



Development of Mechanistic Models

Mechanistic Model for Roskilde Fjord

Technical documentation on biogeochemical model

Prepared for Danish EPA (Miljøstyrelsen, Fyn)

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Eelgrass in Kertinge Nor Photo: Peter Bondo Christensen

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CONTENTS

1	Executive Summary	1
2	Introduction	3
3	Modelling Concept	
3.1	Mechanistic Modelling	
3.2	Model Development	
3.3	Modelling System	5
4	Model Set-up	
4.1	Model Domain	
4.2	Open Boundary Conditions	
4.3	Forcings	
4.4	Sources	
4.5	Initial Conditions	11
5	Model Calibration and Validation	12
5.1	Model Calibration Procedure	12
5.2	Presentation of Key Model Results	12
5.3	Model Performance	
5.3.1	Calibration/Validation at Station ROS60	18
5.3.2	General Calibration/Validation	21
6	Conclusion	26
7	References	27
FIGURE	S S	
Figure 4-1	Model bathymetry of the Roskilde Fjord model with an open boundary towards Isefjorden to the northwest. Water depths refer to MSL.	6
Figure 4-2	Resolution of the horizontal model mesh of the Roskilde Fjord model (Top: full model area, bottom: zoom to the southern inner fjord)	
Figure 4-3	Location of sources in the Roskilde Fjord model. Loadings are scaled to include local run- off and point sources from land to the fjord.	
Figure 5-1	Modelled yearly average bottom water concentrations of dissolved oxygen (DO, mg/l) for 2016.	
Figure 5-2	Modelled yearly average surface water concentrations of chlorophyll-a (CH, mg/l) for 2016.	14
Figure 5-3	Modelled yearly average surface water concentrations of total nitrogen (TN, mg/l) for 2016.	15
Figure 5-4	Modelled yearly average surface water concentrations of total phosphorus (TP, mg/l) for 2016.	16
Figure 5-5	Location of stations used for performance measures in Roskilde Fjord	
Figure 5-6	Comparison of measured and modelled concentrations of dissolved oxygen (DO, mg/l) at station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements,	
	and the solid line shows modelled data for the entire period	18
Figure 5-7	Comparison of measured and modelled concentrations of chlorophyll-a (CH, µg/l) at station ROS60 in surface and bottom (4 m) waters. Dots represent measurements, and	
	solid lines show modelled data for the entire period	19



Figure 5-8	Comparison of measured and modelled concentrations of light attenuation (K _d , m ⁻¹) at station ROS60 in surface water. Dots represent measurements, and solid lines show	
	modelled data for the entire period.	19
Figure 5-9	Measured and modelled concentrations of dissolved inorganic nitrogen (DIN, mg/l) at	
	station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements,	
	and solid lines show modelled data for the entire period	20
Figure 5-10	Measured and modelled concentrations of dissolved inorganic phosphorus (DIP, mg/l) at	
	station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements,	00
Fig 5 44	and solid lines show modelled data for the entire period.	20
Figure 5-11	Comparison of measured and modelled concentrations of total nitrogen (TN, mg/l) at	
	station ROS60 in surface and bottom (4 m) waters. Scatter data represent measurements, and solid lines show modelled data for the entire period	21
Figure 5-12	Comparison of measured and modelled concentrations of total P (TP, mg/l) at station	∠ 1
rigare o 12	ROS60 in surface and bottom (4 m) waters. Scatter data represent measurements, and	
	solid lines show modelled data for the entire period	21
Figure 5-13	Bar chart illustrating all model performances evaluated against three different quality	
	measures and all parameters. The vertical line indicates the aim of 75% being 'excellent',	
	'very good' or 'good'	22
TABLES		
Table 2-1	Water bodies included in the Roskilde Fjord model.	3
Table 5-1	Review of model performance at station FRB65 based on measured and modelled data	
	for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green	
	indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a	
	'poor' model	23
Table 5-2	Review of model performance at station FRB75 based on measured and modelled data	
	for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green	
	indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a 'poor' model.	24
Table 5-3	Review of model performance at station ROS60 based on measured and modelled data	24
Table 5-5	for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green	
	indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a	
	'poor' model	25
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1 Executive Summary

The model development presented in this technical note represents the biogeochemical model development for Roskilde Fjord. The Roskilde Fjord model is part of a large 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 Roskilde Fjord, together with a quality assessment of the model performance. This specific model includes two Danish water bodies:

