to simulate the year 2012 and 2013.

The model describes three types of pelagic algae (phytoplankton), benthic diatoms, light climate and extended nutrient cycles in the water and sediment. It is driven by modelled hydrodynamics and suspended sediment concentrations for 2012 and 2013, and uses observations for the year 2012 and 2013 regarding boundary conditions, meteorological forcing and river loads.

For the calibration year 2012, the suspended sediment concentration needed adjustment in order to produce extinction values that were consistent with measurements. The adapted model produced on average good results for extinction, chlorophyll-a and nutrients. Variability of chlorophyll-a was overestimated. For the validation year 2013, the sediment concentrations were directly taken from the sediment model and produced extinction values consistent with measurements. Also average chlorophyll-a concentrations matched measurements, but variability was overestimated, similar as for 2012.
With the current forcing of the model, it is not possible to fit the model for chlorophyll-a both in the inner and outer parts of the estuary. It has been concluded that on a time scale at which chlorophyll-a is evaluated as a Water Framework Directive indicator (summer half-year) the model performs well except for the shallow and dynamic Dollard region.

A first comparison of area-integrated primary production with extrapolations from measurements show that, in most areas, model results are in a similar range, but lower than results from measurements, except the inner part of the Dollard. One explanation for the difference between model result and measurements is the different methods to spatially integrate primary production.

References
Offertenummer 1205711-000-ZKS-0004, toekenningbrief RWS/WD-2011/3497

Version	Date	Author	Initials	Review	Initials	Approval	Initials
0.1	April 2013	dr. W. Stolte					
0.2	June 2013	dr. W. Stolte					
1.0	Nov. 2013	dr. W. Stolte		dr. F.J. Los			
2.0	Oct. 2014	dr. W. Stolte		dr. F.J. Los			
3.0	Feb. 2015	dr. A. de Kluijver		dr. F.J. Los		MSc. F.M.J. Hoozemans	
4.0	June 2015	dr. W. Stolte		dr. F.J. Los		MSc. F.M.J. Hoozemans	

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Contents

1 Introduction

The Water Framework Directive (WFD) requires EU member states to achieve good ecological and chemical status of all designated water bodies (rivers, lakes, transitional and coastal waters) by 2015. Therefore Rijkswaterstaat has initiated the project ‘Research mud dynamics Ems Estuary’ (*Onderzoek slibhuishouding Eems-Dollard*). The aim of this project is to (I) determine if and why the turbidity in the Ems Estuary (Figure 1.1) has changed, (II) to determine how the turbidity affects primary production, and (III) to investigate and quantify measures to reduce turbidity and improve the ecological status of the estuary – see also the flow chart of the project structure (Figure 1.2).

In the management plan (Rijkswaterstaat, 2009) for the implementation of the WFD (and Natura 2000) in the Netherlands, the context, perspectives, targets and measures for each designated water body (also including the Ems Estuary) have been defined. To achieve a good status of the Ems Estuary (as is required by the WDF), a better knowledge of the mud dynamics in this region needs to be improved. Also triggers for increase in turbidity need to be identified before 2015. Rijkswaterstaat has initiated this project in order to improve the knowledge of the mud dynamics and the impact on the good status of the water bodies.

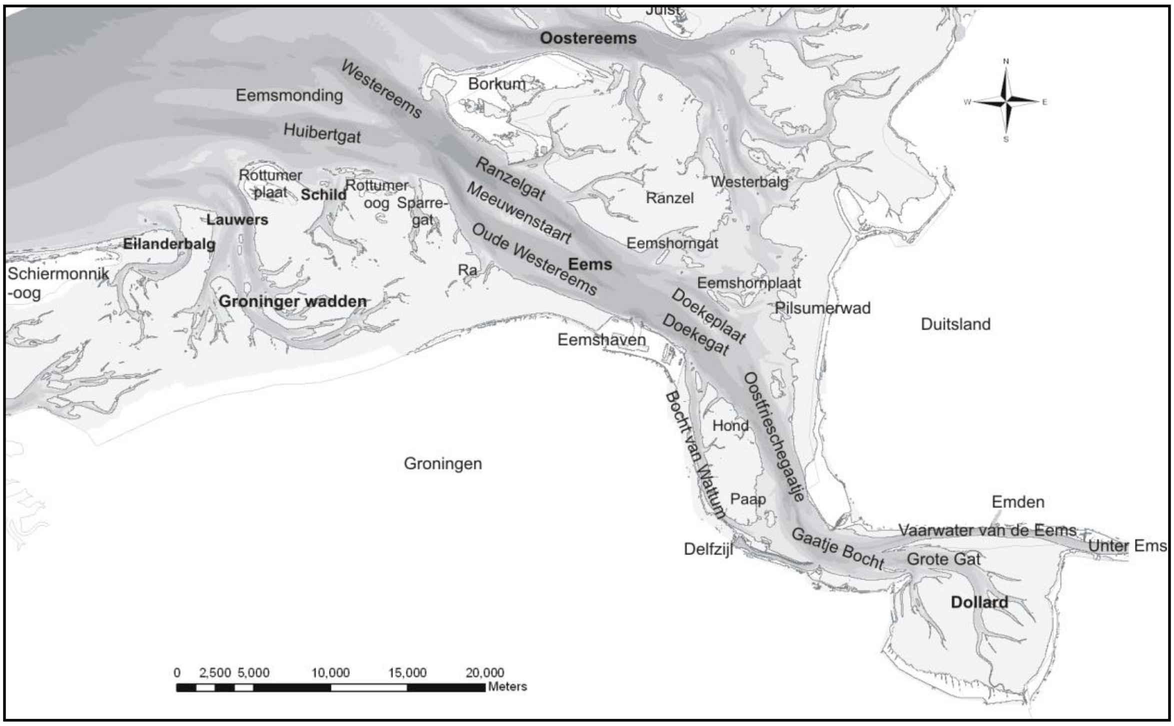

Figure 1.1 Map of Ems Estuary with names of the most important channels and flats (Cleveringa, 2008).

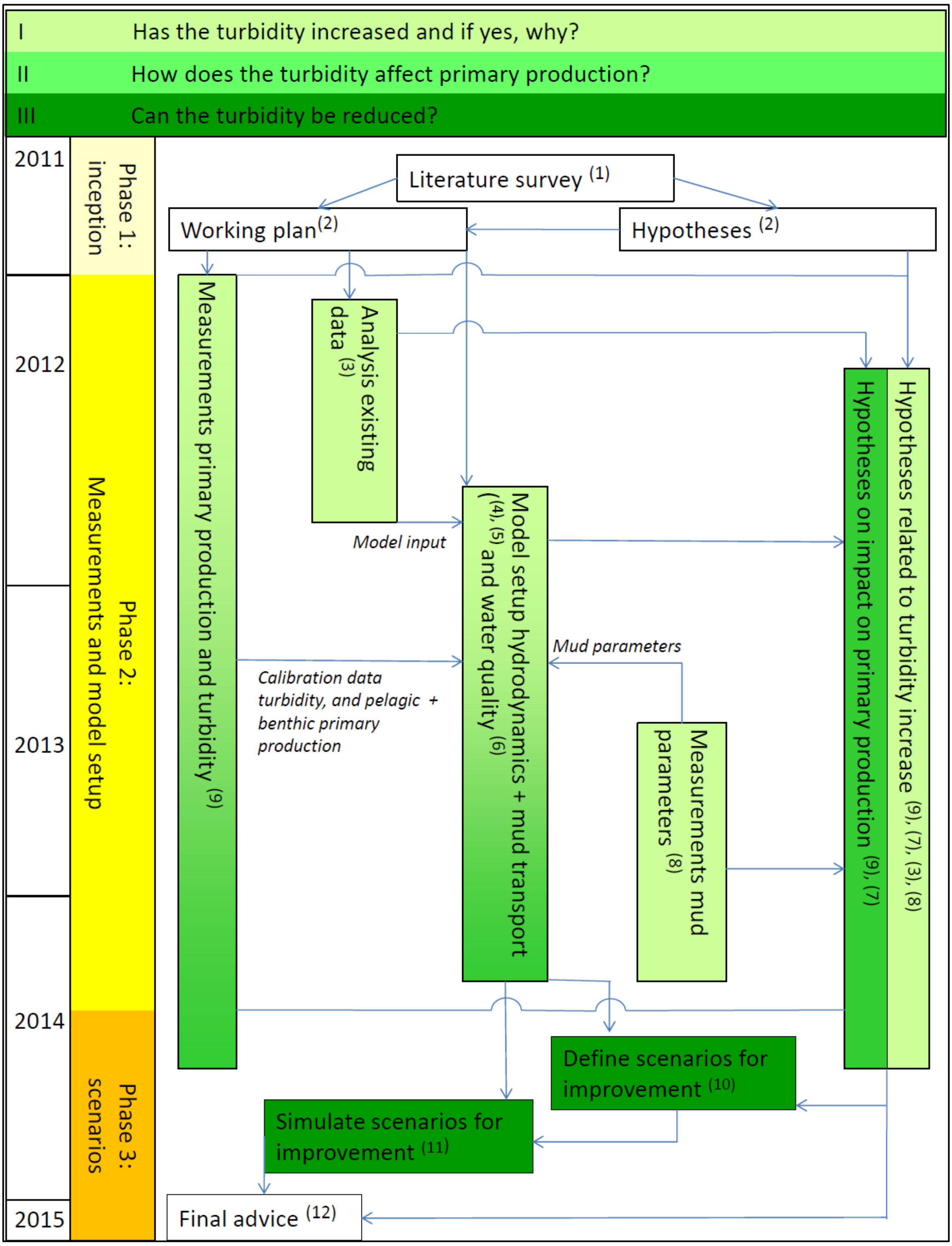

Figure 1.2 Flow chart for the structure and timetable of the study. Green colouring of the phase 2 activities relates to the colour of the main research questions I, II, and III. See Box 1 for a description and Table 1.1 for the references (1) – (12)

This research project explores mechanisms that may be responsible for the present-day turbidity of the estuary and measures to reduce the turbidity. To achieve this, an effect-chain model is setup in which relates human interventions to changes in hydrodynamics, sediment transport, and water quality. This model is supported as much as possible by existing data and new data collected within this project. However, the long-term effect of human interventions on suspended sediment dynamics in an estuary such as the Ems Estuary is complex, and data supporting such an analysis is limited. Although the absolute values of the model predictions should therefore be carefully interpreted, it is a powerful tool to investigate trends. This work provides indicative explanations for the current turbidity patterns and a first exploration of restoration options, but also reveals important gaps in knowledge and next steps to be taken. Additional research is required to further substantiate the results of this project.

The overall study is divided into three stages: an inception phase (phase 1) in which gaps in knowledge are identified and a research approach is defined; phase 2, in which measurements are done and models are set up and calibrated; and phase 3 in which the models are applied to investigate measures to improve the ecological and chemical status of the estuary. The overall structure and timeline of this study is summarized in Figure 1.2 and Box 1. An overview of the deliverables (reports and notes) produced during the project is given in Table 1.1. The numbers 1 to 12 of the deliverables are part of the project layout in Figure 1.2.

BOX 1: SET UP OF THE STUDY (with Figure 1.2; references in Table 1.1)

The primary objective of this study is to address the following:

q1: Has the turbidity increased and why?

q2: If yes, what is the impact on primary production?

q3: Can the turbidity be reduced?

These questions are presented in a flow chart (see Figure 1.2). During phase 1, existing gaps in knowledge were identified (see report 1 in Table 1.1), and a number of hypotheses were formulated related to q1 and q2 (report 2 in Table 1.1), to be addressed during phase 2 of the study.

Phase 2 consists of measurements, model set up and analysis. Measurements of primary production and turbidity are carried out from January 2012 to December 2013, and reported mid 2014 (report 9 in Table 1.1). These measurements are carried out to address hypotheses related to q1 and q2, and to calibrate the sediment transport and water quality models. Existing abiotic data (such as water levels, bed level, dredging, and sediment concentration) are analysed in this phase to address hypotheses related to q1 and to provide data for model calibration (report 3 in Table 1.1). Soil samples in the Ems estuary and Dollard basin have been collected to determine changes in mud content (hypotheses relates to q1) and determine parameter settings of the sediment transport model (report 8 in Table 1.1).

The effect-chain model set up for this study consist of three modules: a hydrodynamic module (report 4 in Table 1.1), a sediment transport module (report 5), and a water quality module (report 6). These models are applied to address the hypotheses related to q1, q2, and q3 (report 7 in Table 1.1).

In phase 3, a number of scenarios are defined to reduce turbidity / improve the water quality (q3) of the estuary (report 10 in Table 1.1). Their effectiveness is tested in reference (report 11). A final report, synthesizing the most important findings and recommendations (report 12) concludes the project.

Table 1.1 Reports / notes delivered during phase 1 to 3 of the Mud dynamics in the Ems estuary project (with numbers referencing to Figure 1.2). The current report is in bold.

Number	Year	Phase	Main research question	Report
1	2011	1	-	Literature study
2	2011	1	-	Working plan phase 2 and 3
3	2012	2	1	Analysis existing data
4	2014	2	-	Set up hydrodynamic models
5	2014	2	-	Set up sediment transport models
6	**2014**	**2**	**-**	**Set up water quality model**
7	2014	2	1, 2	Model analysis
8	2014	2	1	Analysis soil samples
9	2014	2	1, 2	Measurements primary production
10	2014	3	3	Scenario definition (note)
11	2014	3	3	Model scenarios
12	2015	3	1, 2, 3	Final report

In this report #6 the setup of the primary production model is described. Chapter 2 contains a general description of the models and the effect chain. In chapter 3, the general approach for the water quality model is presented. The technical setup of the primary production or water quality model is described in chapter 4. Calibration of the model for the year 2012 is presented in chapter 5. Chapter 6 contains the results of the calibrated primary production model for 2012 and 2013, the validation year. Discussion of model results is presented in chapter 7 and chapter 8 contains references. Details of water quality setup and input are presented in appendices.

2 Description of the models

This chapter provides a brief description of the applied models. More details about each model (such as modelling assumptions, domains, time and resolution etc.) are described in the dedicated model reports to hydrodynamics, sediment transport and water quality (reports 4, 5 and 6 in Table 1.1).

2.1 Introduction

The objective of this study is to determine why turbidity has changed, what the impact is on primary production, and if / how this can be mitigated. These questions can be addressed using a combination of field data and numerical models. The most important gaps in knowledge, as identified in report 1, have been translated into a list of hypotheses (see report 2). These hypotheses cover a range of research objectives related to hydrodynamics, sediment transport, and water quality. For research questions addressing hydrodynamic processes, a hydrodynamic model is used. Modelling turbidity requires the use of a sediment transport model in combination with the hydrodynamic model. Primary production is dependent on turbidity, and therefore primary production is modelled with a hydrodynamic-sediment transport- primary production model. This is known as an effect-chain model, which is described in more detail in section 2.2.

The hypotheses formulated in report 2 will be addressed with the numerical models in report 7. The hydrodynamic model, the sediment transport model, and the water quality model (report 4, 5, and 6, resp.) should therefore be able to simulate the processes relevant for these hypotheses. The most important processes (see for details report 1) can be summarized as:

a) Tidal propagation and changes in tidal propagation in the Ems Estuary and lower Ems River as a result of deepening
b) Residual flows resulting from wind and salinity, and changes therein as a result of deepening
c) Sediment transport mechanisms and typical sediment concentration levels as a result of tides, waves, and density-driven flows
d) Sediment trapping in ports and the long-term effect of subsequent dredging and dispersal on the suspended sediment concentration in the estuary.
e) Pelagic and benthic primary production under influence of light and nutrient availability

In each of the relevant reports, the applicability of the model to address the processes above will be addressed: a) and b) in report 4 and 7; c) and d) in report 5 and 7; e) in report 6 and 7.

The starting point for the effect-chain model is a numerical model developed within previous studies (see e.g. Van Kessel et al. (2013) for an overview) which is originally based on a model developed by Alkyon. This model is hereafter referred to as the WED model (Wadden Sea Ems Dollard). The original WED model was initially set up for the year 2005. In this project a large amount of monitoring data has been generated for the year 2012 en 2013. This includes the primary production and turbidity data, but also the continuous measurements collected near Eemshaven in the first half of 2012. Therefore, the model is recalibrated for the year 2012. In addition, also some aspects of the model required further improvement. These improvements are explained in more detail in section 2.3.

The WED model is set up to simulate relatively long time periods and large spatial scales. Some of the research questions to be addressed cover smaller spatial scales and different process formulations, and these questions require the use of more detailed models. For this purpose, two new models were set up: the ERD (Ems River Dollard) and the ER (Ems River) model – see Figure 2.1 for the layout of the models and section 2.4 for details. These models have a hydrodynamic module (ERD) and a hydrodynamic- and sediment transport module (ER). See Table 2.1 for an overview of the modules for each model.

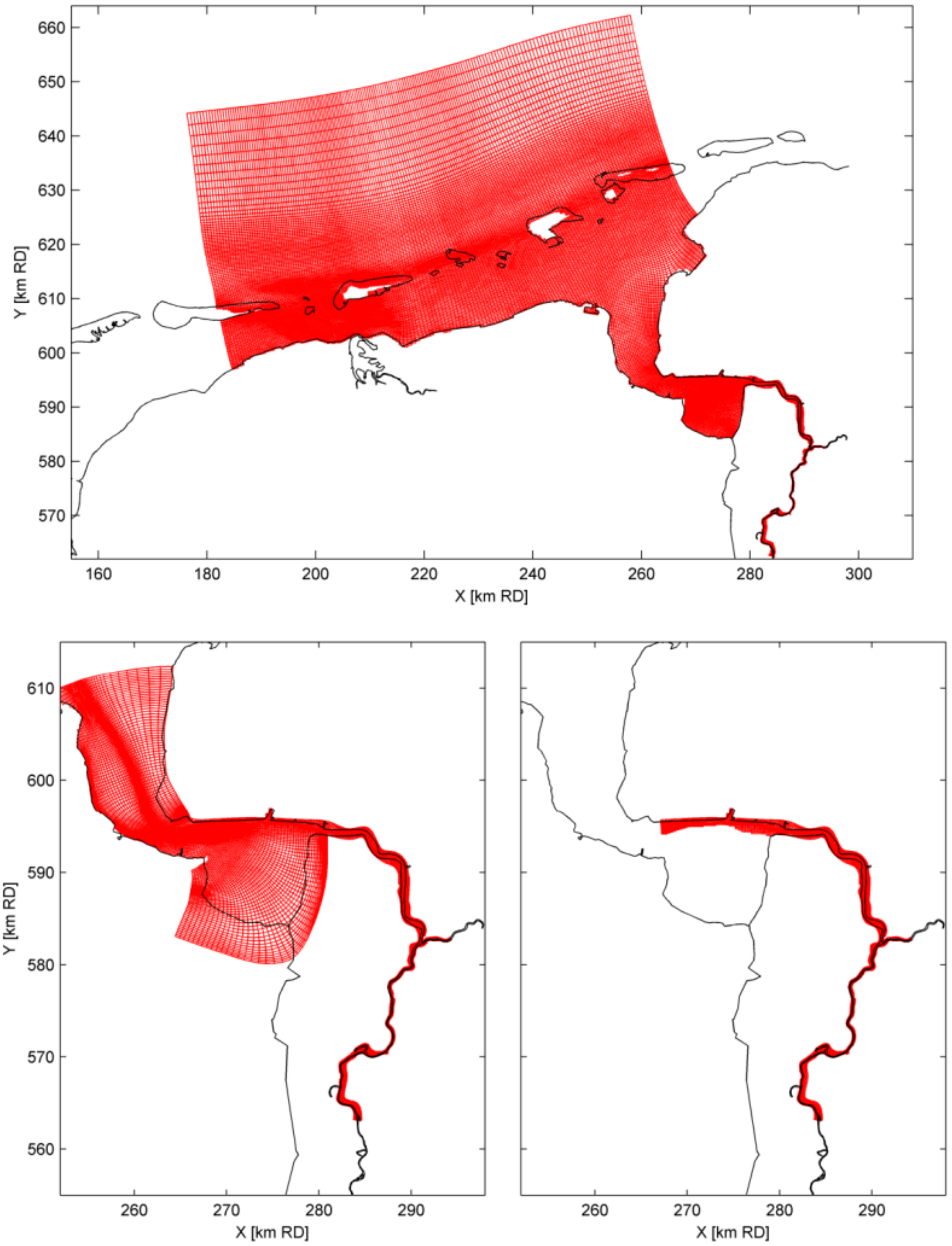

Figure 2.1 Computation grid of the WED model (top), the ERD model (lower left), and the ER model (lower right).

Table 2.1 Models adapted (WED) or developed (ER, ERD) within this project

Model	Hydro	Sediment transport	Waves	Water quality	Purpose
WED	yes	yes	yes	Yes	Set up of an effect chain model to simulate long-term hydrodynamic, sediment transport, and water quality changes
ERD	yes	no	no	no	Simulate tidal processes in parts of the Ems Estuary, the Dollard, and the lower Ems River.
ER	yes	yes	no	no	Quantify tidal and sediment transport processes within the lower Ems River and changes in sediment exchange between Ems river and Ems estuary

2.2 Effect chain models

An effect chain module contains various models to describe the effect of changes in the physical and morphological environment on chemical and biological variables in a complex environment. The model application must therefore be able to perform accurate calculations over several subject domains. For this purpose, an effect chain model is used to link different topic-specific models, each describing different processes in a chain of events. The basic idea of running different models is that each model component in itself can be optimally configured describing a limited set of processes. The alternative, one model describing all processes in one run, will have a higher computational demand and less flexibility, or a lower accuracy. Combining the results of the different models in a chain is necessary in order to take into account all relevant processes. In this study, the following three models were "chained" (Figure 2.2):

- A hydrodynamic model, producing time-dependent three-dimensional (3D) fields of salinity, temperature and other physical parameters such as bottom friction. This model was run using the open-source software Delft3D-Flow.
- A sediment model describing the transport and distribution of fine sediments, using the output of the hydrodynamic model as an input. This model was run using the open-source software Delft3D-WAQ configured for fine sediments.
- A water quality/primary production model describing cycling of nutrients, light distribution in the water, and primary production by phytoplankton and microphytobenthos. This model was run using the open-source software Delft3D-WAQ configured for ecological processes. The water quality/primary production model component uses the output of both the hydrodynamic model and the sediment model as an input.

For addressing the questions in this study, we follow an approach in which we assume that there is no significant feedback between hydrodynamics, sediment transport and water quality. This is elaborated in more detail in section 2.3. Therefore the coupling between the models is done off-line, meaning that each model is executed separately, using the output of the previous model in the chain as input. The hydrodynamic model exports files with hydrodynamic variables which are input for the sediment transport model. Subsequently, the sediment transport model generates files with sediment concentration fields that are (together with the hydrodynamic input files) used by the water quality model. This big advantage of this offline approach is that computational times remain manageable.

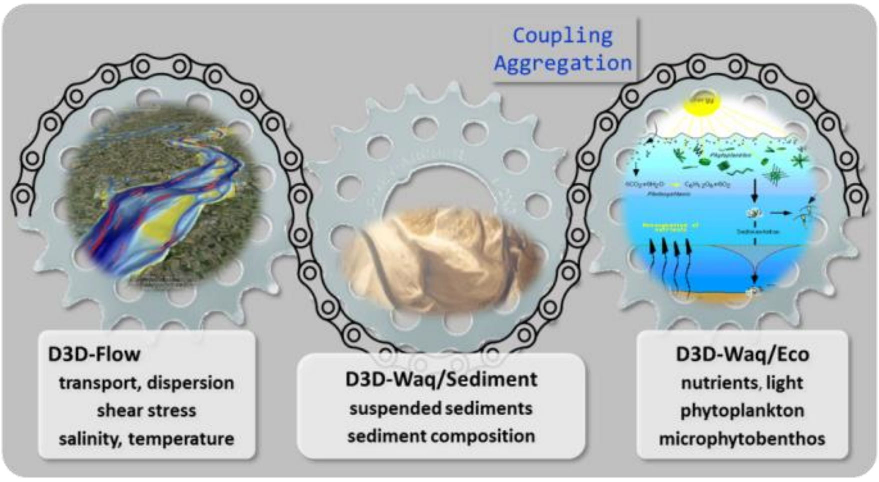

Figure 2.2 General set up of a linear effect-chain model.

2.3 The Waddensea Ems Dollard (WED) model

The WED model is the effect-chain aiming to relate (changes in) large-scale hydrodynamic to (changes in) turbidity and primary production (see Figure 2.1). This model is used to determine the effects of dredging and dumping, the role of ports and access channels, and changes in the Wadden Sea or North Sea on turbidity and primary production. For primary production changes in nutrients are also important variables. In the water quality module the limiting factors for primary production are nutrients (determined by nutrient supply and dispersion) and light (determined by turbidity). An important question is in which part of the estuary (and during which part of the year) primary production is nutrients-limited and which parts are light-limited. In order to adequately address the research questions formulated for this study (see Report 2, Table 1.1), the WED model developed in the previous KPP studies needed to be improved on several aspects:

In the initial results of the **hydrodynamic model** of the KPP studies, the computed salinity deviates considerably from the observed salinity. As salinity is a good approximation of computed dispersion and mixing, the salinity modelling needs to be improved for the current study. The mismatch in the model is probably the result of over-simplified boundary conditions and therefore the freshwater sources are now more accurately implemented. In addition, the computed salinity is now also verified with continuous measurements collected in the German part of the estuary and close to Eemshaven in addition to data collected at the Dutch MWTL stations). A second major improvement in the hydrodynamic model is the computation of wave-induced bed shear stresses with the SWAN wave model, instead of the less accurate fetch-length wave approach that was initially applied. The SWAN model generates a stronger along-estuary gradient in wave height and bed shear stress, which promotes up-estuary sediment transport.

The WED **sediment transport model** computed the transport of fine sediment (mud). One of the shortcomings of the initial sediment transport model was that the residual transport of sediment was directed down-estuary, whereas observations indicate that the Ems Estuary is importing. To better reproduce this, the wave model was improved, dredging and dumping was integrally modelled (sediment depositing in ports is regularly dredged and disposed on dumping locations through a dredging routine), and the sediment settings of the model were modified. Also, the original sediment transport model was only limitedly compared to observations. New observations were generated within the mud sampling programme (Report 8), the primary production measurements (Report 9), and the GSP measurements collected near Eemshaven. The model is recalibrated and the results are compared to a wider range of suspended sediment transport observations. In addition to the turbidity measurements, the model accuracy is determined by comparing modelled sediment fluxes with estimated sediment fluxes, through ADCP transects or port siltation rates. Finally, the modelled sediment deposition is compared with observed sediment distribution patterns.

The WED sediment transport model is coupled off-line (in Delft3D-WAQ), which means there is no dynamic feedback between morphology, water density, and the hydrodynamics. A coupling between hydrodynamics and morphology is needed when bed level changes significantly influence the hydrodynamics within the modelled timeframe, which is usually only required for sand and for decadal timescales. Morphological changes resulting from fine sediment erosion or deposition usually have limited impact on hydrodynamics. Fine sediment may influence the vertical mixing through suppression of turbulence at concentrations exceeding several 100 mg/l. This may play a role in the Dollard, and will certainly influence sediment dynamics in the lower Ems River. However, a fully coupled model is approximately 10 times slower than a non-coupled model, and multi-year simulations are not feasible with a fully coupled model because of the associated computational times. Multi-year simulations are needed to develop a sediment transport model which is in dynamic equilibrium (where computed sediment concentrations are independent of initial conditions but determined by hydrodynamics, model settings, and boundary conditions), which is needed to compute the effect of perturbations to the system. In the majority of the Ems Estuary the concentrations are below several 100 mg/l, and the bed level changes low, and therefore the long computational times are considered more important than a full coupling. In addition to the computational period, also the sediment transport processes available in Delft3D-WAQ are important. In Delft3D-WAQ, the buffering of fine sediment is simulated using the model developed by van Kessel et al. (2011), which are important for estuarine sediment dynamics, and probably more important than the sediment-induced density effects (which are included in the fully coupled model). Based on the computational effort and available transport formulations, the WED sediment transport model is coupled off-line to hydrodynamic model.

The **water quality/primary production model** was further developed using a more detailed process description (Report 6 in Table 1.1), and using newly available monitoring data (Report 9). The implementation of a more detailed description of nutrient cycles including layered sediment with early diagenesis of organic material resulted in a major improvement in the calculation of phosphate compounds. The phosphate compounds show a strong sediment flux in summer in the inner parts of the estuary. Secondly, the monitoring programme carried out by IMARES (Report 9) provided a better approximation of phytoplankton growth process parameters, and validation data additional to the national monitoring programme.

The combination of the hydrodynamic, sediment transport, and water quality models (the effect-chain model) will be used to explore the effects of natural variation and man-made changes in the nutrient loads and sediment dynamics of the estuarine waters on turbidity, primary production and phytoplankton biomass. This provides a tool which can be used to better understand the historic changes in the Ems Estuary (Report 7) but also to estimate the effect of proposed measures to improve the turbidity and primary production (Report 11).

2.4 The Ems River (ER) and Ems River Dollard (ERD) models

It is known that the lower Ems River became significantly more turbid in the last decades (e.g. de Jonge et al., 2014). At present the lower Ems River is considered as a hyper-concentrated system with very limited ecological value. The ecological state of the lower Ems River is not part of the current study. However, the exchange of sediment between the lower Ems River and the Ems Estuary may be important for the sediment dynamics in the Ems Estuary, and part of the hypotheses formulated in report 2 (Table 1.1). Also a more quantitative understanding of changes in the lower Ems River is needed to understand the current state of the Ems Estuary.

The resolution of the WED model is insufficient to accurately model the dynamics in the lower Ems River and the exchange with the Ems Estuary. In order to better understand the changes in the lower Ems River (and exchange with the Ems Estuary), two models were set up: the Ems River Dollard (ERD) model and the Ems River (ER) model (see Figure 2.1). The ERD model covers the Dollard and the Ems Estuary up-estuary of Eemshaven, whereas the ER model only covers the lower Ems River and the Emden navigation channel. The ERD model can be applied to model (for instance) the effects of channel morphology and land reclamations in the lower Ems River, but also parts of the Ems Estuary (such as the Dollard), on the tidal dynamics.

The ER model only covers the lower Ems River and the Emden navigation channel, and is specifically set up to model the changes in tidal dynamics and sediment transport mechanisms, as a result of deepening of the Ems River. As described in section 2.3 the sediment module of the WED model is executed in an off-line mode without a dynamic feedback between hydrodynamics, sediment concentration, fluid density, and morphology. In the lower Ems River, such a simplification is not valid, and therefore the hydrodynamics, morphology, and water density in the ER model are fully coupled.

3 General approach for Water Quality model set-up

3.1 Development history of the water quality and primary production model

The development of the model described in this study started in a previous project (Stolte et al., 2012). The model was set up for the year 2001, and some relatively simple scenarios regarding effects of changing suspended sediment concentrations were run. In the current project, this model was further developed, and set up for the years 2012 - 2013. At the same time, a monitoring program was started, gathering primary production and supporting monitoring data for the years 2012 and 2013. The goal of this study was to use the newly gathered data to improve the input and to calibrate and validate the model to answer the hypotheses. The TO-KPP model had the following main characteristics:

- Coupling to hydrodynamic model for transport, dispersion, fresh water loads and temperature for the year 2001.
- Coupling to output of sediment model to force the concentration of suspended sediments for 2001.
- Wind and solar irradiance observations were included as physical forcings
- Nutrient loads from the Ems river and polders were calculated using measured concentrations
- Boundary concentrations were included based on MWTL monitoring at Terschelling 10 (North Sea boundary) and Zoutkamperlaag (Wadden Sea boundary).
- Water quality processes included nitrification, denitrification, nutrient uptake by phytoplankton, phytoplankton growth, mortality and sedimentation and remineralisation of dead phytoplankton. Sediment processes were simulated by a single sediment layer with simplified formulations for nutrient remineralisation, nitrification and denitrification. The model processes and constants were chosen essentially the same as used in the North Sea model (Blauw, et al. 2008, Los et al. 2008)
- Benthic diatoms were modelled as other algae, which cannot be transported.

The above model was validated with respect to concentrations of nutrients and chlorophyll a. The results were reasonable for chlorophyll a and phytoplankton biomass. However, nutrients, and especially phosphorus concentrations were not well described.

3.2 General concepts and specific choices for the Ems- estuary water quality model

3.2.1 Focus

This project is specifically designed to test hypotheses (see section 2.1) and to calculate scenarios as expressed in the WFD river basin management plan for the estuary. The most relevant scenarios with respect to primary production are those with changes in sediment dynamics, since the Ems estuary is extremely turbid and primary production is overall light limited. The focus of the model setup is therefore on the relation between sediment, extinction and light availability and primary production. Also the effect of changing sediment concentrations on the relation between benthic and pelagic primary production was considered an important aspect. In addition, scenarios with reduced nutrient loads are used to explore the sensitivity of the model to changes therein. So, proper setup of nutrient loadings is another focus of the model setup.

3.2.2 Light availability and primary production

Primary production is dependent on light availability and nutrient concentrations. Contrary to nutrient availability, light availability varies with depth. Light is extinguished exponentially with depth and varies in time (day-night cycle). The value of the extinction coefficient is determined by the properties of the water and the substances. Total extinction is calculated as the sum of extinction by sediment, organic fractions (detritus and phytoplankton), dissolved substances and background extinction. The extinction coefficient is used to calculate how much light is available at a certain depth with Lambert-Beer law:

$I_d = I_0 * e^{(-E*d)}$
where
I_d = light intensity at depth d (W m^{-2}) or in % relative to surface light
I_0 = light intensity at the surface (W m^{-2}) or as 100%
E = extinction coefficient (m^{-1})
d = depth (m)
Light limited phytoplankton can benefit directly from an increase in light or a reduction in extinction. Microphytobenthos are positioned at the bottom and will only react to changes in extinction if light can reach the bottom in the first place.

3.2.3 Spatial scale and resolution

There is a difference in temporal and spatial scale on which processes work and substances are present. In systems with steep gradients, such as the Ems Estuary, resolution of the grid will influence the results of some processes (Los and Blaas 2010). This is important to mention for interpretation of the results. For example, phytoplankton biomass (chlorophyll-a) is an integrated product of primary production and other processes and transport. The result is relatively independent of resolution. The same holds for nutrients. Extinction and primary production on the other hand are local instant processes that are sensitive to resolution. In systems with large gradients, high resolution is recommended, but can result in different spatial patterns between chl *a* (large scale product that can be transported and mixed over the estuary) and primary production (which is a local process, that can instantly change when water and phytoplankton is transported to an other environment).

3.2.4 Temporal scope of the model application

During 2012, a pelagic monitoring programme was carried out by IMARES within the current project. This monitoring programme was especially designed to fill the gaps in knowledge, i.e. it gathers data to estimate the primary production rates and phytoplankton biomass during two complete years every two weeks and at 6 stations in a gradient through the estuary (Figure 4.17). Primary production, light extinction, suspended sediment concentration, and limiting factors for phytoplankton were measured at 6 stations along the estuarine gradient, while continuous (1/min) measurement of phytoplankton pigment fluorescence was done in a transect along the estuarine gradient. These measurements and the continuous transect provide a unique opportunity to validate the model on a relatively fine spatial scale. During 2013, also benthic primary production and phytobenthos biomass was measured in a cross transect through the estuary (report 9).

In order to optimally benefit from this monitoring programme, the TO-KPP model was set-up for the years 2012 and 2013. This means that the model now was forced by new hydrodynamic and suspended sediment forcing, representing the conditions for those years. Also, boundary conditions, physical forcings, loads and validation data were defined for these years.

