Development of Mechanistic Models

Mechanistic Model for the Smålandsfarvandet

Technical documentation on biogeochemical model

The expert in **WATER ENVIRONMENTS**

DHI

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| Prepared for | Danish EPA (Miljøstyrelsen, Fyn) |
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Eelgrass in Kertinge Nor
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1 Executive Summary

The model development presented in this technical note represents the biogeochemical model development for the Smålandsfarvandet and surrounding water bodies (the SMF model). The SMF model is part of a larger model complex comprising several mechanistic models developed by DHI and a number of statistical models developed by Aarhus University (AU), Bioscience.

The model complex is developed with the overall aim to support the Water Framework Directive (WFD) by introducing mechanistic models in as many Danish water bodies as possible and integrating with Bayesian statistical modelling, and cross-system modelling carried out by AU, Bioscience.

Here we present the overall biogeochemical model set-up covering the Smålandsfarvandet and the surrounding water bodies, together with a quality assessment of the model performance. This specific model includes 18 Danish water bodies:

Water Body[*]	Number	Water Body[*]	Number
Korsør Nor	16	Langelandsbælt, øst	41
Basnæs Nor	17	Grønsund	45
Holsteinsborg Nor	18	Præstø Fjord	47
Skælskør Fjord og Nor	25	Stege Bugt	48
Smålandsfarvandet, syd	34	Stege Nor	49
Karrebæk Fjord	35	Smålandsfarvandet, åbne del	206
Dybsø Fjord	36	Nakskov Fjord	207
Avnø Fjord	37	Fehmarnbelt	208
Guldborgssund	38	Rødsand	209

[*] Water bodies defined for the River Basin Management Plans 2015-2021

The SMF biogeochemical model builds on the developed hydrodynamic model of the Smålandsfarvandet and is developed to describe the biogeochemistry within the model domain with a focus on parameters relevant for WFD, including dynamics in nutrients, phytoplankton, primary production, dissolved oxygen, organic matter and benthic vegetation.

The model quality is evaluated from three model performance measures: Percent Bias (P-Bias), Spearman Rank Correlation, and Cost Function (CF). According to DHI (2019b), Model Efficiency Factor (MEF) was suggested initially, but during the model development, it was concluded that MEF is not suitable to evaluate this kind of biogeochemical models, why Cost Function (CF) is introduced. The quality measure CF was used in Erichsen et al. 2017 as part of an international evaluation (Hermann et al. 2017). As described in DHI (2019b), the MEF evaluates the Root Mean Square Error (RMSE) to the standard deviation (based on measurements). As model results are compared against measurements at the exact point in time in dynamic estuarine systems with strong gradients, the MEF has proven not to be suited (due to its dependency on entirely right timing). The CF assesses the fit/misfit between measurements and observations also normalized to the standard deviation (based on measurements) why it is decided to use this measure in the overall assessment of model performance.

Concerning the performance measures, our ambition is to have 75% of all measures (Percent Bias, Spearman Rank Correlation and Cost Function) meet 'excellent', 'very good', or 'good' for all parameters and stations (lumped).

As can be seen from the present technical note, 80% of all data sets meet the success criteria when evaluated against the three performance measures, and 75% when assessing both annual performance and summer/winter performance of all data. The average model performance, evaluated at 11 stations within the model domain, for the biogeochemical model of the Smålandsfarvandet and surrounding water bodies, is summarized below:

- Model performance measures for dissolved oxygen (DO) are on average 3.2% (P-Bias), 0.9 (Spearman Rank Correlation) and 0.5 (CF). The average model performance for this parameter is categorized to be 'excellent' (P-Bias) and 'very good' (Spearman Rank Correlation and CF).
- Model performance measures for chlorophyll-a (CH) are on average 66.5% (P-Bias), 0.0 (Spearman Rank Correlation) and 1.1 (CF). The average model performance for CH is categorized to be 'good' (CF) and 'poor' (P-Bias and Spearman Rank Correlation).
- Model performance measures for light attenuation coefficient (K_d) are on average 27.3% (P-Bias), 0.1 (Spearman Rank Correlation) and 1.1 (CF). The average model performance for K_d is categorized to be 'good' (P-Bias and CF) and 'poor' (Spearman Rank Correlation).
- Model performance measures for dissolved inorganic nitrogen (DIN) are on average 24.2% (P-Bias), 0.7 (Spearman Rank Correlation) and 0.5 (CF). The average model performance for DIN is categorized to be 'very good' (Spearman Rank Correlation and CF) and 'good' (P-Bias).
- Model performance measures for dissolved inorganic phosphorus (DIP) are on average 83.5% (P-Bias), 0.4 (Spearman Rank Correlation) and 1.6 (CF). The average model performance for this parameter is categorized to be 'good' (Spearman Rank Correlation and CF) and 'poor' (P-Bias).
- Model performance measures for total nitrogen (TN) are, on average, 13.3% (P-Bias), 0.5 (Spearman Rank) and 0.6 (CF). The average model performance is categorized to be 'very good' (P-Bias and CF) and 'good' (Spearman Rank Correlation).
- Model performance measures for total phosphorus (TP) are, on average, 22.7% (P-Bias), 0.2 (Spearman Rank) and 0.9 (CF). The average model performance for TP is categorized to be 'very good' (CF), 'good' (P-Bias) and 'poor' (Spearman Rank Correlation).

The details behind the above performance are available in Table 5-1, Table 5-2 and Table 5-3. Time-series comparisons are available here: rbmp2021-2027.dhigroup.com (Google Chrome only).

The ambition of meeting 'excellent', 'very good', or 'good' for 75% of all parameters and stations (lumped) has been reached. The SMF model will be applied in the Danish waterbodies of the Smålandsfarvandet and the surrounding seas. In this technical note, we conclude that the SMF biogeochemical model has been developed successfully for modelling nutrient scenarios in the assessment and maximum allowable inputs (MAI).

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2 Introduction

The model development presented in this technical note represents the biogeochemical model development for the Smålandsfarvandet and surrounding water bodies (SMF model) and builds on top of the SMF hydrodynamic model (DHI 2019d). Documentation on the model application will be presented in the following reports. The biogeochemical model is part of the mechanistic model complex development, which includes two regional models, three local-domain models, and six estuary specific models. The model complex is developed with the overall aim to support the Water Framework Directive (WFD) by introducing mechanistic models in as many Danish water bodies as possible and integrating with Bayesian statistical modelling and cross-system modelling carried out by AU, Bioscience.

Here we present the overall biogeochemical model set-up covering the Smålandsfarvandet and surrounding water bodies, together with a quality assessment of the model performance. The SMF model includes the 18 Danish water bodies listed in Table 2-1 below. The location of the Danish water bodies is documented in Erichsen et al. (2019).

Table 2-1   Water bodies included in the SMF model.

Water Body[*]	Number	Water Body[*]	Number
Korsør Nor	16	Langelandsbælt, øst	41
Basnæs Nor	17	Grønsund	45
Holsteinsborg Nor	18	Præstø Fjord	47
Skælskør Fjord og Nor	25	Stege Bugt	48
Smålandsfarvandet, syd	34	Stege Nor	49
Karrebæk Fjord	35	Smålandsfarvandet, åbne del	206
Dybsø Fjord	36	Nakskov Fjord	207
Avnø Fjord	37	Fehmarnbelt	208
Guldborgssund	38	Rødsand	209

[*] Water bodies defined for the River Basin Management Plans 2015-2021

The biogeochemical model computes the development during the modelling period in ecological parameters, including concentrations of nutrients, dissolved oxygen, and organic matter and the Secchi depth, due to, e.g. primary production. The results represent short term changes due to specific weather events, seasonal variations and interannual trends. This project will focus on summer chlorophyll-a and parameters influencing distribution and growth of eelgrass. A detailed description of the specific state variables included in the SMF biogeochemical model can be found in DHI (2019c).