Water body*)	ID Number
Roskilde Fjord, ydre	1
Roskilde Fjord, indre	2

^{*)} Water bodies defined for the River Basin Management Plans 2015-2021

The Roskilde Fjord biogeochemical model builds on the developed hydrodynamic model of Roskilde Fjord and is developed to describe the biogeochemistry within the model domain with 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 was not suitable to evaluate this kind of estuarine biogeochemical models, why Cost Function (CF) was introduced. The quality measure CF was used in Erichsen and Timmermann (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 the full 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 measurements (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, 91% of all annual data set meet the success criteria when evaluated against the three performance measures, and 86% when assessing both annual performance and summer/winter performance of all data. The average model performance for the biogeochemical model of Roskilde Fjord is summarized below:

 Model performance measures for dissolved oxygen (DO) are 1% (P-Bias), 0.9 (Spearman Rank Correlation) and 0.3 (CF). The average model performance for DO is categorized to be 'excellent' (P-Bias, Spearman Rank Correlation and CF).



- Model performance measures for chlorophyll-a (CH) are on average 42% (P-Bias), 0.3 (Spearman Rank Correlation) and 0.9 (CF). The average model performance for CH is categorized to be 'very good' (CF) and 'poor' (P-Bias and Spearman Rank Correlation).
- Model performance measures for light attenuation coefficient (K_d) are on average 18% (P-Bias), 0 (Spearman Rank Correlation) and 1.3 (CF). The average model performance for K_d is categorized to be 'very good' (P-Bias), 'good' (CF) and 'poor' (Spearman Rank Correlation).
- Model performance measures for dissolved inorganic nitrogen (DIN) are on average 10% (P-Bias), 0.8 (Spearman Rank Correlation) and 0.3 (CF). The average model performance for DIN is categorized to be 'excellent' (CF) and 'very good' (P-Bias and Spearman Rank Correlation).
- Model performance measures for dissolved inorganic phosphorous (DIP) are on average 18% (P-Bias), 0.6 (Spearman Rank Correlation) and 0.9 (CF). The average model performance for DIP is categorized to be 'very good' (P-Bias, Spearman Rank Correlation and CF).
- Model performance measures for total nitrogen (TN) are on average 20.4% (P-Bias), 0.7 (Spearman Rank Correlation) and 0.6 (CF). The average model performance for TN is categorized to be 'very good' (Spearman Rank Correlation and CF) and 'good' (P-Bias).
- Model performance measures for total phosphorous (TP) are on average 10.9% (P-Bias),
 0.7 (Spearman Rank Correlation) and 0.6 (CF). The average model performance for TP is categorized to be 'very good' (P-Bias, Spearman Rank Correlation and CF).

The details behind the above performance are available in Table 5-1 to 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 well reached. Hence, in this technical note, we conclude that the Roskilde Fjord biogeochemical model has been developed successfully for Roskilde Fjord water bodies and will be applied for modelling nutrient scenarios in these water bodies in the assessment of maximum allowable inputs (MAI).



2 Introduction

The model development presented in this technical note represents the biogeochemical model development for Roskilde Fjord and builds on top of the Roskilde Fjord 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 Roskilde Fjord, together with a quality assessment of the model performance. The Roskilde Fjord model includes two 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 Roskilde Fjord model.

Water body*)	ID Number
Roskilde Fjord, ydre	1
Roskilde Fjord, indre	2

^{*)} 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 Roskilde Fjord 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 was not suitable to evaluate this kind of estuarine biogeochemical models. As described in DHI (2019b), the MEF evaluates the RMSE as 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 system with strong gradients and variable dynamics, the MEF has proven not to be suited (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. The CF measure was also used in Erichsen & Timmermann (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 Roskilde Fjord. The Roskilde Fjord 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 Roskilde Fjord model is defined as an estuary specific model. The mechanistic model complex development as part of the present 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 Seamodel, and the Baltic Sea, which is covered by the IDW-model (Inner Danish Waters).
 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: Six specific estuary (fjord) 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 Roskilde Fjord 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, 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 the technical report DHI (2019c).



4 Model Set-up

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

For the present project, the model is set up for the period 2002-2016, which means that all model input data need to cover this period.