Water quality and primary production models have been set up for a variety of systems in the Netherlands and abroad using the Delft-3D software used in this study. Although Deltares strives to use generic process formulations where possible, systems may differ in regulatory processes, which then drive the choices of processes in the model set-up.

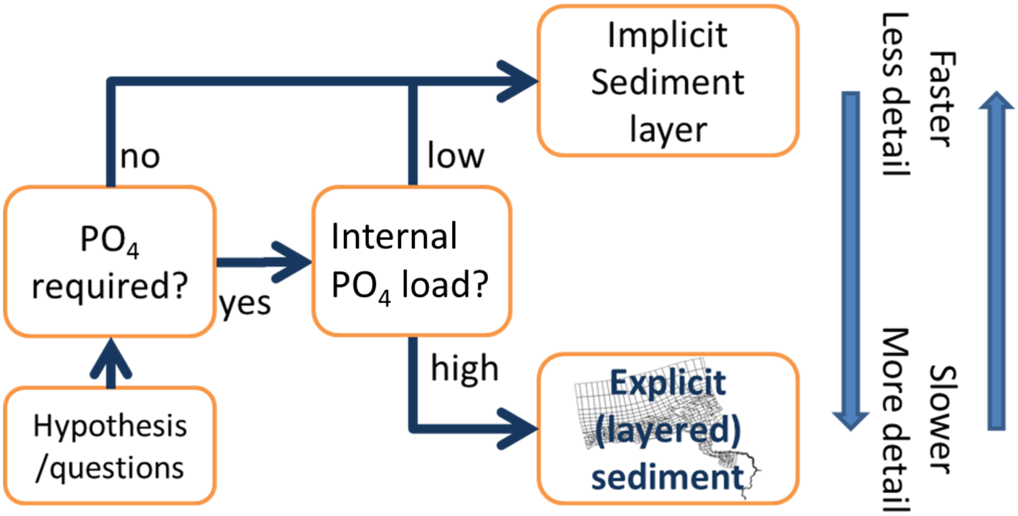

Figure 3.1 Decision scheme for the choice of sedimentprocesses to be included in the model. A trade off between a faster model with less detail, and a slower model with higher detail in processes is considered. The addition of detail is motivated by the choices in the scheme.

In similar systems in the Netherlands (e.g. Schelde estuary, Western Wadden Sea) where models are set up for the same type of purposes, phosphate loads and concentrations have been reduced to such low levels during the last decades that the effect of phosphate return fluxes in summer from the sediments are diminished to a negligible level. However, phosphate itself is still important and can be a limiting factor (e.g. in the Wadden Sea). As opposed to the Schelde and the western Wadden Sea, the Ems estuary is characterized by a high phosphate load from the Ems river. This has as a consequence that there is a large surplus of phosphate in the system and subsequent high concentrations of adsorbed phosphate in the sediment. In combination with relatively high organic loads, sediments in the Dollard contain may release large amounts of phosphate during summer, leading to high concentrations in the water. The Ems Estuary water quality model formulation has therefore been made suitable to simulate phosphate return fluxes from the sediment (Figure 3.1). This implies the use of a larger set of biogeochemical processes and a more detailed vertical resolution in the sediment.

The advantages of this choice as opposed to a simpler approach are:

- ⊕ Mineralization of organic matter can be modelled in more detail, including the use of alternative electron acceptors (most notably denitrification, sulfate reduction). Although the primary goal is not to model sulfate reduction itself, it is necessary to calculate the redox state of the sediment, which determines the phosphate adsorption capacity.
- ⊕ Due to the layered sediment and calculation of electron acceptors in the sediment, sediment-water fluxes of especially phosphate can be modelled more realistically than with a simple bottom layer model set-up.
- ⊕ Scenarios concerning nutrient reduction, especially in combination with reduction in turbidity will be possible

However, there are also some drawbacks to this choice including:

- ⊙ Longer calculation time (appr. 4 x longer) because of the layered sediment
- ⊙ Higher degree of over-parameterization. Although many of the parameters are generic and well-documented, some need to be calibrated. There are no recent measurements of concentrations of substances in the sediment in the area.

Therefore, processes and substances in the sediment were calibrated to match the concentrations in the water column. In the current version of the model, benthic primary production is modelled as a function of available light and nutrients at the bottom water layer. At a later stage, microphytobenthos may be included as process in the sediment rather than in the bottom water layer as it is described in the current model (Blauw, 2003).

Following the requirements for the project and the known difficulties from earlier studies, the following steps have been made to improve the model set-up as compared to the earlier version (TO-KPP study, Stolte et al., 2012) based on the North Sea model description:

- Boundaries, loads, meteorology, hydrodynamic and sediment forcing were set up for more recent years, namely 2012 and 2013.
- Sediment-water exchange and the mineralization of organic matter in the sediment has been set up using a layered sediment (9 layers) and a set of equations describing the chain of electron-acceptors to mineralize organic matter as a function of available oxygen in the sediment layers.

4 Modelling software, model schematization and predefined processes

The software used to model water quality and primary production in this study is DELWAQ. DELWAQ is the engine of the D-Water Quality and D-Ecology programmes of the Delft3D modelling suite. It is based on a rich library from which users and developers can pick relevant substances and processes to quickly put water and sediment quality models together. For the current modelling work, DELWAQ version nr 5.00 (more exact: 5.00.00.2393:2512M) is used. The software can be downloaded from http://oss.deltares.nl.

4.1 Grids

4.1.1 Water

The schematization describes the distribution of computational cells over de model domain. For the water phase, the schematization has been extensively described in Stolte et al., (2012). Due to strong vertical mixing, a 2D model grid is sufficient. An additional advantage is shorter calculation times. For questions needing vertical detail in the water column, a 3D version with 8 sigma-layers (constant relative thickness) is available. Comparison of the 3D and 2D version showed that the 3D version of the model showed more detail in the calculated salinity distribution, but that hardly any vertical stratification occurred (Figure 4.1). Also, the 2D model captured sufficiently the overall salinity gradient through the estuary (Figure 4.1). It was therefore concluded that for the current study, a 2D version was sufficient.

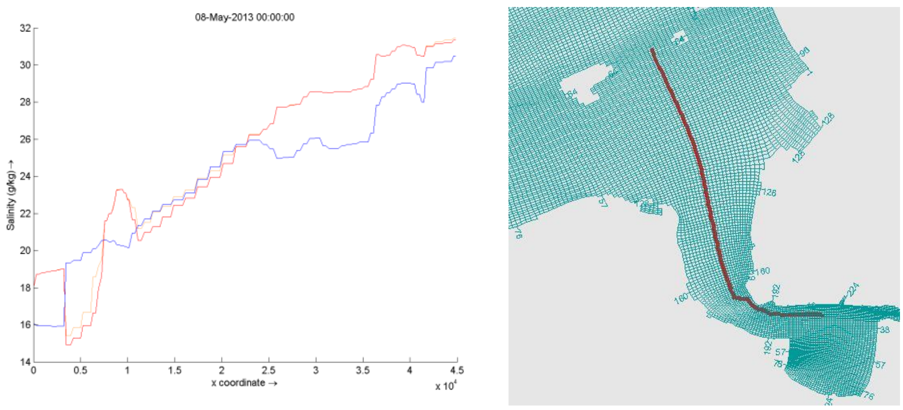

Figure 4.1 Blue: 2D recalculated salinity; red: 3D recalculated top layer; orange: 3D recalculated bottom layer. Date: 1 May 2012 over the transect shown in the right panel.

Hydrodynamic conditions for 2012 and 2013 (described in report 4) were aggregated horizontally (Figure 4.2) by 2x2 in deep waters (>= 5m), and by 4x4 in shallow (< 5m) water and vertically (resulting in one layer, thus a 2D model). Locations for open boundaries and points for nutrient loading were defined according to earlier versions of the water quality model (Figure 4.2). As compared to the TO-KPP version, one extra loading point was added at the German side of the estuary (Knocker Tief).

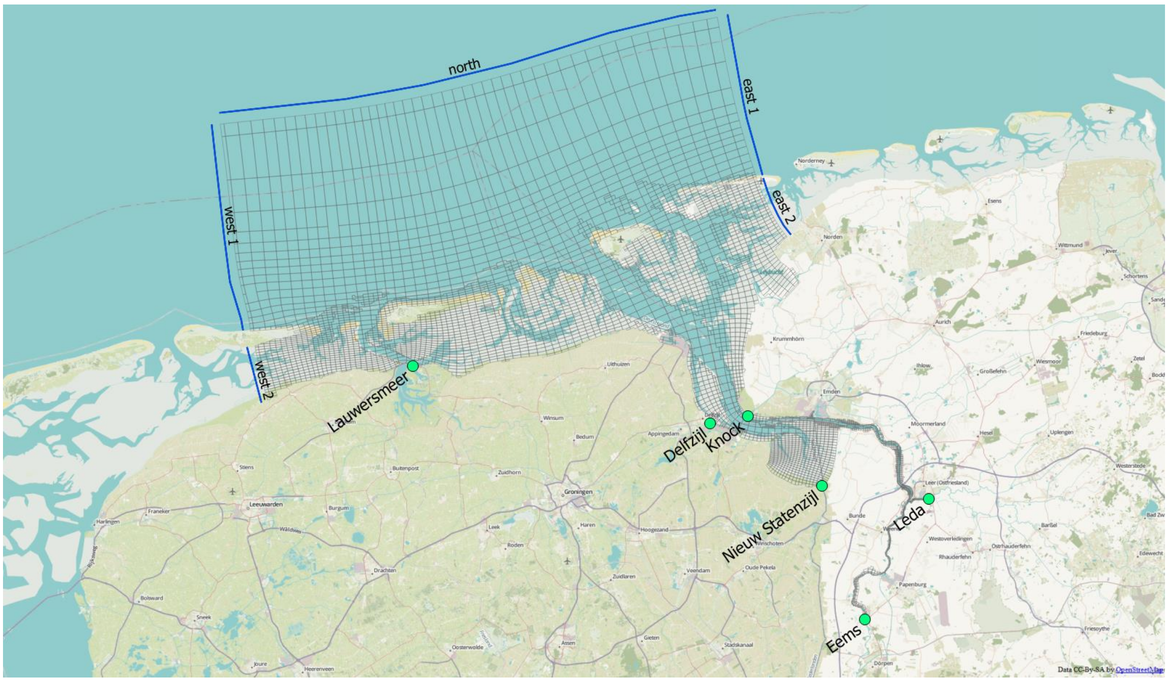

Figure 4.2 Computational grid (blue solid lines) with open boundaries and loading locations for the Ems-Dollard water quality model. The grid is aggregated as compared to the hydrodynamic grid (black dotted lines) by factor 4x4 for areas deeper than 5 m, and 2x2 for shallower areas.

4.1.2 Sediment grid

The water column schematization has been extended with a vertically layered sediment grid which allows for transport of particulate and dissolved substances through the water-sediment interface. Including 9 layers in the sediment results in an increase in computation time. The total thickness is 0.4 m. The sediment is horizontally aggregated as compared to the water grid, for performance purposes. Horizontally, the sediment grid was aggregated 8x8 hydrodynamic grid cells for deeper parts (>= 5 m depth) and 4X4 grid cells for shallower parts (< 5 m depth) (Figure 4.3).

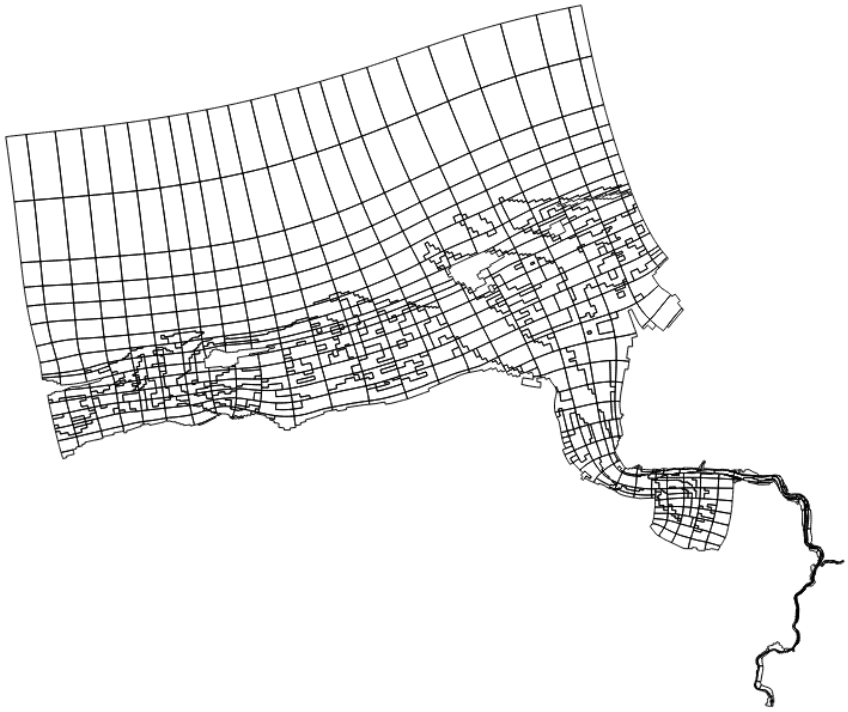

Figure 4.3 Horizontal lay-out of the computational grid for the sediment.

4.2 Selection of substances and processes

The predefined processes of the water quality and primary production model described in Stolte et al., (2012) were taken as a starting point for the current model. The current model description overlaps in many aspects with this previous description, but there are also some differences. These differences are described below

The model is set up and calibrated for 2012, and validated for 2013. This section describes the set-up, and will refer to earlier version (TO-KPP study, Stolte et al., 2012) of the water quality model set-up where appropriate.

4.2.1 Model configuration

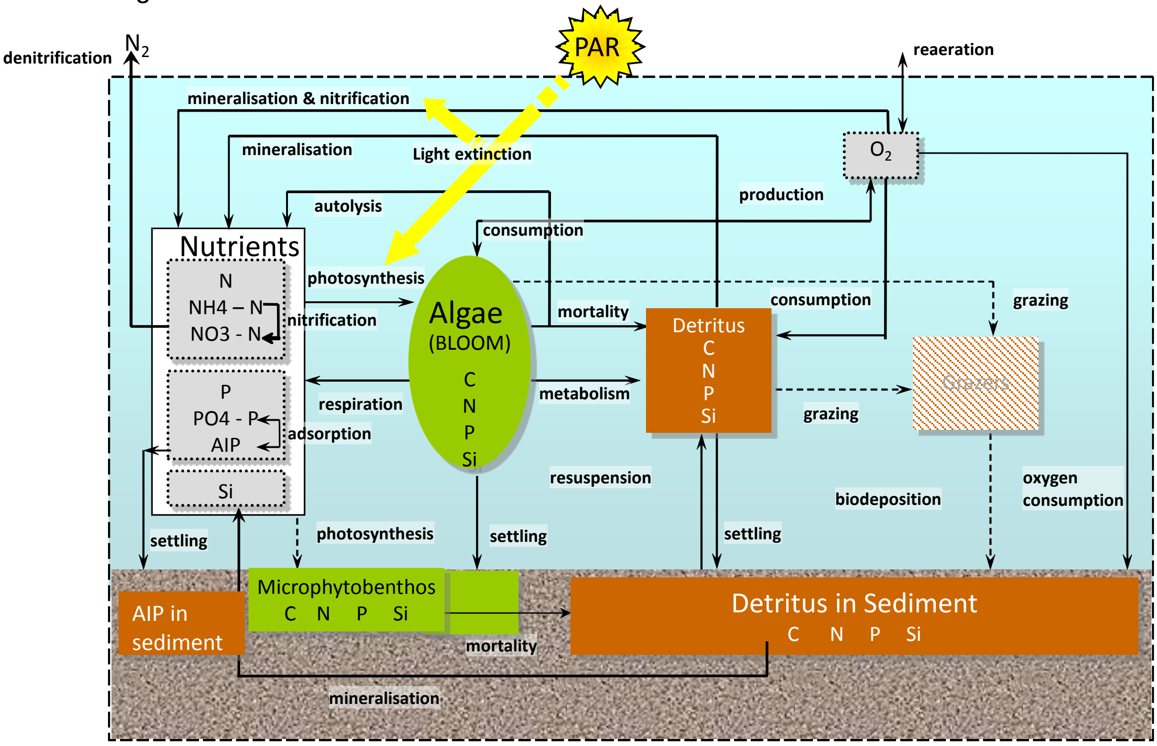

Figure 4.4 Generic Ecological Modelling configuration for modelling eutrophication effects in marine environments, for example used in the North Sea model. This scheme contains a simplified sediment nutrient model. For the current version of the model described here, nutrient cycling in the sediment has been modelled explicitly using several layers (see text and Figure 4.5).

The generic configuration for eutrophication (Blauw et al., 2008), which has been applied in numerous other model applications, has been used as a starting point in earlier versions of this model. This previous model included primary production by different phytoplankton species, including marine diatoms, flagellates, and *Phaeocystis* spp., full cycles of nutrients in the water phase and simplified nutrient cycles in the sediment (Figure 4.4).

The sediment grid provides a sediment column below each water column (or each set of water columns). Layers are sufficiently thin to generate steep concentration gradients across the sediment-water interface. Processes added as compared to the TO-KPP model version related to the speciation of phosphate and the redox potential dependent vertical concentration profiles in the sediment bed were added (Figure 4.5, Smits & Van Beek, 2013). All processes included in the model application proceed in both water grid cells and sediment grid cells, using generic process formulations.

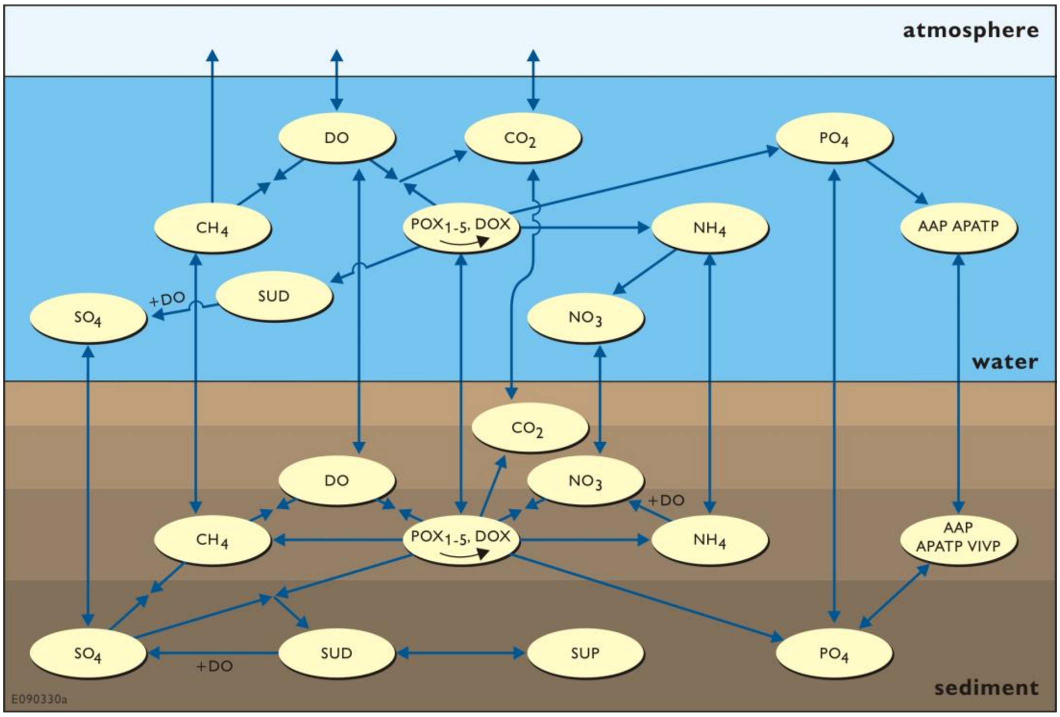

Figure 4.5 The water and sediment quality processes in the model version with extended sediment processes (except silicon related processes).

The different detritus substances and processes in the previous model were replaced by four detritus components, two "fast" decomposing components dominant in the water column, and two "slow" decomposing components dominant in the sediment bed. Opal silicate replaces the detrital silicate component. Adsorbed P, vivianite-P, apatite-P were added as additional phosphate components. Sulphate, dissolved and particulate sulphide, detrital sulphur and methane are expected to play a minor role in the Ems-Dollard but were included in the model to maintain overall consistency in mass and fractionation of electron acceptor usage in the decomposition of organic matter (Figure 4.5). Because carbon dioxide is assumed to be of no influence on the other processes, (e.g. Kromkamp et al. 1995), it was not included as a state variable.
DOC is the refractory dissolved organic matter. Silt and sand in the bed sediment are simulated as IM1 and IM2, respectively. IM3 is used for the forcing of suspended sediment (silt). IM3 is calculated as sum of the two different fractions of suspended sediment that were used in the sediment model. The extinction associated with suspended inorganic material is calculated as the extinction-weighted sum of the two fractions of suspended sediment from the sediment model, to account for the different extinction coefficients for the two fractions (section 4.4).

Thus, substances presently included in the Ems-Dollard model are:

- The organic carbon in the biomass of 3 selected marine phytoplankton groups (marine diatoms, marine flagellates, *Phaeocystis* spp.) and one group of micro-phytobenthos (marine diatoms). Each group consists of 3 types (N-, P-, and light-limited). Detrital organic matter (for carbon POC and DOC; for nitrogen PON and DON; for phosphorus POP and DOP; for sulphur POS and DOS). Methane (CH4).
- Ammonium (NH4) and nitrate (NO3).
- Dissolved phosphate (PO4), adsorbed phosphate (AAP), vivianite-P (VIVP) and Apatite-P (APATP).

- Dissolved silicate (Si) and opal silicate (OPAL).
- Dissolved oxygen (OXY).
- Sulphate (SO4), dissolved sulphide (SUD) and particulate sulphide (SUP).
- Inorganic sediment fractions (IM1 and IM2) in the bed.
- Inorganic sediment suspended in the water phase as the sum of two fractions from the sediment model (IM3)
- Salinity (Salinity).

The processes included in the present Ems-Dollard model with extended biogeochemical processes are described in Smits and van Beek (2013).
The vertical mass transport in the sediment results from advection and dispersion. Advection arises from burial (or digging) and seepage (tidally induced). Seepage is ignored in the present model, whereas only net settling (no resuspension) is included in the model. Dispersion results from bioturbation of particulate matter, and from bio-irrigation, flow induced micro-turbulence and molecular diffusion.
A generic description of all processes in D-Water Quality is provided by Deltares (2013).
The process formulations are used to calculate mass fluxes ($g.m^{-3}.d^{-1}$) for each of the water and sediment quality processes. These fluxes are added to an advection and diffusion mass transport equation, which is solved numerically. Although processes and formulations are generic in the sense that they are applied equally to the water column and the sediment bed, local conditions such as the presence or absence of dissolved oxygen determine the relative importance of processes.
All process coefficients are included in Tables A.1-4. Most process coefficients have been derived from calibration for Lake Veluwe (Smits and Van Beek, 2013) and for the western Wadden Sea (Delft hydraulics 2006).

4.2.2 Phytoplankton species composition

Marine diatoms, marine flagellates and *Phaeocystis* were included in the model. Freshwater species were not considered, because there is no fresh water (<5 promille) at any time in the estuary. In the river, freshwater species may occur, but suspended sediment concentrations are so high that significant growth will probably not occur.
Dinoflagellates, normally included in the North Sea models, do not occur in the Ems Estuary (Figure 4.6) and were therefore excluded. The parameter values for phytoplankton composition were taken from the North Sea standard setup.

4.2.3 Microphytobenthos

As described above, the updated present model for the Ems estuary maintains the (modified) BLOOM “Ulva” species to simulate “microphytobenthos” (Stolte et al., 2012). In the current 2D version of the model, the microphytobenthos is fixed to the lower 10 % of the total water depth, effectively experiencing light at the sediment-water interface. A clear simplification of the model as compared to nature is that nutrients are taken up directly from the water phase, and that oxygen is released in the water directly. The method has proven to give qualitatively correct results in the previous model version (Stolte et al., 2012).

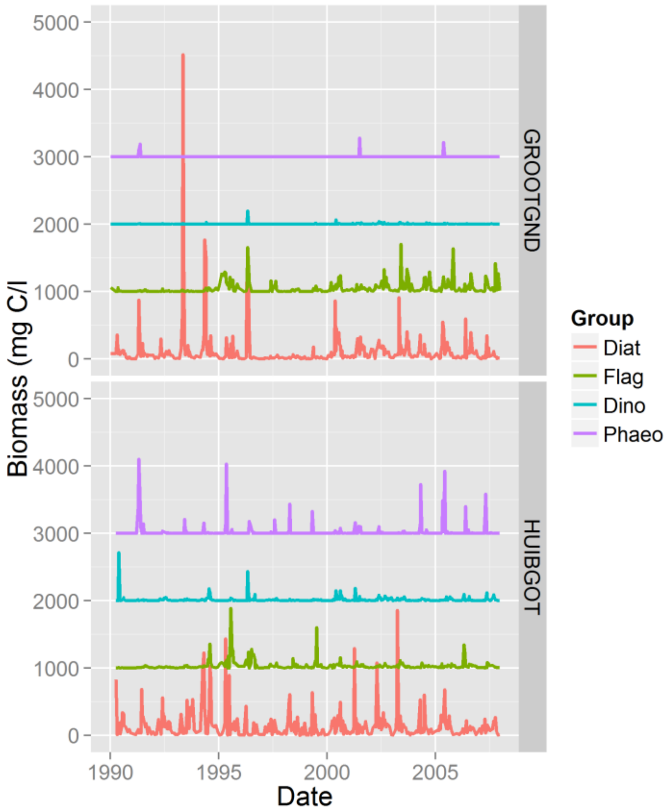

Figure 4.6 Historical development of phytoplankton groups (diatoms, flagellates, dinoflagellates, Phaeocystis spp.) at the stations Groote Gat Noord and Huibertgat Oost. For clarity, vertical scales have been shifted for each algal group. It is important to notice that the biomass contribution of dinoflagellates is minimal during the last 10 years. Source: Rijkswaterstaat Helpdesk water (DONAR), grouping according to Koeman et al., 2005.

4.3 Time steps

The time step used in the water-quality simulations is 5 minutes. The time step was chosen to offer the best compromise between accuracy and computing time.

4.3.1 BLOOM time step

The highly dynamic environment of the Ems estuary with steep gradients in light climate, salinity and currents resulting in highly fluctuating light climate has led to reconsideration of the time step for BLOOM, the module responsible for phytoplankton growth calculation. Generally, BLOOM is run with time steps of 24 hours. For every BLOOM time step, budgets of primary production and nutrients are calculated and fed back to the other processes in the water quality model. Internally, primary production within the BLOOM routine is calculated with a time step of 30 minutes to compensate for fluctuations in light availability over the day. However, in an intertidal area the average experienced light regime of a phytoplankton population fluctuates not only due to daily variation of incident radiation, but also due to lateral transport over mud flats and gullies. This variation is not accounted for internally by BLOOM, because the light history of a segment is accounted for only in a particular segment while, by tidal transport, phytoplankton are travelling through areas with different depth and therefore light availability. Potentially, a too long BLOOM time step can therefore lead to very high production over mud flats (where light is ample available), and underestimation of production and biomass in the deep parts. The experience in the current study is that this may result in high fluctuations in phytoplankton biomass. Furthermore, the effect of the tide becomes more visible with larger time-steps and a spring-neap cycle becomes visible. For those reasons, we have tested a shorter time step of the BLOOM module. In the previous model (model scenarios 2002), a time step of 8 hours had been used. In the current model setup, this still resulted in very high fluctuations of chlorophyll-a in the inner part of the estuary. Therefore even smaller time steps were tested (Figure 4.7). Finally, a time step of 1 h was chosen in order to prevent unnecessary high fluctuations due to “bursts” of growth at calculating time steps. This choice was based on the results in this study alone, and it should be investigated further how the BLOOM module may be improved in general to better deal with variation of light availability due to lateral transport[1].

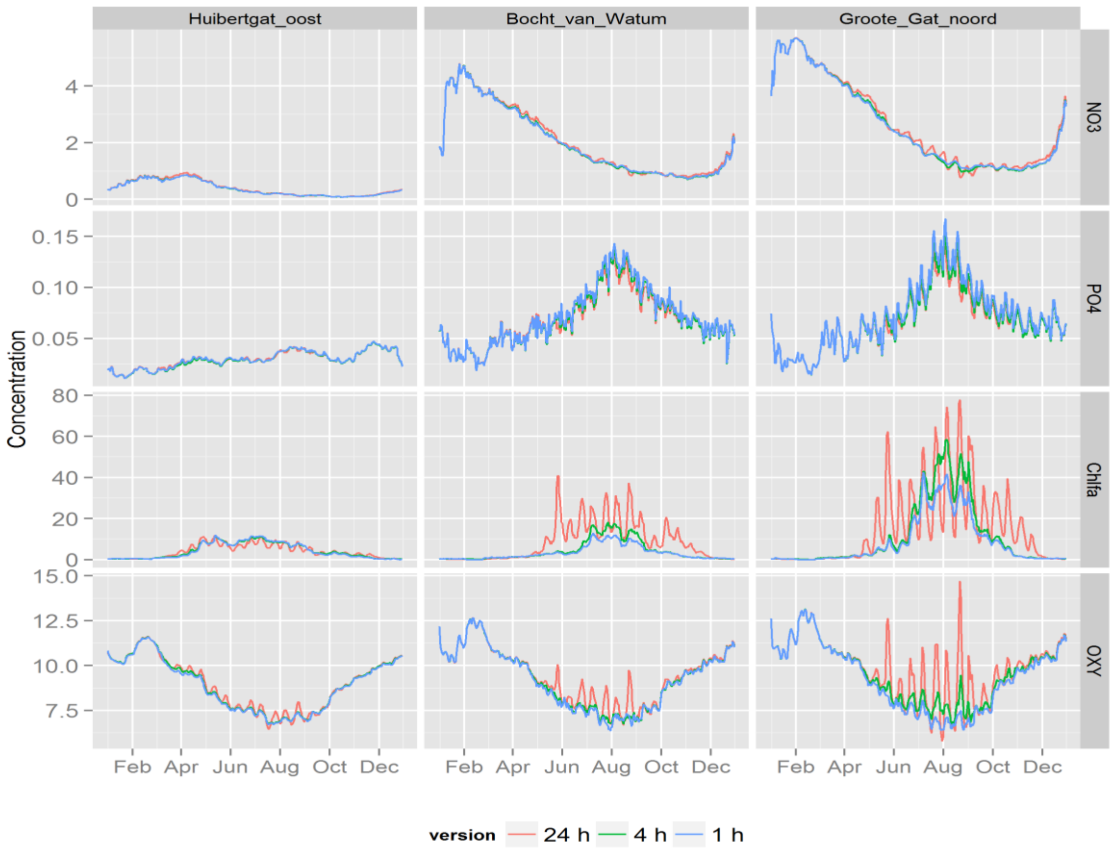

Figure 4.7 Comparison of daily averaged model results using a BLOOM time step of 24 h, 4 h, or 1 h. Large fluctuations with an approximate periodicity of the spring-neap cycle occur at time step of 4 hours and longer. From these results, it was decided to use a 1h time step.

[1] *Currently, a software development is going on to let BLOOM account for the variation in available light due to horizontal transport of water and algae in estuary with steep depth gradients. This is initiated by the current modelling work in estuaries. It is expected that this software development will improve the calculation of primary production in highly varying environments like the Ems estuary without having to decrease the BLOOM time step.*

4.4 Physical forcings

4.4.1 Suspended sediment forcing

Suspended sediment (or suspended particulate matter, SPM) concentrations are extremely important for primary production modelling, because this is the main factor for light attenuation in the water column. Therefore, the primary production results are likely to be very sensitive to this parameter. At the same time, it is very difficult to estimate the spatial distribution of SPM in the whole estuary from e.g. MWTL measurements which are only done in the channels, at three locations (MWTL stations).The SPM concentrations were derived from the calibrated and validated sediment model output. The sediment model is calibrated on these 3 MWTL locations and other measurements as well (see sediment model report 5). The base of the suspended sediment forcing is the model output per hour of IM1 and IM2 (two fractions of suspended sediment). Sediment forcing and light extinction for each time step and grid cell was obtained in the following steps

- Horizontal aggregation to the water quality model water grid
- Vertical aggregation to one layer (2D) was done by averaging the sediment concentration from the top 50% (corresponding to layers 1 and 2 in the sediment model). The reason for this is that the top layer is relevant in comparison with MWTL and IMARES monitoring at 1.5 m depth. Also, this part of the water column is expected to be of highest importance for phytoplankton production.
- IM1 and IM2 were summed as input for total suspended sediment IM3 in the water quality model

For consistency of the model chain, the final sediment model runs in the accompanying sediment model report (report 5) have been used as input into the water quality and primary production model.

As an alternative for direct coupling of sediment model output, a cosine function for sediment dynamics is often used as input for water quality, in many of the North Sea studies (Los, Villars and van der Tol, 2008, Deltares rapport 2012). This is done to correct for small model artefacts in the sediment model that have a large influence on primary production. Briefly, the seasonal dynamics of sediment is determined with a cosine function, the average and amplitude come from the silt model and measurements. The wind field is used to include short term variation. The cosine function is included in the calibration procedure (section 5).

4.4.2 Light extinction of suspended sediment

Extinction of light is simulated by the model software by adding up the calculated extinction caused by phytoplankton, suspended sediments, dissolved organic matter and a background extinction. In the current model set-up, light extinction due to suspended sediment is pre-processed together with a background extinction (0.08 m-1), and used in the model as a time- and space-dependent input (segment function). For both suspended sediment fractions, a specific extinction coefficient of 0.025 was used (Los and Blaas 2010).

- The contribution of SPM to the light extinction coefficient (K_{spm} in m^{-1}) was calculated using the specific extinction coefficients (K_1 and K_2 in m^2 mg^{-1}) for the two suspended sediment fractions IM1 and IM2 (in mg m^{-3}) by $K_{spm} = K'_1*IM1 + K'_2*IM2$ for each segment and time step. This is similar for the cosine function.
- In the Ems river, suspended sediment concentrations as modelled by the WED model were unrealistically low. This is mainly because the WED model is not suitable to model the special conditions in the Ems river. In order to prevent algal growth in this part of the model, the minimum extinction was set to 20 for the Ems river. This effectively prevented phytoplankton completely.

- For a selection of segments in the Dollard, also quite low suspended sediment concentrations were calculated with the WED model. This led occasionally to very high phytoplankton concentrations at the edges of the Dollard (Figure 4.8), which does not seem to be realistic. To effectively stop pelagic primary production in those areas, a minimum extinction was calibrated to 20.