According to DHI (2019b), the quality measure Model Efficiency Factor (MEF) was suggested as a quality measure initially, but during the biogeochemical model development, it was concluded that MEF is unsuitable for evaluating this kind of biogeochemical models. As described in DHI (2019b), the MEF evaluates the RMSE to the standard deviation (based on measurements). As we compare model results to the measurements at the exact point in time in a number of estuary systems with strong gradients and variable dynamics, the MEF has proven to be unsuited (due to its dependency on entirely right timing). For the validation of the biogeochemical models, we have included the quality measure Cost Function (CF) in replacement of MEF (Table 5-3). The CF measure was also used in Erichsen et al. 2017 and describes how the difference between measured and modelled values is related to the inherent variation in field observations.

3 Modelling Concept

3.1 Mechanistic Modelling

The present technical note represents the biogeochemical part of the model complex covering the Smålandsfarvandet and the surrounding water bodies (SMF model). The SMF model is one model out of eleven mechanistic models developed to increase the knowledge of pressures and status in Danish marine waters and to provide tools for the Danish EPA as part of the implementation of the WFD. Mechanistic models enable dynamic descriptions of ecosystems and interactions between natural forcing and anthropogenic pressures. Hence, mechanistic models can be applied for predictions of changes in specific components, like chlorophyll-a concentrations, due to changes in, e.g. anthropogenic pressures.

The SMF is defined as a local domain model. The mechanistic model complex development as part of the current projects includes two regional models, three local-domain models, and six estuary-specific models:

- The regional models cover both specific Danish water bodies and regional waters, such as the North Sea and a small part of the North Atlantic, which are included in the North Sea-model, and the Baltic Sea, which are covered by the IDF-model. These models provide model results for specific water bodies but, equally important, give boundaries to local-domain models and estuary-specific models.
- Local-domain models are developed to allow for resolving most small and medium-sized water bodies in the north-western Belt Sea, the south-western Belt Sea and the water bodies in and around Smålandsfarvandet.
- Estuary-specific models are developed to allow for detailed modelling of specific estuaries.

The ecological conditions in marine waters are determined by several different natural factors like water exchange, stratification, water temperature, nutrient availability, sediment characteristics, the structure of the food web, etc. On top of that, several anthropogenic factors like nutrient loadings, fishery, etc., also impact the ecosystem and potentially the ecological status.

The model developed in this specific project aims at supporting the Danish EPA's implementation of the WFD. During this project, the models are developed to represent the present period (2002-2016) evaluated against NOVANA measurements. Here we use current data on solar radiation, current nutrient loadings, etc.

After the models are developed, they will be applied for scenario modelling with changed nutrient loading to assess the Maximum Allowable nutrient Inputs (MAIs).

3.2 Model Development

The model development consists of a 3D hydrodynamic model describing the physical system (water levels, current, salinity and water temperatures), and a 3D biogeochemical (ecosystem) model describing the governing biogeochemical pelagic and benthic parameters and processes like phytoplankton, dissolved oxygen, primary production, etc. The model structure is modular, meaning that a hydrodynamic model is developed independently of the biogeochemical model (for further information about the hydrodynamic model see DHI (2019a)). A more detailed description of the biogeochemical model is available in DHI (2019c), and the underlying SMF hydrodynamic model is described in DHI (2019d).

All mechanistic models have been set up and calibrated/validated for the period 2002-2016 and reported according to the performance measures P-Bias, Spearman Rank Correlation and CF (DHI 2019b). Results from the entire modelling period are furthermore presented as time series in a WEB-tool (rbmp2021-2027.dhigroup.com, Google Chrome only) with a few examples included in section 5.3. Most data used for calibration and validation originate from the national monitoring programme NOVANA (see http://odaforalle.au.dk for more details). For some models and some parameters, other data are included, and the specific origin of those data will be referenced when used.

3.3   Modelling System

The biogeochemical model is based on the 3D modelling software MIKE 3 HD FM (version 2017) developed by DHI together with the numerical 3D equation solver MIKE ECO Lab to describe the relevant biogeochemical processes in the modelling system. The MIKE 3 FM modelling system is based on a flexible mesh approach with horizontal mesh elements of varying size within the modelling domain. The water column is resolved by multiple layers. The modelling system has been developed for applications within oceanographic, coastal and estuarine environments.

The scientific documentation of MIKE 3 HD FM is given in DHI (2019a).

The main components and processes determining the status of the water quality and the response in the ecosystem (e.g. changes in eelgrass biomass) are included in the biogeochemical model. They are based on external factors (meteorology and nutrient supply). The model describes the turnover of organic material and nutrients (dissolved inorganic nitrogen, phosphate and silicate), both in the pelagic (water column) and the benthic phase (seabed or sediment). The pelagic phase includes phytoplankton and nutrients, and the benthic department covers sediment pools of nutrients and the exchange of nutrients between the sediment and water phase. Furthermore, the benthic part of the model describes the biomass and growth of benthic vegetation at the sea bed. The mechanisms behind the biogeochemical model and the ECO Lab templates used are described in DHI (2019c).

4 Model Set-up

The biogeochemical model for the Smålandsfarvandet and the surrounding water bodies builds on top of the hydrodynamic model (HD) and an integrated transport model (AD). The set-up and calibration/validation of the physical Smålandsfarvandet model (HD and AD) are documented in technical notes (DHI 2019d).

For the current project, the model is set up for the period 2002-2016, which means that all model input data need to cover this period.
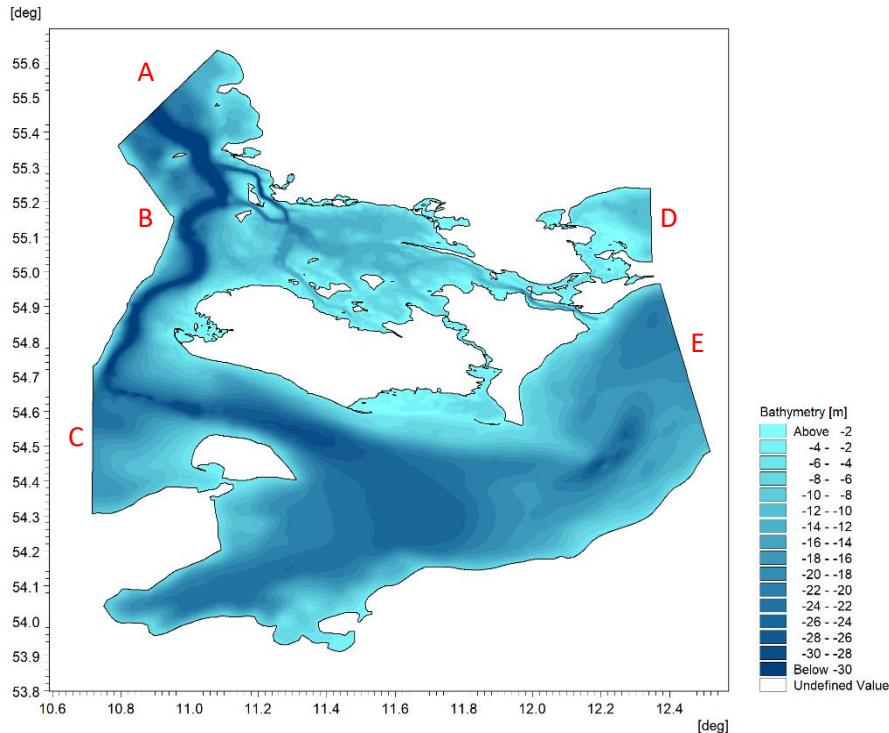
Figure 4-1   Model bathymetry of the SMF model. Water depths refer to DVR90. The model includes 5 open boundaries: A) Storebælt boundary, B) Northern Langeland boundary, C) Southern Langeland (Kiel Bugt) boundary, D) Faxe Bugt boundary, E) Østersø boundary.

4.1 Model Domain

The model domain is determined in accordance with the area of interest of the modelling study. Also, considerations of the area of influence, being the surrounding areas that affect the area of interest, and suitable open boundary locations, affect the choice of the model domain.

For the SMF model being one of DHI's general local models, the model domain focuses on water bodies around Lolland, Falster, Southern Sjælland and surrounding smaller islands. The model has 5 open boundaries that can be seen in Figure 4-1.