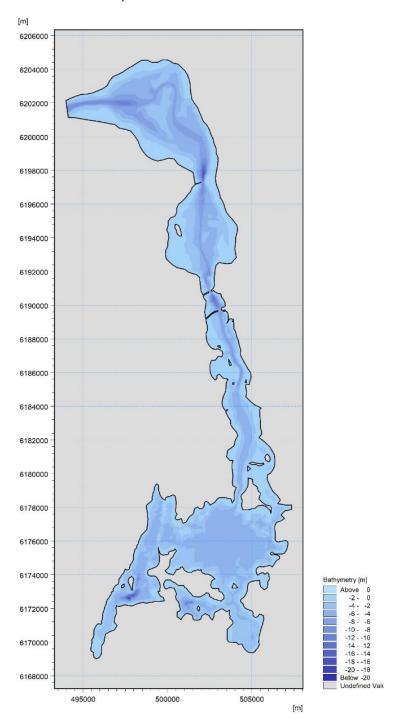


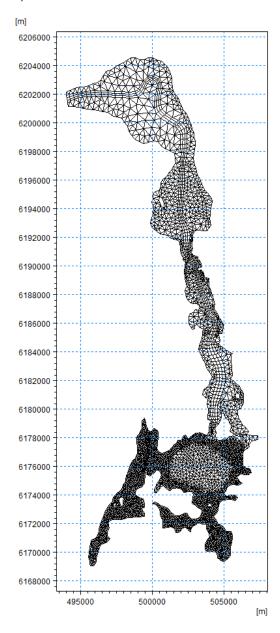
Figure 4-1 Model bathymetry of the Roskilde Fjord model with an open boundary towards Isefjorden to the northwest. Water depths refer to MSL.



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.

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 model. The bathymetry of the Roskilde Fjord model is shown in Figure 4-1, whereas Figure 4-2 shows the resolution of the horizontal mesh. A total of 22 combined sigma resolves the vertical of the water column- and z- layers. Two sigma-layers resolve the water column from surface to -2m below MSL (or local depth if less than 2m), and the water column below is resolved by up to 20 z-layers (depending on local water depth), each of 0.5 m thickness. Further documentation on model mesh and horizontal/vertical resolution of the Roskilde Fjord HD model can be found in DHI (2019d).





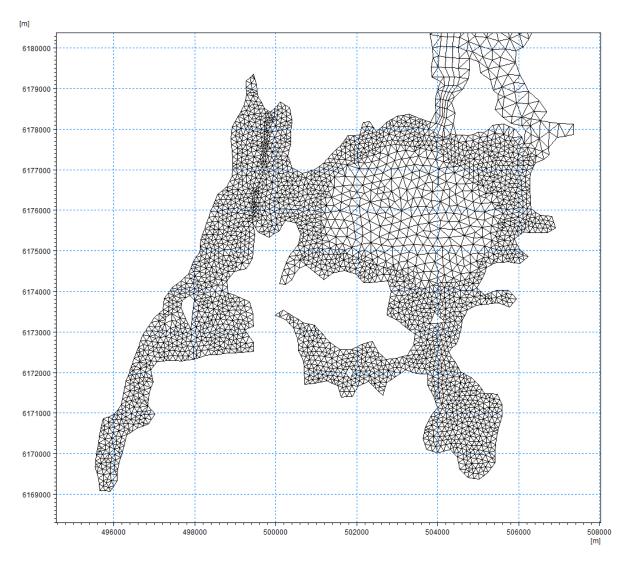


Figure 4-2 Resolution of the horizontal model mesh of the Roskilde Fjord model (Top: full model area, bottom: zoom to the southern inner fjord).

4.2 Open Boundary Conditions

The Roskilde Fjord model has one open boundary towards Isefjorden, located to the northwest of the model domain. Profiles of biogeochemical state variables at the boundary were extracted from DHI's existing regional model. 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 temporally varying forcing.

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, 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 Roskilde Fjord model includes sources with land-based nutrient loadings. In Figure 4-3, the location of the sources is shown. Freshwater run-off from land is included in the hydrodynamic module.

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 data from DCE/AU, Department of Bioscience on a 4th order water body level.

More details are included in DHI (2020).



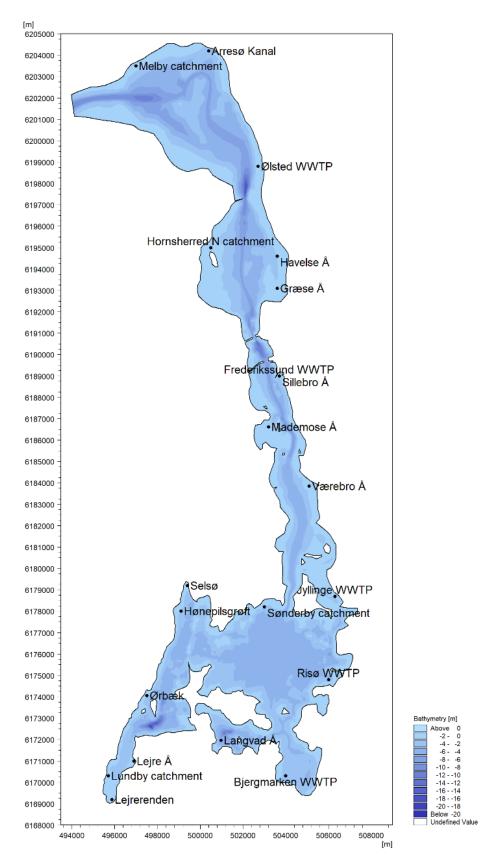


Figure 4-3 Location of sources in the Roskilde Fjord model. Loadings are scaled to include local run-off and point sources from land to the fjord.