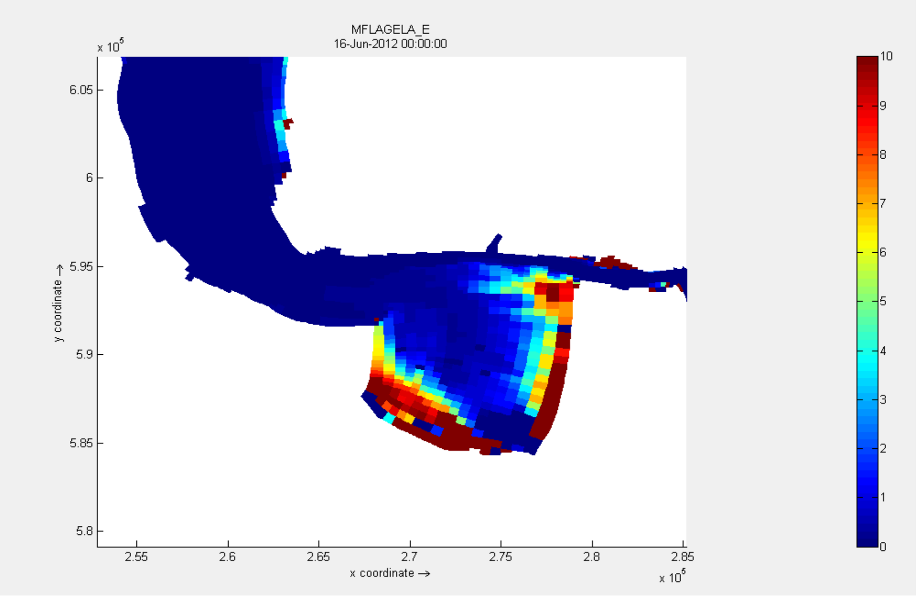

Figure 4.8 Occasional high biomass of phytoplankton (in this case, flagellates in g C /m3) at the edge of the Dollard. Although the contribution to total biomass is limited due to the shallow depth, it has a great influence on modelled phytoplankton concentrations at station Groote Gat Noord.

4.4.3 Meteorological forcings

Water temperature - The water temperature used in the water quality and primary production model is taken as the average of the three MWTL stations within the estuary. The sediment bed has the same temperature as the water column. Locally, especially in shallow areas and during drying of mud flats, temperatures may deviate from this average, causing an under- or overestimation of process rates. This has not been investigated further.

Wind velocity - Daily measurements of wind speeds for year 2012 at “Nieuw Beerta” were obtained from the KNMI database. Wind velocity is assumed to be spatially constant but temporally variable specified as time series measurements. Wind velocity is included in the water quality model since it is used to determine oxygen re-aeration between the water surface and the overlying atmosphere and vice-versa (see Delft3D technical reference manual for details).

Surface irradiance - Surface radiation values ($J/m^2/d$) obtained from the KNMI station “Nieuw Beerta” for the year 2012 were converted to daily averaged fluxes (W/m^2). It is assumed that the surface radiation varies in time but is spatially constant. A comparison with stations nearby (Terschelling and Lauwersoog) verified this assumption (Figure 4.9).

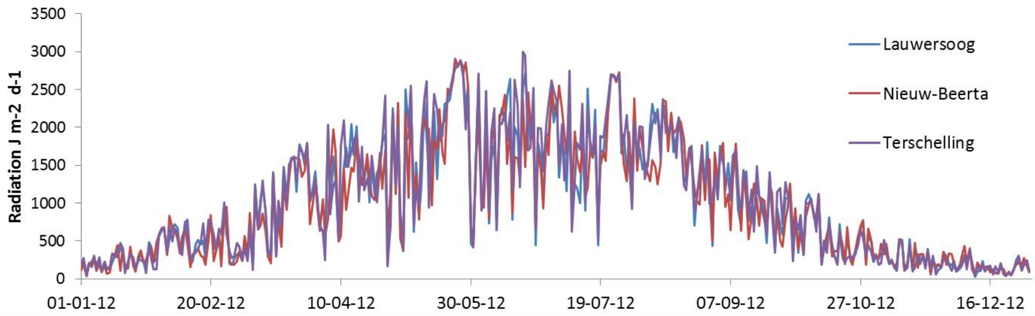

Figure 4.9 Total radiation at the surface used for the Ems-Dollard grid derived from radiation at KNMI stations Lauwersoog, Nieuw Beerta and Terschelling. Data from Nieuw Beerta are used as incident radiation forcing.

4.5 Boundary conditions

4.5.1 Open boundaries

The transport of substances over the boundaries is calculated using the water transport from the hydrodynamic model, and concentrations based on the Rijkswaterstaat MWTL monitoring station Terschelling10 has been used for forcing of substance concentrations at the western, northern and eastern boundary (Figure 4.10). This is the station closest to the Wadden Sea, but still outside the model grid, containing measurements in 2012. This station is representative for nutrient fluxes coming from lake IJssel and the Wadden Sea.

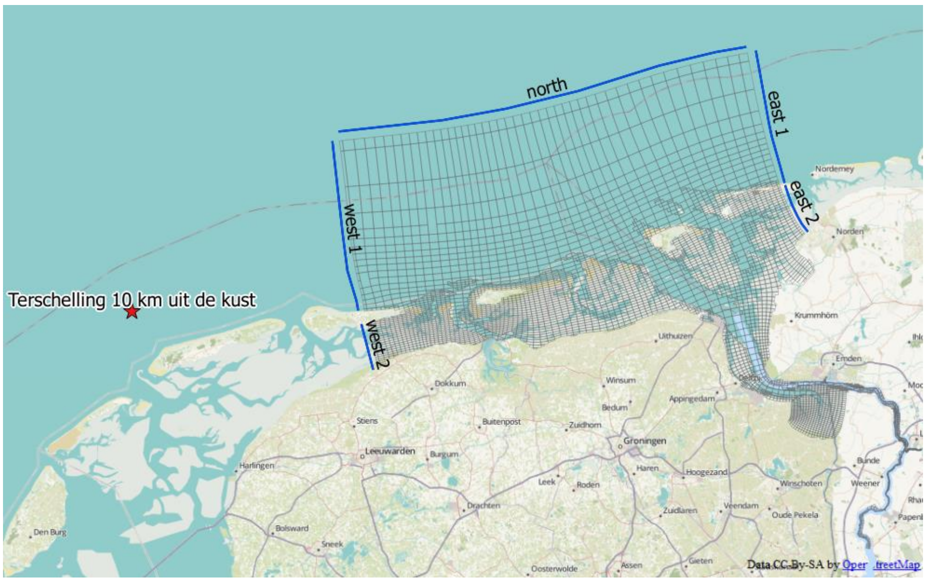

Figure 4.10 Data from the MWTL station "Terschelling 10 km uit de kust" (red star) was used to define boundary conditions.

Concentrations of relevant substances at the open North Sea boundaries from the available monitoring data were obtained by the following steps:

a) Missing measurement data were replaced by linear interpolation.
b) Measured variables were, where necessary, converted into the explicitly simulated variables. Variables without matching observed variables were estimated from other variables. This is explained in the text.

The boundary for the total amount of particulate detrital organic carbon was determined as measured TOC minus Algal C (determined from chlorophyll-a).
Constant N/C, P/C and S/C ratios were used to calculate the total amounts of nutrients in particulate and dissolved detrital organic matter and algae biomass assuming light limitation in algae.

Application of these kind of rules may sometimes result in negative numbers which are replaced by zero values. This has no negative effect on model performance.
The yearly net transport of total nitrogen and phosphorus based on the described model input is visualized in Figure 4.12. Yearly net transport over the boundaries is 35 and 25 times higher for nitrogen and phosphorus respectively as compared to the loads from the Ems (Figure 4.13).

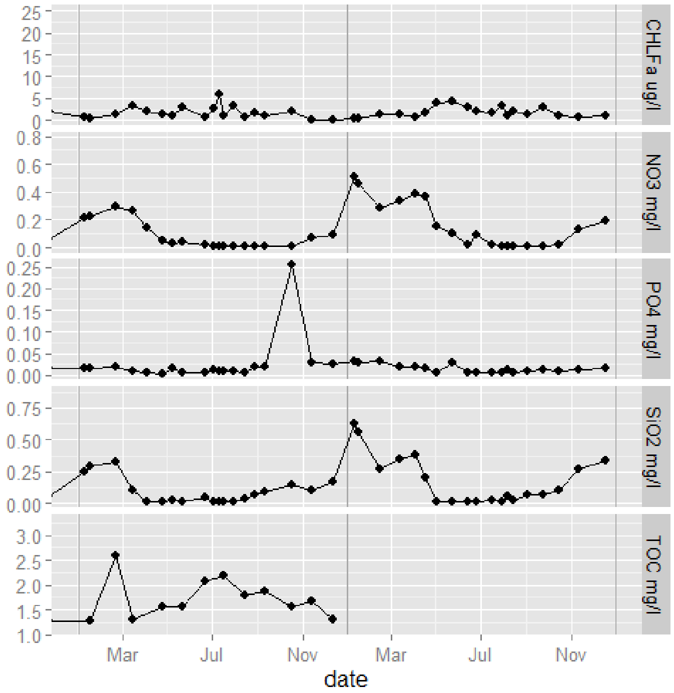

Figure 4.11 Dissolved reactive nutrients and chlorophyll-a at Terschelling 10, used for boundary concentration definition. The values of PO4 in October 2012 is considered to be an outlier.

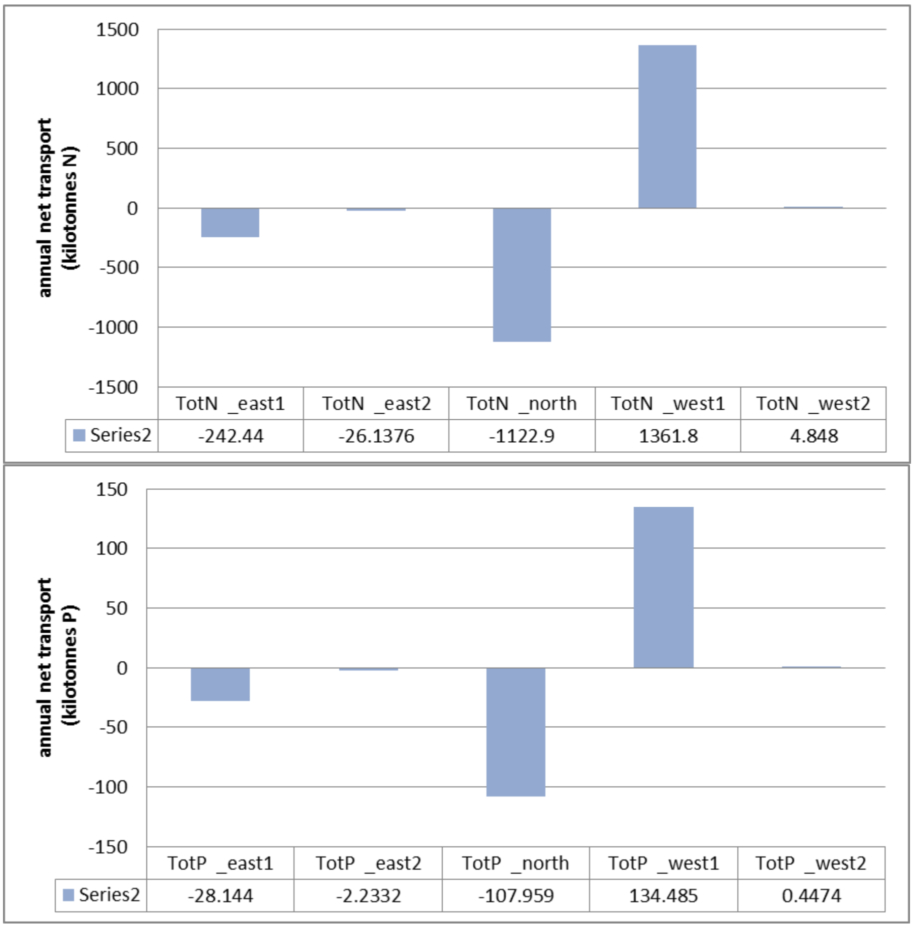

Figure 4.12 Total net transport of nitrogen (above) and phosphorus (below) over the open boundaries (boundaries indicated in Figure 4.2). Positive values indicate net inward transport, negative values represent net outward transport. For comparison, the net inward transport over the west1 boundary is approximately 35 and 25 times higher than the yearly load of nitrogen and phosphorus respectively from the Ems river (compare to combined loads of Ems and Ems/Leda, Figure 4.13).

4.5.2 Loads

Atmospheric deposition of nitrogen is applied as in a previous version of the model (Stolte et al., 2012). It is assumed to be constant in time and space at values derived from EMEP modelled deposition maps, collated using the Baltic Nest application (nest.su.se). The deposition distinguishes between reduced nitrogen (as ammonium, 0.0024 gN/m2/d) and oxidized nitrogen (as nitrate, 0.0016 gN/m2/d).

External surface water loads of substances on the Ems-Dollard arise from the following sources:

- the River Ems
- the River Leda
- the catchment of the Westerwoldse Aa discharging at Nieuw-Statenzijl,
- Dutch polders discharging at Delfzijl
- German polders discharging at Knock
- Dutch polders discharging via Lauwersmeer

The total loads of nitrogen and phosphorus are visualized in Figure 4.13. It is obvious that the Ems loads for nitrogen and phosphorus are dominating. The smaller loads, however, may have influence on a local scale.

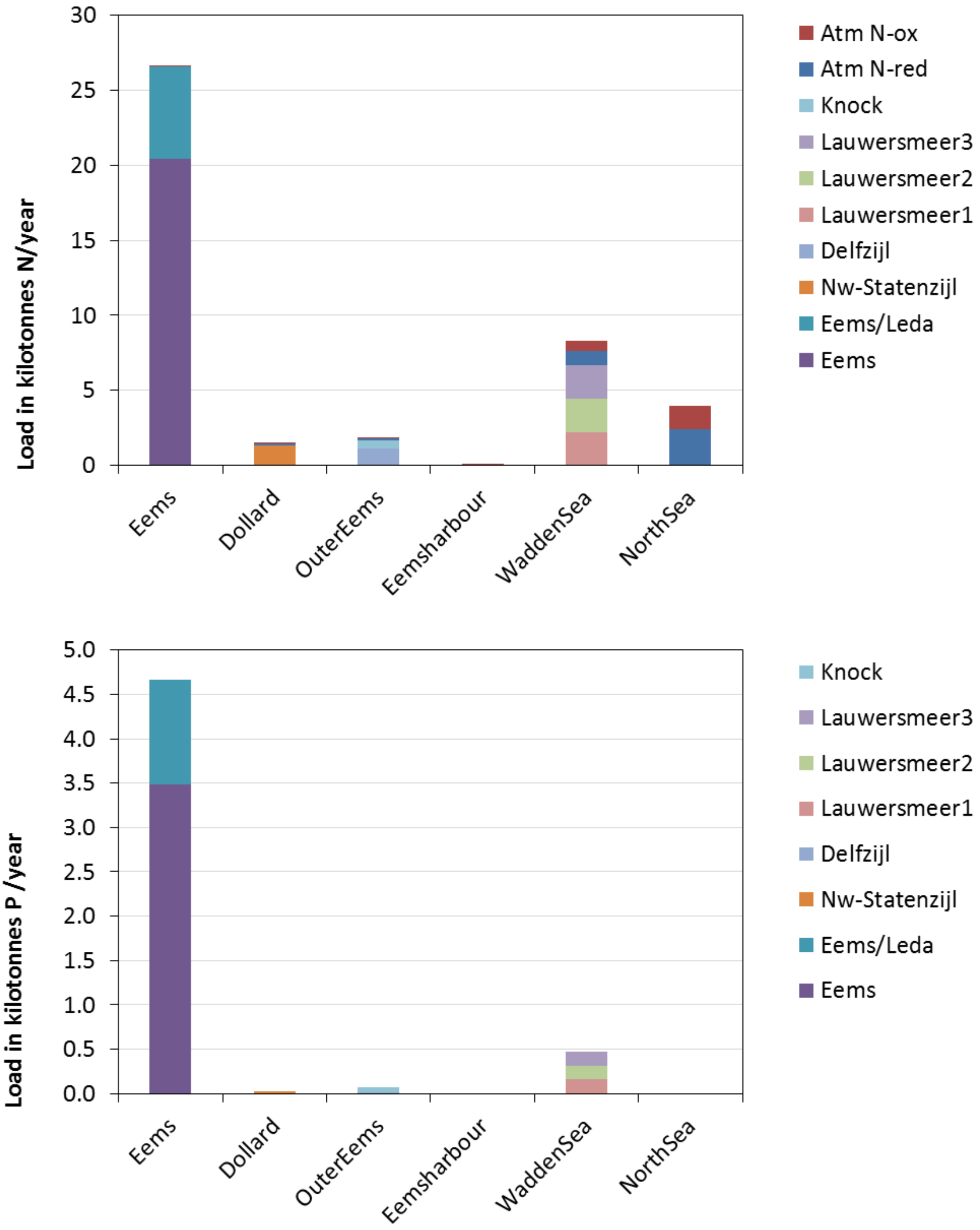

Figure 4.13 Loads of total nitrogen (above) and phosphorus (below) used in the model. The Ems/Leda merges into the Ems before the outflow into the Dollard. This makes the total load from the Ems at least 10 times higher than any of the other loads. Loads are organized per area as defined in Figure 4.20.

The loads are imposed on the model as the result of flow rates and concentrations. The following general steps have been taken to derive the concentrations of relevant substances for these loads using the available monitoring data (for details, see text in next section):

a) Concentrations from the monitoring point “Leerort” (Figure 4.14) have been used to define the concentrations in the rivers Ems and Leda, as they both discharge via this monitoring location.
b) Polder water discharges were included at Delfzijl, Knock and Lauwersmeer.
c) The same 2010 data have been used for the loads from Lauwersmeer as were used for previous modelling, because the 2012 data for Lauwersmeer were not available.
d) Missing data were interpolated.
e) Data “below detection limit” were set at half the detection limit.
f) Because the measured variables are partially not the same as the simulated variables, the non-matching measured variables were converted into the simulated variables (appendix C).
g) A priori guesses were made for simulated variables that have no matching observed values. This is further explained in the text and appendix C.

Water quality loads were obtained after request from Water Board of Hunze en Aas and Noorderzijlvest in case of the Dutch polder loads, and from NLWKN Niedersachsen for the German data on Ems water quality (pers. Comm.).

The following paragraphs present information on the water quality variables representing the Ems and Ems/Leda, and conversion into the concentrations of the simulated substances. The model produces the loads by multiplication of concentrations and flow rates. The latter are imposed on the water quality model as delivered by the Delft3D-FLOW hydrodynamic model. The concentrations and formulations for the smaller loads are presented in Appendix B-1.

Similar as for the boundary conditions the concentrations of a number of simulated substances are set equal to zero for all loads. This includes IM1, IM2, SUD, SUP, CH4, VIVP, APATP, OPAL, POC4 as well as all algae species. The concentrations of these substances are negligibly low in the water column. Freshwater algae die when discharged into saline water. In the model all algae biomass in the freshwater loads is instantly turned over into the detritus pools (POX).

4.5.2.1 Rivers Ems and Leda loads

The monitoring locations are shown in Figure 4.14. Figure 4.15 show a selection of the 2012 data relevant for the waterquality study for of the monitoring locations in River Ems. The monthly data from location “Leerort” downstream of the confluence of the rivers Ems and Leda have been used for the sum of the loads of both rivers.

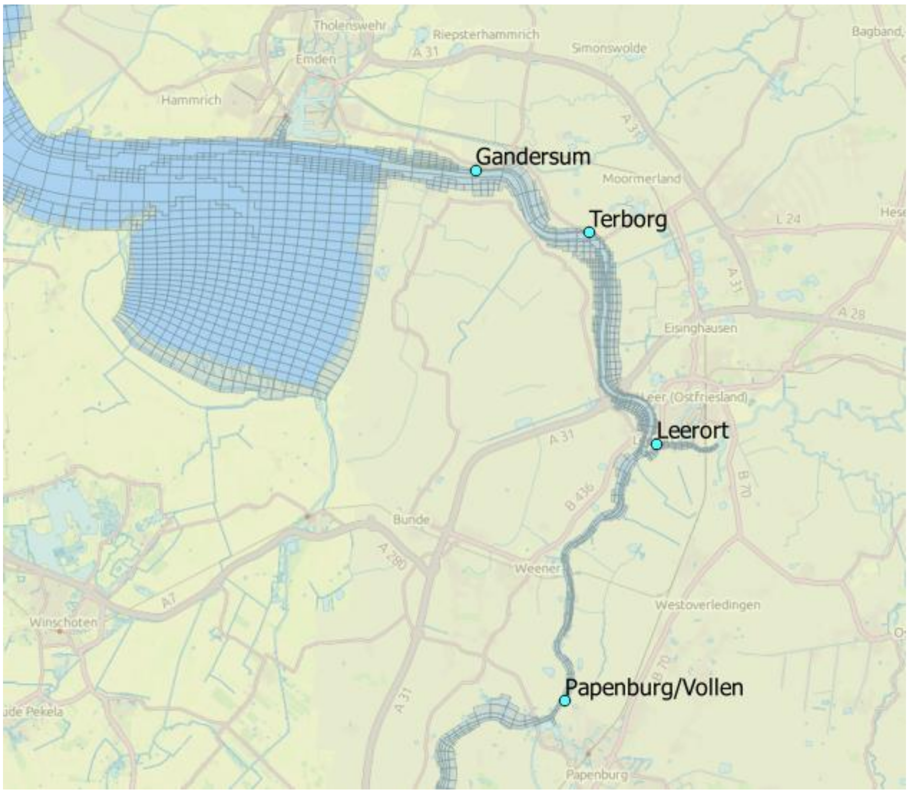

Figure 4.14 Overview of monitoring stations in the Ems River. Concentrations at Leerort were used to define concentrations for the river loads from Ems and Leda.

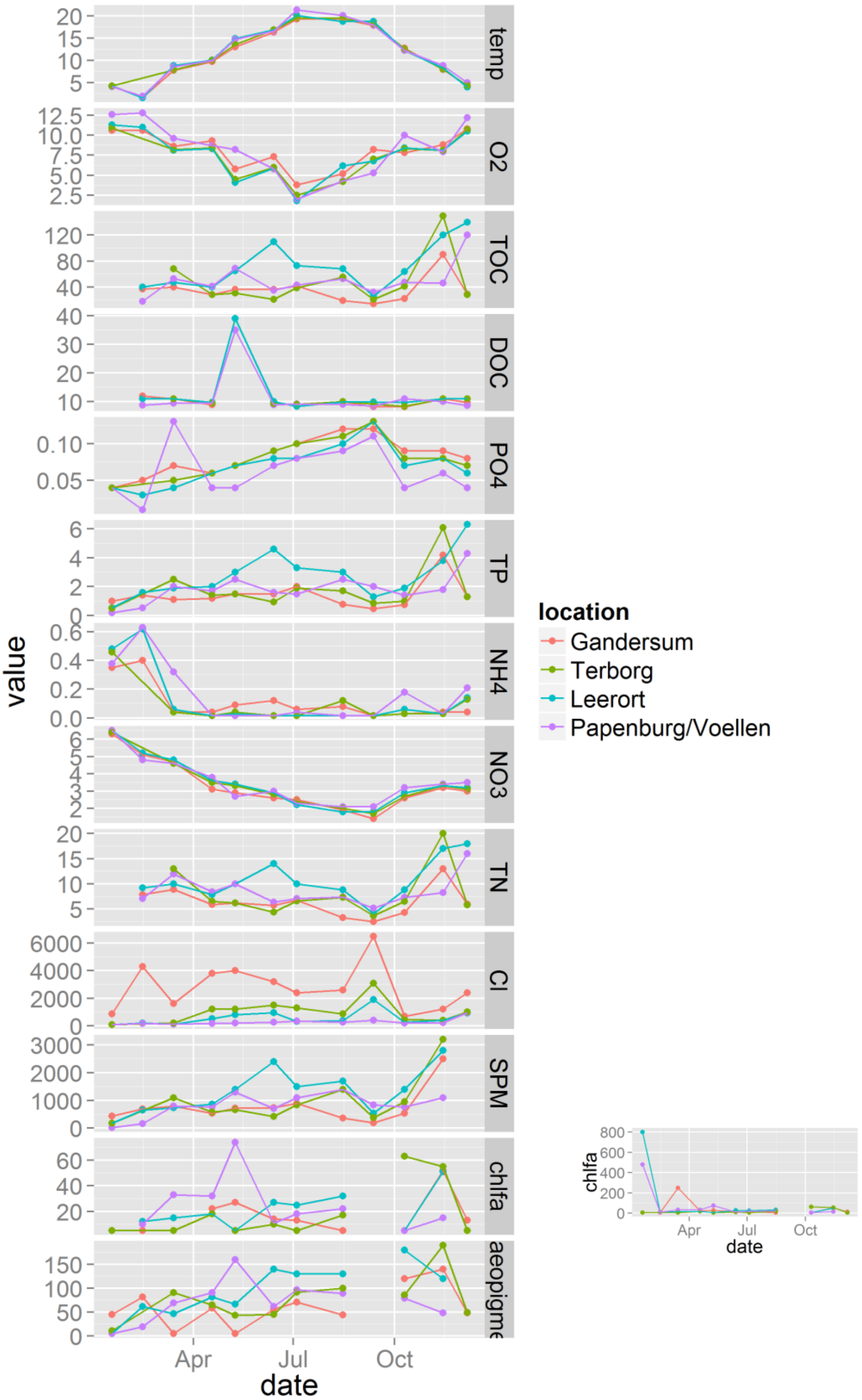

Figure 4.15 Concentration at the different loading locations in the Ems. Three very high chlorophyll a values (>200 ug/l) in January and March were removed, because they were considered unrealistic (see small graph). For September, no measurements were available. Locations are shown in figure 5.6

Silicate observation data were not available for the Ems river (personal correspondence with NLWKN) and was therefore estimated by extrapolation of Si concentration to a value at zero salinity for each month (Figure 4.16 and Table 4.1).

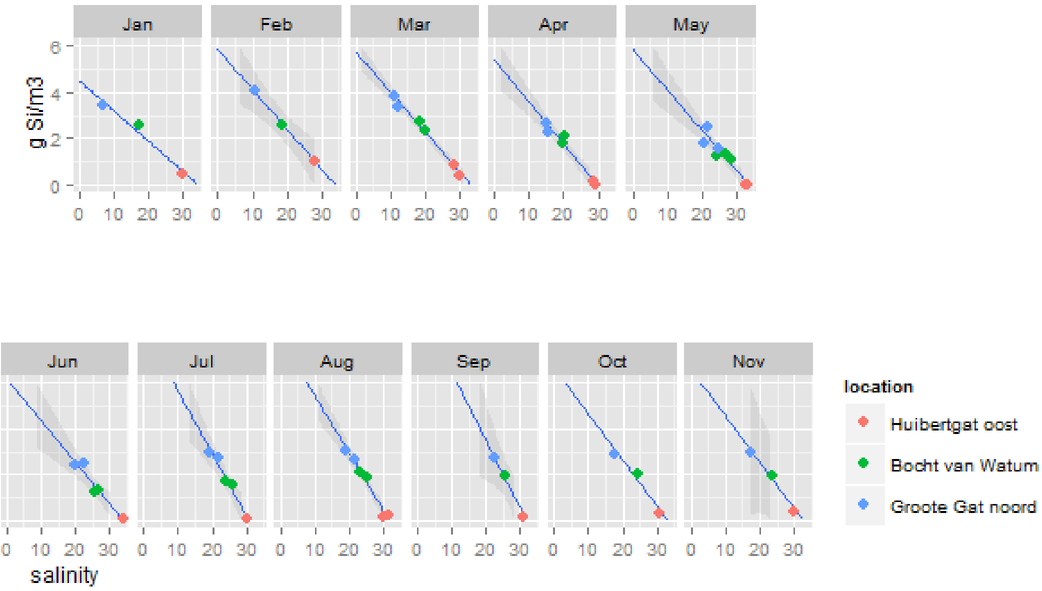

Figure 4.16 Dissolved reactive Si (MWTL) as a function of salinity, fitted with a linear model. The dark grey area indicates the 95% prediction interval (could not be calculated in Jan and Oct).

Table 4.1 The estimated silicate values in mg Si/l in the Ems river, based on extrapolation of MWTL measurements to zero salinity based on linear regression.

month	value	Std. Error	P-value
Jan	4.46	0.31	4.44E-15
Feb	5.81	0.41	8.66E-15
Mar	5.69	0.30	0.00E+00
Apr	5.36	0.40	4.06E-14
May	5.81	0.54	9.60E-12
Jun	5.92	0.50	7.08E-13
Jul	8.29	0.74	2.76E-12
Aug	7.90	0.59	3.91E-14
Sep	9.39	1.08	1.12E-09
Oct	6.60	0.69	1.19E-10
Nov	6.54	0.66	5.56E-11

Detailed information on quantitatively less important loads are given in Appendix 8BC.

4.6 Initial water and sediment composition

4.6.1 The water body concentrations

The initial composition of the water body was determined in two steps. The realistic concentration fields of the substances resulting from the previous model version for the end of the 2001 simulation (31 December) were converted into tentative initial concentration fields of the substances in the new model starting at 1 January 2012. The resulting concentration fields were used as initial composition in the first 2012 simulation with the new model. In a second step, it was assumed that water concentrations in 2012 are cyclic, and the concentration fields that resulted from the new model for the end of 2012 (31 December) were taken as initial composition input file in 4 successive year simulations. This resulted in a stable initial composition that returns at the end of a year simulation.

4.6.2 The sediment bed

The initial composition of the substances in the sediment bed was derived as a function of silt content of the bed. The observed and the simulated silt content fields in the Ems estuary, (report 5) were used for this purpose. These fields are quite similar but the simulated field has lower silt contents in the central part of the estuary. Since no data on the relation between silt content and sediment composition were available for the Ems estuary, sediment composition data for the Western Wadden Sea from studies by Delft Hydraulics (1983) and RIKZ Rijkswaterstaat (1988) were used to prepare regression analysis of relevant substances with silt content. These regression equations were then used to derive initial sediment composition from the sediment silt concentration field generated with the Delft3D-WAQ sediment model (report 5).

The regression equation details are further explained in Appendix D.

Silicate return flux as a result of release of adsorbed silicate (a process not covered yet by the model) was approximated by enhancing the initial OPAL-Si concentration in the sediment. This has no consequences for other processes.

Furthermore, the model was run by a number of years by using the output of the model at 31st December 2012 as initial situation input for the next model run, assuming that the year behaves more or less cyclic. In total, 4 cycles were run after which the conditions at the end of a year did not deviate from start conditions.

4.7 Monitoring stations and areas

4.7.1 Observation points for validation

Figure 4.17 Location of different validation measurements. Three MWTL stations (green) will be used (Groote Gat Noord, Bocht van Watum and Huibertgat Oost). As part of this project a monitoring program has run during 2012 with primary production measurements (blue), and Pocket Ferrybox monitoring of several parameters, including phytoplankton fluorescence (line).

4.7.2 Processing of observations at IMARES monitoring stations

During 2012, monitoring additional to the MWTL long-term monitoring was performed by IMARES as part of this project. The stations that were sampled approximately every two weeks during 2012 are located as a transect of 6 stations through the estuary and are especially suitable to validate the longitudinal patterns that the model produces. .

4.7.3 Observation points for phytobenthos biomass

During 2013, microphytobenthos biomass and production was measured by IMARES in this project (report 9). The segments in which the monitoring positions were located are presented in Figure 4.18 More than for pelagic monitoring stations, the spatial variability of biological processes in general, and primary production in particular can be expected to be very high, because there is no horizontal dispersion of importance in the sediment.

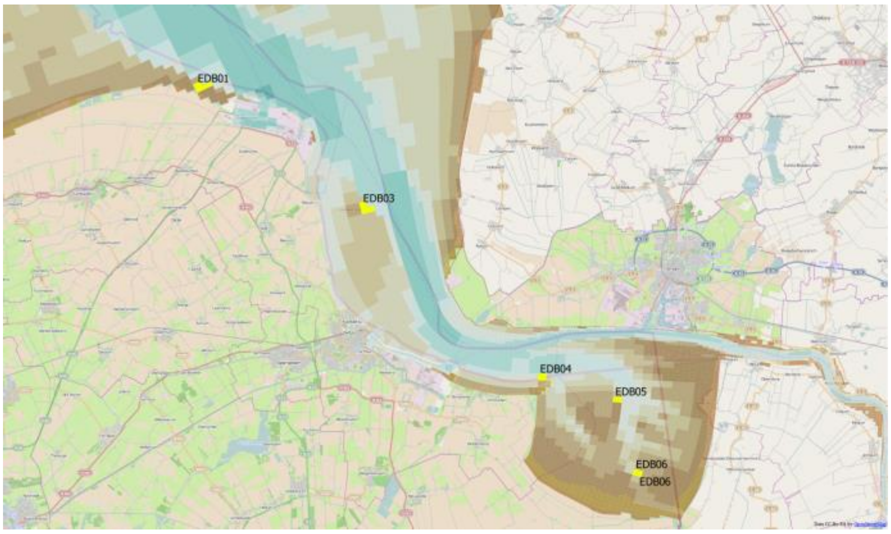

Figure 4.18 Segments (in yellow) in which monitoring stations were located for microphytobenthos biomass and production.

The values obtained for a segment are representatives for the whole segment, and do therefore not necessarily conform exactly to the conditions of the observation station with respect to depth, and therefore light climate, phytobenthos biomass and production. Validation of these variables can therefore be expected to be less strict with regard to exact numbers, and should be focussed at relative values and the general pattern of variables in time for example. Observation areas are defined to calculate overall fluxes of substances through the estuary and to calculate area-integrated fluxes like net primary production. Also, average concentration of substances are produced for each area. Three sets of observation areas were defined and used for reporting.

1 Grid-covering areas for total balances of substances. These areas were used to calculated fluxes of nutrients through the estuary (Figure 4.19).

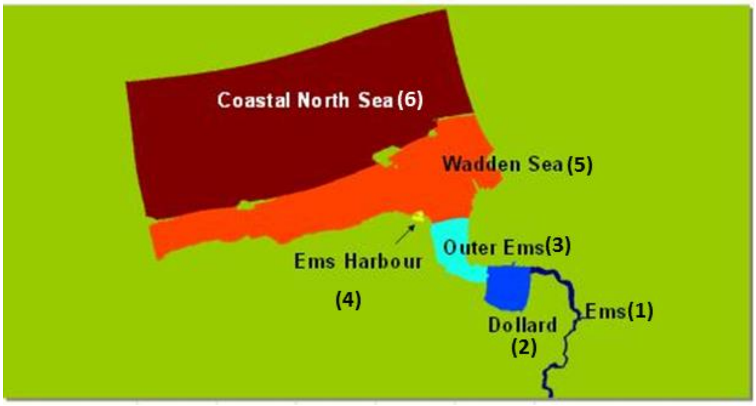

Figure 4.19 Observation areas used for calculating nutrient fluxes throughout the estuary.

2 Areas for comparison with IMARES primary production calculations. These areas correspond to the areas that were used by IMARES to calculate integrated primary production (Figure 4.20). Modelled yearly balances for primary production by algae were calculated for each area to compare with results from measurements.

Figure 4.20 Observation areas to compare integrated model results with areas used by IMARES to calculate primary production.

5 The calibration procedure

The first test to judge whether the coupling of the water quality and primary production model to the hydrodynamic model works well is to visualize the values of continuity and salinity over the grid.