The model mesh is the representation of the model domain. More specifically the model mesh defines the model area, the location of the open boundaries, the land-water boundaries, the horizontal and vertical model resolution (discretization), and the water depths (bathymetry) of the area. The bathymetry of the SMF model is shown in Figure 4-1, whereas Figure 4-2 shows the resolution of the horizontal mesh. For the SMF model, the horizontal mesh mainly consists of triangular elements of varying sizes, but also quadrangular elements have been applied for resolving deep channels. The horizontal resolution varies gradually from 100-200 m in the coastal areas around Lolland, Falster, Zealand, and surrounding smaller islands to 1.2-2 km in the deep areas and along the German coast. In the vertical mesh, the water column is resolved

by 10 sigma-layers at down to -10 m depth (or where water depth is smaller) and up to 35 z-layers with a thickness of 1 m from level -10 m to the local seabed level. Further documentation on model mesh and horizontal/vertical resolution of the SMF HD model can be found in DHI (2019d).
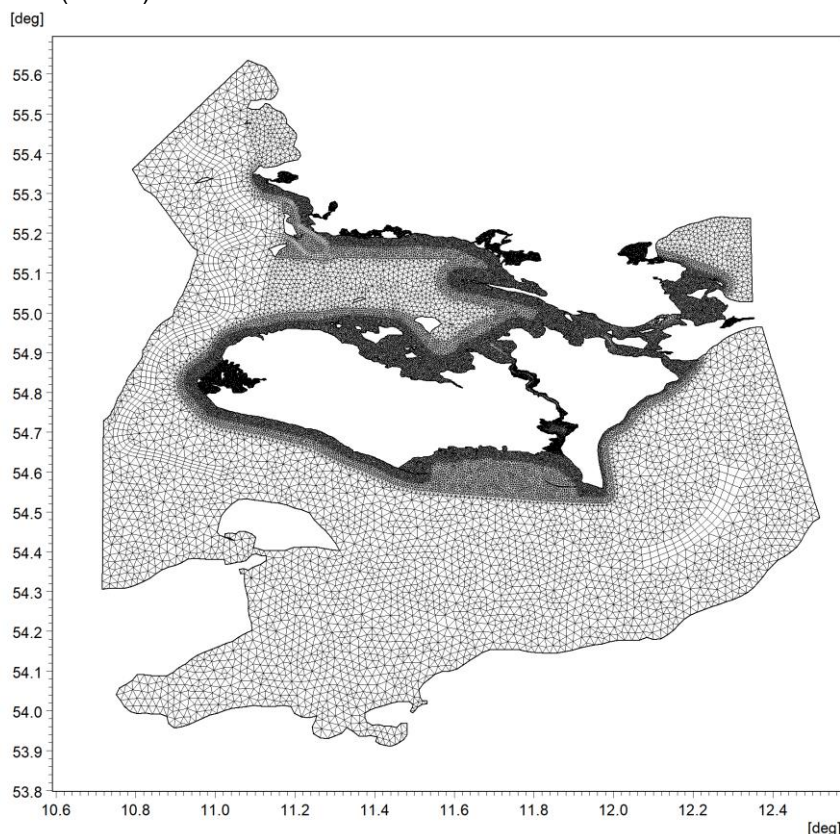
Figure 4-2   Resolution of the horizontal model mesh of the SMF model.

4.2   Open Boundary Conditions

The SMF model has 5 open boundaries (see Figure 4-1) connecting the model domain to surrounding Danish waters. The biogeochemical data for the boundary conditions are extracted from DHI's Inner Danish Waters model (the DKBS2-HD75). Documentation on boundary conditions for the biogeochemical model development is given in DHI (2020).

4.3   Forcings

Data on solar radiation are calculated from clearness percentages and applied as a spatial and temporally varying forcing covering the entire model domain.

Area-distributed atmospheric deposition of nitrogen (N) is provided by AU, Department of Environmental Science, and aligned with HELCOM depositions (see DHI 2020).

To estimate suspended sediment concentrations, a dynamic bottom shear stress information is needed. Wave parameters from a Spectral Wave model are included as model forcing, including significant wave height, wave period and mean wave direction, together with current conditions from the hydrodynamic model results.

Documentation on model forcing is given in DHI (2020).

4.4 Sources

The SMF model includes sources with land-based nutrient loadings. In Figure 4-3, the location of the sources is illustrated. Freshwater run-off from land is included in the hydrodynamic module. In Denmark, 4th order area run-off distributed to main rivers and streams is applied.

The model sources are specified as time series with daily loadings of inorganic and organic nutrients, including also total nitrogen (TN) and total phosphorus (TP). The land-based nutrient loadings are based on the following data sources:

- DCE (Danish Centre for Environment and Energy) – Danish run-off
- E-HYPE (http://hypeweb.smhi.se/europehype/time-series/) – Non-Danish run-off

More details are included in DHI (2020).
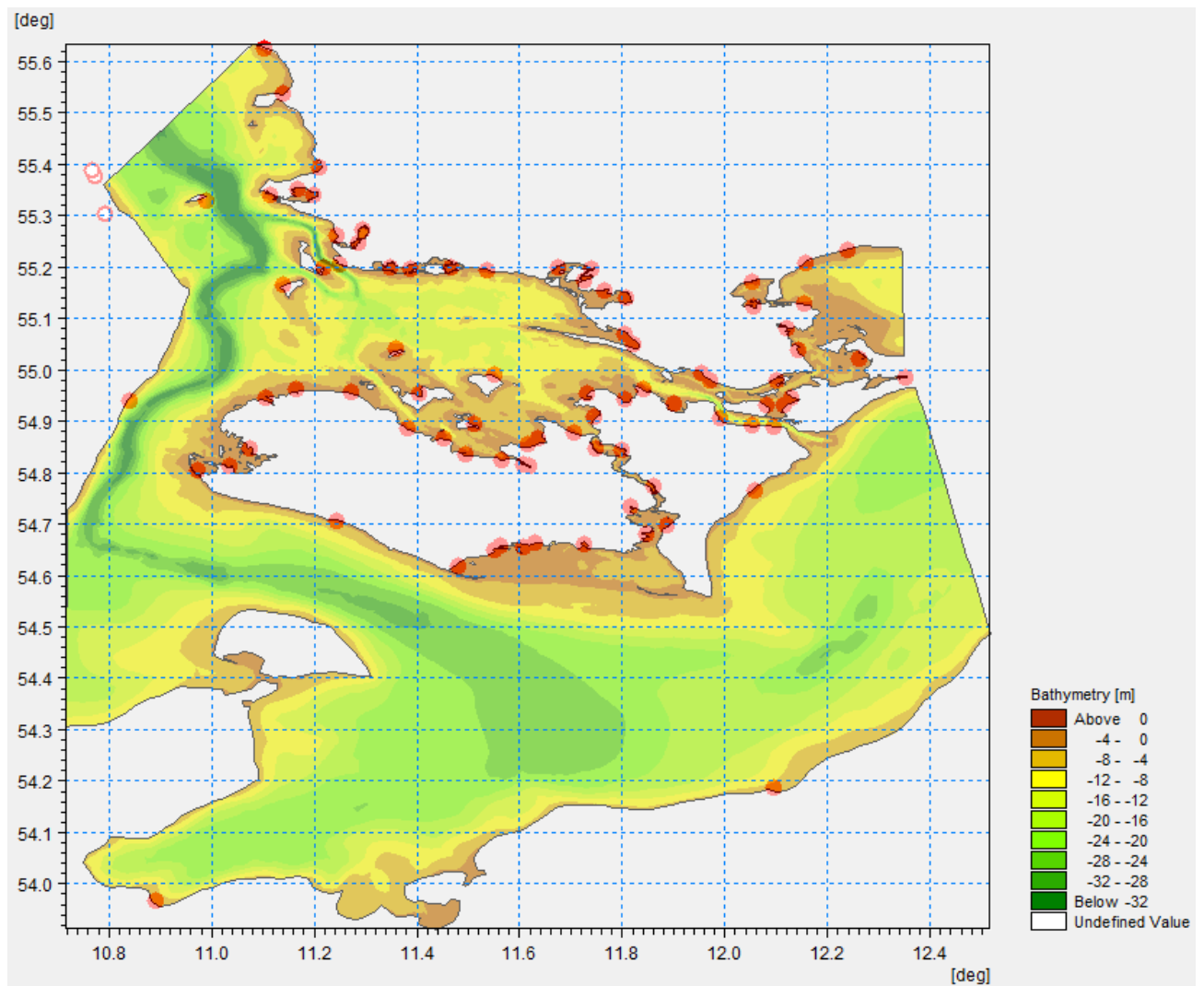
Figure 4-3   Illustration of the location of sources in the SMF model. The sources' positions represent the main rivers, but loadings are scaled to include all local run-off and point sources from land to sea. In Denmark, 4th order area run-off distributed to main rivers and streams is applied. Closed circles - included sources, open circles - not included sources.