4.5 Initial Conditions

To properly initiate a model simulation, the model requires initial conditions for the various state variables. Initial values in the pelagic phase applied in the Roskilde Fjord model were estimated based on measurements within the Roskilde Fjord area. The available measurements from around 2002 were applied as uniform values in the entire model domain, and the model was spun-up by four times run for the year 2002 before being used for calibration/validation.

Initial fields of seabed substrates are based on mud-data from EMODNET (2016). Initial values of benthic vegetation (e.g. eelgrass) 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 & Timmermann 2017). As such, the model validation constitutes the final documentation of the model performance.

The Roskilde Fjord 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 given for the entire period using a WEB-tool (rbmp2021-2027.dhigroup.com, Google Chrome only).

5.1 Model Calibration Procedure

Calibration of the biogeochemical Roskilde Fjord 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, within the water bodies covered by the model domain, will be given.



Average concentrations of dissolved oxygen in bottom waters during 2016 range from 8.0 mg/l in the inner part and between 8.8-10.4 mg/l in the outer part of Roskilde Fjord (Figure 5-1).

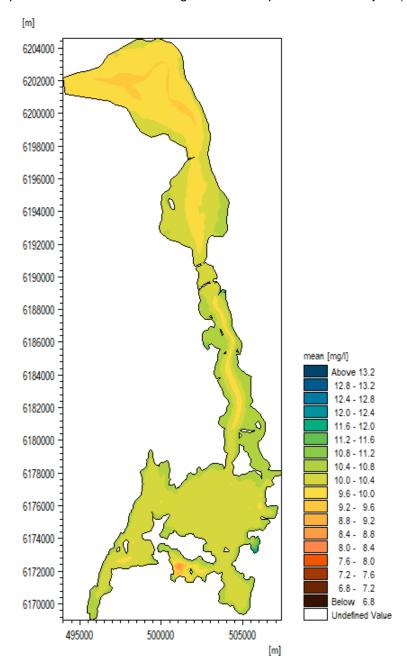


Figure 5-1 Modelled yearly average bottom water concentrations of dissolved oxygen (DO, mg/l) for 2016.



Yearly average concentrations of surface chlorophyll-a during 2016 range from minimum values of 0.0004 mg/l to maximum values of 0.0048 mg/l (Figure 5-2).

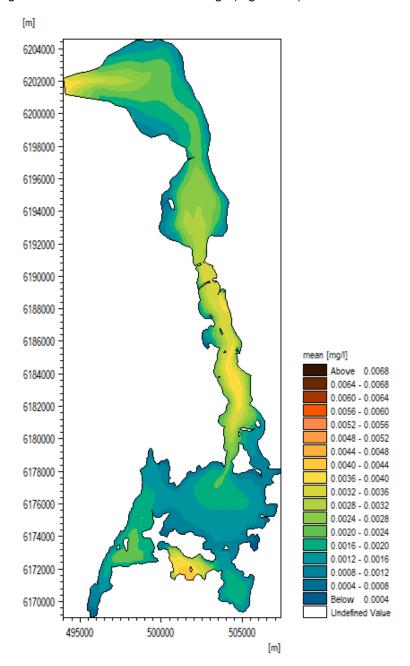


Figure 5-2 Modelled yearly average surface water concentrations of chlorophyll-a (CH, mg/l) for 2016.



Yearly average concentrations of surface total phosphorus during 2016 range between 0.4 mg/l to 1.1 mg/l (Figure 5-3). Highest values are observed in the central and southern inner part.

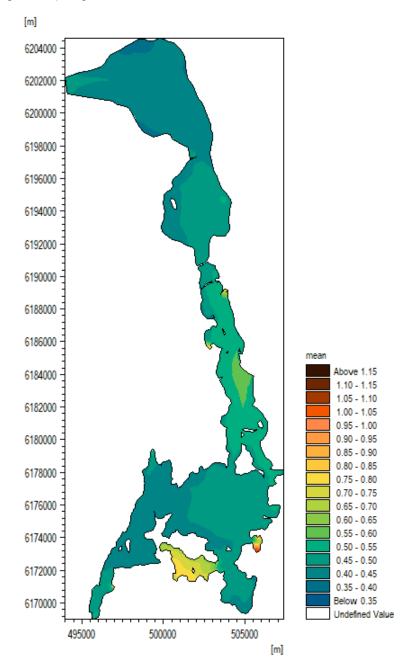


Figure 5-3 Modelled yearly average surface water concentrations of total nitrogen (TN, mg/l) for 2016.