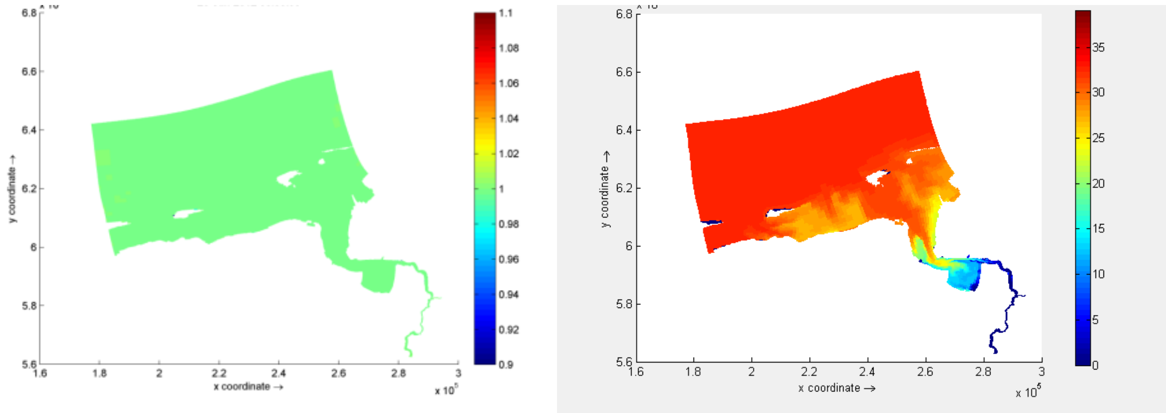

Figure 5.1 Distribution of continuity (left) and salinity (right) throughout the model grid for 28th June 2012 (randomly chosen). Continuity of 1 means that water transport phenomena from FLOW are implemented correctly in the water quality model.

The transport and dispersion of conservative tracers is modelled correctly, by checking a tracer which is added to the model in concentration 1, called continuity. This can be regarded as a numerical check of the coupling procedure. For the current set-up, continuity was 1 in all the segments of the model (Figure 5.1), indicating no numerical abnormalities due to the coupling. Furthermore, recalculated salinity distributes over the estuary in a normal pattern (Figure 5.1).

5.1 Calibration and results presentation

The results are presented as time series comparing modelled and observed values, while the goodnes of fit (GoF) has been illustrated in so called “target diagrams”. In a target diagram, the normalized unbiased Root Mean Square Difference (nuRMSD or uRMSD*) is projected on the horizontal axis, showing the over- or under-estimation of variability of the model results as compared to the observations. On the vertical axis, the normalized Bias (nBias or Bias*) is projected, indicating the over- or underestimation of the average values. Negative values indicate underestimation, positive values indicate over-estimation by the model. For specific purposes, the nuRMSD and nBias can be calculated over relevant time periods, e.g. summer or winter. Important underlying assumptions of the interpretation are:

- The model variable is well represented by the observation variable
- The observation value represents the “true” value

In a target diagram, all points within the widest circle are regarded as a “reasonable fit”, while points within the smaller (striped) circle are regarded as “good fit” (**Error! Reference source not found.**). The criterium “good fit” is based on the relation between RMSD’* en R^2 and a circle with diameter of 0.67 compares to $R^2 = 0.74$ (Los & Blaas, 2010, Jolliff et al., 2009).

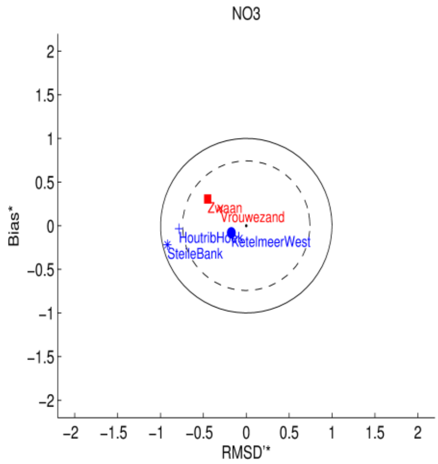

Figure 5.2 Example of target diagram, in this case for nitrate concentrations in Lake Ijssel.

5.2 The calibration procedure and use of monitoring data

For calibration of the model, results for 2012 were compared to MWTL measurements for the three available stations. An important step in the calibration procedure is the adaptation of the suspended sediment field from the sediment transport model. As described in report 5, various suspended sediment concentration observations were mutually inconsistent, with suspended sediment concentrations measured at MWTL stations being lower than measured at Imares stations and at GSP stations. These latter two sources were primarily used for calibration of the sediment model, whereas the availability of extinction measurements makes MWTL stations more useful for the extinction modelling. To reproduce the extinction at these MWTL stations accurately, it was necessary to lower the suspended sediment concentration fields. The calibration was done according to the following steps:

1. Compensation of overestimation of chlorophyll-a at Groote Gat Noord by artificially raising the light extinction in the Ems and in shallow parts of the Dollard. The rationale behind this is explained in section 4.4.
2. Because modelled suspended sediment concentrations (sediment model) and resulting extinction (WQ model) were approximately 2x higher than measured at MWTL stations, the suspended sediment forcing from the sediment model was reduced by a factor 2. Modification was done by only applying a constant factor over the whole model domain.
3. In order to better describe the seasonal variation of extinction, the concentration of suspended sediment from the sediment model was redistributed in time by applying a cosine distribution on the average suspended sediment concentration for each model segment. This improved the seasonal distribution as judged from time series comparison.

   Modelled pelagic chlorophyll-a was compared to measured values. At this stage, it appeared that at locations where average extinction was modelled correctly, average pelagic chlorophyll-a was modelled correctly too. It was decided to not further calibrate any phytoplankton characteristics.
4. Modelled benthic chlorophyll-a concentrations were compared to measured values and calibrated by adjusting phytobenthos growth parameters.

After these steps, no further calibration was done to improve the modelled nutrient concentrations. As it appeared, light was the main regulating factor for primary production in the estuary, and nutrients are always available in ample amounts in the estuary plume.

In the following part, the calibration procedure is shown in steps, by showing time graphs and target diagrams of extinction and chlorophyll-a at MWTL stations for 2012. Two different target diagrams are shown:

- A target diagram showing one dot for each station and substance. Here the deviation is shown for each station.
- A target diagram with only one dot. The variation between stations is also taken into account in the target diagram. This type also gives an answer on how well the between-station variation is described by the model.

The different plots tell different stories. A time plot is subjective, but it may be used to judge the models performance to reproduce patterns. The first target diagram explains objectively how well the substance is modelled for each station, and the second target diagram shows how well the estuarine gradient (if any) is reproduced by the model. Similar plots are used in the results section.

Initial result with uncalibrated model

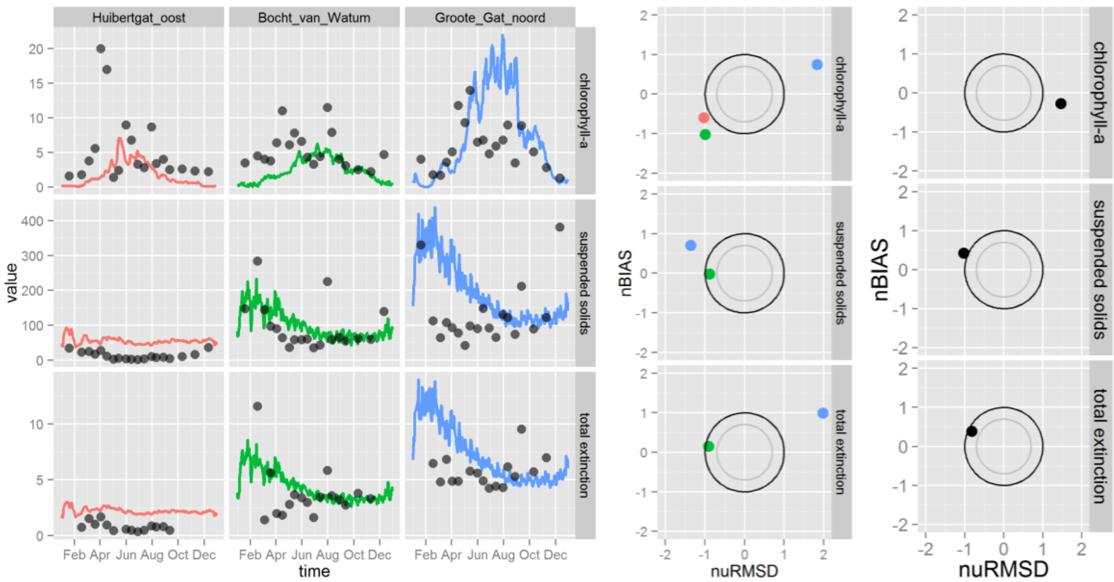

Figure 5.3 Uncalibrated version of the model showing chlorophyll-a, suspended sediment and extinction for 2012 with target diagrams.

When using standard parameter settings, and suspended sediment were applied directly from the sediment model, extinction is highly overestimated at all three stations, and most at Huibertgat Oost, concurrent with an overestimation of suspended sediments as compared to MWTL measurements. This led to underestimation of chlorophyll-a at Huibertgat Oost and Bocht van Watum. At Groote Gat Noord, chlorophyll-a was highly overestimated in summer, which is not in line with the overpredicted extinction. This overprediction could be explained by low suspended sediment, low extinction and therefore high production in areas closeby, most notably in the Ems river, and in the shallowest areas of the Dollard. These are known issues of the sediment model, because it is not designed to reproduce the suspended sediment concentrations in the river Ems, and in very shallow parts, suspended sediments seem to be underestimated.

Step 1 Correction of high chlorophyll-a in the Dollard at station Groote Gat Noord

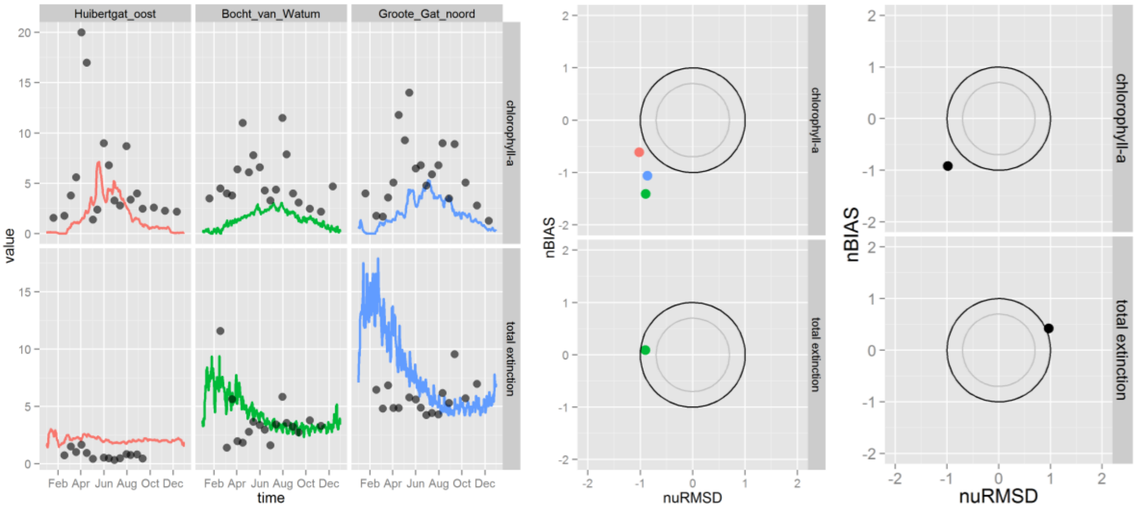

Figure 5.4 Model version after step 1 (correction of overestimated chlorophyll in the Dollard) showing chlorophyll-a and extinction for 2012 with target diagrams.

When applying a minimum extinction of 20 in River Ems and shallow parts of the Dollard (see section 4.4), the high chlorophyll-a concentrations in summer at Groote Gat Noord disappeared completely and target diagrams for chlorophyll-a improved. It had no effect on extinction, which was expected.

Step 2. Calibration to measured extinction

The goal was here to reduce the difference between modelled and measured extinction by adjustments of the suspended sediment field from the sediment model.

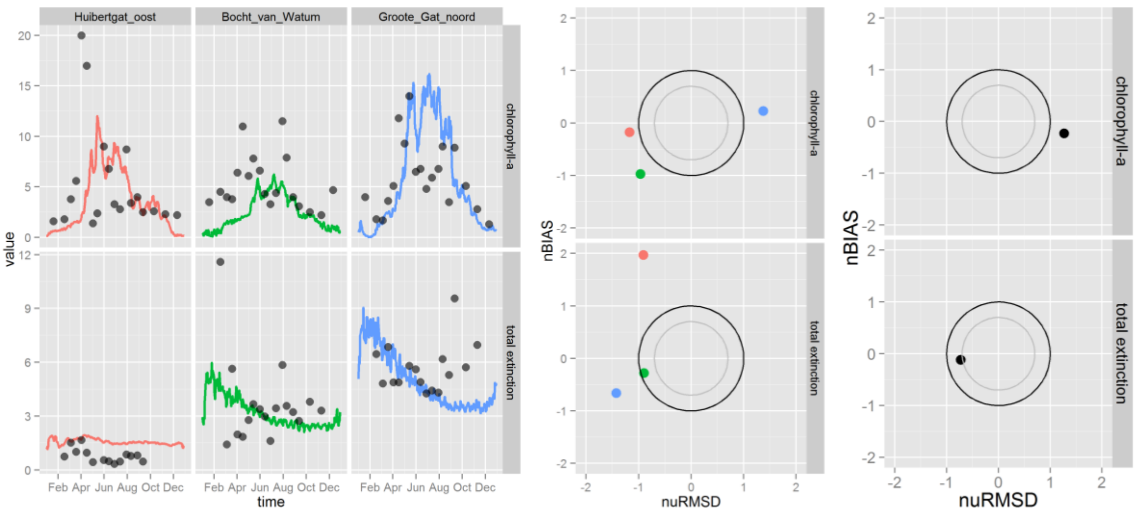

Figure 5.5 Model version after step 2, showing chlorophyll-a and extinction for 2012 with target diagrams.

In order to fit the measured extinction, the suspended sediment concentration was reduced with a factor 2 before using it as a forcing for the primary production model. This adaptation of suspended sediment concentration reduced the total extinction by almost a factor 2 (Figure 5.5). Average extinction was now simulated well at Groote Gat Noord and Bocht van Watum.

Average chlorophyll-a is simulated well. The variability of chlorophyll-a within stations is underestimated as compared to the observations for Bocht van Watum and Huibertgat Oost (middle graph) and overestimated for Groote Gat Noord. The variation of extinction between stations is captured well, for chlorophyll-a, this variation is slightly overestimated (right graph).

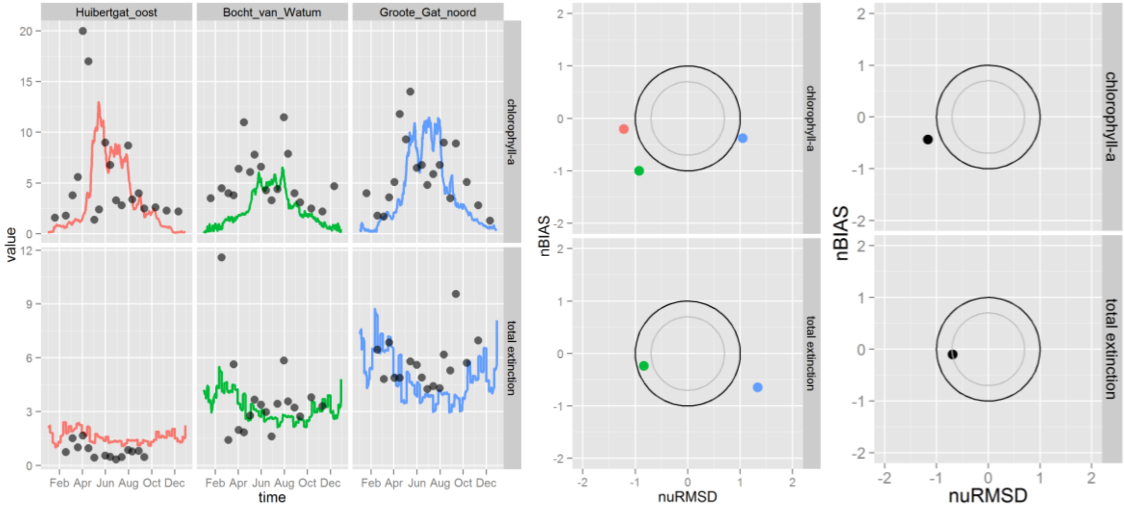

Figure 5.6 Model version after step 3 showing chlorophyll-a and extinction for 2012 with target diagrams.

Step 3 redistribution of suspended sediment
In step 3 (Figure 5.6), the suspended sediment concentrations were redistributed over the year for each grid cell in order to better fit the observed values. A cosine function in combination with a wind-related function was used to construct a time series for each grid cell based on the average concentration calculated with the sediment model. Like in previous versions, a general reduction of suspended sediment of a factor 2 was applied. The objective model qualification in the target diagrams did not clearly improve as compared to the previous version, but on the basis of the time plots, this version was judged to better describe chlorophyll-a in the Ems estuary because it better describes the timing of the spring bloom.

Step 4 Calibration of benthic chlorophyll-a
Standard settings of the process calculating the benthic diatoms in the current model appeared not suitable without calibration. Observations were used from the monitoring programme carried out by IMARES in this project. There were a number of difficulties hampering a direct comparison:

- Since the primary production measurements were not considered to be comparable to earlier measurements, only benthic chlorophyll-a measurements were used for calibration.
- Benthic chlorophyll-a was only measured during 2013, and not during 2012, the calibration year.
- Benthic chlorophyll-a is known to be very patchy distributed, and very dependent on the exact position with respect to the water level. The exact level of the measurement was not known, and the model grid cells are much bigger than the sampled sediment. Also, model grid cells are assumed to be homogeneous. It was decided to calculate benthic chlorophyll-a for an area around the monitoring station, to account for some of the variability due to these unknown factors.
- It was further taken care of that benthic primary production was in the same order of magnitude as pelagic primary production and in the range of what has been measured before, namely between 50 and 250 g C m^{-2} y^{-1} (Colijn & De Jonge, 1984).

The calibration is therefore done with the aim to produce benthic chlorophyll-a concentrations that are in the same order of magnitude as the 2013 measurements and to produce benthic primary production that was in the same order of magnitude as pelagic primary production for the different areas (De Jonge, 1995). The only constants that were used for calibration were the two constants that regulate benthic diatom growth rate as a function of temperature (slope and offset) (Figure 5.8).
Possibly, a better calibration might be obtained when also considering other constants, and/or other calibration procedure, but given the quantity and quality of available measurements, it is questionable whether this would be the best way forward towards better benthic primary production model results.

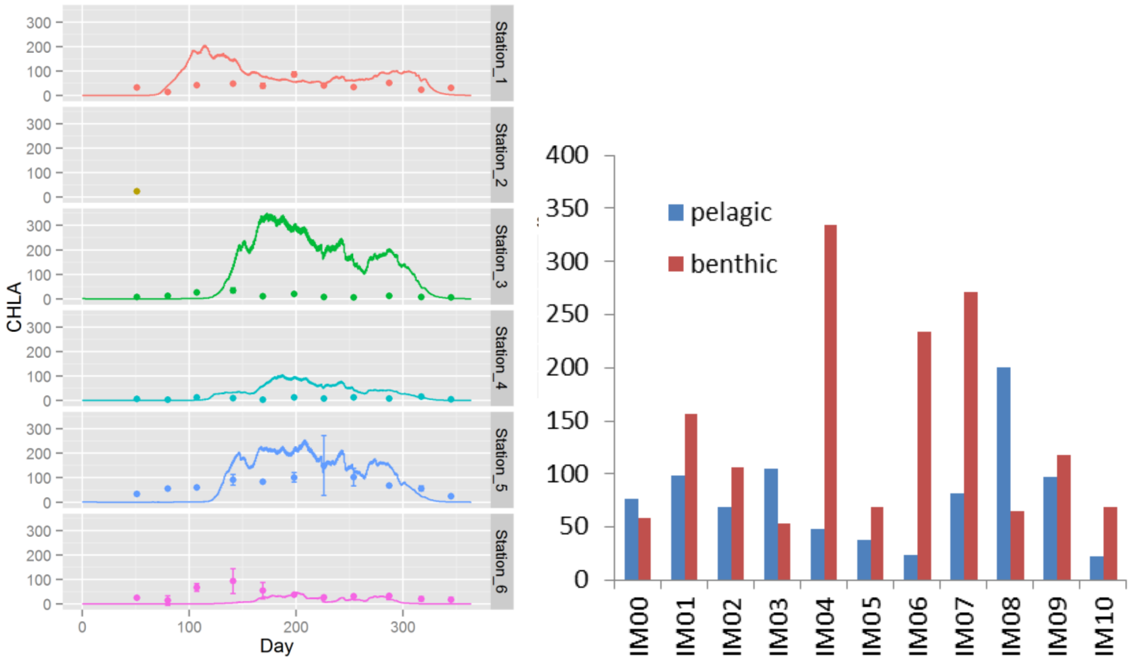

Figure 5.7 Chlorophyll a in mg/m3 (left), modelled and measured (2013) at the 6 benthic stations, and primary production in g/m2/y (right) for the different areas defined in the monitoring programme.

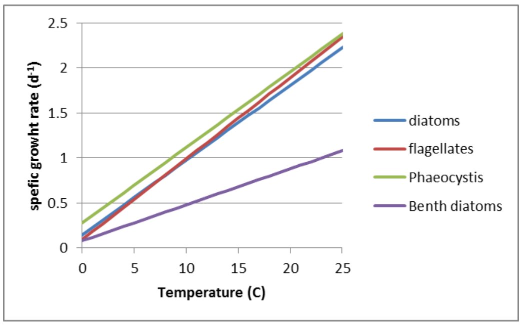

Figure 5.8 Relationship of maximum specific growth rate with temperature for benthic diatoms after calibration as compared to the other algal groups in the model.

Benthic chlorophyll-a in the calibrated model did not match the measured values well, but was in most cases (except station 3) in the right order of magnitude (Figure 5.7). Benthic primary production was with those settings in most areas in the same order as the pelagic primary production, calculated as $gC/m^2/y$. The conclusion is then that benthic primary production model results could not be calibrated more quantitatively. Any scenario results for benthic production related variables should therefore be interpreted as relative changes, rather than absolute values.

The calibration was finalized by running the model for one extra year, and using the end situation of 2012 as a start for a new 2012 run. Also, with the reduced benthic primary production after calibration, pelagic chlorophyll-a apparently increased as compared to the version before the calibrated benthic primary production (Figure 5.9), most likely due to a higher availability of nutrients, caused by decreased competition with benthic diatoms.

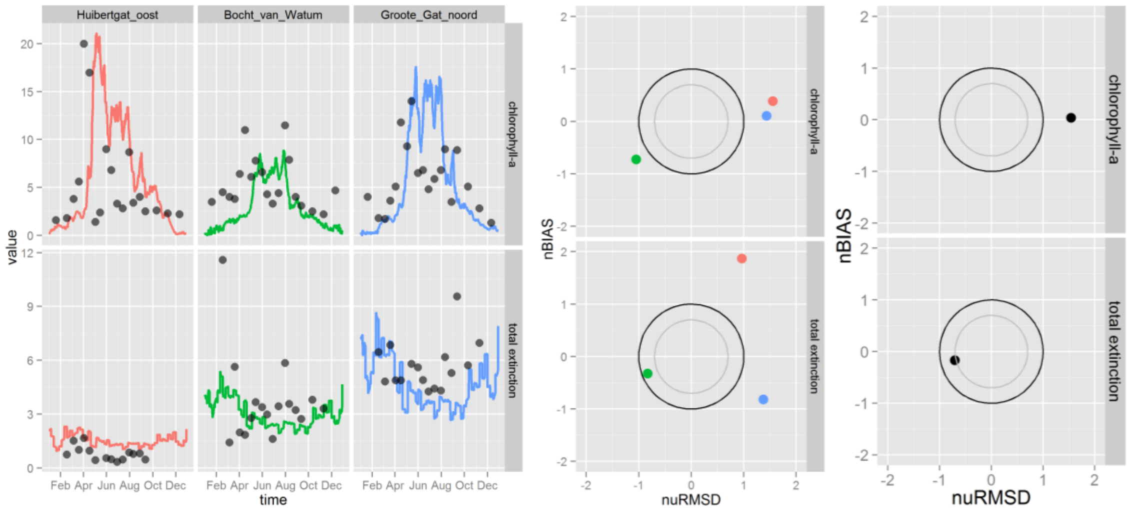

Figure 5.9 Model version after step 4 with adapted parameters for benthic diatoms. The chlorophyll- peak in spring is now more pronounced, and closer to the observations. The objective model qualification in the target diagrams do not improve as compared to the previous version, but on the basis of the time plots, this version was judged to better describe chlorophyll-a in the Ems estuary.

In order to illustrate the relation between the water quality modelling efforts (this report) and the monitoring programme by RWS (MWTL), IMARES (IMARES report) and others, we present an overview of which monitoring results have contributed to the modelling study and for what purpose (Table 5.1).

Table 5.1 Overview of coupling between the monitoring study and the modelling study.

Monitoring data set	**Model set-up/ calibration**	**Validation 2012**	**Validation 2013**
MWTL WQ (nutrients, SPM, E, Chlorophyll)			
Terschelling 10	Boundary conditions		
HBo, BvW, GGn	Ems river loads (silicate) Calibration 2012: Extinction, Chlfa		validation
MWTL phytoplankton			
HBo, GGn		validation	not available
NLWKN WQ + water boards			
Nutrients	River and polder loads		
IMARES programme			
Pocketbox data		validation (chla, spm, extinction)	validation (chla, spm, extinction)
Station bottle data		validation (SPM, nutrients)	validation (SPM, nutrients)
benthic survey	calibration(2013 chlfa)		
Phytoplankton composition		not used	not used

6 The results of the calibrated model

6.1 Salinity

Simulated salinity in the Ems estuary agrees well with observed salinity from MWTL and IMARES measurements (Figure 6.1). The simulation results show the dilution of saline North Sea water with freshwater from the Ems River, the Westerwoldse Aa and the Dutch and German polders bordering the estuary. Whereas dilution is minimal in Huibertgat due to the strong mixing with North Sea water, dilution is strong in the Dollard in particular during high discharges in the winter (Figure 6.2). At the highest discharge in the beginning of February the salinity drops to below 7 psu at Groote Gat (Figure 6.1). During high discharges the water quality in the Dollard is consequently strongly affected by the external loads from the river and the polders.

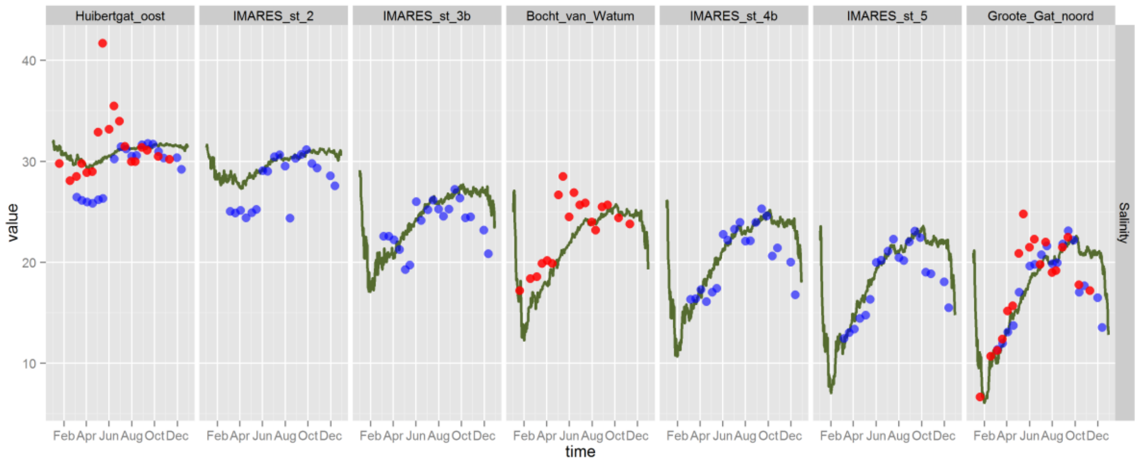

Figure 6.1 Simulated salinity (psu) in the Ems estuary for 2012, at MTWL stations Huibertgat, Bocht van Watum and Groote Gat and additional IMARES stations 2, 3b, 4b and 5. The green line represents modelled daily averages, filled red circles (●) and blue circles (●) indicate measurements from the MWTL program and IMARES, respectively.

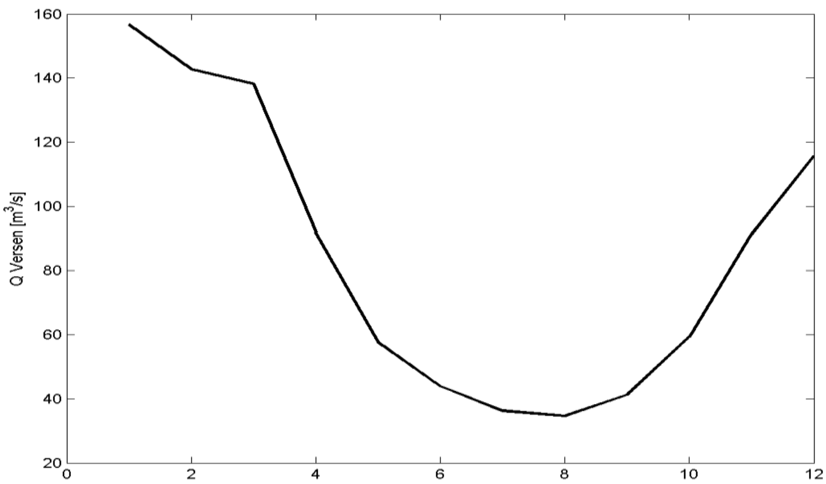

Figure 6.2 monthly discharges of the Ems river at Versen.

Judged from the target diagrams, the model represents salinity reasonably well (Figure 6.3). At Huibertgat Oost, some MWTL salinity measurements deviate strongly from the modelled values and IMARES measurements (Figure 6.3). Especially the value > 40 PSU seems unrealistically high. We have not further investigated the possible source of error in the measurements. Taken over the whole gradient, the model simulates salinity well (Figure 6.3).

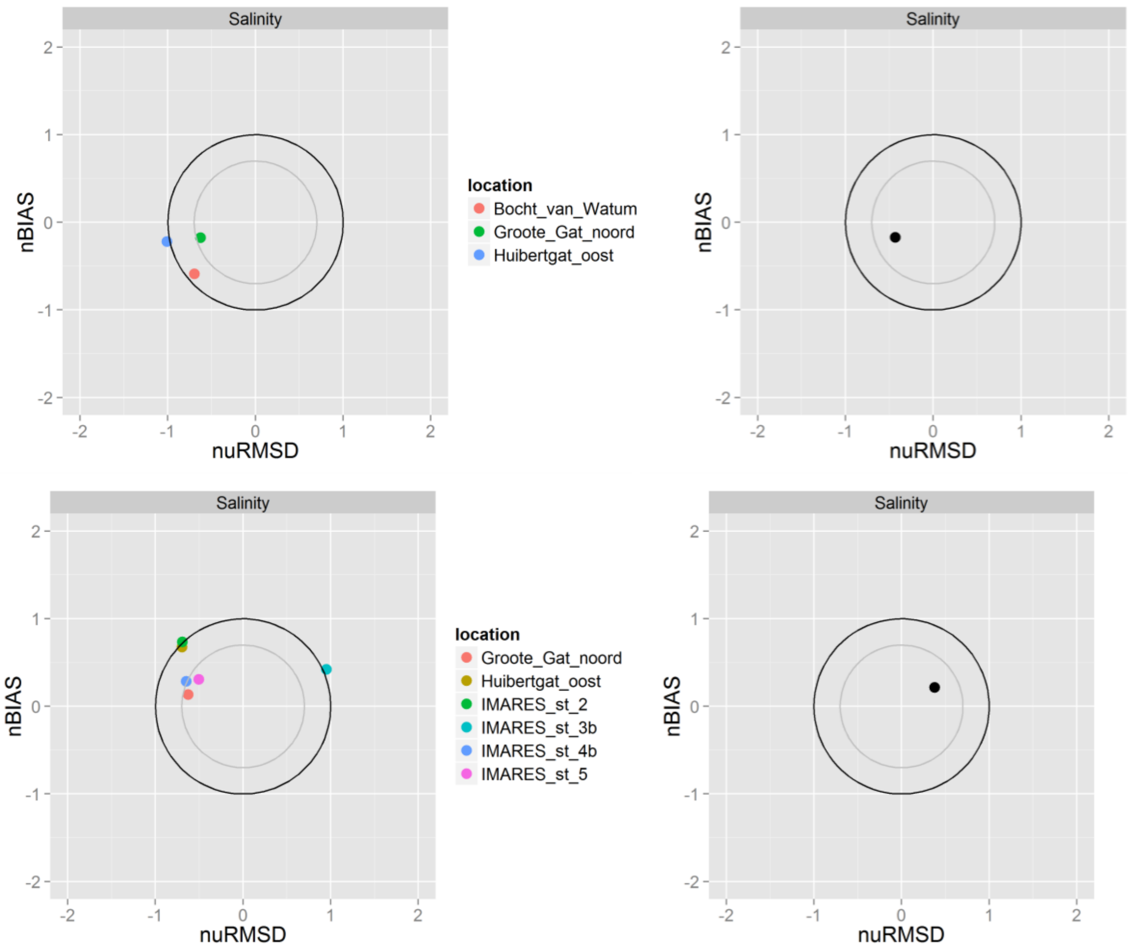

Figure 6.3 Target diagrams of salinity in 2012 for the three MWTL stations separate as indicated by color (upper panel left) and combined (black dot, upper panel right). Panels below are similar for IMARES stations, left panel has stations separated and indicated by color, right panel shows stations combined. Measurements and simulated values are compared on an hourly basis.

6.2 Extinction

Total extinction of light is caused by individual fractions of substances, such as suspended sediment (inorganic matter), phytoplankton and detritus (dead organic matter). In the Ems estuary most of the light extinction is caused by suspended sediment (Figure 6.4). Due to the strong light extinction by suspended sediment the total extinction coefficient is high in the Dollard as appears from Figure 6.4 and Figure 6.5 in Groote Gat Noord. With an average extinction of 5.6 m^{-1} at Groote Gat Noord, light availability is only 5.8% of surface light at 0.5 m depth (Figure 6.8). So even though the water column is mostly shallow in the Dollard, light limitation is the most important growth limitation for phytoplankton in the Ems estuary. The target diagrams show that modelled extinction is slightly underestimated and has higher variability compared to measured extinction at Groote Gat Noord (Figure 6.6).

Extinction decreases seawards in the estuary (Figure 6.5), so light availability in the water column increases. However, even at Huibertgat Oost average light availability is 45% at 1 m depth (Figure 6.8). Extinction is predicted reasonable at Bocht van Watum and IMARES station 2 (Figure 6.6). Extinction is on average over-predicted at Huibertgat Oost by the model (Figure 6.6) and this has a large negative effect on average light availability (Figure 6.8). When the variability and bias over all stations is considered, also covering the spatial variability the extinction is reasonably predicted (Figure 6.7).