4.5 Initial Conditions

To properly initiate a model simulation, the model requires initial conditions for the various state variables.

Initial fields of seabed substrates are based on shear stress and sediment type (sedimentation-, transportation- or erosion area), which were related to empirical relationships to measured sediment data across Denmark. Initial values of benthic vegetation (e.g. eelgrass) and pelagic phase were estimated by running a MIKE ECO Lab model with defined initial biomass for the entire model domain for a three-year simulation period.

In DHI (2020) further details on initial model values are given.

5 Model Calibration and Validation

After set-up of the model, calibration and validation of the model are undertaken. The model **calibration** is the process of adjusting model process settings and model constants within the literature range to obtain satisfactory agreement between observations and model results in the local modelling domain. In practice, the model set-up and the model calibration are often performed iteratively, since a good comparison between observations and model results requires a well-proportioned model domain as well as adequate model forcings.

The model **validation** is the process of comparing observations and model results qualitatively and quantitatively for a different period from the calibration period, to demonstrate the suitability of the calibrated model more generally. The qualitative comparison is typically made graphically, and the quantitative comparison is usually made using specific performance (goodness of fit) measures (DHI 2019b; Erichsen et al. 2017). As such, the model validation constitutes the final documentation of the model performance.

The SMF model was run for the period 2002-2016, and the entire period is used for a combined calibration and validation effort, due to lack of enough observation data for separate calibration and validation tasks. Consequently, model performance measures are presented for this period. The model results compared with observations of the different biogeochemical parameters are presented for the entire period using a WEB-tool (rbmp2021-2027.dhigroup.com, Google Chrome only).

5.1 Model Calibration Procedure

Calibration of the biogeochemical SMF model is achieved by tuning model constants to optimize model results on calibration parameters compared to measured data. The constants adjusted in the calibration procedure are numerous. They include, e.g. phytoplankton growth rates, grazing rates, mortality rates (phytoplankton and zooplankton), light attenuation constants, sedimentation rates, re-suspension rates, mineralization rates (pelagic and sediment), denitrification rates (pelagic and sediment).

The key parameters to optimize in the calibration procedure include dissolved oxygen, chlorophyll-a, light attenuation, inorganic nutrients, total nitrogen and total phosphorus. After each adjustment of calibration constants, the model is run, and time-series are compared to measured data at selected stations. The procedure is iterated until model results and measured data compare in both time and space.

5.2 Presentation of Key Model Results

During the model calibration procedure, an extensive amount of data on state variables and processes is produced. To allow for a smooth and homogeneous quality assurance, few standard plots and time series are generated automatically and evaluated during the baseline and scenario execution.

Examples of modelled key validation parameters are presented as 2D fields in Figure 5-1 to Figure 5-4 and illustrate the spatial variation of the validation parameters. In the following, a brief assessment of the spatial distribution of key parameters will be given.

Average concentrations of dissolved oxygen in bottom waters during 2016 range from a minimum of 5 mg/l in the deeper waters of Lübeck Bay/Mechlenburg Bay and of Storebælt to maximum values of 10-13 mg/l found in the coastal areas of Lolland, Falster, Zealand and surrounding smaller islands (Figure 5-1).

Figure 5-1   Modelled yearly average bottom water concentrations of dissolved oxygen (DO, mg/l) for 2016.

Yearly average concentrations of surface chlorophyll-a during 2016 range from 1.6 μg/l to 3.6 μg/l in the modelling area (Figure 5-2). The highest average concentrations of chlorophyll-a in the surface during 2016 are observed in the Lübeck Bay, Nakskov Fjord, Karrebæk Fjord, Dybsø Fjord and Avnø Fjord.

Figure 5-2   Modelled yearly average surface water concentrations of chlorophyll-a (CH, mg/l) for 2016.

Yearly average concentrations of surface total nitrogen during 2016 are highest in Lübeck Bay, Dybsø Fjord, Karrebæk Fjord, Præstø Fjord and Avnø Fjord, with values ranging between 0.5 – 2.5 mg/l (Figure 5-3). In the open waters of the model domain, average surface concentrations of total nitrogen range between 0.29 - 0.31 mg/l.
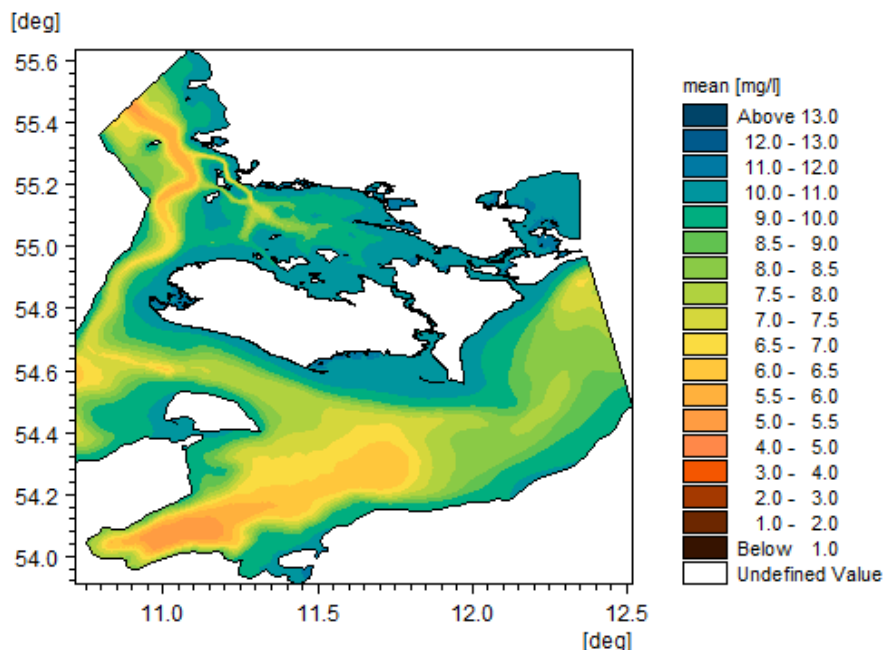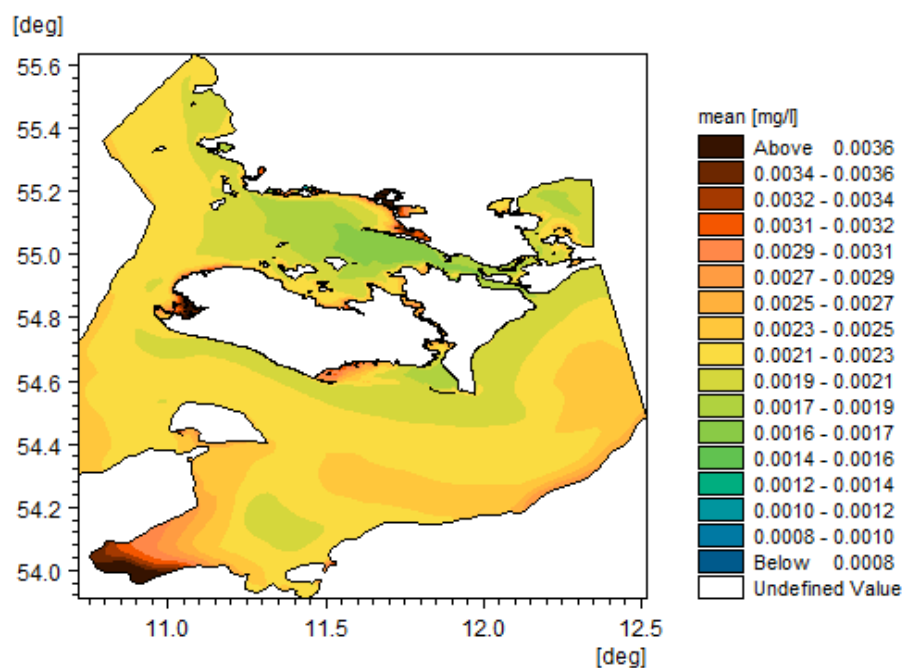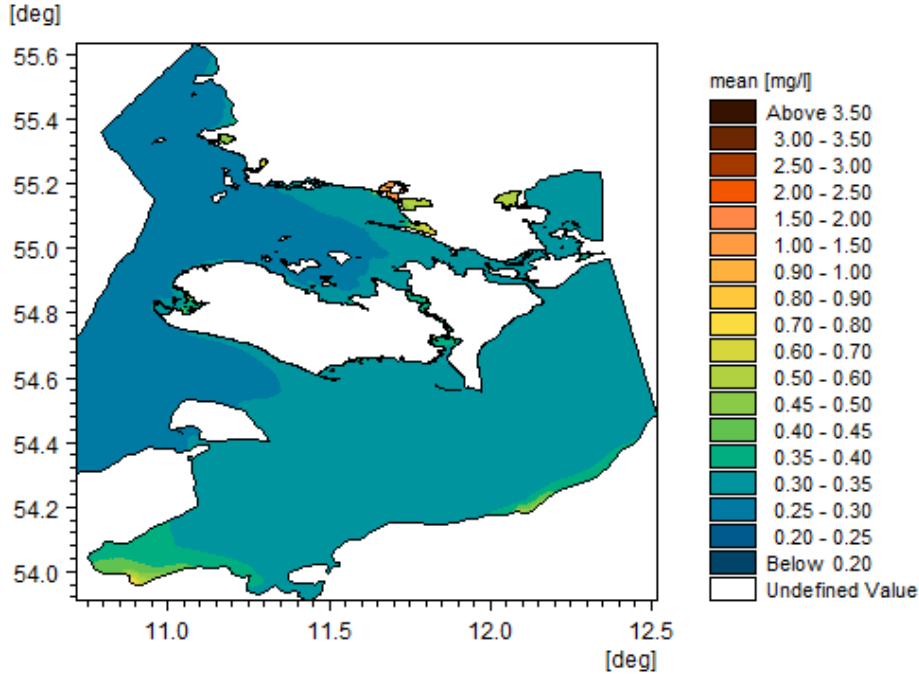