Yearly average concentrations of surface total phosphorus during 2016 range between 0.2 mg/l to 1.3 mg/l (Figure 5-4). Highest values are observed in the inner part of the fjord.

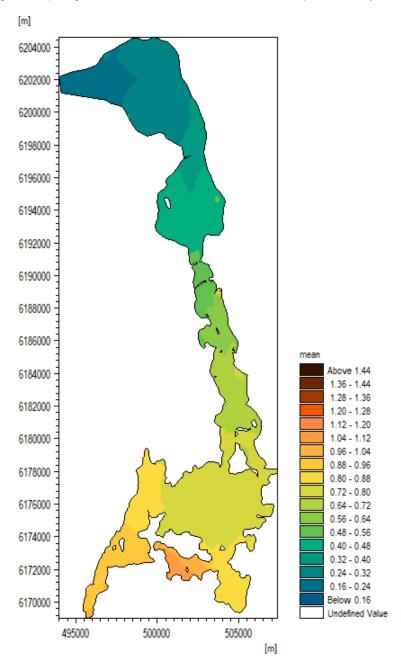


Figure 5-4 Modelled yearly average surface water concentrations of total phosphorus (TP, mg/l) for 2016.

5.3 Model Performance

The Roskilde Fjord biogeochemical model was calibrated and validated against measured data (observations) on modelled ecosystem parameters at selected stations within the model domain. Figure 5-1 shows the location of three stations within the model domain. All stations within the model domain 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 Roskilde Fjord model compares well to the measurements in terms of model parameters (see Figure 5-3 to Figure 5-9), 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 stations used for performance measures in Roskilde Fjord.



5.3.1 Calibration/Validation at Station ROS60

In the following, we present an example of the calibration/validation from Roskilde Fjord at station ROS60 and refer to rbmp2021-2027.dhigroup.com (Google Chrome only) for more details on the Danish measurement stations. The location of station ROS60 is shown in Figure 5-5.

The comparison at station ROS60 shows a good agreement between the measurements and the Roskilde Fjord model for 90.5% of the parameters according to the three performance measure P-Bias, Spearman Rank Correlation and CF (see Table 5-3 together with DHI (2019b) and Erichsen *et al.* (2017) regarding the applied measures).

In Figure 5-6, measured and modelled concentrations of dissolved oxygen (DO) at station ROS60 in the surface and bottom (here 4 m) waters are shown. From the figure, it is seen that for DO the variability and seasonality of the surface and bottom (4 m) waters are well represented by the model. This is in agreement with the statistical performance measures (see Table 5-3), where measured and modelled DO compares 'excellent' (P-Bias and CF) and 'very good' (Spearman Rank Correlation) at station ROS60.

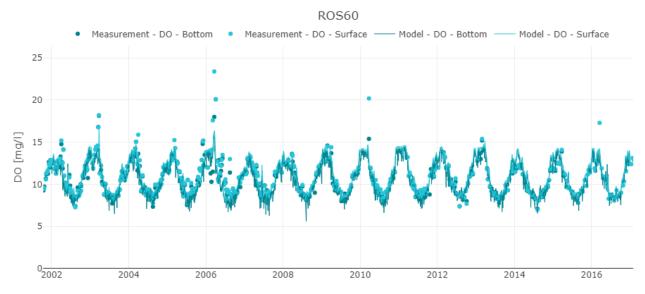


Figure 5-6 Comparison of measured and modelled concentrations of dissolved oxygen (DO, mg/l) at station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements, and the solid line shows modelled data for the entire period.

For chlorophyll-a (CH), the dynamics in seasonality are also well represented by the model (see Figure 5-7). From the statistical performance measures, annual CH compares 'very good' (CF), 'good' (Spearman Rank Correlation) and 'poor' (P-Bias) (see Table 5-3).