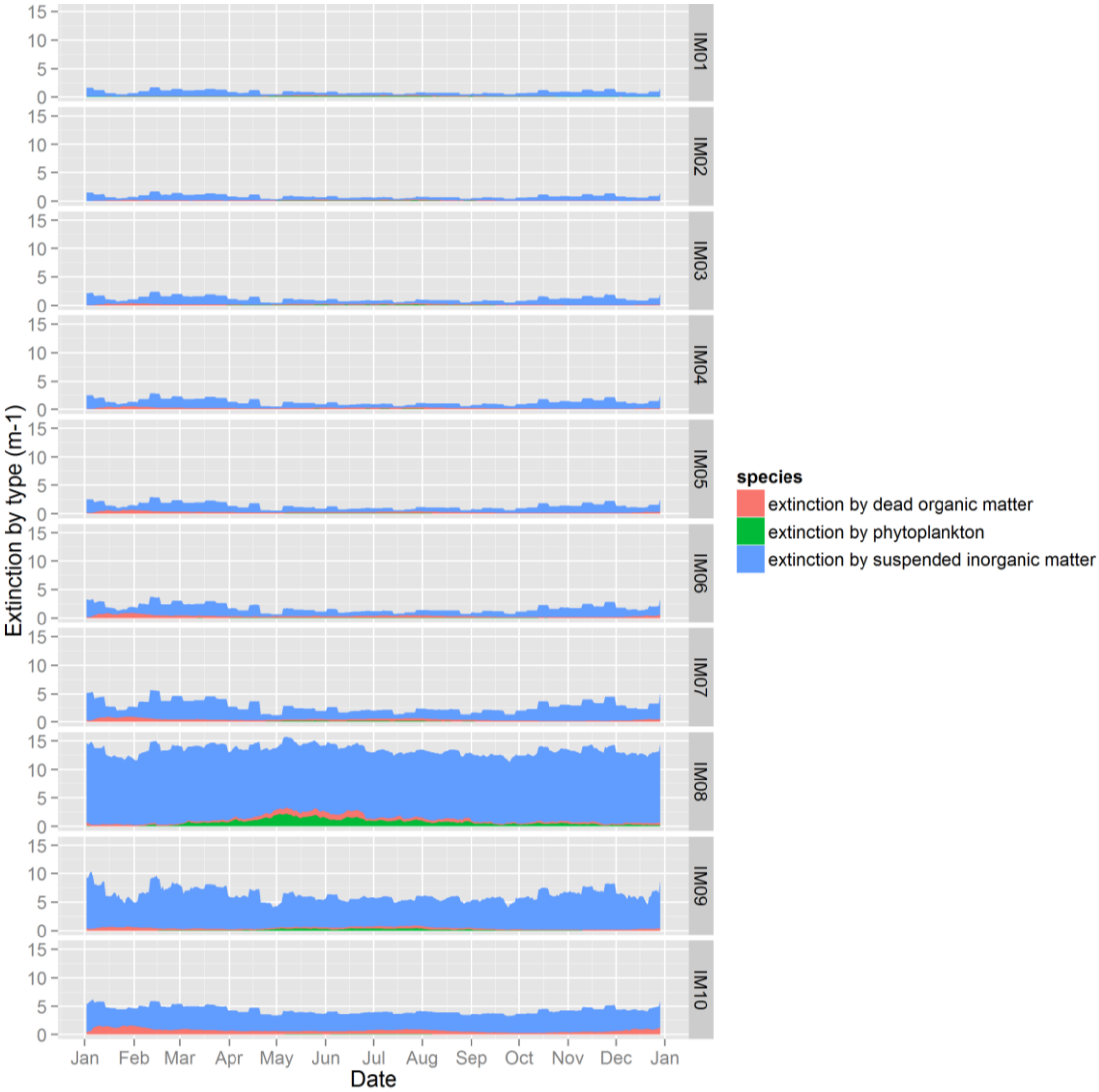

Figure 6.4 Extinction by different substances at different areas in 2012 (Figure 4.20). The sum is total extinction.

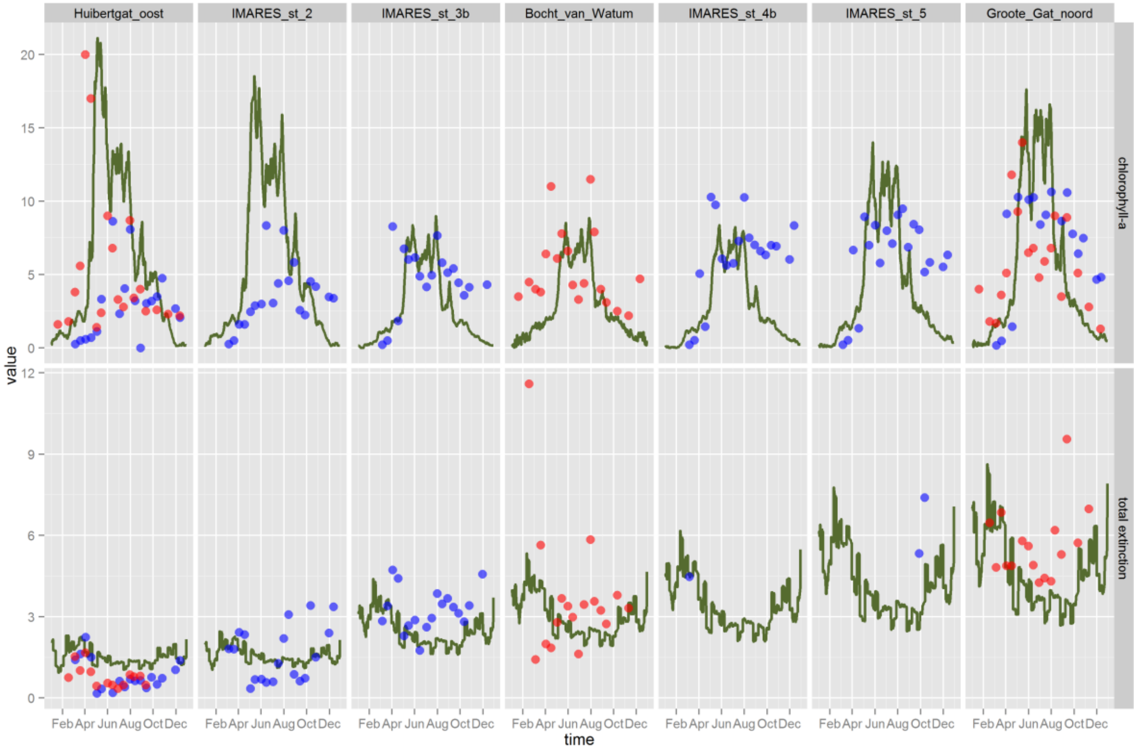

Figure 6.5 Simulated chlorophyll a (µg/L) and total extinction (m^{-1}) in the Ems estuary for 2012, at MTWL stations Huibertgat, Bocht van Watum and Groote Gat and additional IMARES stations 2, 3b, 4b and 5. The green line represents modelled daily averages, filled red circles (●) and blue circles (●) indicate measurements from the MWTL program and IMARES, respectively.

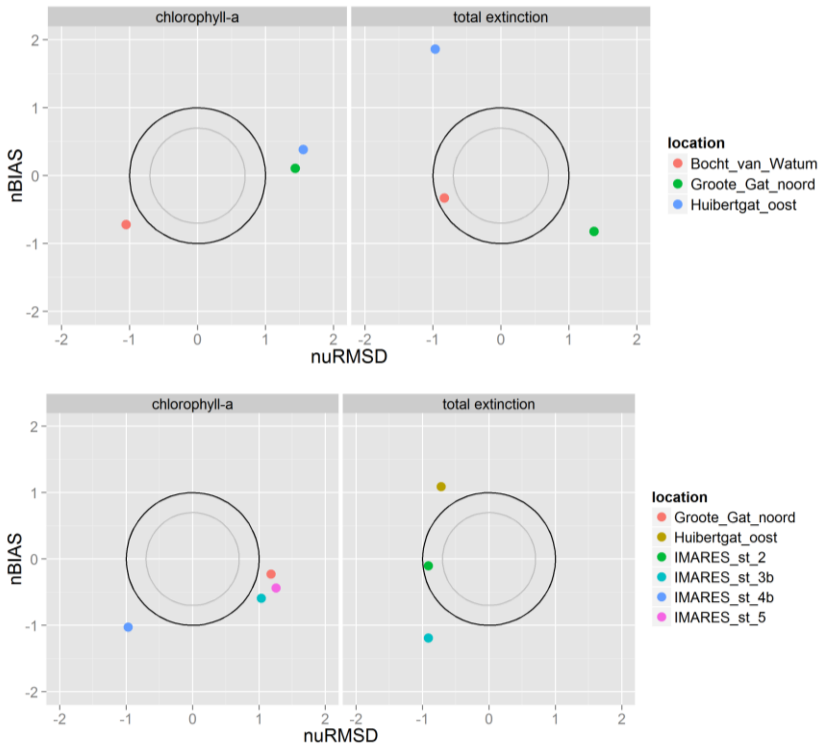

Figure 6.6 Target diagrams of chlorophyll-a and extinction in 2012 for the three MWTL stations (upper panel) and IMARES stations (lower panel), indicated by color (left panel). The comparison is done on an hourly basis.

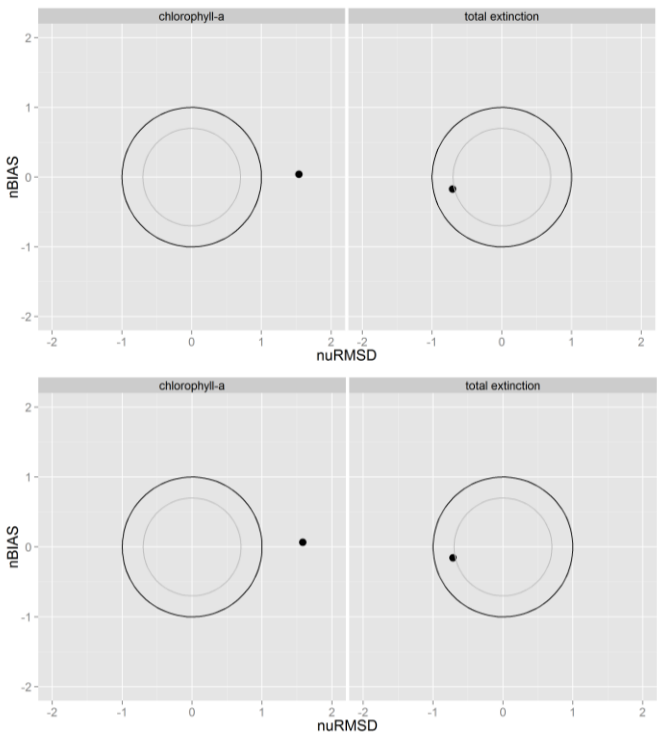

Figure 6.7 Target diagrams of chl a and extinction in 2012 for all stations combined. Upper panel are MWTL stations and lower panel are Imares stations. The comparison is done on an hourly basis.

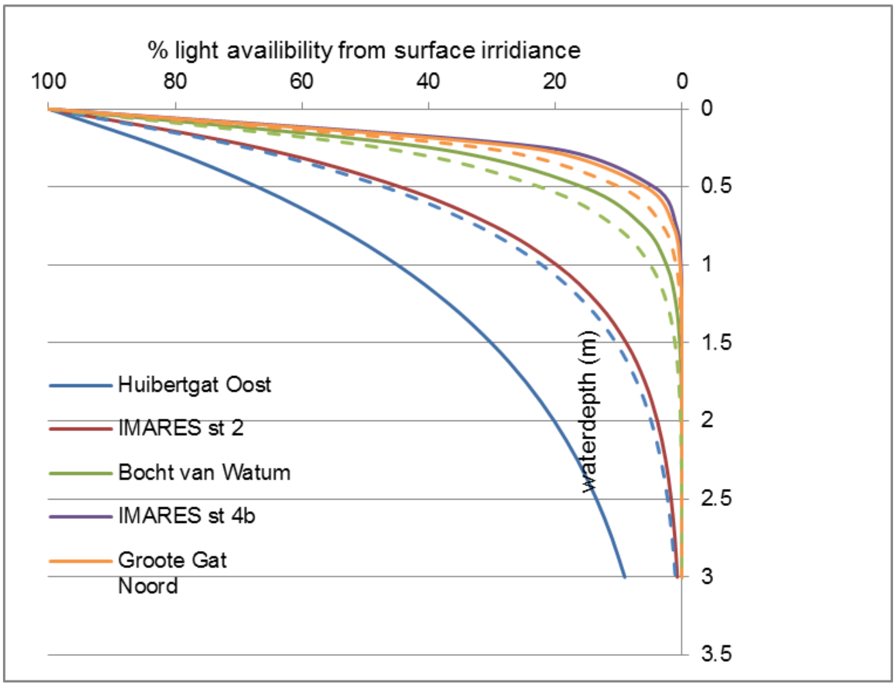

Figure 6.8 Light availability as % of surface irradiance through the water column calculated from average extinction coefficients in 2012, see section 4.4 for the equation. Solid lines and dashed lines are calculated from average measured values and modelled values, respectively.

6.3 Phytoplankton

6.3.1 Chlorophyll-a

Phytoplankton biomass as determined by chlorophyll *a* is very low during most of the winter due to low temperature and strong light limitation (Figure 6.5). In spring, when light availability and temperature increase, phytoplankton concentrations increase as well. Phytoplankton concentrations decline steadily towards winter.

In general, variation of phytoplankton and thus chlorophyll-a is a result of production/mortality and transport. This causes differences in the patterns of phytoplankton production and biomass, because primary production occurs in shallow (intertidal) areas. Produced chlorophyll-a is transported and dispersed, a process where strong gradients of chlorophyll-a are eroded. Thus, mismatches between the simulated and measured spring bloom at monitoring locations can be caused by

- Uncertainties in primary production elsewhere
- Uncertainties in transport and dispersion

The only station with a distinct measured spring bloom peak and decline is Huibertgat Oost, towards the sea (Figure 6.5). Note that this peak is measured by MWTL, but not by IMARES, showing some inconsistency between measurements. A bloom peak at Huibertgat Oost is also simulated by the model, but a month later. This could be explained by an overestimation of extinction by the model in spring (Figure 6.5). However, simulated primary production at Huibertgat Oost is zero throughout the year (Figure 6.9), so local phytoplankton concentrations are produced elsewhere. Although the overall impression of the time-series plots is fairly well, the target diagram indicates that average value and variability is too low at Huibertgat Oost (Figure 6.6). Tests have shown that the under-prediction of chlorophyll a at Huibertgat Oost during spring (time series graph) cannot be relieved easily, as during that period, very low light levels were available for phytoplankton (see radiation curve in Figure 4.9). The dip in irradiance is seen at all stations in this part of the Netherlands (Lauwersoog, Terschelling), and is therefore likely to really have occurred in the modelled area.

Also at IMARES_st_3b, Bocht van Watum, IMARES station 4b and Groote Gat Noord the simulated bloom is delayed compared to the measured bloom (Figure 6.5). At Bocht van Watum, the delay in spring bloom is unexpected, since simulated extinction is lower than measured extinction, so the model actually overestimates light availability (Figure 6.5). At IMARES station 2 a spring bloom is simulated, but not measured, while extinction is simulated well. This illustrates that local concentrations are an integrated result of processes happening in different space and time.

Groote Gat Noord is located in a very turbid area and has no simulated primary production (Figure 6.9). However, according to the measurements, positive values of chlorophyll-a are present throughout the year (Figure 6.5). This has probably been produced in the shallow areas in the Dollard and transported to the channel. The simulated bloom peak is higher than measured. Over-prediction of phytoplankton in the model may be caused by growth and subsequent transport of very high biomass of phytoplankton at the edges of the Dollard, where water depth is very low, light availability is high, and nutrients are still in ample supply. It is not clear whether and to what extent this phenomenon is occurring in reality. However, the biomasses currently calculated by the model at the station Groote Gat Noord seem unrealistically high. The target diagrams show that average values and variability in the model are higher than measurements from both MWTL and IMARES (Figure 6.6), even though both measurements show a different pattern (Figure 6.5).

In winter, simulated values are lower than measured values at IMARES station 3b, 4b and 5 and Groote Gat Noord (Figure 6.5). One possibility to explain the differences between modelled and observed chlorophyll a in winter is that resuspension of benthic diatoms and other algae may occur in winter due to strong winds. Microphytobenthos chlorophyll-a is present during winter (Boer, 2000), and resuspension has been demonstrated (De Jonge & Van Beusekom, 1992).This is visible as chlorophyll-a in observations, but is not taken into account in the model. Also, the first half of February 2012 was a very cold period (water temperature below zero) with possible ice cover in the inner parts of the Dollard, which may have scraped off sediment and attached algae, causing enhanced chlorophyll-a concentrations in the water.

The target diagrams also considering spatial variation show that average chlorophyll-a values are simulated well, compared to both MWTL and IMARES measurements (Figure 6.7). But variability is over predicted relative to both measurement series (Figure 6.7). Proper simulation of average phytoplankton concentrations is most relevant for WFD quality objectives and for carrying capacity and food availability for higher trophic levels.

6.3.2 Limiting factors

In Figure 6.9, phytoplankton limitation factors are plotted for a number of segments with the model domain. In the deep parts, phytoplankton growth is limited by light throughout the year, and hardly any net primary production occurs.
In shallower areas, light is only limiting during winter. At shallow locations outside the Ems plume (“Ra” and “Lauwers_oos”), phosphorus and later also nitrogen become limiting during summer. Silicate is only limiting during summer at the most westerly stations plotted here.

In Figure 6.10, phytoplankton limiting factors are plotted as an average for all segments within the 11 “IMARES areas”. All areas are on average strongly light-limited during the whole year.

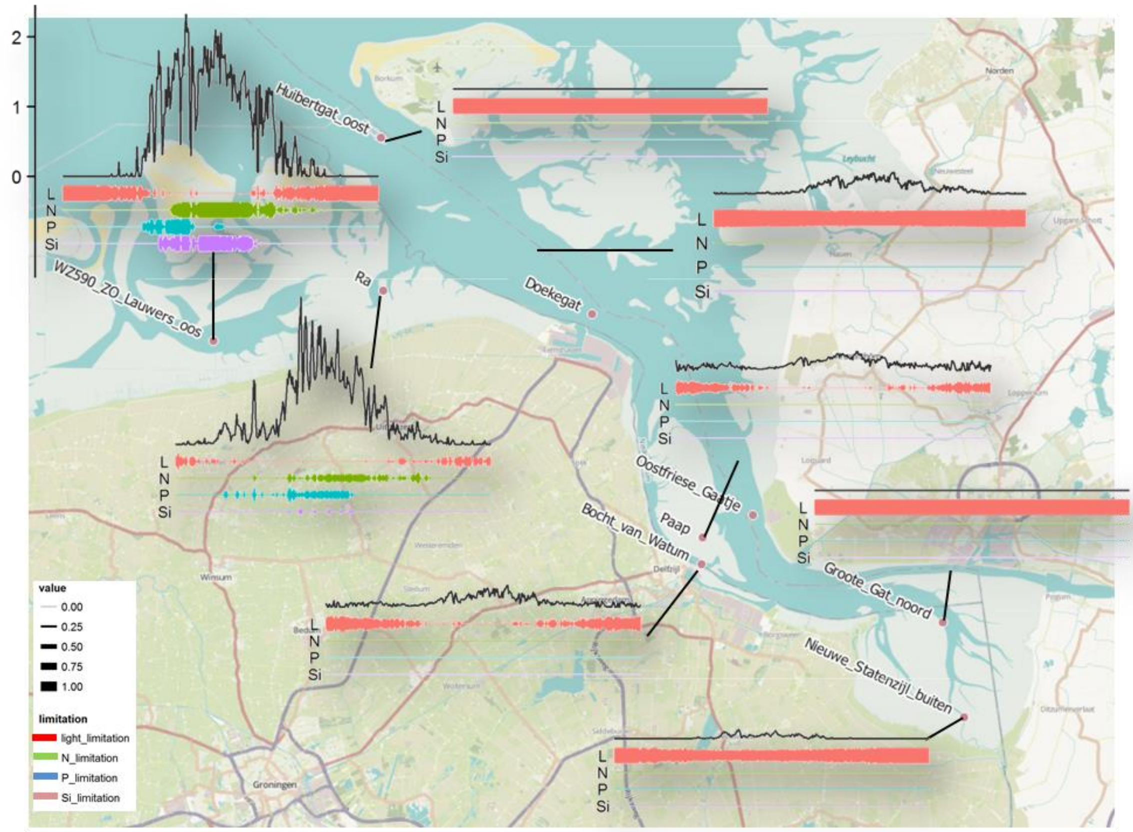

Figure 6.9 Presentation of net primary production(gC/m2/d) (black line) and limiting factors modelled for the present situation. Coloured horizontal lines indicate the variation of limiting factors over the year. Limiting factors could occur for pelagic or benthic algae and the strength of limitation is indicated by the thickness of the coloured line. Scales are equal for all plots. L = light limitation (red), N = nitrogen limitation (green), P = phosphorous limitation (blue), Si = silica limitation (purple).

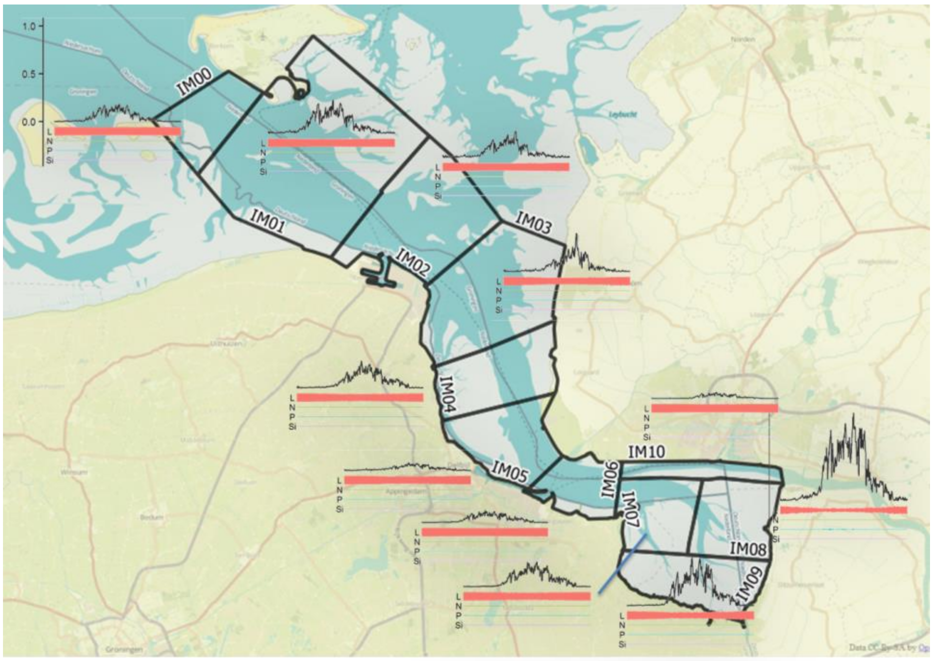

Figure 6.10 Plots with primary production (gC/m^2/day) over the year and the limiting factors for primary production or phytoplankton growth at averaged over IMARES areas. Values are daily averages of hourly model output. Limitation values vary from 0 (no limitation) to 1 (limitation).

The limiting factors for benthic primary production can differ from those for primary pelagic primary production. To see whether nutrients are limiting benthic production, the biomass together with nutrient concentrations at each station is shown in Figure 6.11. In station EDB01, silicate becomes exhausted, indicating silicate limitation. In all other stations none of the nutrients become exhausted, so light combined with growth is likely limiting..

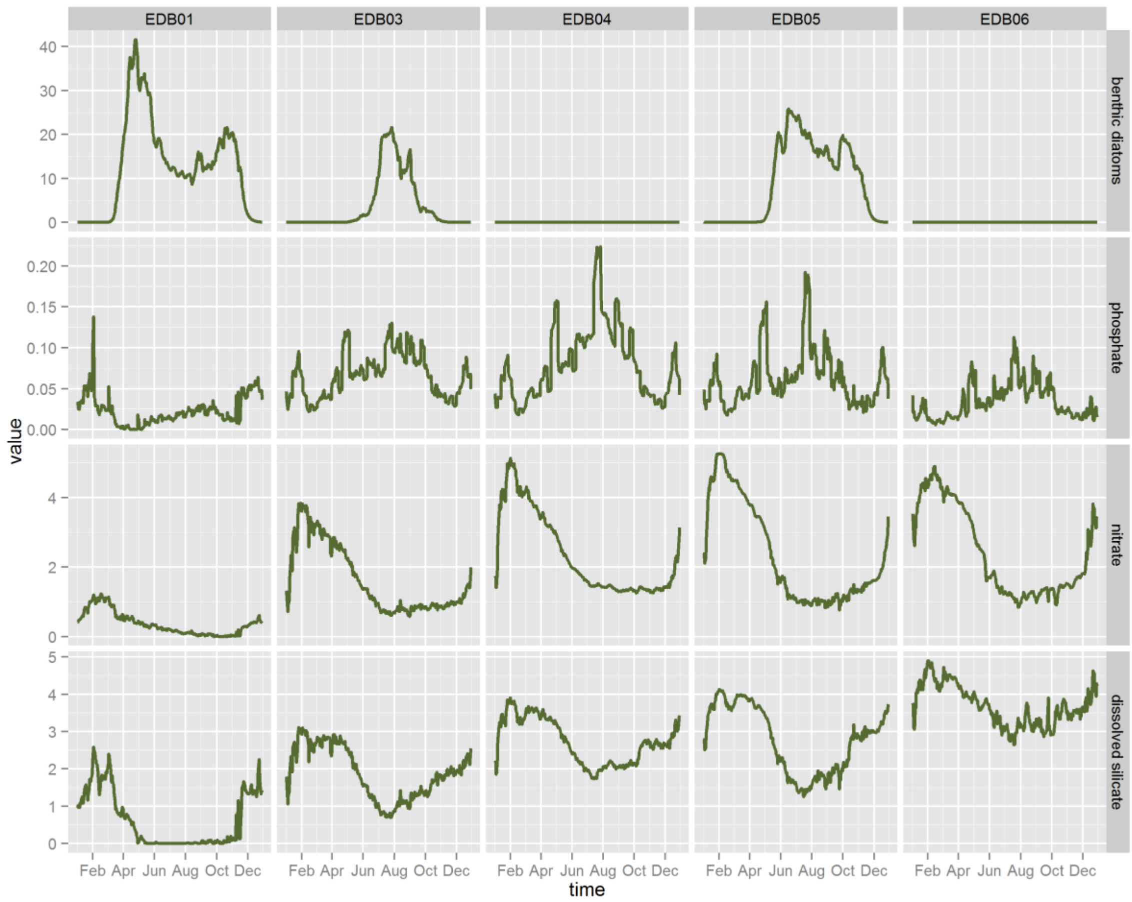

Figure 6.11 Modelled benthic diatoms and reactive nutrients at the stations where benthic primary production was measured. Silicate is the most likely limiting nutrient, and is completely exhausted in the outermost station EDB01 in summer. Since nutrients are available in ample amount at most places, light and growth are likely the most important limiting factor for microphytobenthos.

6.3.3 Pelagic primary production

Pelagic primary production measurements were based on biweekly sampling at different locations by IMARES. Samples were incubated, after which the photosynthetic parameters were estimated (maximum photosynthesis/chlorophyll-a and the light dependency of photosynthesis). These parameters were then used to calculate total primary production per area by taking into account irradiance, measured turbidity at the station, and bathymetry of the areas (Figure 6.12). Using the model, net primary production was calculated for the same areas.

Modelled and measured pelagic area-specfic primary production range from 20-160 $gC/m^2/year$ and both results show that primary production is higher towards the sea than in the inner estuary (Figure 6.12). Measured primary production is higher than modelled primary production in IM00 and IM01 (Figure 6.12), what is contradictory to chlorophyll-a results, which are higher in the model for Huibertgat Oost and Imares station 2 (Figure 6.12, Figure 6.5). Also in area IM04 and IM06, measured primary production values are higher than modelled values, but here chlorophyll-a is higher as well (Figure 6.12, compare with Imares station 3b and 4b in Figure 6.5). In IM07 modelled primary production is higher than measured primary production, even though the model underestimates chlorophyll-a at Groote Gat Noord (Figure 6.5, Figure 6.12).

The differences between modelled and measured primary production could be attributed to:

- Differences between the used bathymetry and/or integration over depth for the areas. Measured primary production is calculated as the average of low and high tide integrated values, while the modelled values are integrated over time, taking into account the depth variation and horizontal transport and dispersion due to the tides
- In the model, extinction due to suspended solids is calculated and implemented spatially over the whole grid. In contrast, primary production calculated from measurements assume a uniform distribution of extinction based on the extinction measurements at the monitoring stations located in the deeper parts of the estuary. In shallow areas which generally show higher extinctions due to resuspended material, primary production from measurements may therefore be overestimated as compared to the modelled values.
- Possible differences in temperature and light availability. Since both modelled and measured primary production are based on measured temperature and light, these factors are probably not very important.

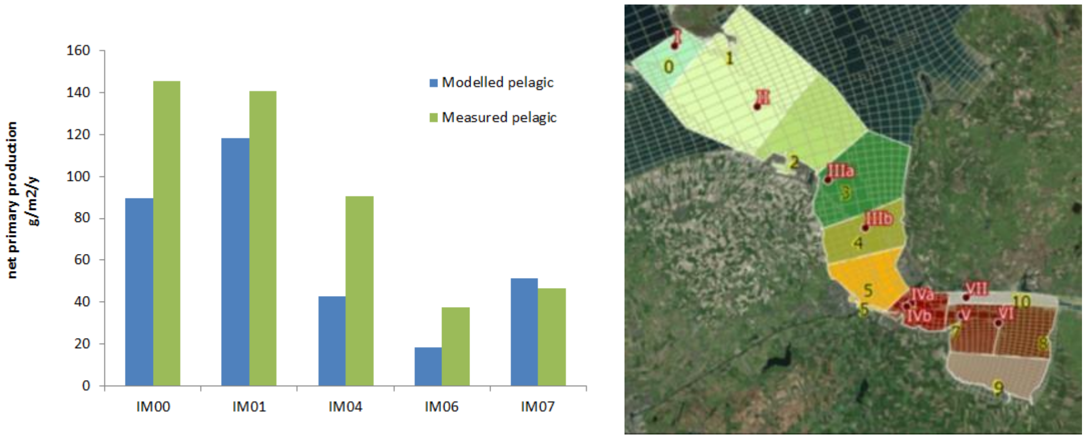

Figure 6.12 Integrated modelled pelagic primary production and comparison with measured estimates.

6.4 Oxygen

Modelled daily average dissolved oxygen reproduces the observations most of the year with higher values in winter and lower values in summer (Figure 6.13). In winter and spring, modelled values are lower than MWTL measured oxygen, especially at station Huibertgat Oost. However, the model results are in the same range as measurements from IMARES (Figure 6.13).

In general, dissolved oxygen concentration is sensitive to:

- Temperature
- Salinity
- Primary production
- Respiration and mineralisation
- Reaeration, and thus to wind speed

Given these sources of variation, the target diagrams for oxygen show a good or reasonable fit to measurements (Figure 6.14). Also the overall fit of the model to measurements is good (MWTL) or reasonable (IMARES) (Figure 6.15).

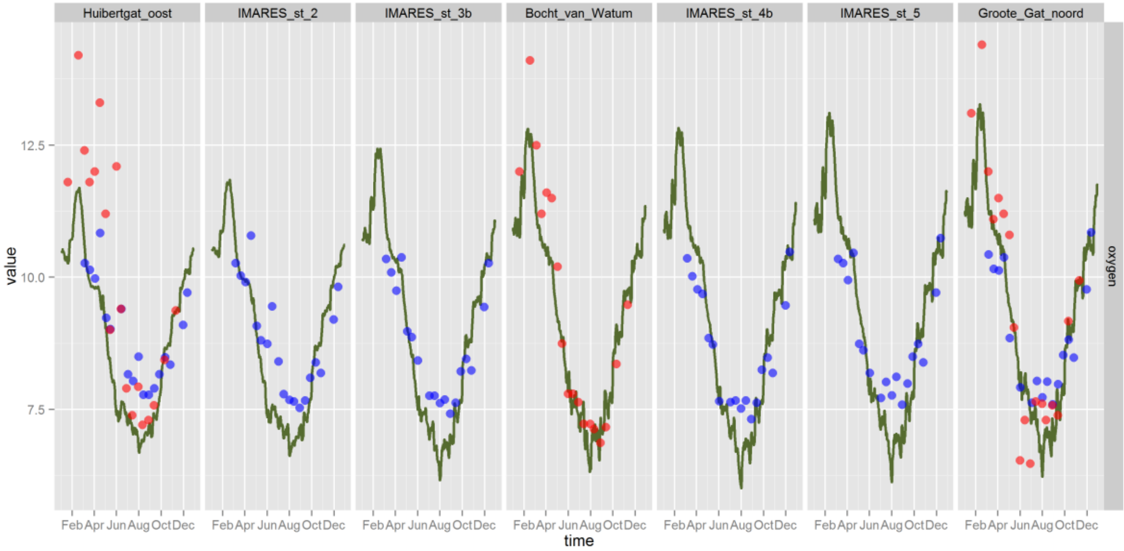

Figure 6.13 Simulated oxygen (mg/L) in the Ems estuary for 2012, at MTWL stations Huibertgat, Bocht van Watum and Groote Gat and additional IMARES stations 2, 3b, 4b and 5. The green line represents modelled daily averages, filled red circles (●) and blue circles (●) indicate measurements from the MWTL program and IMARES, respectively.

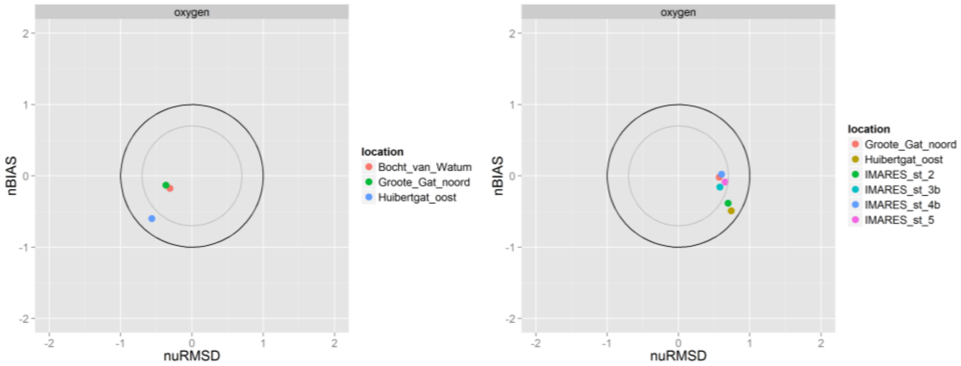

Figure 6.14 Target diagrams of oxygen in 2012 for the three MWTL stations (left panel) and IMARES stations (right panel), indicated by color. Comparison is done on an hourly basis.

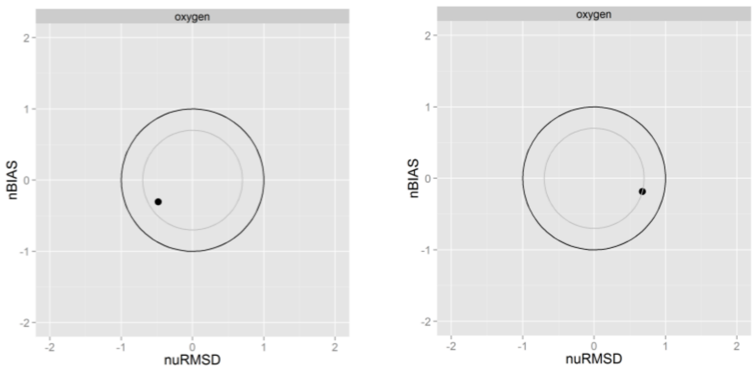

Figure 6.15 Target diagrams of oxygen in 2012 for all stations combined. Left panel shows MWTL stations and right panel shows Imares stations. Comparison is done on an hourly basis.

6.5 Nutrients

Nutrients show a clear gradient from high concentrations in the Dollard to low concentrations in the lower part of the estuary and this is also captured by the model (Figure 6.17). The typical pattern of low summer values for nitrate and ammonium, as well as the increase of phosphate in summer due to internal loads from the sediment are both predicted well by the model (Figure 6.17).