Figure 5-3   Modelled yearly average surface water concentrations of total nitrogen (TN, mg/l) for 2016.

Yearly average concentrations of surface total phosphorus during 2016 are between 0.014 mg/l to 0.14 mg/l with highest values in Karrebæk Fjord (Figure 5-4).
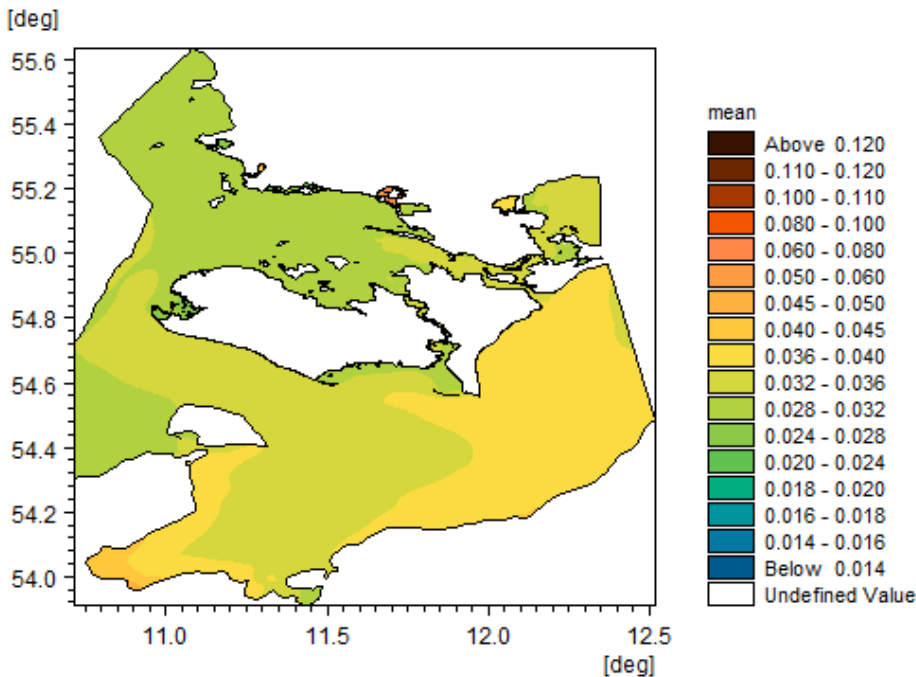
Figure 5-4   Modelled yearly average surface water concentrations of total phosphorus (TP, mg/l) for 2016.

5.3 Model Performance

The SMF biogeochemical model was calibrated and validated against measured data (observations) on modelled ecosystem parameters at selected stations within the model domain. Figure 5-5 shows the location of all 20 monitoring stations within the model domain. Out of all stations, 11 stations had enough measurement data in the period 2002-2016 to be included in the model calibration and validation (at least one year of weekly or bi-weekly data). The biogeochemical calibration/validation parameters include dissolved oxygen (DO), chlorophyll-a (CH), light attenuation (K_d), dissolved inorganic nitrogen (DIN), dissolved inorganic phosphorus (DIP), total nitrogen (TN) and total phosphorus (TP). Generally, the SMF model compares well to the measurements in terms of model parameters (see Figure 5-1 to Figure 5-4 and Figure 5-6 to Figure 5-12), and the overall performance measure (summarized in Table 5-1 to Table 5-3) confirms a statistically good agreement between measurements and model results.
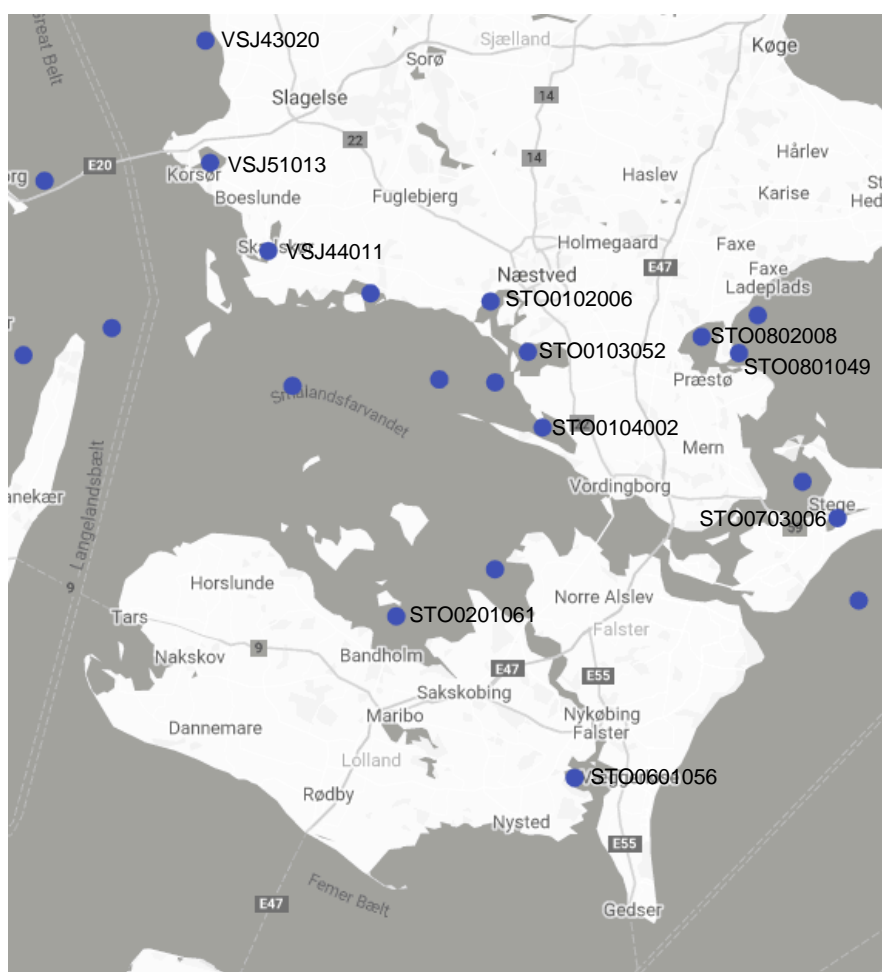
Figure 5-5   Location of the different calibration and validation stations used in the SMF-model performance (only stations with ID are used).