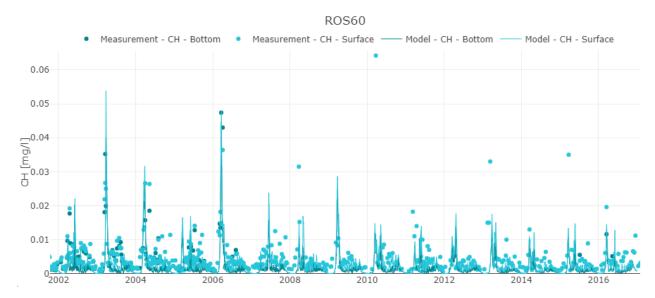


Figure 5-7 Comparison of measured and modelled concentrations of chlorophyll-a (CH, μg/l) at station ROS60 in surface and bottom (4 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

For light attenuation coefficient (K_d), the majority of the seasonality is well represented by the Roskilde Fjord model (see Figure 5-9). From the statistical performance measures annual K_d compares 'very good' according to P-Bias, 'good' based on CF and 'poor' according to Spearman Rank Correlation, and summer K_d compares 'excellent' (P-Bias) (Table 5-3).

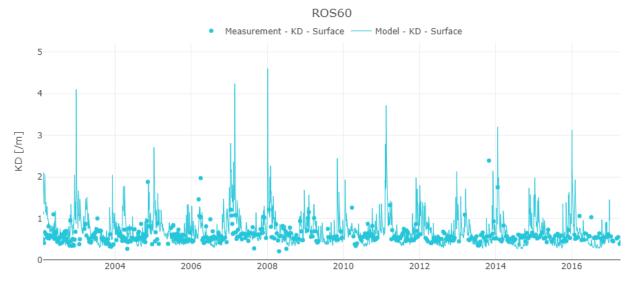


Figure 5-8 Comparison of measured and modelled concentrations of light attenuation (K_d, m⁻¹) at station ROS60 in surface water. Dots represent measurements, and solid lines show modelled data for the entire period.

For dissolved inorganic nitrogen (DIN), the structure in the seasonality is well represented by the Roskilde Fjord model (see Figure 5-9). This is further supported by the statistical performance measures where annual DIN compares 'excellent' according to P-Bias and CF, and 'very good' according to Spearman Rank Correlation (see Table 5-3). For winter DIN the model performance is 'excellent' for all quality measures at station ROS60 (Table 5-3).



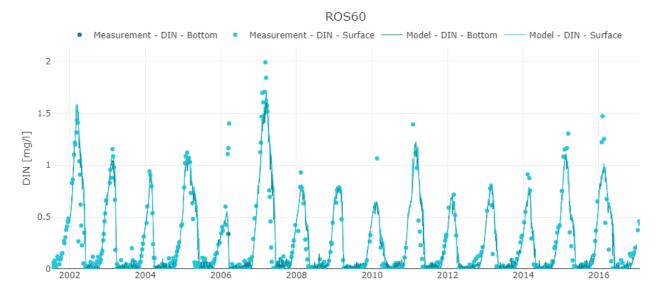


Figure 5-9 Measured and modelled concentrations of dissolved inorganic nitrogen (DIN, mg/l) at station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

When comparing measured and modelled concentrations of DIP (see Figure 5-10), we see relatively similar winter concentrations and a definite drop in spring. The overall patterns are well represented by the model, which is further supported by the statistical performance measures, where the model performance for annual DIP is 'very good' (P-Bias, Spearman Rank Correlation and CF).

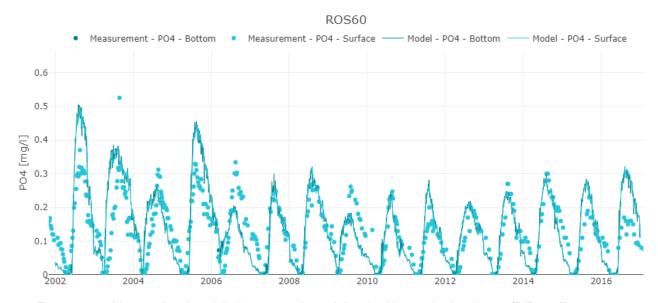


Figure 5-10 Measured and modelled concentrations of dissolved inorganic phosphorus (DIP, mg/l) at station ROS60 in the surface and bottom (4 m) waters. Dots represent measurements, and solid lines show modelled data for the entire period.

In Figure 5-11, comparisons of measured and modelled total nitrogen (TN) at station ROS60 in surface water and bottom water are shown. For TN, the variability in time and through the water column is well represented by the model. The statistical performance measures support this (see Table 5-3), where measured and modelled TN compare 'very good' (P-Bias, Spearman Rank and CF) at station ROS60.