6.5.1 Nitrogen

On average, ammonium is slightly under-predicted at Huibertgat Oost, while nitrate is over-predicted in the estuary (Figure 6.17). The over-prediction is also visible in the target diagrams for IMARES stations, but not for MWTL stations (Figure 6.18). This over-prediction seems to be caused by an overestimated load from the river Ems in winter, possibly due to linear interpolation of monthly water quality data. The importance of correct nitrogen concentration depends on whether this nutrient can become limiting for phytoplankton growth. The model does not predict any nitrogen-limited phytoplankton in most of the Ems estuary (Figure 6.9 and Figure 6.10), but in adjacent parts of the Wadden Sea the model predicts some nitrogen limitation during summer. Although the individual stations show some deviations between measured and simulated values, the overall score of nitrate is reasonable (Figure 6.19).

6.5.2 Phosphate

Dissolved phosphate from the model reproduces observed dissolved phosphate on average, but the simulated variability is too high in the upper part of the estuary (Bocht van Watum, Imares station 4b and 5 and Groote Gat Noord) (Figure 6.18). Over the whole gradient, average concentrations are good with zero bias, and variability is reasonable with slight overestimation (Figure 6.19). Due to the high concentrations of inorganic suspended sediment a large percentage of phosphorus in the water column is present as adsorbed phosphate (Figure 6.16). The settling of adsorbed phosphate is a major component of the sediment-water exchange flux of phosphorus. Because the summer level of dissolved phosphate is primarily determined by internal loading from the sediment, the accurate prediction of dissolved phosphate points at realistic simulation of the P-return flux from the sediment. Phytoplankton is not phosphorus limited in most of the Ems estuary, and only incidentally phosphorus limited in the spring in the adjacent parts of the Wadden Sea (Figure 6.10.).

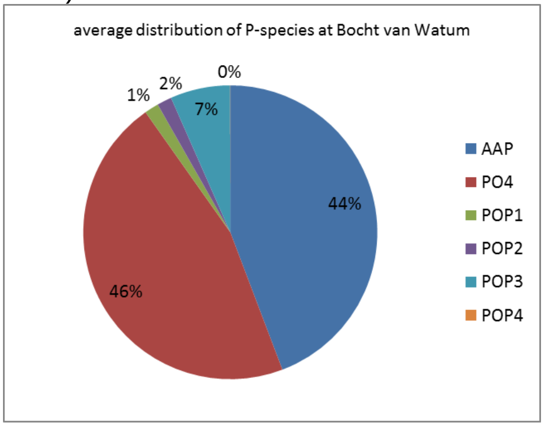

Figure 6.16 average distribution of different phosphate species at Bocht van Watum in 2012. Approximately half (46%) is made up by inorganic reactive phosphate (PO4). Adsorbed anorganic phosphate (AAP) is only slightly less (44%). Particulate species POP1 – POP4 make up the rest.

6.5.3 Silicate

The gradient over the estuary and pattern in dissolved silicate (silica in short) is reproduced by the model, but with a time shift, i.e. modelled concentrations decline 1 – 2 months later than measured silica values (Figure 6.17). This can be explained by the observed shift in start of the phytoplankton bloom (Figure 6.5), the contribution of diatoms, or the silicate requirements of diatoms. Also, there is uncertainty about the actual loads via the Ems (section 4.5.2.1).This has not been further addressed at this stage. Average values are predicted well at most stations (Figure 6.18) and spatial variation is captured well (Figure 6.19). Modelled variability is too low at Groote Gat Noord and too high at the other stations (Figure 6.18). Variability over the whole estuary shows a reasonable to good fit to measurements (Figure 6.19).

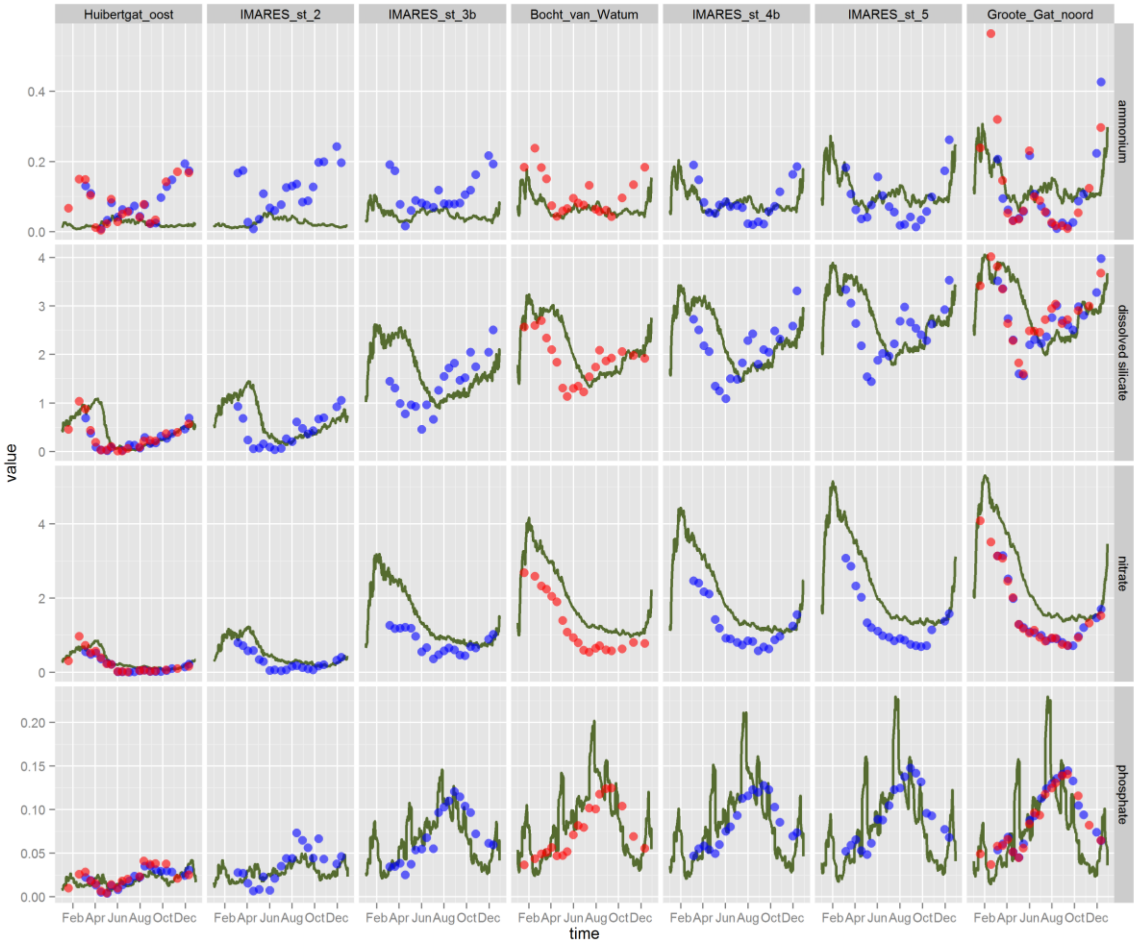

Figure 6.17 Simulated and observed ammonium, dissolve silicate, nitrate and phosphate (all in mg/l) in the Ems estuary for 2012, at MWTL and IMARES stations. The green line presents modelled daily averages. The filled red circles (●) and blue circels (●) indicate measurements from the MWTL program and IMARES program, respectively.

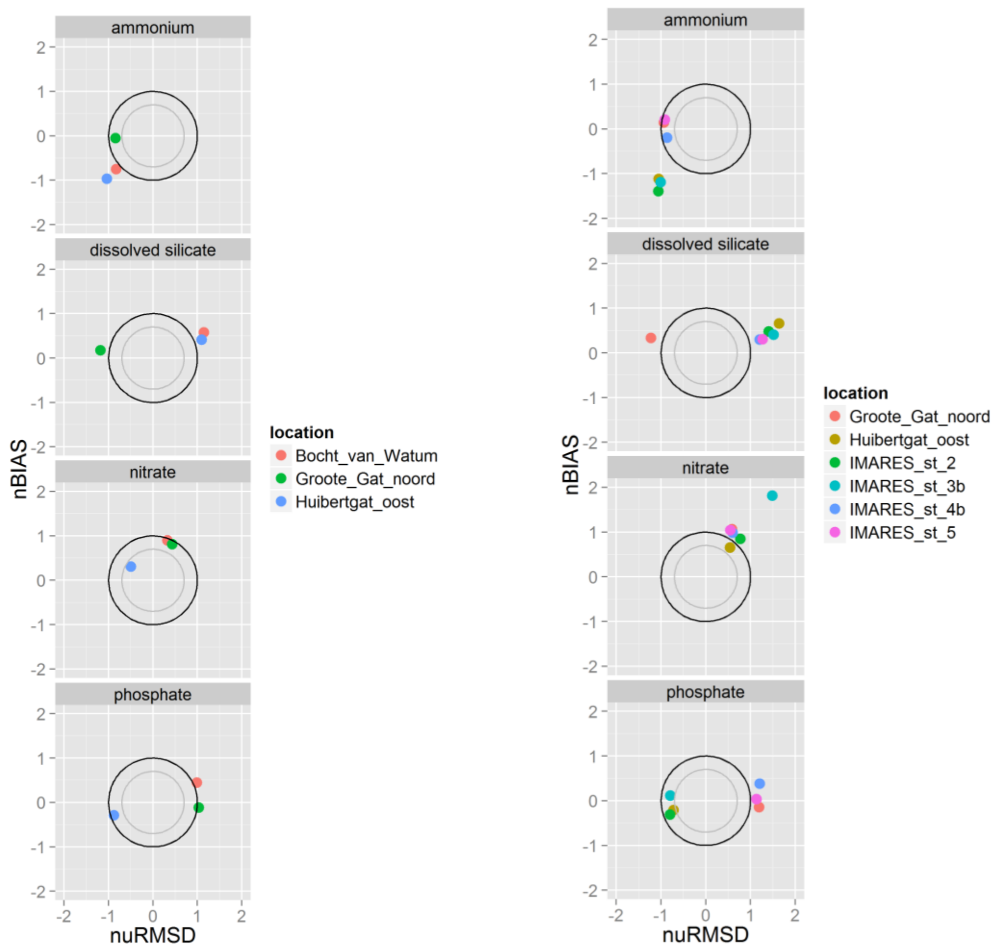

Figure 6.18 Target diagrams of nutrients in 2012 for the three MWTL stations (left panel) and IMARES stations (right panel, indicated by color. Measurements and simulated values are compared on an hourly basis.

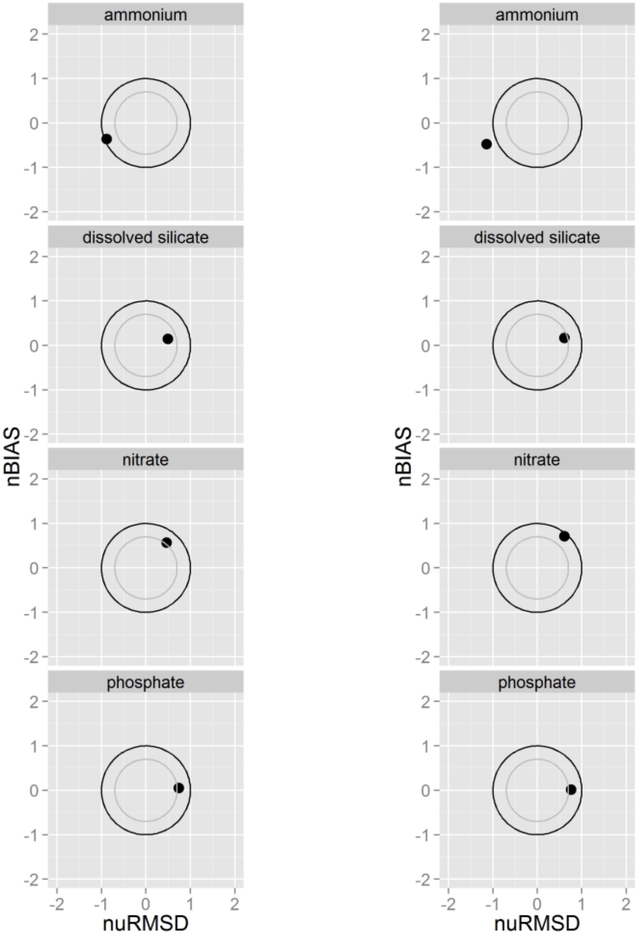

Figure 6.19 Target diagrams of nutrients for all stations combined. Measurements and simulated values are compared on an hourly basis.

6.6 Organic carbon fractions

Simulated TOC, POC and DOC agree reasonably well with the measurement data. This implies that the model has a good balance between the production (primary production and external loading) and the loss (decomposition and settling) of organic matter. Only at Groote Gat Noord, the highest measured values are not reproduced by the model. Since phytoplankton is slightly overestimated by the model at Groote Gat Noord (Figure 6.5), so this should be dead organic matter.

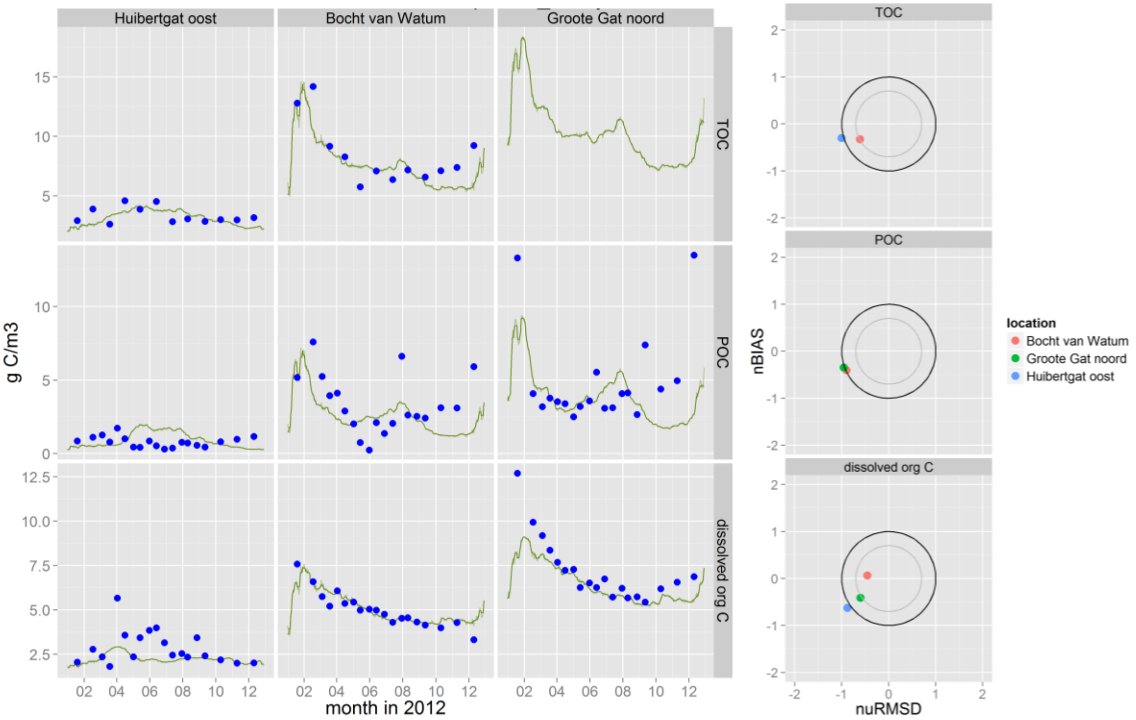

Figure 6.20 Simulated and observed Total Carbon, Particulate Carbon and dissolved organic carbon g/m^3) in the Ems estuary for 2012 at MWTL stations. The line presents daily average model values, blue dots (•) indicate measurements from the MWTL program.

Right panel: Target diagrams of water quality parameters for the three MWTL stations (indicated by color). Measurements and model results were compared per hour.

6.7 Phytobenthos biomass

Validation of microphytobenthos was done on the basis of chlorophyll-a per m^2. Model results from 2012 are here compared with measurements from the year 2013. When comparing the single segments in which benthic monitoring stations were located, it can be observed that for station 1-5, the model predicts too high chlorophyll a concentrations (Figure 6.21). Only at station 6 the model simulates too low values. The over- and underestimation makes it difficult to further calibrate growth parameters to better fit the model. While phytoplankton measurements and model results are assumed to represent a larger area, the phytobenthos values present local values. So measurements and modelled values in an adjacent cell can be very different. Hence it remains difficult to judge large scale model results based on small scale measurements.

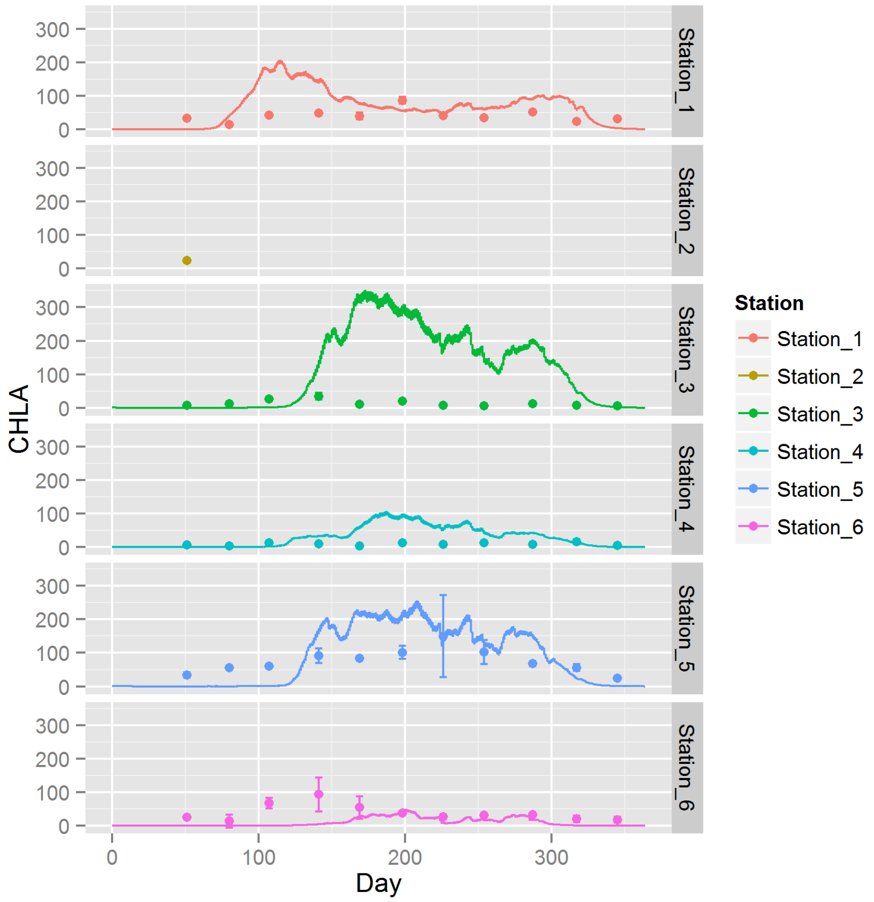

Figure 6.21 Comparison of modelled (lines) and observed (points +/- sd) microphytobenthos (expressed as mg chl a/ m^2) in the segment in which the exact monitoring position was located (left panel)

6.8 Nutrient fluxes through the estuary

Nutrient fluxes and balances will be evaluated based on the areas defined in Figure 6.22. In Figure 6.23 and Figure 6.24, net fluxes of total nitrogen and phosphorus, respectively, are presented. The net fluxes are calculated as the difference between all ingoing and outgoing fluxes. For boundaries, gross fluxes may be orders of magnitude larger than the net fluxes, due to tidal transport of water and substances.

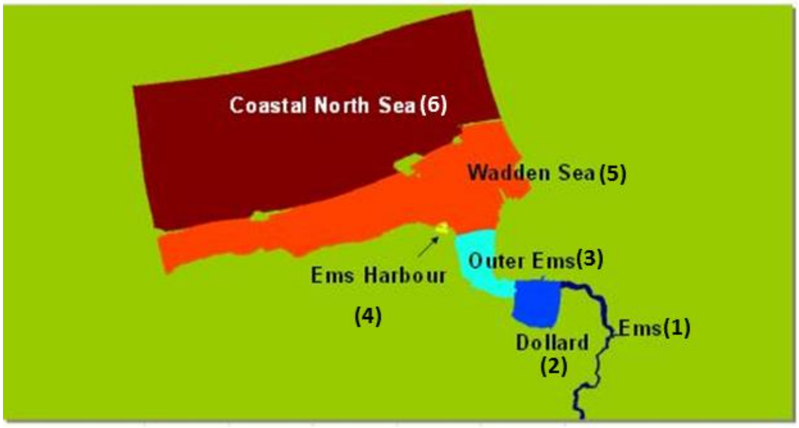

Figure 6.22 Areas used for calculating fluxes of nutrients through the estuary.

Nitrogen is transported through the estuary with highest net input into the system via the Ems river. The Dollard and Outer Ems are areas where the flux of nitrogen into the bottom sediment is approximately equal to the external loads, which means that there is no net retention of nitrogen here. Therefore, almost the total flux of nitrogen from the Ems River to the estuary is net transported into the Wadden Sea. The Wadden Sea part of the estuary receives more nitrogen via loads from polders (22.6 tons/day) than is transported to the sediment (14.8 tons/day). From the Wadden sea area, there is a net transport of approximately 11 tons/day to the North Sea.

Denitrification occurs effectively only in the sediment, since oxygen concentrations in the water are so high that they prohibit this process. In reality, denitrification in the water may occur in hypoxic (micro)zones, but this has not been included in the model. In the sediment, denitrification is an important process. In total, the modelled estimate is that 33 tons N/day disappears through denitrification in the sediment for the model domain excluding the large North Sea area.

The term “storage” is the closing term of the budgets for all compartments. It can be regarded as a measure of the difference of mass at the end and beginning of the model run, which covers one complete year. It is usually low in water, because water phase is well mixed and exchange of mass between the compartments is very high. In the sediment, this value is typically much higher, and it could be an indication of non-steady state. Often, storage terms get smaller when rerunning the model several times. However, it could also point to other causes for difference of circumstances between the end and beginning of the model run. The total balance of nitrogen is lower than 0.5 % of the gross transport over the boundaries. Theoretically, this value should be zero, but some numerical inaccuracy (rounding errors) may explain the small difference.

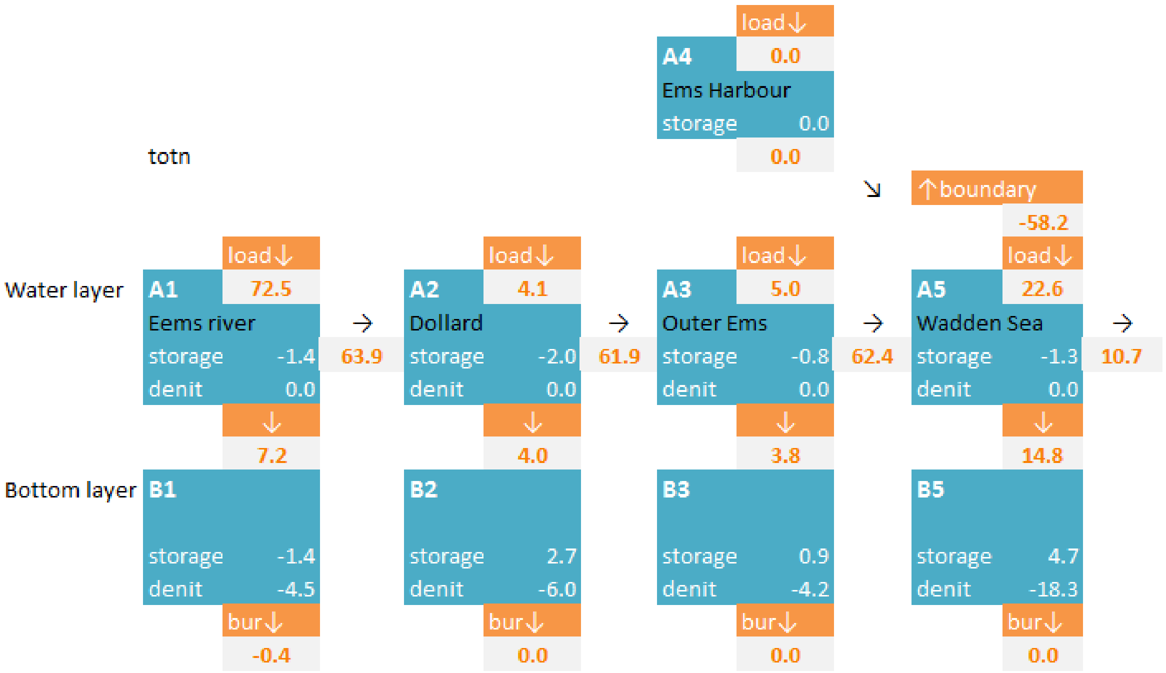

Figure 6.23 Net balances for total nitrogen in tons N/day. Loads include atmospheric deposition. Storage is a measure of the difference between mass at the end and start of the run (one full year), and should be zero if the model is in perfect steady state. "denit" = denitrification, "bur" stands for burial to deep sediment.

Phosphorus is transported through the estuary with highest input into the system via the Ems river (Figure 6.24). The Dollard and Outer Ems are areas where influx of phosphorus into the bottom sediment is larger than the external loads, which means that there is a certain net retention of phosphorus here. The Dollard and outer Ems therefore act as sinks of phosphorus, and reduce the amount of phosphorus that is net transported from the river to the Wadden Sea. In the Wadden Sea area there is only very little net transport of phosphorus to the sediment (0.1 tons/day) as compared to the flux to the North Sea and the boundaries. In total, around 5 tons P/day are transported out of the estuary to the Wadden Sea. Finally, from the Wadden Sea compartment, a net transport of 0.6 tons P per day is calculated to the North Sea, which is half of the calculated polder loads of phosphorus to the Wadden Sea (1.3 tons per day). There is net retention of phosphorus in the Wadden Sea part of the model domain.

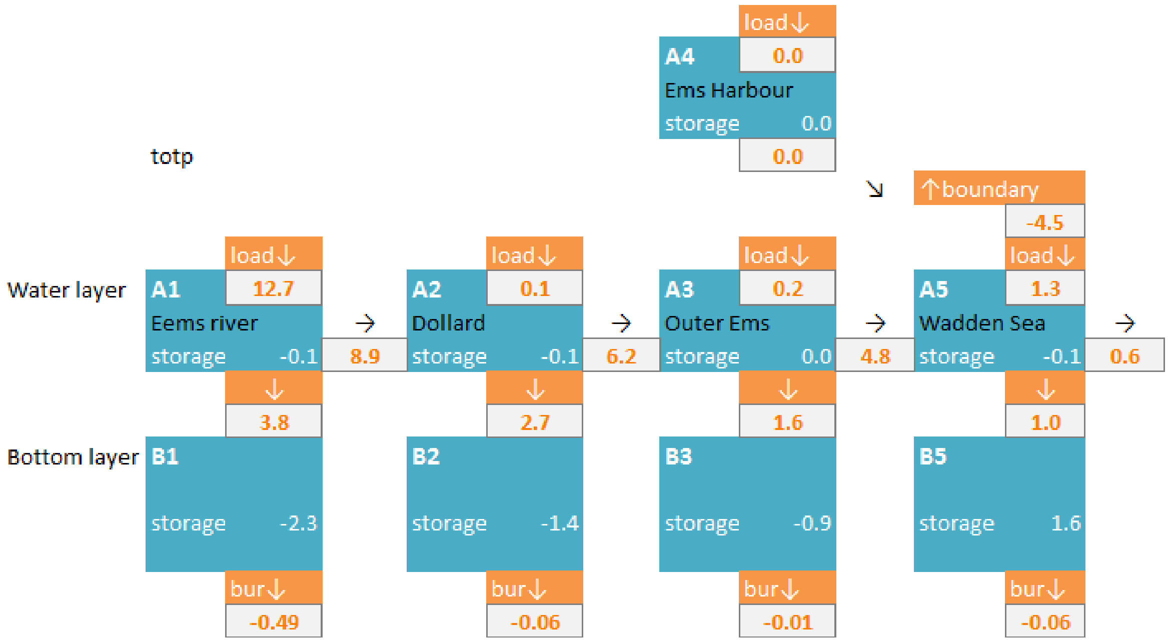

Figure 6.24 Net balances for total phosphorus in tons P/day. Storage is a measure of the differen between mass at the end and start of the run (one full year), and should be zero if the model is in perfect steady state. "bur" stands for burial to deep sediment.

6.9 Validation of 2013 results

The model calibrated for 2012 was applied to the 2013 conditions, and results of 2013 were compared to MWTL and Imares measurements of 2013. For 2013, the model was set up using the exact same parameter values as the 2012 model, but loads, boundaries, and meteo including daily irradiance were applied using data from 2013. Furthermore, hydrodynamics and sediment forcing functions were taken from respectively Delft3D-Flow and Delft3D sediment for 2013, described elsewhere.

Using suspended sediment concentrations directly from the sediment model already provided a good fit of extinction with the available measurements (Figure 6.25). Therefore, no modification of the suspended sediment concentration from the sediment model was done, apart from aggregation to the water quality grid. So, no correction factor was used, and no redistribution in time of suspended sediments. For the Ems river and the shallow parts of the Dollard, a minimum extinction was set of 20, identical as for the 2012 calibration/validation.

6.9.1 Extinction

Overall, results of 2013 are comparable to 2012 results and also the performance of the model compared to measurements. Extinction shows a similar gradient in the estuary as in 2012, with highest values in the Dollard, at Groote Gat Noord (Figure 6.25). However, measured and modelled extinction is on average higher in 2013 compared to 2012. The fit of extinction is reasonable for Groote Gat Noord and Bocht van Watum (Figure 6.26), but is overestimated for Huibertgat Noord (Figure 6.25, not seen in target diagram because of scale). Modelled extinction shows a positive bias (overestimated average) and an underestimation of variability compared to Imares measurements at stations Huibertgat Oost, 2 and 3b. The other stations have no or few measurements.

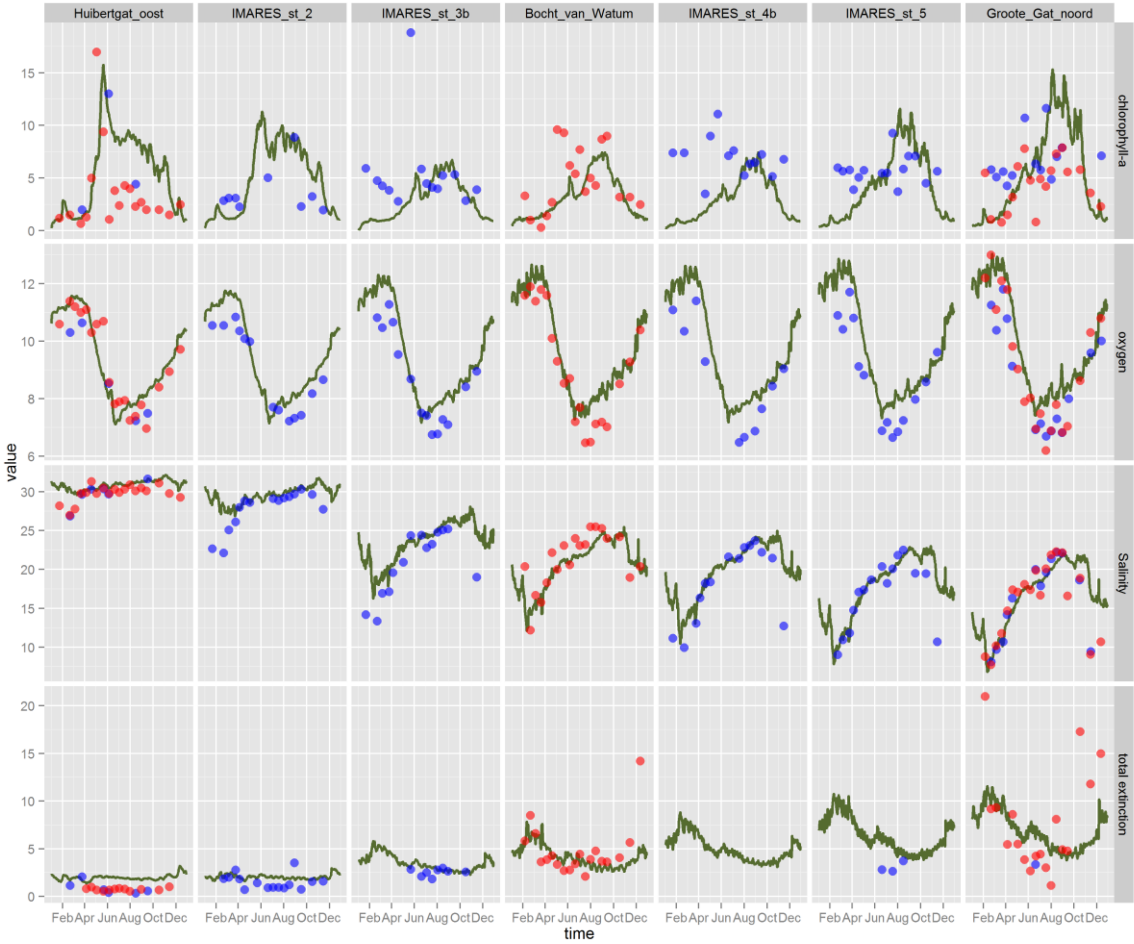

Figure 6.25 Simulated chlorophyll a (µg/L), oxygen (mg/L), salinity (psu) and total extinction (m^{-1}) in the Ems estuary for 2013, at MTWL stations Huibertgat, Bocht van Watum and Groote Gat and additional IMARES stations 2, 3b, 4b and 5. The green line represents modelled daily averages, filled red circles (●) and blue circles (●) indicate measurements from the MWTL program and IMARES, respectively.

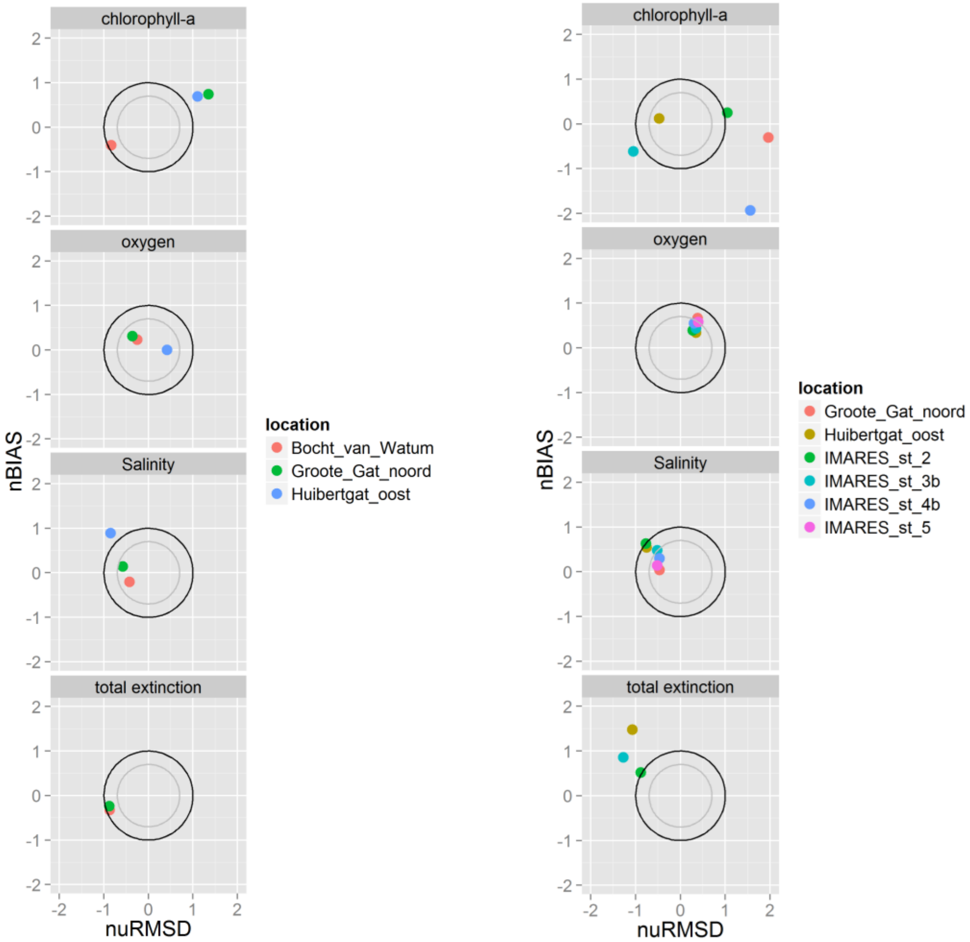

Figure 6.26 Target diagrams of water quality parameters in 2013 for the three MWTL stations (left panel) and IMARES stations (right panel), indicated by color (left panel). Measurements and simulated values are compared on an hourly basis.