5.3.1 Calibration/Validation at Station VSJ51013

In the following, we present an example on the calibration/validation from the model domain at station VSJ51013 and refer to rbmp2021-2027.dhigroup.com (Google Chrome only) for more details on the Danish measurement stations. The location of station VSJ51013 is shown in Figure 5-5.

The comparison at station VSJ51013 shows a good agreement between the measurements and the SMF model for 79% of the parameters according to the three performance measure P-Bias, Spearman Rank Correlation and CF (see Table 5-1, Table 5-2 and Table 5-3).

In Figure 5-6 measured and modelled concentrations of dissolved oxygen (DO) at station VSJ51013 in the surface and at bottom waters (here 2 m) are shown. From the figure, it is seen that for DO, the variability and seasonality of the surface and bottom waters are well represented by the model. This is in agreement with the statistical performance measures (see Table 5-1 to Table 5-3), where measured and modelled DO compares 'excellent' (P-Bias) and 'very good' (Spearman Rank Correlation and CF) at station VSJ51013.

Figure 5-6   Comparison of measured and modelled concentrations of dissolved oxygen (DO, mg/l) at station VSJ51013 in the surface and bottom (2 m) waters. Dots represent measurements, and the solid line shows modelled data for the entire period.

For chlorophyll-a (CH), the dynamics in seasonality are presented in Figure 5-7. The model tends to overestimate spring concentrations of CH. From the statistical performance measures, annual CH compares 'very good' (CF) and 'poor' according to P-Bias and Spearman Rank Correlation, and summer concentrations of CH compare 'very good' (P-Bias), 'good' (CF) and 'poor' (Spearman Rank Correlation) (see Table 5-1 to Table 5-3).

Figure 5-7   Comparison of measured and modelled concentrations of chlorophyll-a (CH, mg/l) at station VSJ51013 in surface and bottom (2 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

The measured light attenuation coefficient (K_d) and model prediction are presented in Figure 5-8. From the figure, it is seen that the model captures the absolute values of K_d. The statistical performance for the annual period for this parameter is 'excellent' (P-Bias), 'very good' (CF), and 'poor' (Spearman Rank Correlation) (see Table 5-1, Table 5-2 and Table 5-3).
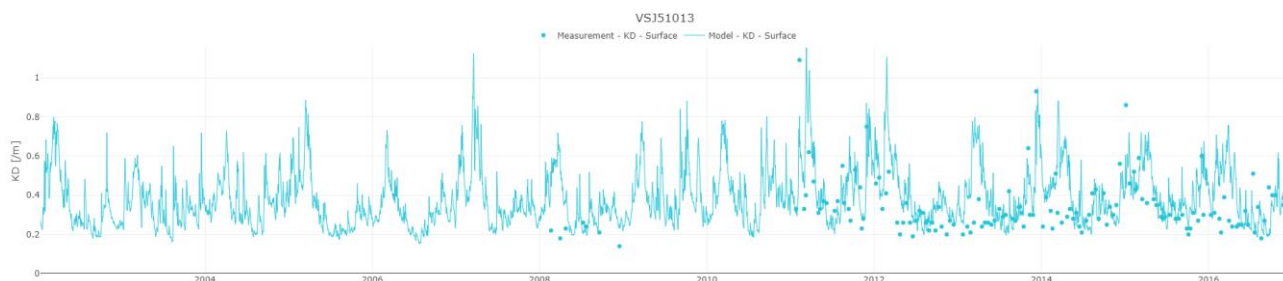
Figure 5-8   Comparison of measured and modelled light attenuation coefficient (K_d, m^{-1}) at station VSJ51013 in the surface waters. Dots represent measurements, and the solid line shows modelled data for the entire period.

For dissolved inorganic nitrogen (DIN), the structure in the seasonality at station VSJ51013 is well represented by the SMF model (see Figure 5-9), with a tendency to overestimate winter concentrations. From the statistical performance measures, annual DIN compares 'very good' (Spearman Rank Correlation and CF) and 'poor' (P-Bias) (see Table 5-1, Table 5-2 and Table 5-3).
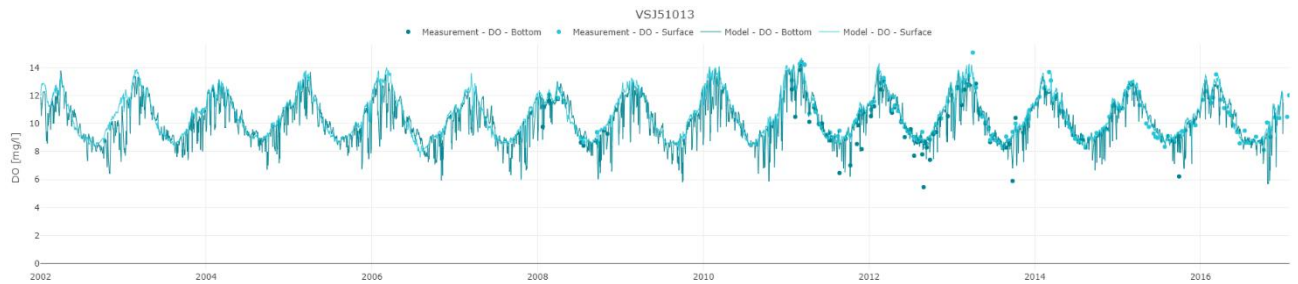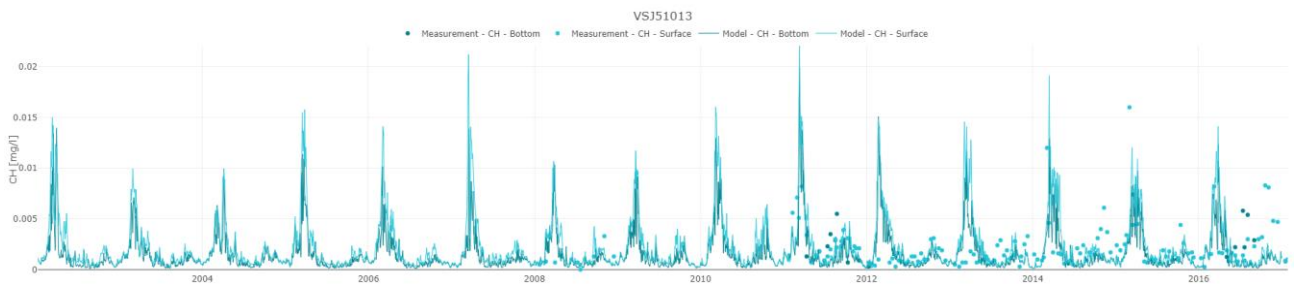

Figure 5-9   Measured and modelled concentrations of dissolved inorganic nitrogen (DIN, mg/l) at station VSJ51013 in the surface and bottom (2 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

When comparing measured and modelled concentrations of DIP (see Figure 5-10), we see relatively similar concentrations with a tendency of the model to overestimate winter concentrations of DIP. The model performance for annual DIP is 'good' according to all quality measures at VSJ51013 (Table 5-1 to Table 5-3).