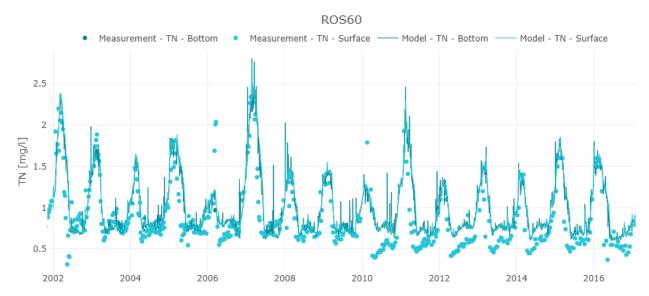


Figure 5-11 Comparison of measured and modelled concentrations of total nitrogen (TN, mg/l) at station ROS60 in surface and bottom (4 m) waters. Scatter data represent measurements, and solid lines show modelled data for the entire period.

The seasonal dynamics in TP predicted by the model (see Figure 5-12) compare well with measured data on TP. The model performance for TP at station ROS60 is 'excellent' (P-Bias and R²), 'very good' (Spearman Rank Correlation and CF) and 'good (MEF).

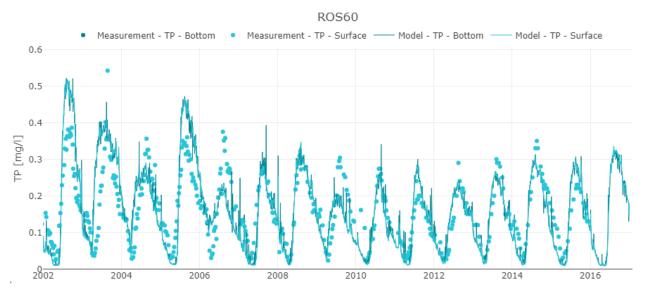


Figure 5-12 Comparison of measured and modelled concentrations of total P (TP, mg/l) at station ROS60 in surface and bottom (4 m) waters. Scatter data represent measurements, and solid lines show modelled data for the entire period.

5.3.2 General Calibration/Validation

For the calibration/validation period (2002-2016), all 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. Figure 5-5 shows the three 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 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 Roskilde Fjord, 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 three stations were found to be 'excellent', 'very good' or 'good' for 86% 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 91% of the measurements.

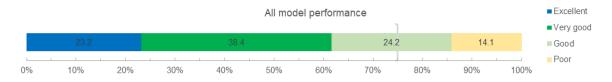


Figure 5-13 Bar chart illustrating all model performances evaluated against three different quality measures and all parameters. The vertical line indicates the aim of 75% being 'excellent', 'very good' or 'good'.

According to P-Bias (Table 5-1, Table 5-2 and Table 5-3), the model meets 'excellent', 'very good' or 'good' for 85% of all measurements (including specific winter and summer evaluations) and 86% 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. In general, the P-Bias obtains negative values for most of the parameters, indicating that the model underestimates observed values. On average, P-Bias evaluates the model performance for dissolved oxygen to be 'excellent'; for K_d, DIN, DIP and TP model performance is on average 'very good'; for TN the average model performance is 'good'. The model performance for CH evaluated from P-Bias is on average 'poor'.

From the quality measure Spearman Rank Correlation (Table 5-1 to Table 5-3) the model performance meets 'excellent', 'very good' or 'good' in 73% of all measurements (including specific winter and summer evaluations) and 86% in the annual measurements. A good annual correlation obtained from the Spearman Rank Correlation 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 to be 'excellent'; for DIN, DIP, TN, and TP the model performance is on average 'very good'. The average model performance for K_d and CH evaluated from Spearman Rank Correlation is on average 'poor'.

According to the performance measure CF (Table 5-1 to Table 5-3), the model meets 'excellent', 'very good' or 'good' in 100% of all measurements at the three stations (**Error! Reference s ource not found.** to Table 5-3). 67% of all measurements and 81% of annual measurements at the stations meet 'excellent', 'very good', or 'good'. On average, the Cost Function evaluates DO and DIN to be 'excellent'. For CH, DIP, TN, and TP, the model performance is categorized to be 'very good' on average for all measures and 'good' for K_d.



Table 5-1 Review of model performance at station FRB65 based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a 'poor' model.

Parameter	P-Bias (%)	Spearman Rank Correlation	CF	Number of observations
TN annual	-16.4	0.67	0.57	380
TP annual	-8.7	0.58	0.65	380
DIP annual	6.0	0.60	0.77	378
DIP winter ^a	-19.7	0.29	0.97	84
DIN annual	-10.9	0.80	0.22	380
DIN winter ^a	-2.0	0.87	0.34	85
CH annual	-41.0	0.38	0.69	313
CH summer ^b	-60.6	0.12	1.30	148
DO annual	1.8	0.92	0.34	506
K _d annual	24.6	-0.18	1.60	287
K _d summer ^c	0.5	-0.17	1.24	177

^a January, February, December

^b May-September

^c March-September



Table 5-2 Review of model performance at station FRB75 based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a 'poor' model.