6.9.2 Phytoplankton

Similar to 2012, the only station with a real measured spring bloom in 2013 is Huibertgat Oost, although at Imares station 3b one high value was measured (Figure 6.25). The phytoplankton bloom is reproduced by the model, but at most stations (except Huibertgat Oost and Imares stations 2) the bloom seems to be quite late compared to 2012 model and observed results and measurements in 2013 (Figure 6.25). The reason is the higher extinction in 2013. Target diagrams show that modelled chlorophyll-a has a reasonable fit for Bocht van Watum (MWTL), but the model over-predicts the average and variability of MWTL measured chl *a* at Huibertgat Oost and Groote Gat Noord (Figure 6.26). Contrary, the model shows a good fit to Imares measurements at Huibertgat Oost (Figure 6.26). Modelled values are on average too low at Imares station 3b, 4b and Groote Gat Noord and the fit to station 2 is (close to) reasonable (Figure 6.26).

6.9.3 Primary production

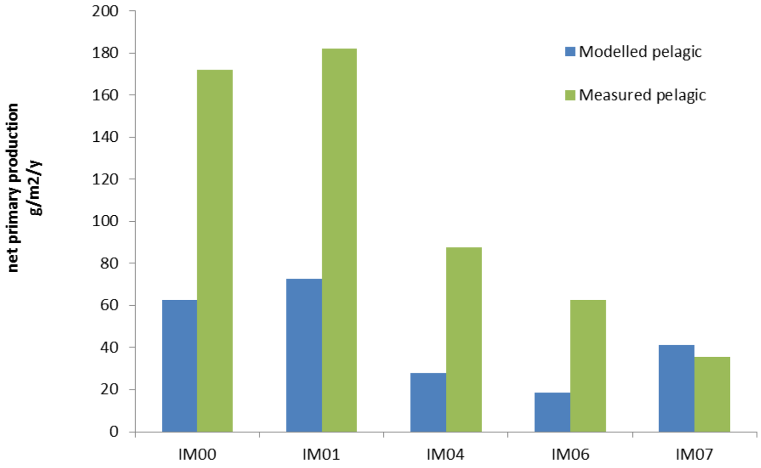

Figure 6.27 Integrated modelled pelagic primary production for 2013 and comparison with estimates derived from measurements.

The validation of pelagic primary production for 2013 is not as good as for the calibration year 2012. The gradient of primary production through the estuary is correct, i.e. there is highest production towards the seaward side of the estuary. Simulated primary production is however, 4 – 5 times lower than the estimates from measurements (Figure 6.27). When comparing 2012 with 2013 primary production, it can be noticed that:

- In 2013, measured pelagic primary production was higher than in 2012, (e.g. 170 instead of 140 for IM00).
- The modelled primary production for 2013 is lower than those in 2012 (e.g. 60 instead of 80 for IM00).
- Extinction coefficients for the different stations are higher in 2013 as compared to 2012 (Figure 6.25 and Figure 6.5).

Since light is the predominant limiting factor for primary production in 2013 (Figure 6.28) primary production in 2013 is expected to be lower than in 2012. The lower modelled primary production in 2013 as compared to 2012 is consistent with the extinction measurements The higher measured production in 2013 as compared to 2012 can be explained by higher specific (per chlorophyll-a) maximum primary production rates and not by variation in licht extinction coefficients (measurements primary production report nr 9). There is no direct explanation for the variation in specific primary production between 2012 – 2013, and it may well be within the natural variation within years and between stations.

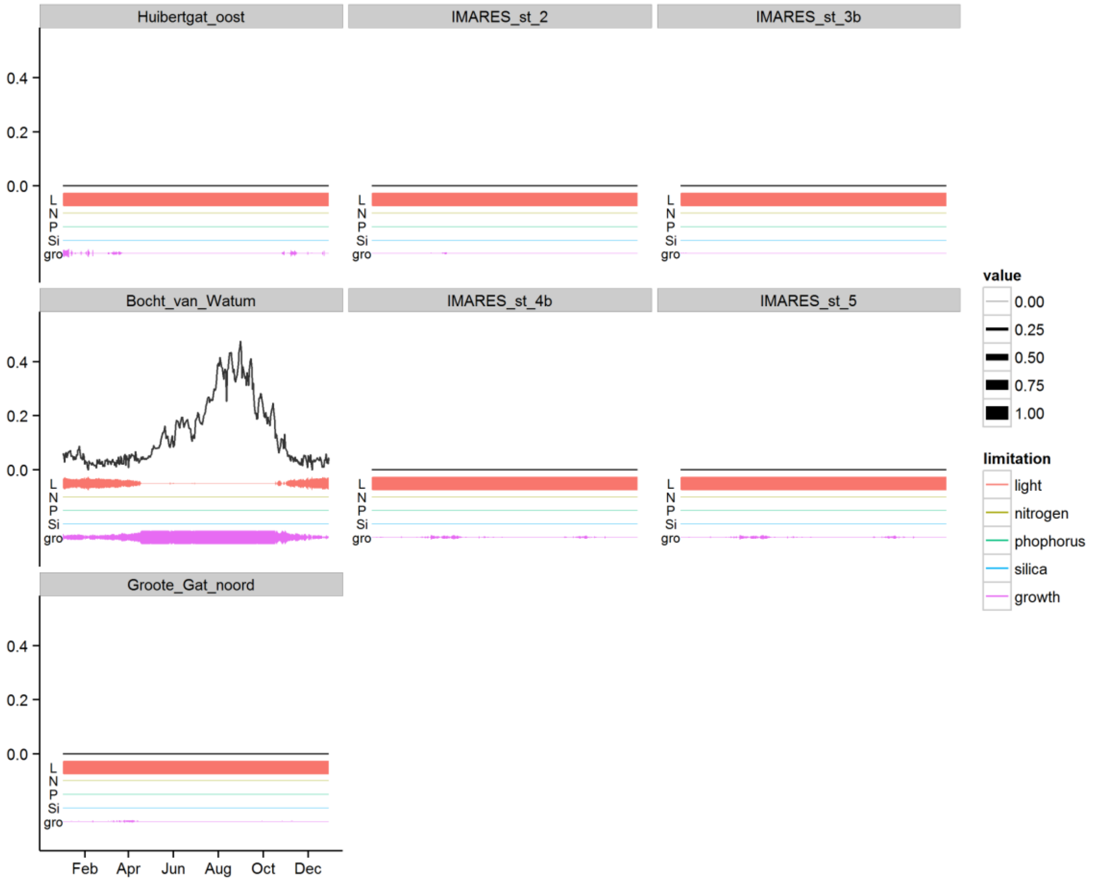

Figure 6.28 Plots with primary production (gC/m²/day) for the year 2013 and the limiting factors for primary production or phytoplankton growth at the three MWTL stations and additional IMARES stations. Values are daily averages of hourly model output. Values vary from 0 (no limitation) to 1 (limitation). For the stations in the Ems-Dollard Plume, light is the dominant limiting factor. At Bocht van Watum, a relatively shallow station, primary production is possible and light is not limiting during summer. Growth limitation indicates that phytoplankton growth is only limited by their intrinsic growth rate (which is dependent of temperature).

7 General discussion

The current water quality and primary production model for the Ems estuary enables the simulation of primary production, phytoplankton biomass, nutrient concentration, benthic primary production and phytobenthos biomass in the area. The performance with respect to the different modelled variables is varying and to a high degree dependent on the quality of the input to the model. These inputs are in order of decreasing importance:

- Hydrodynamic processes, transport and dispersion derived from the hydrodynamic model (3D, 200x200m, 8 layers in vertical) and aggregated to the water quality model grid (2D, horizontally aggregated by 2x2 (shallower than 5 m), 4x4 (deeper parts)). This affects all variables. Mixing in the estuary is highly driven by tidal processes, determining the distribution of all solutes and suspended matter. Salinity is a good proxy for how well mixing is modelled. Apart from the distribution of solutes, horizontal mixing also influences the light availability to phytoplankton since water with phytoplankton is transported from shallow areas with ample light available to deeper areas where, on average, much less light is available. For benthic primary production, drying of mudflats is important, since in these turbid waters, benthic primary production can only occur when there is no overlying water. Drying and flooding of areas is also determined by the hydrodynamic model. However, in shallow areas, notably the drying mudflats, the hydrodynamic model could not be validated because there are nomonitoring stations Since net primary production is highest in those shallow areas, it is important to better validate e.g. the time that areas are flooded (and net pelagic primary production occurs).
- Suspended sediment concentrations necessary to drive the underwater light climate for phytoplankton production originates from the sediment model. The spatial and temporal patterns of suspended sediment concentration are calculated by the sediment model and used as input to the water quality model after aggregation to the primary poduction model grid. In the vertical, only the top two layers (0 – 50% of the total depth) of the sediment model were used for aggregation to the 2D primary production model. Also, like for hydrodynamics, the suspended sediment concentrations in shallow areas could not be validated due to lack of measurements in those areas. Also, the continuous progress made in this type of modelling (sediment model report 5) requires a continuous process of testing, validation and possibly recalibration of the water quality and primary production model.
- The specific extinction coefficient of suspended sediment, derived from measurements and/or literature values defines the relation between suspended sediment concentrations and the light extinction in the water column. Different values have been reported in the literature. In the current study, a literature value of 0.025 /m has been used regardless of size classes distribution of SPM.
- Phytoplankton process parameters define the reaction of algae to the environment, most importantly (in this study) to underwater light availability. In the current study, standard parameter values have been used for phytoplankton. For phytobenthos, parameters have been adapted in the calibration process so that the production of phytobenthos accounted for approximately 50 % of the total production.

The most crucial factor for modelling primary production was the light climate, and thus by the concentration of suspended sediment that was used as input in the model. Although over the whole model grid and year, the sediment model was concluded to perform reasonably, there are some aspects that hamper the modelling of primary production. These were

1 An overestimated concentration of suspended sediment measured by MWTL at Huibertgat Oost. This area is very important for primary production in the estuary, because it is relatively clear with potentially high production. Uncertainty in light climate in this part of the model is expected to have large consequences for total production in the estuary.
2 Overestimation of suspended sediment at Groote Gat Noord, as compared to MWTL measurements during spring. During the second half of the year, the modelled suspended sediment agrees better with the MWTL observations. For the 2012 run, suspended sediment concentrations were redistributed in time so that the overestimation in spring was spread out over the year. This did improve the model, and especially the timing of the spring bloom.
3 Model results show that light limitation is the regulating factor for pelagic primary production in the Ems estuary. In the Ems river, and at shallow areas, most notably in the Dollard, suspended sediment concentrations may be underestimated. The primary production model predicted very high biomass in those areas (Figure 4.8), whereas there is no field information that could support this. Moreover, these high biomasses were transported to Groote Gat Noord, causing unrealistic high chlorophyll-a concentrations at that station (Figure 5.5). The Ems river is not the primary target of the used sediment model (WED), and it is also otherwise not an area of interest for primary production. For both cases, the high production was effectively suppressed by applying an artificial minimum extinction to prevent high biomass productivity spreading out to deeper areas.

A general conclusion on the performance of the primary production model should be done regarding the calibration procedure. During the calibration procedure, the first goal was to reproduce the extinction values measured at the MWTL stations. Therefore, the suspended sediment concentrations from the sediment model for 2012 were reduced by a factor of 2, before using it as input in the water quality model (Figure 5.5). Moreover, the overestimation of suspended sediment during spring for 2012 was improved by redistribution of suspended sediment (F. Los et al., 2008) over the year using a cosine function in combination with a wind-driven variation (Figure 5.6). For the validation year 2013, both these adaptations were not necessary to improve suspended sediment concentration and/or light extinction coefficient, therefore suspended sediment concentrations from the sediment model were used without conversion. For scenarios, this means that the processes resulting from changes in suspended sediment and extinction are clearly well-understood and represented in the model.

We conclude that the primary production model responds well to changes in suspended sediment concentration, and therefore can be used to simulate the effect of (changes in) suspended sediment concentrations and pelagic primary production. We also conclude that a correct simulation of pelagic primary production and chlorophyll-a is dependent on a correct estimation of light extinction coefficient in the water. In order to do this for the year 2012, it was necessary to modify the suspended sediment fields by a few controlled, previously applied steps, that can easily be repeated to simulate scenarios. For 2013, these adaptations were not necessary, the suspended sediment fields led to realistic extinction coefficients as compared to measurements. The above, and the fact that 2013 is a validation year so the model is not calibrated towards it, leads to the conclusion that 2013 is a better reference year for scenarios than 2012. However, in 2013, simulated annual primary production deviated from the estimation based on measurements. Currently, we cannot explain this deviation in terms of variation of light climate between the years.

The uncertainty of scenario simulation cannot be completely estimated from the calibration/validation quality only. Different calibration procedures might be necessary such as the difference between calibration for light extinction in 2012 and 2013. Morover, there could be different sets of parameter values that would result in similar validation quality for a given year. In order to get a grip on the reliability of scenarios, multiple calibration versions of one and the same year could be used as a reference for further scenario simulation. This would give a more complete image of the uncertainty of scenarios than the validation quality alone.

For benthic production, light is also a limiting factor, but nutrient limitation can be present as well. In particular, silicate became limiting in the Wadden Sea area during early summer of the estuary. Benthic primary production is restricted to tidal flats, where enough light is available during drying, and is therefore only partly determined by the turbidity of the overlying water. Any change in turbidity in the estuary is therefore likely to have effects on primary production, but more on pelagic than on benthic production, unless turbidity is reduced to such a degree that more light can reach the bottom.

Nutrient concentrations were modelled reasonable to well for 2012, although the model was not specifically calibrated for nutrients. Since nutrients do not limit primary production in the Ems estuary on a large scale, no further effort has been put in optimizing nutrient model results.

The calibration of the water quality model showed that the suspended sediment concentration in 2012 and the resulting extinction was overestimated, especially during the first half of the year (Figure 5.5) as compared to MWTL measurements. A possible explanation could be that in the sediment model, the resuspension of fine sediment is overestimated during the winter and spring. In nature, resuspension may be influenced by biological structures such as benthic diatom mats, which are not taken into account in the sediment model.

Given the above adaptations of the suspended sediment forcing, average chlorophyll-a concentrations were predicted well in 2012 and 2013 at the MWTL and IMARES stations. The variability of chlorophyll-a was overestimated in most stations, with relatively high values in summer and low values in winter as compared to measurements. An explanation for the underestimation in winter could be that in the current model, no sheer-stress induced resuspension of benthic algae is incorporated. Especially in winter, when wind velocities are high, this may account for some of the chlorophyll observed in the water column (De Jonge & Van Beusekom, 1995, De Jonge & Van Beusekom, 1992).

Pelagic primary production from the model was compared to IMARES measurements in those areas where measurements were made (Figure 6.12). Overall, the longitudinal transect through the estuary was reproduced well. Measured primary production were comparable (40 – 140 g C m^{-2} y^{-1}) to modelled values for 2012 (20 – 120 g C m^{-2} y^{-1}). Both measured and modelled production is lower than primary production rates observed in the late 70’s (Colijn et al., 1987): see report 9 for an extensive comparison primary production in the 70’s and 2012-2013.

The primary production of microphytobenthos in the present model is approximated by an additional species in the BLOOM sub-model. This methodology makes the calculation of microphytobenthos conceptually compatible with the growth of other algae in the system. In principle, microphytobenthos is then allowed to resuspend and compete with phytoplankton for light and nutrients in a generic way. There are however some shortcomings of this approach which should be taken into account when interpreting the results. Effectively, microphytobenthos is confined to a water layer just above the sediment. Consequently, nutrients are taken up from the water, and oxygen is released to the water. In reality, these processes are at least partly directed to the shallow sediment layers. It has not been investigated if this has an influence on the calculation of benthic primary production or biomass. A future development might be to replace the current microphytobenthos by an alternative method. One candidate is an existing module MICROPHYT that has been developed to be used in combination with layered sediment. This module simulates two benthic diatom groups, represented by an epipelic (migratory) and an epipsammic species. The module has not been tested with recent Delft3D software versions, and further testing is needed before use.

In this model application, an advanced sediment compartment with 9 layers in the vertical has been added to the water quality model, in combination with a consistent set of biogeochemical processes for the degradation of organic material as a function of gradients in oxygen concentration or redox condition. Such processes can improve model behaviour with respect to phosphate return fluxes in areas with high import and production of organic material, such as the Ems estuary.

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A Input process coefficients for the water and sediment quality sub-model

Table A.1 Input process coefficients for the decomposition of organic matter.

Name	Process / Definition of parameter	Source[1]	Model Value	Range	Units
	Decomposition of organic matter				
ku_dFdec20	max. min. rate fast decomp. detr. POC1 at 20^o C	2/3/5	0.20	0.2-0.05	d^{-1}
kl_dFdec20	min. min. rate fast decomp. detr. POC1 at 20^o C	2/3/5	0.15	0.2-0.05	d^{-1}
ku_dMdec20	max. min. rate medium dec. detr. POC2 at 20^o C	1/4/5	0.025	0.08-0.001	d^{-1}
kl_dMdec20	min. min. rate medium dec. detr. POC2 at 20^o C	1/4/5	0.025	0.08-0.001	d^{-1}
ku_dSdec20	max. min. rate slow dec. detritus POC3 at 20^o C	1/4/5	0.0012	0.003-0.0003	d^{-1}
kl_dSdec20	min. min. rate slow dec. detritus POC3 at 20^o C	1/4/5	0.0012	0.003-0.0003	d^{-1}
k_dprdec20	min. rate part. refractory detritus POC4 at 20^o C	1/4/5	0.000035	0.0003-0.000002	d^{-1}
k_DOCdec20	min. rate diss. refractory detritus DOC at 20^o C	1/4/5	0.0035	0.0003-0.000002	d^{-1}
au_dNf	max. stoich. constant nitrogen in fast dec. detritus	2/3/5	0.15	0.18-0.12	$gN.gC^{-1}$
al_dNf	min. stoich. constant nitrogen in fast dec. detritus	2/3/5	0.075	0.12-0.07	$gN.gC^{-1}$
au_dNm	max. st. constant N in medium slow dec. detritus	2/3/5	0.12	0.18-0.12	$gN.gC^{-1}$
al_dNm	min. st. constant N in medium slow dec. detritus	2/3/5	0.06	0.12-0.06	$gN.gC^{-1}$
au_dNs	max. st. constant N in slow decomposing detritus	2/3/5	0.12	0.18-0.12	$gN.gC^{-1}$
al_dNs	min. st. constant N in slow decomposing detritus	2/3/5	0.006	0.12-0.06	$gN.gC^{-1}$
a_dNpr	stoich. constant nitrogen in refractory detritus	1/5	0.07	0.07-0.015	$gN.gC^{-1}$
au_dPf	min. stoich. constant phosphorus in fast dec. detritus	2/3/5	0.015	0.025-0.015	$gP.gC^{-1}$
al_dPf	min. stoich. constant phosphorus in fast dec. detritus	2/3/5	0.0075	0.015-0.008	$gP.gC^{-1}$
au_dPm	max. st. constant P in medium slow dec. detritus	2/3	0.012	0.020-0.012	$gP.gC^{-1}$
al_dPm	min. st. constant P in medium slow dec. detritus	2/3/5	0.006	0.012-0.006	$gP.gC^{-1}$
au_dPs	max. st. constant P in slow dec. detritus	2/3/5	0.012	0.020-0.012	$gP.gC^{-1}$
al_dPs	min. st. constant P in slow dec. detritus	2/3/5	0.006	0.012-0.006	$gP.gC^{-1}$
a_dPpr	stoich. constant phosphorus in refractory detritus	1/5	0.007	0.007-0.002	$gP.gC^{-1}$
a_dSpr	stoich. constant sulphur in refractory detritus	4/5	0.005	-	$gS.gC^{-1}$
b_ni	attenuation constant for nitrate as electron acceptor	1/4	1.0	1.0-0.8	-
b_su	attenuation constant for sulphate as electron acceptor	1/4	1.0	1.0-0.5	-
b_poc1poc2	conv. fraction fast dec. detr. into medium dec. detr.	1/4/5	0.3	0.4-0.2	-
b_poc2poc3	conv. fraction medium dec. detr. into slow dec. detr.	1/4/5	0.2	0.4-0.2	-
b_poc2doc	conv. fraction medium dec. detr. into diss. refr. detr.	4/5	0.15	0.2-0.1	-
b_poc3poc4	conv. fraction slow dec. detr. into part. refr. detr.	4/5	0.2	-	-
b_poc3doc	conv. fraction slow dec. detr. into diss. refr. detr.	4/5	0.15	-	-

1) 1=SWITCH (Delft Hydraulics, 1994 and 1998), 2=ECO (MARE, 2002), 3=DBS (Delft Hydraulics, 1995), 4=expert estimate, 5=literature (inclusive of publication ECO in PLOS ONE 2013)

Table A.2 Input process coefficients for the consumption of electron-acceptors and the production of methane.

Name	Process / Definition of parameter	Source[1]	Preferred Value	Range	Units
	Consumption of electron-acceptors, methanogenesis				
KsOxCon	half saturation constant for oxygen limitation	4/5	1.0	1.0-0.05	$gO_2.m^{-3}$
KsNiDen	half saturation constant for nitrate limitation	4/5	0.25	0.4-0.05	$gN.m^{-3}$
KsSuRed	half saturation constant for sulphate limitation	4/5	2.0	5.0-0.05	$gS.m^{-3}$
KsOxDenInh	half sat. const. for DO inhibition of denitrification	4/5	2.0	2.0-0.1	$gO_2.m^{-3}$
KsNiSRdInh	half sat. const. for nitrate inhib. of sulph. reduction	4/5	0.02	0.2-0.02	$gN.m^{-3}$
KsSuMetInh	half sat. const. for sulphate inhib. of methanogenesis	4/5	1.0	1.0-0.05	$gS.m^{-3}$
CoxDenInh	critical diss. oxygen conc. inhibition of denitrification[2]	4/5	1.0/10.0	1.0-5.0	$gO_2.m^{-3}$
CoxSRedInh	critical diss. oxygen conc. inhibition of sulphate red.	4/5	0.05	0.1-0.01	$gO_2.m^{-3}$
CoxMetInh	critical diss. oxygen conc. inhib. of methanogenesis	4/5	0.02	0.1-0.01	$gO_2.m^{-3}$
CniMetInb	critical nitrate conc. inhibition of methanogenesis	4/5	0.05	0.1-0.01	$gN.m^{-3}$
RedFacDen	correction factor for denitr. below crit. temperature	4	1.25	1.25-0.0	-
RedFacSRed	correction factor for sulph. red. below crit. temp.	4	1.25	1.25-0.0	-
RedFacMet	correction factor for methanogen. below crit. temp.	4	1.25	1.25-0.0	-
CTBactAc	critically low temp. for specific bacterial activity	1/2	2.0	4.0-0.0	^oC

1) 1=SWITCH (Delft Hydraulics, 1994 and 1998), 2=ECO (MARE, 2002), 3=DBS (Delft Hydraulics, 1995), 4=expert estimate, 5=literature (inclusive of publication ECO in PLOS ONE 2013)

2) First preferred value concerns water column, second value concerns the sediment

Table A.3 Input process coefficients for processes of ammonium, sulphide and methane.

Name	Process / Definition of parameter	Source[1]	Preferred Value	Range	Units
	Nitrification				
RcNit20	MM nitrification rate in water/sediment	4/5	0.2/22.0	0.05-25.0	$gN.m^{-3}.d^{-1}$
KsAmNit	half saturation constant for ammonium limitation	5	0.4	0.7-0.1	$gN.m^{-3}$
KsOxNit	half saturation constant for oxygen limitation	5	1.0	1.0-0.05	$gO_2.m^{-3}$
CoxNit	critical DO concentration for nitrification	4	0.0	1.0-0.0	$gO_2.m^{-3}$
CTNit	critically low temperature for nitrification	1/2	0.0	4.0-0.0	^oC
	Oxidation, precip., dissolution, speciation sulphide				
RcSox20	pseudo second-order sulphide oxid. rate at 20 ^oC	5	10.0	85.0-2.0	$gO_2^{-1}.m^3.d^{-1}$
CoxSUD	critical dissolved oxygen concentration	4	0.0	1.0-0.0	$gO_2.m^{-3}$
DisSEqFeS	eq. dis. free sulph. conc. for amorph. iron sulphide	4/5	$0.2\ 10^{-10}$	$2.0\text{-}0.2\ 10^{-10}$	$mole.l^{-1}$
RcDisS20	dissolution reaction rate	4/5	$2.0\ 10^6$	-	d^{-1}
RcPrecS20	precipitation reaction rate	4/5	$1.0\ 10^6$	-	d^{-1}
pKhs	neg. log. of eq. constant for HS^- (see directives!)	5	-14.0	-	$-log(l.mole^{-1})$
pKh2s	neg. log. of eq. constant for H_2S (see directives!)	5	-7.1	-	$-log(l.mole^{-1})$
pH	acidity in the water column/sediment bed	5	8.1/8.1	9.0-6.5	-
	Oxidation, ebullition, volatilisation of methane				
RcMetOx20	MM-rate for methane oxid. with oxygen at 20 ^oC	4/5	0.1	0.5-0.05	$gC.m^{-3}.d^{-1}$
RcMetSu20	MM-rate for methane oxid. with sulphate at 20 ^oC	4/5	0.05	0.3-0.03	$gC.m^{-3}.d^{-1}$
CoxMet	critical DO concentration for methane oxidation	4	0.0	2.0-0.0	$gO_2.m^{-3}$
CsuMet	critical sulphate conc. for methane oxidation	4	0.0	2.0-0.0	$gS.m^{-3}$
KsMet	half saturation constant for methane consumption	4/5	0.5	1.0-0.2	$gC.m^{-3}$
KsOxMet	half saturation constant for DO consumption	4/5	1.0	2.0-0.05	$gO_2.m^{-3}$
KsSuMet	half saturation constant for sulphate consumption	4/5	1.0	2.0-0.05	$gS.m^{-3}$
CTMetOx	critically low temperature for methanogenesis	1/2	3.0	4.0-2.0	^oC
fScEbul	scaling factor for the methane ebullition rate	4	1.0	1.0-0.0	-

1) 1=SWITCH (Delft Hydraulics, 1994 en 1998), 2=ECO (MARE, 2002), 3=DBS (Delft Hydraulics, 1995), 4=tentative estimate, 5=literature

Table A.4 Input process coefficients for processes of phosphate and silicate.

Name	Process / Definition of parameter	Source[1]	Preferred Value	Range	Units
	Adsorption, precipitation, dissolution of phosphate				
KadsP_20	molar adsorption equilibrium constant	2/5	1800.0	3000-1000	$(mole.l^{-1})^{a-1}$
a_OH-PO4	stoichiometric reaction constant for pH-dependency	5	0.2	0.3-0.1	-
fr_FeIM1	fraction reactive iron in silt, inorganic matter IM1	6	0.035	0.075-0.025	$gFe.gDW^{-1}$
fr_FeIM2	fraction reactive iron in sand, inorganic matter IM2	6	0.0	0.05-0.0	$gFe.gDW^{-1}$
fr_FeIM3	fraction reactive iron in silt, inorganic matter IM3	6	0.035	0.075-0.025	$gFe.gDW^{-1}$
fr_Feox	fraction ox. iron (III) in the reactive iron fraction	1/4/5	0.3	0.5-0.1	-
Cc_oxPsor	critical DO concentration for iron reduction	1/4	1.0	1.5-0.1	$gO_2.m^{-3}$
Cc_oxVivP	critical DO concentration for presence reduced iron	4	0.25	0.5-0.01	$gO_2.m^{-3}$
RCAdPO4AAP	sorption reaction rate	4	10.0	10.0-1.0	d^{-1}
RcPrecP20	vivianite precipitation reaction rate	5	0.6	0.8-0.1	d^{-1}
RcDissP20	vivianite dissolution reaction rate	1/4/5	0.05	0.1-0.005	$m^3.gO_2^{-1}.d^{-1}$
EqVIVDisP	equilibrium diss. phosphate conc. for vivianite	1/4/5	0.15	0.25-0.05	$gP.m^{-3}$
RatAPandVP	ratio of apatite and vivianite precipitation rates	5	2.0	2.0-0.0	-
RcDisAP20	apatite dissolution reaction rate	4/5	0.0025	0.01-0.001	$m^3.gP^{-1}.d^{-1}$
EqAPATDisP	equilibrium dissolved phosphate conc. for apatite	5	0.15	0.25-0.05	$gP.m^{-3}$
	Dissolution of opal silicate				
Ceq_DisSi	equilibrium dissolved silicate conc. saline water	5	17.0	10.0-20.0	$gSi.m^{-3}$
RcDisSi20	dissolution reaction rate	5	0.00005	0.005-0.00005	$m^3.gSi^{-1}.d^{-1}$

1) 1=SWITCH (Delft Hydraulics, 1994 en 1998), 2=ECO (MARE, 2002), 3=DBS (Delft Hydraulics, 1995), 4=tentative estimate, 5=literature (inclusive of publication ECO in PLOS ONE 2013), 6=measurements.

B Formulation for concentration of substances for open boundaries

At location Terschelling10, 19 samples were taken in 2012 (monthly in the winter half year and fortnightly in the summer half year). One missing value was added for dissolved phosphate (PO4) and total phosphorus (TOTP), two missing values for total nitrogen (TOTN) and three missing values for dissolved oxygen (DO). 7 values of total organic carbon (TOC) were added by means of adding the available data of particulate organic carbon (POC) and dissolved organic carbon (DOC).

For the quantification of the boundary concentrations of the simulated parameters the following formulations have been applied (all units are $g.m^{-3}$):

IM1 = 0.0
IM2 = 0.0
Salinity = 32.5
SO4 = 820.0
SUD = 0.0
SUP = 0.0
CH4 = 0.0
OXY = DO

NH4 = NH4N
NO3 = NO3N
PO4 = PO4P
AAP = 0.0
VIVP = 0.0
APATP = 0.0
Si = DSi
Opal = 0.0

POC1 = TOC * 0.3 - DOC * 0.3 - CHLPHLL * 0.3 / 0.025 / 1000
POC2 = TOC * 0.6 - DOC * 0.6 - CHLPHLL * 0.6 / 0.025 / 1000
POC3 = TOC * 0.1 - DOC * 0.1 - CHLPHLL * 0.1 / 0.025 / 1000
POC4 = TOC * 0.0 - DOC * 0.0 - CHLPHLL * 0.0 / 0.025 / 1000

PON1 = TOTN * 0.40 - DOC * 0.3 * 0.11 - CHLPHLL * 0.3 * 0.185/0.025/1000 - NH4N * 0.40 - NO3N * 0.40
PON2 = TOTN * 0.53 - DOC * 0.6 * 0.11 - CHLPHLL * 0.6 * 0.185/0.025/1000 - NH4N * 0.53 - NO3N * 0.53
PON3 = TOTN * 0.07 - DOC * 0.1 * 0.11 - CHLPHLL * 0.1 * 0.185/0.025/1000 - NH4N * 0.07 - NO3N * 0.07
PON4 = TOTN * 0.00 - DOC * 0.0 * 0.11 - CHLPHLL * 0.0 * 0.185/0.025/1000 - NH4N * 0.00 - NO3N * 0.00

POP1 = TOTP * 0.40 - DOC * 0.3 * 0.005 - CHLPHLL * 0.3 * 0.026 / 0.025 / 1000 - PO4P * 0.40
POP2 = TOTP * 0.53 - DOC * 0.6 * 0.005 - CHLPHLL * 0.6 * 0.026 / 0.025 / 1000 - PO4P * 0.53
POP3 = TOTP * 0.07 - DOC * 0.1 * 0.005 - CHLPHLL * 0.1 * 0.026 / 0.025 / 1000 - PO4P * 0.07
POP4 = TOTP * 0.00 - DOC * 0.0 * 0.005 - CHLPHLL * 0.0 * 0.026 / 0.025 / 1000 - PO4P * 0.00

POS1 = TOC * 0.3 * 0.016 - DOC * 0.3 * 0.005 - CHLPHLL * 0.3 * 0.0175 / 0.025 / 1000
POS2 = TOC * 0.6 * 0.012 - DOC * 0.6 * 0.005 - CHLPHLL * 0.6 * 0.0175 / 0.025 / 1000
POS3 = TOC * 0.1 * 0.008 - DOC * 0.1 * 0.005 - CHLPHLL * 0.1 * 0.0175 / 0.025 / 1000
POS4 = TOC * 0.0 * 0.005 - DOC * 0.0 * 0.005 - CHLPHLL * 0.0 * 0.0175 / 0.025 / 1000

DOC = DOC * 1.5
DON = DOC * 0.11 * 1.5
DOP = DOC * 0.005 * 1.5
DOS = DOC * 0.005 * 1.5

MDIATOMS_E = CHLPHLL * 0.4 / 0.0533 / 1000
MDIATOMS_N = CHLPHLL * 0.0 / 0.015 / 1000
MDIATOMS_P = CHLPHLL * 0.0 / 0.015 / 1000
MFLAGELA_E = CHLPHLL * 0.6 / 0.0228 / 1000
MFLAGELA_N = CHLPHLL * 0.0 / 0.01 / 1000
MFLAGELA_P = CHLPHLL * 0.0 / 0.01 / 1000
PHAEOCYS_E = CHLPHLL * 0.0 / 0.023 / 1000
PHAEOCYS_N = CHLPHLL * 0.0 / 0.007 / 1000
PHAEOCYS_P = CHLPHLL * 0.0 / 0.007 / 1000

NB1: The names at the left hand side of the above formulations refer to simulated substances, the names at the right hand side to measured parameters.

C Concentrations of substances for polder loads

C.1.1 Ems and Leda loads

For the river load concentrations of simulated parameters the following formulations have been applied (all units are $g.m^{-3}$).