Figure 5-10   Measured and modelled concentrations of dissolved inorganic phosphorus (DIP, mg/l) at station VSJ51013 in the surface and bottom (2 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

In Figure 5-11 comparisons of measured and modelled total nitrogen (TN) at station VSJ51013 in surface water and bottom (2 m) water are shown. The SMF model well represents both surface and bottom concentrations of TN. From the statistical performance measures (see Table 5-1 to Table 5-3), measured and modelled TN compares ''very good' (CF) and 'very good' (P-Bias and Spearman Rank Correlation) at station VSJ51013.

Figure 5-11   Comparison of measured and modelled concentrations of total nitrogen (TN, mg/l) at station VSJ51013 in surface and bottom (2 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

The seasonal dynamics in TP predicted by the model (see Figure 5-12) compare well with measured data on TP with a tendency to overestimate summer concentrations. According to the quality measures, the model performance for TP is 'excellent' (P-Bias), 'very good' (CF) and 'good' (Spearman Rank Correlation).
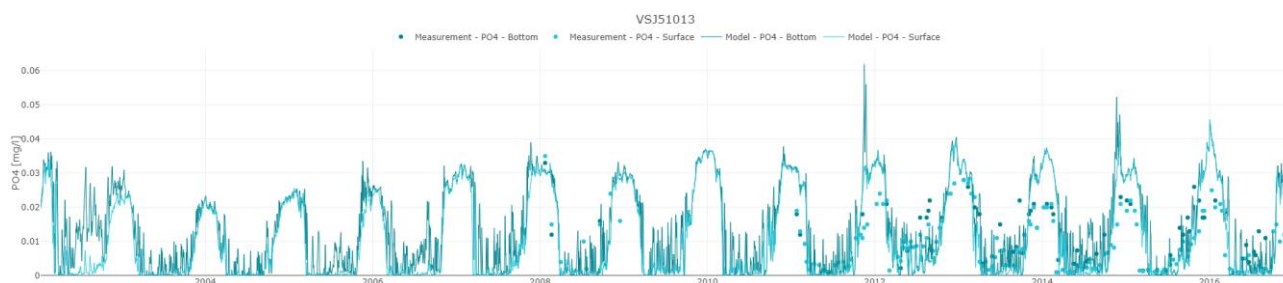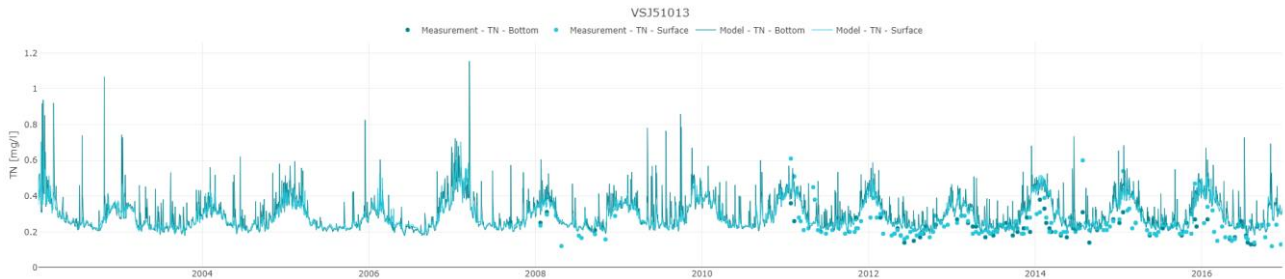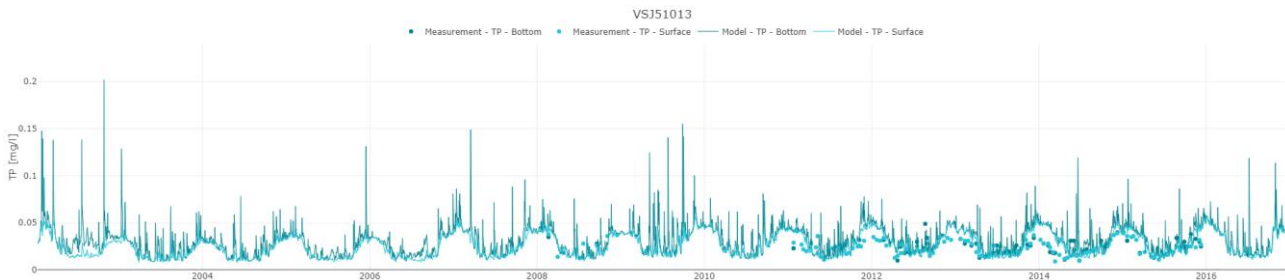

Figure 5-12   Comparison of measured and modelled concentrations of total P (TP, mg/l) at station VSJ51013 in surface and bottom (2 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

5.3.2   General Calibration/Validation for Danish Waters

For the calibration/validation period (2002-2016) 11 out of the 20 monitoring stations had a sufficient amount of measurement data (at least one year of weekly or bi-weekly data) to be included in the model performance analysis (stations listed in, e.g. Table 5-1). Figure 5-5 shows the different Danish locations with measurements on ecosystem parameters (chlorophyll-a (CH), light attenuation (K_d), dissolved oxygen (DO), dissolved inorganic phosphorus (DIP), dissolved inorganic nitrogen (DIN), total nitrogen (TN), and total phosphorus (TP)) during the period 2002-2016. Time series data are presented using the WEB-tool (http:// rbmp2021-2027.dhigroup.com).

In Table 5-1 to Table 5-3 the model performance is evaluated according to DHI (2019b) based on three performance measures: P-Bias, Spearman Rank Correlation and CF. In the tables, colour codes are included to highlight the overall model performance as 'excellent', 'very good', 'good' or 'poor'. For the biogeochemical model covering the Smålandsfarvandet and surrounding seas, we aim at 'excellent', 'very good' or 'good' model performance for 75% of the data sets on measures. All model performances (both annual and summer/winter) evaluated against the three different quality measures at 11 stations were found to be 'excellent', 'very good' or 'good'

for 75% of the measurements (see Figure 5-13 and Table 5-1 to Table 5-3). The annual model performance was found to be 'excellent', 'very good' or 'good' for 80% of the measurements.

All model performance

Excellent	Very good	Good	Poor
13.5	32.8	28.4	25.3

Figure 5-13   Bar chart illustrating all model performance evaluated against three different quality measures and all parameters. The vertical line indicates the aim of 75% being 'excellent', 'very good' or 'good'.
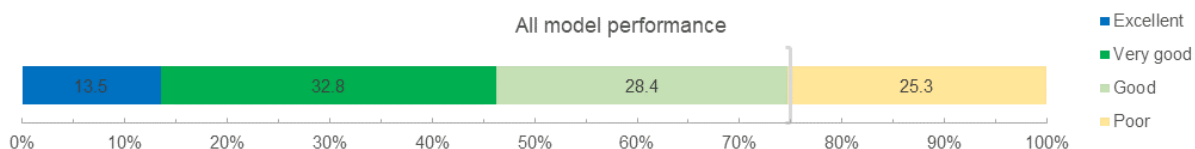
According to P-Bias (Table 5-1), the model meets 'excellent', 'very good' or 'good' for 69% of all measurements (including specific winter and summer evaluations) and 77% when evaluating the annual measurements only. A 'good' model performance measured by P-Bias for summer and winter measurements indicates that the predicted absolute values of summer chlorophyll-a, summer light attenuation, and winter inorganic nutrient concentrations correspond well to the observed values. On average, P-Bias evaluates the model performance for dissolved oxygen to be 'excellent'; for TN the model performance is on average 'very good' and for K_d, DIN and TP the average performance is 'good'. The model performance for CH and DIP is on average 'poor'.

From the quality measure Spearman Rank Correlation (Table 5-2) the model performance meets 'excellent', 'very good' or 'good' in 55% of all measurements (including specific winter and summer evaluations) and 62% in the annual measurements. A good annual correlation obtained from the Spearman Rank measure indicates a good seasonal correlation, where the predicted dynamics correspond well with the observed seasonal variability. On average, the Spearman Rank Correlation evaluates the model performance for dissolved oxygen and DIN to be 'very good'. For DIP and TN, the average performance is 'good'. The model performance for all CH, K_d and TP evaluated from Spearman Rank Correlation is on average 'poor'.