Parameter	P-Bias (%)	Spearman Rank Correlation	CF	Number of observations
TN annual	-28.2	0.76	0.86	291
TP annual	-20.2	0.60	0.69	290
DIP annual	-14.0	0.69	0.61	287
DIP winter ^a	-34.4	0.65	0.74	70
DIN annual	-16.8	0.84	0.24	291
DIN winter ^a	-13.9	0.85	0.38	71
CH annual	-23.7	0.46	0.50	229
CH summer ^b	-34.5	0.40	0.92	103
DO annual	0.9	0.92	0.30	424
K _d annual	44.3	0.04	1.63	217
K _d summer ^c	23.7	0.14	1.11	131

^a January, February, December

^b May-September

^c March-September



Table 5-3 Review of model performance at station ROS60 based on measured and modelled data for the validation period 2002-2016. Blue colour indicates an 'excellent' model; dark green indicates a 'very good' model; light green indicates a 'good' model, and yellow indicates a 'poor' model.

Parameter	P-Bias (%)	Spearman Rank Correlation	CF	Number of observations
TN annual	16.7	0.61	0.50	477
TP annual	3.7	0.83	0.59	455
DIP annual	11.9	0.80	0.66	479
DIP winter ^a	-21.7	0.65	1.68	91
DIN annual	9.1	0.77	0.27	477
DIN winter ^a	-7.4	0.95	0.23	89
CH annual	-42.8	0.38	0.59	592
CH summer ^b	-49.1	-0.01	1.11	287
DO annual	-0.4	0.88	0.35	883
K _d annual	15.4	0.15	1.15	443
K _d summer ^c	-0.8	0.09	1.08	284

^a January, February, December

^b May-September

^c March-September



6 Conclusion

This technical note shows that the model performance for the biogeochemical model covering Roskilde Fjord meets the performance measure 'excellent', 'very good' or 'good' for 91% of the annual measures and 86% for both yearly and summer/winter measurements evaluated against five quality measures. The ambition is to meet the above criteria in 75% of all measures for all parameters and all stations (lumped). Hence, we conclude that the biogeochemical model covering Roskilde Fjord is well suited for modelling scenarios as part of the overall development of mechanistic models towards the RBMP 2021-2027.



7 References

DHI (2019a). MIKE 21 & MIKE 3 Flow Model FM. Hydrodynamic and Transport Module. Scientific Documentation

(http://manuals.mikepoweredbydhi.help/2019/Coast_and_Sea/MIKE_321_FM_Scientific_Doc.pd f)

DHI (2019b). Development of Mechanistic Models. Assessment of Model Performance. DHI technical report (project no. 11822245)

DHI (2019c). Development of Mechanistic Models. Short Technical Description of the Biogeochemical Models Applied for the Mechanistic Model Development. DHI technical report (project no. 11822245)

DHI (2019d). Development of Mechanistic Models. Mechanistic Model for Roskilde Fjord. Hydrodynamic model documentation. DHI report (project no. 11822245)

DHI (2020). Development of Mechanistic Models. Short Technical Description of the Biogeochemical Models Input Data. DHI technical report (project no. 11822245)

EMODnet Bathymetry Consortium (2016). EMODnet Digital Bathymetry (DTM) (http://doi.org/10.12770/c7b53704-999d-4721-b1a3-04ec60c87238, link working 15-11-2018).

Erichsen AC, Møhlenberg F, Timmermann K, Christensen JPA & Göke C (2019). Gennemgang af grundlaget for afgrænsning, karakterisering og typeinddeling af kystvande i vandområdeplanerne. Rapport. https://mst.dk/media/187927/afgraensning-karakterisering-typologi.pdf

Erichsen AC (Ed.), Timmermann K (Ed.), Christensen JPA, Kaas H, Markager S, Møhlenberg F (2017). Development of models and methods to support the Danish River Basin Management Plans. Scientific documentation. Aarhus University, Department of Bioscience and DHI, 191 pp.

Herman P, Newton A, Schernewski G, Gustafsson B & Malve O (2017). International Evaluation of the Danish Marine Models. Miljøstyrelsen

(https://mfvm.dk/fileadmin/user_upload/MFVM/Nyheder/Bilag_1_Evalueringsrapport_om_de_danske_kvaelstofmodeller__10._oktober_2017-2.pdf)