Salinity = CL * 0.002
SO4 (mg S/l) = SO4 (mg SO_4/l) * 0.333
OXY = DO

NH4 = NH4N
NO3 = NO3N
PO4 = PO4P
AAP = TOTP * 0.8 - DOC * 0.007 * 0.8 - PO4P * 0.8
Si = (time series derived from MWTL measurements, see report)

POC1 = TOC * 0.05 - DOC * 0.05
POC2 = TOC * 0.05 - DOC * 0.05
POC3 = TOC * 0.90 - DOC * 0.90
POC4 = TOC * 0.00 - DOC * 0.00

PON1 = TOTN * 0.07 - DOC * 0.07 * 0.07 - NH4N * 0.07 - NO3N * 0.07
PON2 = TOTN * 0.06 - DOC * 0.06 * 0.07 - NH4N * 0.06 - NO3N * 0.06
PON3 = TOTN * 0.87 - DOC * 0.87 * 0.07 - NH4N * 0.87 - NO3N * 0.87
PON4 = TOTN * 0.00 - DOC * 0.00 * 0.07 - NH4N * 0.00 - NO3N * 0.00

POP1 = TOTP * 0.07 * 0.2 - DOC * 0.07 * 0.007 * 0.2 - PO4P * 0.07 * 0.2
POP2 = TOTP * 0.06 * 0.2 - DOC * 0.06 * 0.007 * 0.2 - PO4P * 0.06 * 0.2
POP3 = TOTP * 0.87 * 0.2 - DOC * 0.87 * 0.007 * 0.2 - PO4P * 0.87 * 0.2
POP4 = TOTP * 0.00 * 0.2 - DOC * 0.00 * 0.007 * 0.2 - PO4P * 0.00 * 0.2

POS1 = TOC * 0.05 * 0.016 - DOC * 0.05 * 0.005
POS2 = TOC * 0.05 * 0.016 - DOC * 0.05 * 0.005
POS3 = TOC * 0.90 * 0.016 - DOC * 0.90 * 0.005
POS4 = TOC * 0.00 * 0.016 - DOC * 0.00 * 0.005

DOC = DOC
DON = DOC * 0.07
DOP = DOC * 0.007
DOS = DOC * 0.005

(NB: The names at the left hand side of the above formulations refer to simulated substances, the names at the right hand side to measured parameters.)

Adsorbed phosphorus (AAP) is estimated as 80% of total phosphorus (TOTP) minus dissolved dissolved phosphorus (DOP + PO4). The other 20% is allocated to particulate organic phosphorus (POP1-4) (knowledge developed in previous projects). This resulted in a realistic P/C ratio in organic matter as represented by particulate organic carbon (POC1-4 as TOC-DOC).

It is assumed that river algae die instantly when discharged into saline water, and therefore, that all algae biomass is part of particulate detrital organic matter. Consequently, the distribution of particulate detrital organic carbon among the four simulated particulate fractions (POC1-4) is based on TOC-DOC. The distribution fractions of TOC-DOC to POC1-4 reflect the assumption that organic matter in the discharge of the EMS is mainly composed of slowly decomposing detritus, which like inorganic sediment is being recycled between the river and the estuary. The distribution fractions of the organic nutrients are slightly different from the fractions for organic carbon to account for the fact that fast decomposing detritus (POC1 and POC2) has a higher nutrient content than (very) slowly decomposing detritus (POC3 and POC4). It was verified that distribution fractions add up to one. The N/C, P/C and S/C ratios used are representative of detrital organic matter and are in line with the ratios used by the model.

It was verified that the distribution formulations would not lead to negative concentrations of adsorbed phosphorus (AAP) and particulate detrital organic components (POC, PON, POP, POS) by checking that the sum of substances would not exceed TotN, TotP en TOC. No negative values remained for the final set of ratios after verification.

C.1.2 Dutch polder and Westerwoldse Aa loads

Figure 8.1 shows the locations of fresh water discharges from the Dutch polders and the Westerwoldse Aa along the Dollard. The water quality monitoring locations near the discharge locations are indicated. The 2012 monitoring data for a selection of substances are displayed in Figure 8.2 to Figure 8.6 (data obtained from the Hunze and Aas Water Board). Because the hydrodynamic model has only one water discharge covering all polder discharges located at Nieuw-Statenzijl, all these discharges have been allocated the data for location 5101. The data for location 1103 have been used to quantify the load from the Westerwoldse Aa.

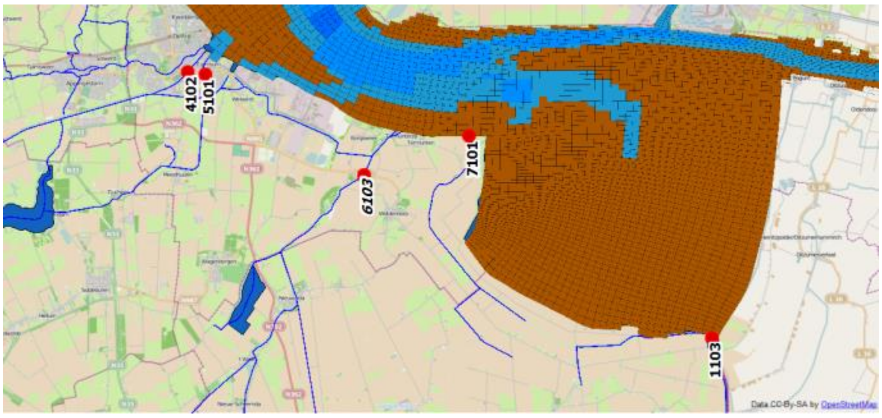

Figure 8.1 Loading locations from the Dutch part of the estuaries. Discharges and nutrient concentrations were kindly provided by the Hunze en Aas Waterboard.

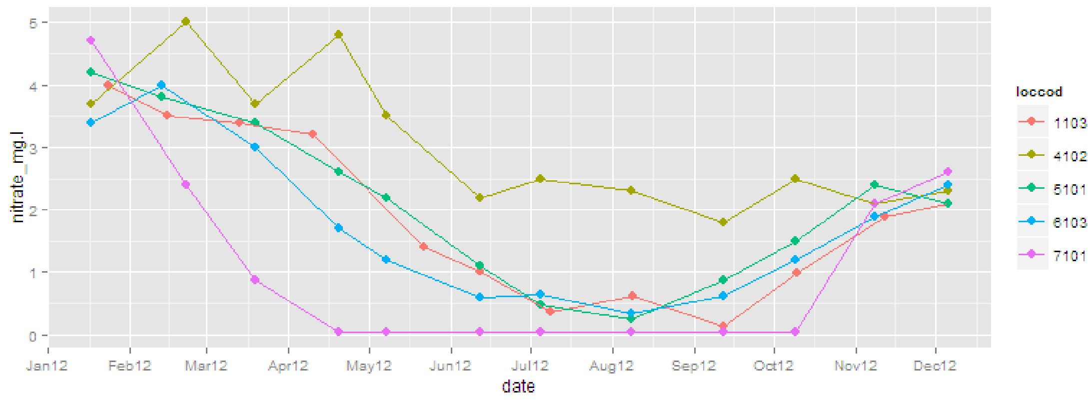

Figure 8.2 Nitrate concentrations at the loading locations on the Dutch part of the estuary.

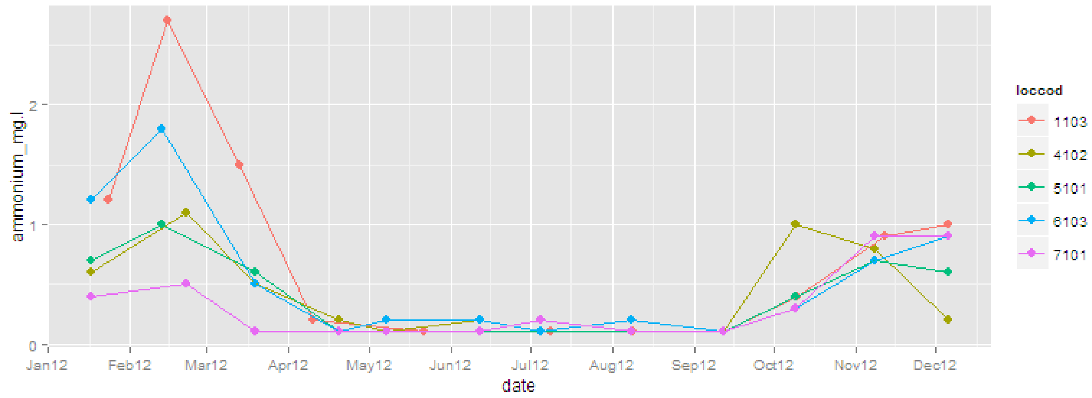

Figure 8.3 Ammonium concentrations at the loading locations on the Dutch part of the estuary.

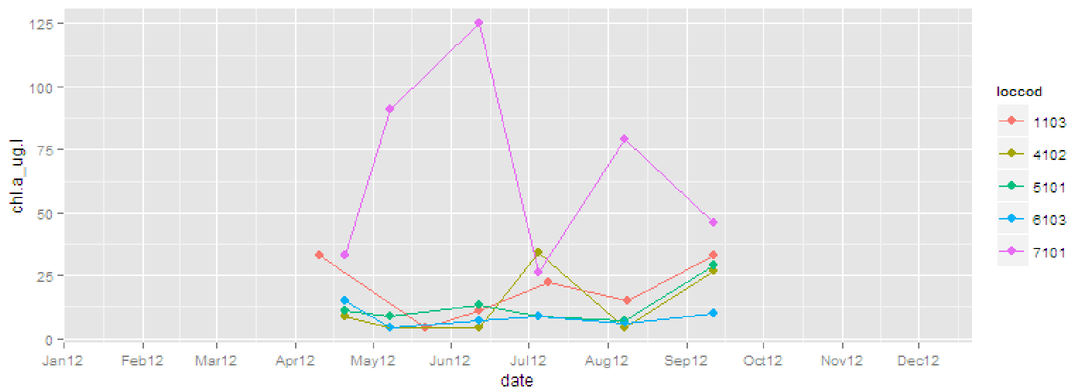

Figure 8.4 Chlorophyll-a concentration at the loading locations on the Dutch part of the estuary.

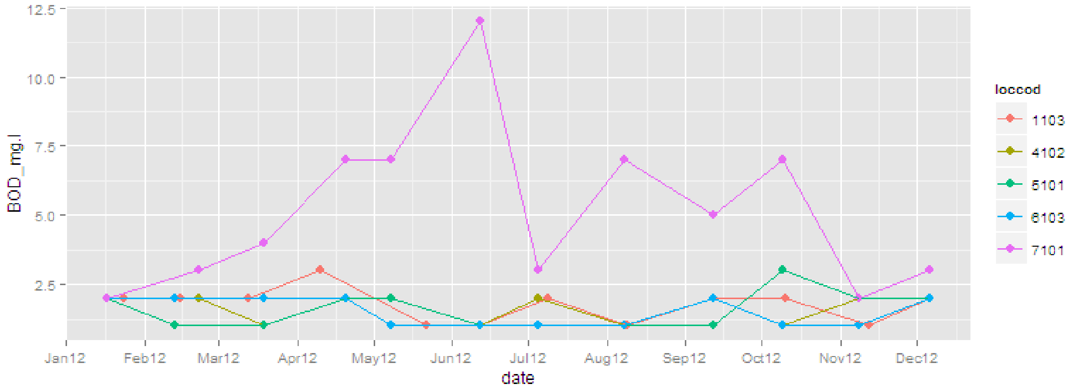

Figure 8.5 Biochemical oxygen demand (over 5 days) at the loading locations on the Dutch part of the estuary.

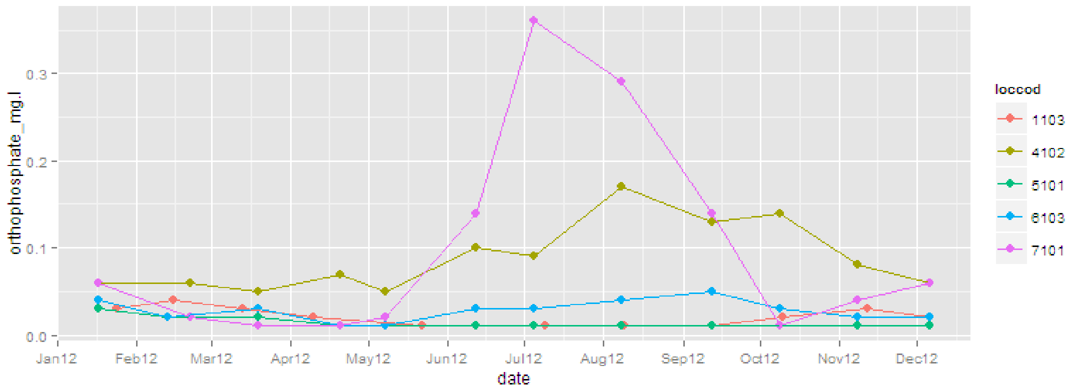

Figure 8.6 Ortho-phosphate concentrations at the loading locations on the Dutch part of the estuary.

Similar monthly data are available for water quality of the polder water at Nieuw-Statenzijl (location 5101) and Delfzijl (location 1103) in 2012, and therefore the following formulations have been applied for the loads from the both Westerwoldse Aa and the polder loads (all units are $g.m^{-3}$):

Salinity = 0.3
SO4 = SO4 * 0.333
OXY = DO

NH4 = NH4N
NO3 = NO3N
AAP = 0.0
PO4 = PO4P
Si = 4.8

POC1 = BOD5 * 0.15 / 0.117 / 2.67
POC2 = BOD5 * 0.15 / 0.117 / 2.67
POC3 = BOD5 * 0.70 / 0.117 / 2.67
POC4 = BOD5 * 0.00 / 0.117 / 2.67

PON1 = TOTN * 0.2 - DOC * 0.2 * 0.1 - NH4N * 0.2 - NO3N * 0.2

PON2 = TOTN * 0.2 - DOC * 0.2 * 0.1 - NH4N * 0.2 - NO3N * 0.2
PON3 = TOTN * 0.6 - DOC * 0.6 * 0.1 - NH4N * 0.6 - NO3N * 0.6
PON4 = TOTN * 0.0 - DOC * 0.0 * 0.1 - NH4N * 0.0 - NO3N * 0.0

POP1 = TOTP * 0.2 - 6.0 * 0.2 * 0.005 - PO4P * 0.2
POP2 = TOTP * 0.2 - 6.0 * 0.2 * 0.005 - PO4P * 0.2
POP3 = TOTP * 0.6 - 6.0 * 0.6 * 0.005 - PO4P * 0.6
POP4 = TOTP * 0.0 - 6.0 * 0.0 * 0.005 - PO4P * 0.0

POS1 = BOD5 * 0.15 * 0.016 / 0.117 / 2.67
POS2 = BOD5 * 0.15 * 0.012 / 0.117 / 2.67
POS3 = BOD5 * 0.70 * 0.008 / 0.117 / 2.67
POS4 = BOD5 * 0.00 * 0.005 / 0.117 / 2.67

DOC = 6.0
DON = DOC * 0.1
DOP = DOC * 0.005
DOS = DOC * 0.005

(NB: The names at the left hand side of the above formulations refer to simulated substances, the names at the right hand side to measured parameters.)

It is assumed that fresh water algae die instantly when discharged into saline water, and therefore, that all algae biomass is part of particulate detrital organic matter (mainly POC1). The distribution of particulate detrital organic carbon among the four simulated particulate fractions (POC1-4) is based on BOD5, whereas it is assumed that BOD5 covers algae biomass and that the contribution of DOC is negligibly small. We ignore the fact that the fraction of POC1 is higher in summer than in winter, and we apply yearly average fractions as calibrated for the observations. Total POC follows from:

$$POC = BODU / 2.67 = BOD5 / (1 - (f1*e^{(-k1*t)} + f2*e^{(-k2*t)} + f3*e^{(-k3*t)} + f4*e^{(-k4*t)})) / 2.67 \qquad (4.23)$$

where,
k1-4 = the degradation rates at 20 ^{o}C in the model; t=5 days
f1-4 = the distribution fractions 0.15 / 0.15 / 0.7 / 0.0
BODU = the ultimate BOD for time t is infinitely long

The distribution fractions reflect the assumption that organic matter in the discharge of the polder water is largely composed of slowly decomposing detritus, which is mainly resuspended bottom detritus. The distribution fractions of the organic nutrients are slightly different from the fractions for organic carbon to account for the fact that fast decomposing detritus (POC1 and POC2) has a higher nutrient content than (very) slowly decomposing detritus (POC3 and POC4). It was verified that distributions fractions add up to one. The N/C, P/C and S/C ratios used are representative of detrital organic matter and are in line with the ratios used by the model.

It was verified that the distribution formulations would not lead to negative concentrations of particulate detrital organic components (PON, POP). The number of negative values was minimized by choosing appropriate nutrient/C ratios. The few very small negative values that remained for POP were made equal to zero.

Additional remarks on the formulations are as follows:

- Salinity is estimated.
- The multiplication constant for SO4 is needed because the data for SO4 are given as mgSO4/L.
- Adsorbed P AAP in polder water may be substantial, but for pragmatic reasons it was ignored for these loads and all particulate P is allocated to organic matter.
- At a lack of data Si is estimated at 4.8 mgSi/L. This value was calibrated after starting with 4 mgSi/L based on data for runoff into Lake Veluwe.

C.1.3 German polder loads to the Dollard

The quality of the German polder water discharged at Knock can be represented by the monthly data collected in 2012 for the sampling location Knockster Tief. However, data for the period September - December were lacking. By means of interpolation one missing value was added for total organic carbon (TOC) and two missing values for dissolved organic carbon (DOC). 4 values smaller than the detection limit were replaced for nitrate (NO3N), 2 for ammonium (NH4N) and one such a value for dissolved phosphate (PO4P).

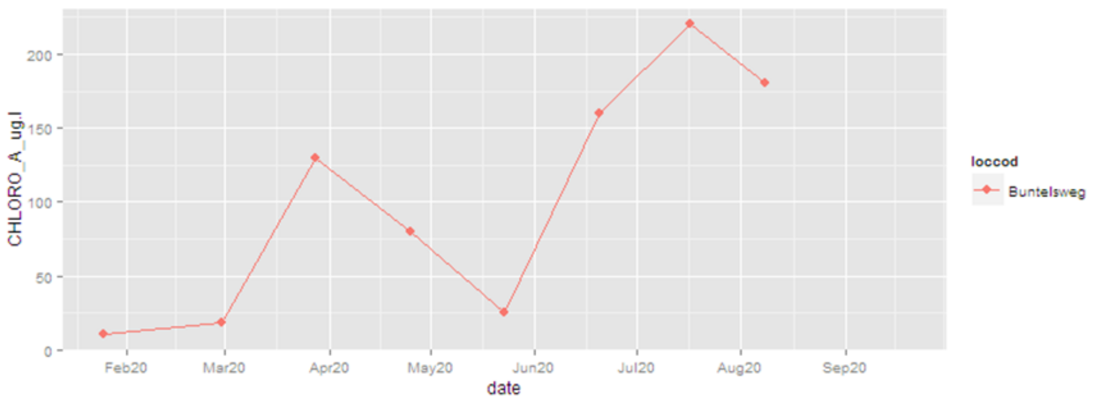

Figure 8.7 Chlorophyll a at the loading location Knock, on the German part of the estuary.

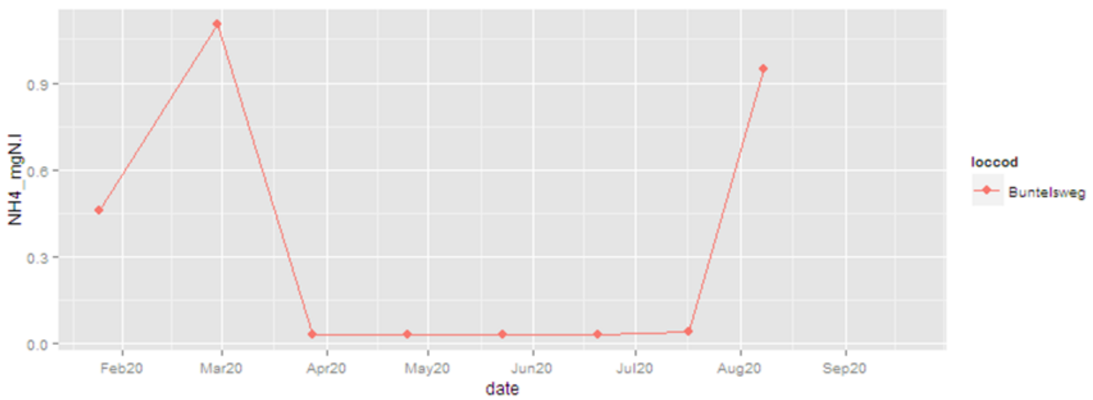

Figure 8.8 Ammonium at the loading location Knock, on the German part of the estuary.

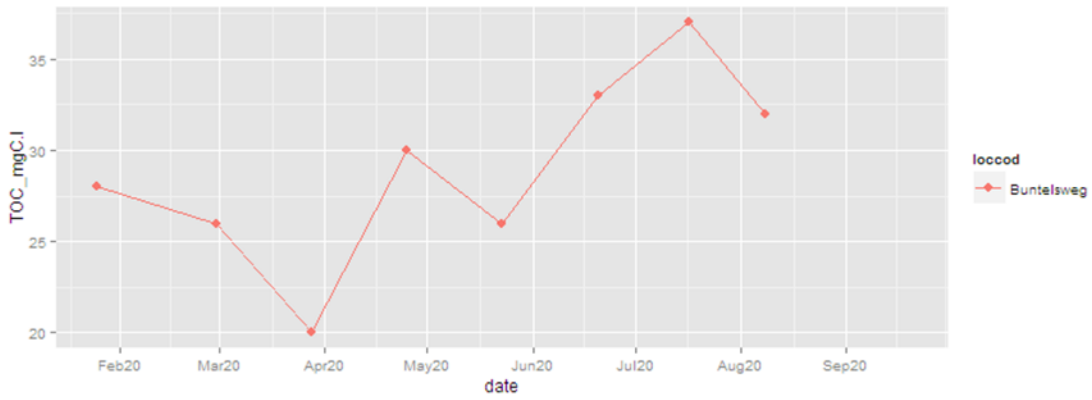

Figure 8.9 Total organic carbon (TOC) at the loading location Knock, on the German part of the estuary.

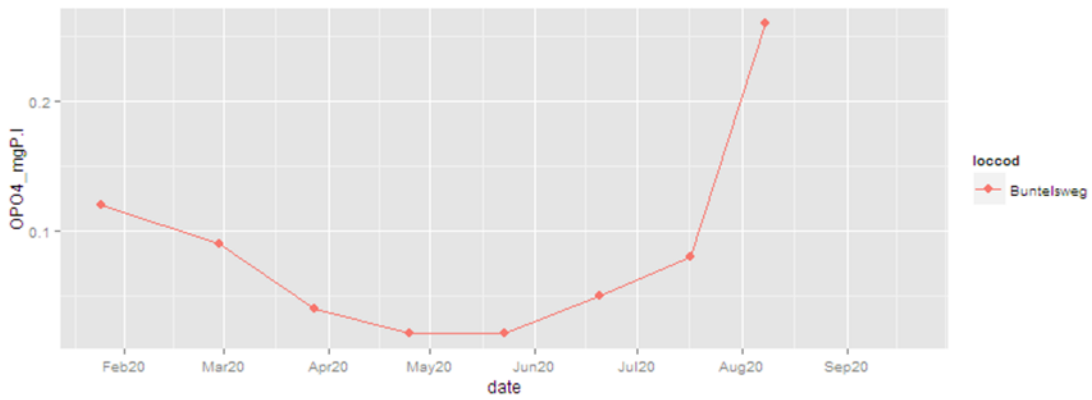

Figure 8.10 Dissolved phosphate at the loading location Knock, on the German part of the estuary.

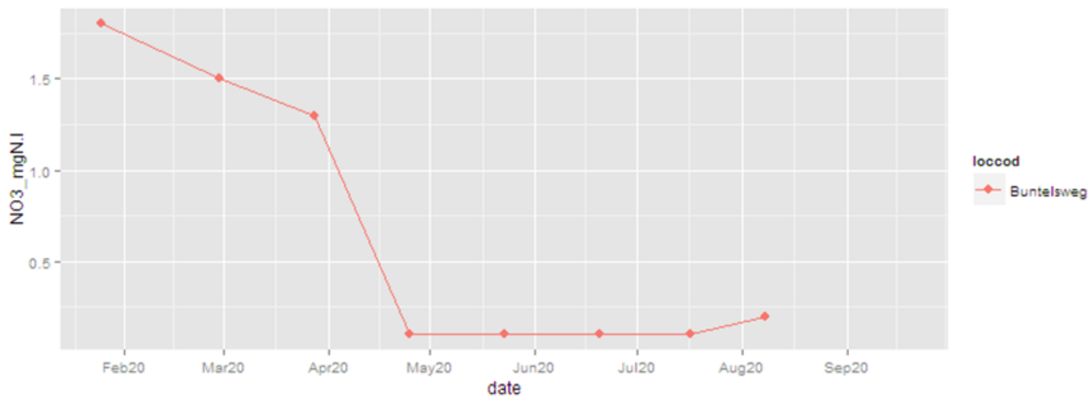

Figure 8.11 Nitrate at the loading location Knock, on the German part of the estuary.

For the quantification of the load concentrations of the simulated parameters in the discharges from the Knockster Tief the following formulations have been applied in line with the formulations used for the loads from the River Ems (all units are g.m^{-3}):

Salinity = CL * 0.002
SO4 = SO4 * 0.333
OXY = DO

NH4 = NH4N
NO3 = NO3N
PO4 = PO4P
AAP = 0.0
Si = 4.8

POC1 = TOC * 0.45 - DOC * 0.45
POC2 = TOC * 0.45 - DOC * 0.45
POC3 = TOC * 0.10 - DOC * 0.10
POC4 = TOC * 0.00 - DOC * 0.00

PON1 = TOTN * 0.53 - DOC * 0.53 * 0.07 - NH4N * 0.53 - NO3N * 0.53
PON2 = TOTN * 0.40 - DOC * 0.40 * 0.07 - NH4N * 0.40 - NO3N * 0.40
PON3 = TOTN * 0.07 - DOC * 0.07 * 0.07 - NH4N * 0.07 - NO3N * 0.07
PON4 = TOTN * 0.00 - DOC * 0.00 * 0.07 - NH4N * 0.00 - NO3N * 0.00

POP1 = TOTP * 0.53 * 0.2 - DOC * 0.53 * 0.007 * 0.2 - PO4P * 0.53 * 0.2
POP2 = TOTP * 0.40 * 0.2 - DOC * 0.40 * 0.007 * 0.2 - PO4P * 0.40 * 0.2
POP3 = TOTP * 0.07 * 0.2 - DOC * 0.07 * 0.007 * 0.2 - PO4P * 0.07 * 0.2
POP4 = TOTP * 0.00 * 0.2 - DOC * 0.00 * 0.007 * 0.2 - PO4P * 0.00 * 0.2

POS1 = TOC * 0.45 * 0.016 - DOC * 0.45 * 0.005
POS2 = TOC * 0.45 * 0.016 - DOC * 0.45 * 0.005
POS3 = TOC * 0.10 * 0.016 - DOC * 0.10 * 0.005
POS4 = TOC * 0.00 * 0.016 - DOC * 0.00 * 0.005

DOC = DOC
DON = DOC * 0.075
DOP = DOC * 0.0075
DOS = DOC * 0.005

(NB: The names at the left hand side of the above formulations refer to simulated substances, the names at the right hand side to measured parameters.)

It is assumed that fresh water algae die instantly when discharged into saline water, and therefore, that all algae biomass is part of particulate detrital organic matter. Consequently, the distribution of particulate detrital organic carbon among the four simulated particulate fractions (POC1-4) is based on TOC-DOC. The distribution fractions reflect the assumption that organic matter in the discharges from the Knockster Tief is mainly composed of algal detritus. The distribution fractions of the organic nutrients are slightly different from the fractions for organic carbon to account for the fact that fast decomposing detritus (POC1 and POC2) has a higher nutrient content than (very) slowly decomposing detritus (POC3 and POC4). It was verified that distributions fractions add up to one. The N/C, P/C and S/C ratios used are representative of detrital organic matter and are in line with the ratios used by the model.

It was verified that the distribution formulations would not lead to negative concentrations of the particulate detrital organic components (POC, PON, POP, POS). The number of negative values have been minimized by choosing more appropriate nutrient/C ratios. The one remaining low negative value for POP has been made equal to zero.

Additional remarks on the formulations are as follows:

- Salinity is calculated proportional to chloride.
- The multiplication constant for SO4 is needed because the data for SO4 are given as mgSO4/L, whereas the model uses mgS/L.
- Adsorbed P AAP in polder water may be substantial, but for pragmatic reasons it was ignored for these loads and all particulate P is allocated to organic matter.
- At a lack of data Si is estimated at 4.8 mgSi/L. This value was calibrated after starting with 4 mgSi/L based on data for runoff into Lake Veluwe.

C.1.4 Lauwersmeer loads

Dutch polders along the Wadden Sea discharge in the model domain via Lauwersmeer at 3 locations. No data were available for these loads from the Lauwersmeer in 2012. Instead the data for 2001 in the previous water quality model were used. This implies the conversion of the organic matter components in the previous model into the components in the current model.

For the quantification of the load concentrations of the simulated parameters in the discharges from the Lauwersmeer the following formulations have been applied (all units are $g.m^{-3}$):

Salinity = Salinity
SO4 = 33.0
OXY = DO

NH4 = NH4N
NO3 = NO3N
PO4 = PO4P
AAP = 0.0
Si = 4.8
Opal = 0.0

POC1 = DETN * 0.45 * 7.0
POC2 = DETN * 0.45 * 9.0
POC3 = DETN * 0.10 * 13.0
POC4 = DETN * 0.00 * 13.0

PON1 = DETN * 0.45 - DOC * 0.45 * 0.1
PON2 = DETN * 0.45 - DOC * 0.45 * 0.1
PON3 = DETN * 0.10 - DOC * 0.10 * 0.1
PON4 = DETN * 0.00 - DOC * 0.00 * 0.1

POP1 = DETP * 0.45 - DOC * 0.45 * 0.005
POP2 = DETP * 0.45 - DOC * 0.45 * 0.005
POP3 = DETP * 0.10 - DOC * 0.10 * 0.005
POP4 = DETP * 0.00 - DOC * 0.00 * 0.005

POS1 = DETN * 0.45 * 7.00 * 0.016
POS2 = DETN * 0.45 * 9.00 * 0.012
POS3 = DETN * 0.10 * 13.0 * 0.008

POS4 = DETN * 0.00 * 13.0 * 0.005

DOC = 7.0
DON = DOC * 0.1
DOP = DOC * 0.005
DOS = DOC * 0.005

(NB: The names at the left hand side of the above formulations refer to simulated substances, the names at the right hand side to measured parameters.)

The loads from the Lauwersmeer in the previous model were only determined for salinity and dissolved oxygen (OXY) and for organic and inorganic nutrients. Consequently, the loads for POC1-4 and POS1-4 had to be deduced from organic nitrogen (DETN = TOTN-NH4N-NO3N). DETN includes the contribution of fresh water algae that will die instantly when discharged into saline water. The distribution fractions reflect the assumption that particulate organic matter in the discharges from the Lauwersmeer is mainly composed of algal detritus. It was verified that distributions fractions add up to one. The N/C, P/C and S/C ratios used are representative of detrital organic matter and are in line with the ratios used by the model.

It was verified that the distribution formulations did not lead to negative concentrations of particulate detrital organic components (PON, POP).

Additional remarks on the formulations are as follows:

- Sulphate SO4 is estimated as an average concentration.
- Adsorbed P AAP in Lauwersmeer water may be substantial, but for pragmatic reasons it was ignored for these loads and all particulate P is allocated to organic matter.
- At a lack of data Si is estimated at 4.8 mgSi/L. This value was calibrated after starting with 4 mgSi/L based on data for runoff into Lake Veluwe.
- Dissolved organic carbon (DOC) was estimated as an average value on the basis of Lake Veluwe data.

D Calculation of initial concentrations in the sediment bed

The regression analysis on the RIKZ (1988) data delivered the following equations concerning the weight percentages of silt:

$$Y = 0.366\,X^{0.953}$$ (R^2=0.83; Y is %<16μ, X is %<63μ) (4.3)

$$X = 3.869\,Y^{0.872}$$ (R^2=0.83; X is %< 63μ, Y is %<16μ) (4.4)

The sediment weight percentages of total organic carbon, total-P and iron can be calculated from the following regression equations derived from the Delft Hydraulics (1983) data:

$$Y = 0.0763\,X + 0.0595$$ (R^2=0.93; Y is % org. carbon, X is %<16μ) (4.5)

$$Y = 0.0028\,X^{1.1247} + 0.009$$ (R^2=0.93; Y is % total-P, X is %<16μ) (4.6)

$$Y = 0.156\,X^{0.811}$$ (R^2=0.97; Y is % Fe, X is %<16μ) (4.7)

(NB: Based on equation 4.6 input coefficient fr_FeIM1 is equal to 0.035.)

In order to calculate the concentrations of particulate organic carbon (POC) and total phosphorus (TOTP) from the silt content (<63μ) as bulk concentration (wet sediment) resulting from the sediment model this content was first converted into a weight percentage with:

% <63μ = 100 * IM1 / (IM1+IM2+OM) (4.8)

where:
IM1 = silt concentration (gDW.m^{-3})
IM2 = sand concentration (gDW.m^{-3})
OM = organic matter concentration (gDW.m^{-3}), approximately equal to 0.0678 * IM1 according to the data in Delft Hydraulics (1983)

Next, regression equation 4.3 is applied to derive %<16μ from %<63μ, equation 4.5 to derive %POC from %<16μ, and equation 4.6 to derive %TOTP from %<16μ. The percentages are converted back into bulk concentrations (g.m^{-3}) using:

POC = %TOC * (IM1+IM2+OM) / 100 (4.9)
TOTP = %TOTP * (IM1+IM2+OM) / 100 (4.10)

The resulting sediment bed average concentrations of POC and TOTP need to be distributed among the various components in the individual sediment layers that shape up a sediment column. This distribution was established as follows. Due to the fact that POC/N/P/S1 and POC/N/P/S2 are decomposed relatively fast these components have very low concentrations compared to POC/N/P/S3 and POC/N/P/S4. This allows us to deal with POC/N/P/S1 and POC/N/P/S2 independently from the total organic matter content of the sediment. We took the concentrations of POC/N/P/S1 and POC/N/P/S2 from a representative sediment column in the western Wadden Sea model, and imposed them equally on all sediment columns in the Ems-Dollard model. For each sediment layer n in each column the concentrations of the other components were scaled on the POC3WW concentration profile in the representative sediment column from the western Wadden Sea model as follows:

$$POC3_n = 0.4 * POC * POC3WW_n / POC3WW_7 \quad (4.11)$$
$$POC4_n = 0.6 * POC * POC3WW_n / POC3WW_7 \quad (4.12)$$
$$PON3_n = PON3WW_n * POC3_n / POC3WW_n \quad (4.13)$$
$$PON4_n = PON3WW_n * POC4_n / POC3WW_n \quad (4.14)$$
$$POP3_n = POP3WW_n * POC3_n / POC3WW_n \quad (4.15)$$
$$POP4_n = POP3WW_n * POC4_n / POC3WW_n \quad (4.16)$$
$$POS3_n = 0.008 * POC3_n \quad (4.17)$$
$$POS4_n = 0.005 * POC4_n \quad (4.18)$$

(NB: The western Wadden Sea model did not include POC4.)

Similarly, TOTP was distributed among components and sediment layers n according to:

$$AAP_n = TOTP_n * AAPWW_n / TOTPWW_n \quad (4.19)$$
$$APATP_n = TOTP_n * APATPWW_n / TOTPWW_n \quad (4.20)$$
$$VIVP_n = TOTP_n * VIVPWW_n / TOTPWW_n \quad (4.21)$$
$$TOTPWW_n = AAPWW_n+APATPWW_n+VIVPWW_n+POP3WW_n \quad (4.22)$$

For all other particulate and dissolved substances the concentrations in the representative western Wadden Sea sediment column were imposed equally on all sediment columns in the Ems-Dollard model. As described for the initial composition of the water column the final step in obtaining a stable initial sediment composition involved taking the concentration fields that resulted from the water and sediment quality model for the end of 2012 (31 December) as initial composition input file in a number of successive simulations.