According to the performance measure CF (Table 5-3), the model meets 'excellent', 'very good' or 'good' in 99% of all measurements and 100% when evaluating the annual measurements only. On average, the Cost Function evaluates DO, DIN, TN and TP to be 'very good'; for CH, K_d and DIP the average model performance is 'good'.

Table 5-1   Review of model performance at station P-Bias (%) based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model (|x|≤10%), dark green indicates a 'very good' model (10<|x|<20%), light green indicates a 'good' model (20<|x|<40%) and yellow indicates a 'poor' model (|x|>40%).

Station	TN	TP	DIP		DIN		CH		DO	K_d		Number of observations	
	Annual	Annual	Annual	Winter[a]	Annual	Winter[a]	Annual	Summer[b]	Annual	Annual	Summer[c]	Annual	Summ/Wint
STO0102006	4.2	8.2	7.0	-6.1	1.5	0.3	250.4	225.0	1.9	39.0	62.0	[139-221]	[49-81]
STO0103052	13.3	15.7	131.1	105.8	94.3	47.1	59.9	-35.6	2.8	-23.2	-29.4	[143-183]	[32-89]
STO0104002	-11.9	28.3	78.6	136.7	-22.8	-13.1	157.6	-12.5	3.0	3.9	-2.4	[106-133]	[21-74]
STO0201061	5.3	9.1	47.4	101.9	10.2	18.6	51.3	-46.5	0.0	-16.1	-18.8	[119-153]	[25-82]
STO0601056	-14.0	24.0	279.6	404.6	-43.6	-39.8	11.8	-64.0	-0.5	-21.9	-37.5	[125-149]	[27-78]
STO0703006	-19.4	-35.8	77.1	156.4	-4.6	16.6	-55.6	-97.6	2.3	-52.5	-62.2	[120-143]	[26-78]
STO0801049	9.2	-9.2	-18.8	28.4	-0.6	24.5	-1.8	-47.8	4.6	22.6	23.2	[223-468]	[55-144]
STO0802008	-2.3	-41.9	-39.2	-8.7	18.7	13.8	-34.6	-80.0	4.9	-31.3	-39.0	[385-710]	[55-144]
VSJ43020	21.5	19.5	21.9	47.0	26.9	19.3	0.5	-22.4	2.5	18.2	21.8	[145-220]	[46-91]
VSJ44011	-19.1	-50.4	29.2	87.6	-4.4	2.0	-46.0	-90.7	5.7	-29.2	-43.5	[56-145]	[30-57]
VSJ51013	26.0	-7.5	21.2	1.6	66.2	42.9	51.3	-19.6	7.1	0.6	-1.6	[138-197]	[50-79]

[a] Jan, Feb, Dec

[b] May-Sep

[c] Mar-Sep

Table 5-2 Review of model performance at station Spearman Rank Correlation (no unit) based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model (≥0.90), dark green indicates a 'very good' model (0.89-0.60), light green indicates a 'good' model (0.59-0.30) and yellow indicates a 'poor' model (<0.30).

Station	TN	TP	DIP		DIN		CH		DO	K_d		Number of observations	
	Annual	Annual	Annual	Winter[a]	Annual	Winter[a]	Annual	Summer[b]	Annual	Annual	Summer[c]	Annual	Summ/Wint
STO0102006	0.88	0.32	0.45	0.47	0.90	0.82	0.33	0.28	0.76	0.20	-0.04	[139-221]	[49-81]
STO0103052	0.38	0.31	0.41	0.58	0.68	0.88	0.23	0.21	0.87	0.06	0.16	[143-183]	[32-89]
STO0104002	0.59	-0.02	0.52	-0.01	0.71	0.46	0.03	0.07	0.89	0.19	0.10	[106-133]	[21-74]
STO0201061	0.33	0.34	0.64	0.05	0.54	0.67	0.29	-0.10	0.86	0.22	0.18	[119-153]	[25-82]
STO0601056	0.36	-0.07	0.27	0.34	0.48	0.74	0.10	0.15	0.85	-0.10	-0.11	[125-149]	[27-78]
STO0703006	0.49	-0.20	0.34	0.44	0.71	0.79	-0.16	-0.03	0.84	0.01	-0.12	[120-143]	[26-78]
STO0801049	0.24	0.29	0.56	0.46	0.64	0.40	-0.08	-0.17	0.85	0.23	0.13	[223-468]	[55-144]
STO0802008	0.53	0.17	0.42	0.20	0.73	0.76	-0.14	-0.08	0.88	0.04	-0.05	[385-710]	[55-144]
VSJ43020	0.53	0.60	0.77	0.30	0.67	0.42	0.14	-0.25	0.95	0.35	0.22	[145-220]	[46-91]
VSJ44011	0.43	-0.04	0.15	0.09	0.73	0.70	-0.09	0.27	0.86	0.30	0.33	[56-145]	[30-57]
VSJ51013	0.56	0.49	0.42	0.63	0.76	0.63	-0.05	-0.31	0.88	-0.04	-0.19	[138-197]	[50-79]

[a] Jan, Feb, Dec

[b] May-Sep

[c] Mar-Sep

Table 5-3   Review of model performance at station Cost Function (CF, no unit) based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model (≤0.40), dark green indicates a 'very good' model (0.40-1.00), light green indicates a 'good' model (1.00-2.99) and yellow indicates a 'poor' model (≥3.00).

Station	TN	TP	DIP		DIN		CH		DO	K_d		Number of observations	
	Annual	Annual	Annual	Winter[a]	Annual	Winter[a]	Annual	Summer[b]	Annual	Annual	Summer[c]	Annual	Summ/Wint
STO0102006	0.32	0.38	0.78	0.72	0.27	0.48	2.36	2.11	0.60	0.96	2.22	[139-221]	[49-81]
STO0103052	0.53	1.02	1.31	1.53	0.48	0.59	1.38	0.79	0.45	0.86	0.96	[143-183]	[32-89]
STO0104002	0.36	1.41	1.26	2.67	0.25	0.60	2.38	1.05	0.40	1.20	1.62	[106-133]	[21-74]
STO0201061	0.63	0.72	1.18	2.58	0.32	0.71	0.72	0.31	0.41	0.89	1.12	[119-153]	[25-82]
STO0601056	0.49	0.86	2.19	4.49	0.28	0.64	1.05	0.75	0.44	1.14	1.31	[125-149]	[27-78]
STO0703006	0.72	0.80	1.14	2.36	0.29	0.61	0.53	0.52	0.47	0.98	1.14	[120-143]	[26-78]
STO0801049	0.84	0.96	0.96	1.15	0.52	0.87	1.07	0.77	0.44	1.13	1.39	[223-468]	[55-144]
STO0802008	0.49	0.75	0.83	0.93	0.33	0.54	0.82	0.76	0.45	0.83	1.17	[385-710]	[55-144]
VSJ43020	0.94	1.05	0.82	2.16	0.45	0.89	0.87	1.03	0.26	0.84	1.33	[145-220]	[46-91]
VSJ44011	0.66	1.02	1.37	2.07	0.33	0.59	0.91	1.08	0.53	0.50	0.50	[56-145]	[30-57]
VSJ51013	0.82	0.86	1.04	0.74	0.65	1.34	0.85	1.45	0.58	0.82	1.06	[138-197]	[50-79]

[a] Jan, Feb, Dec

[b] May-Sep

[c] Mar-Sep

6   Conclusion

This technical note shows that the model performance for the biogeochemical model covering the Smålandsfarvandet and surrounding water bodies meets the performance measure 'excellent', 'very good' or 'good' for 75% of the annual measures and 80% for both yearly and summer/winter measurements evaluated against three quality measures. The ambition is to meet the above criteria in 75% of all measures for all parameters and all stations (lumped).

Few local areas covered by the SMF-model show a lower model performance and hence a higher uncertainty, which will be considered in further analysis. Thus, we conclude that the biogeochemical model covering the Smålandsfarvandet and surrounding water bodies is well suited for modelling scenarios as part of the overall development of mechanistic models towards the RBMP 2021-2027.

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