DHI

Development of Mechanistic Models

Short Technical Description of Biogeochemical Model Input Data

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Short Technical Description of Biogeochemical Model Input Data

Prepared for Danish EPA (Miljøstyrelsen, Fyn)

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Eelgrass in Kertinge Nor

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1 Introduction

As part of the preparation towards the Danish River Basin Management Plans 2021-2027 the Danish Environmental Protection Agency (EPA) has initiated a number of mechanistic model developments with the aim of increasing the spatial coverage of models, improving the calibration/validation and hence the confidence of the Maximum Allowable nutrient Inputs (MAIs).

The mechanistic model complex development includes two regional models, three local-domain models and six estuary specific models.

- Two regional models are being developed: The North Sea model and the model covering the inner Danish waters (IDW). Regional models cover specific Danish water bodies and regional waters, such as the North Sea and a small part of the North Atlantic 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, provide boundaries to local-domain models and estuary specific models.

- Local-domain models: These 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.

- Specific estuary models: Six estuary (fjord) specific models are developed to allow for detailed modelling of the particular estuary.

Each of the different models consists of four specific modules: i) a hydrodynamic module (HD) computing water levels, current (speed and direction), salinity and water temperature, ii) a wave module (SW) computing significant wave heights and wave period, ii) a transport model (or advection/dispersion module - AD) computing the transport and dispersion of a specific biogeochemical component and iv) a biogeochemical module (ECO Lab) computing changes in concentrations of a specific biogeochemical component due to fx primary production of grazing by zooplankton.

The model setup and calibration/validation of the physical models (HD and AD) are reported in a series of model specific technical notes (DHI 2019a – DHI 2019k). The biogeochemical model (ECO Lab)is described in a short technical note (DHI 2019l), whereas the input data to the biogeochemical model is described in the present technical note and the specific model calibration/validation of the biogeochemical models will be reported in a series of model specific technical notes (in progress).

2 Input data

The biogeochemical model development consists of a series of different steps for each of the different model domains: i) setup and calibration of the hydrodynamic model (HD), ii) collection and preparation of input data to the biogeochemical models, iii) calibration and validation of the biogeochemical models and iv) application of the models to ensure the data needed for the estimation of differentiated maximum allowable inputs (MAIs) to the Danish water bodies.

The HD models (including input data and calibration/validation) are reported in a series of model specific technical notes (DHI 2019a – DHI 2019k) and will not be described in more details in this note. Likewise, the results of the calibration/validation of the biogeochemical models will be reported in a series of specific technical notes (in progress) and in the present technical note we will focus on the input data included in the biogeochemical models.

The biogeochemical model (described in more details in DHI 2019l) consists of a range of state variables that all need to be defined and specified:

- In the pelagic phase (water column), the biogeochemical model state variables cover: Phytoplankton carbon (C), nitrogen (N), phosphorous (P) and silicate (Si)[1], chlorophyll-a, zooplankton (C, N and P)[2], particulate organic matter (C, N, P and Si), two fractions of dissolved organic matter (C, N and P) and inorganic nitrogen (DIN), inorganic phosphorous (DIP), inorganic silicate (Si). On top of those state variables the model also include hydrogen sulphide (H_2S), dissolved oxygen (O_2), inorganic suspended material and eelgrass seeds.

- At the seabed the biogeochemical model includes state variables describing two functional groups of macro algae (C, N and P) as well as eelgrass (biomass C, N and P as well as number of shoots). Also, the seabed includes micro benthic algae (C, N and P).

- In the sediment the biogeochemical model includes pools of organic matter (C, N, P and Si) and pools of inorganic nutrient in the porewater (N and P), and iron-bound P. On top of this, pools of inorganic matter are also included.

The above list does not compile all state variables but provide examples of central state variables included in the biogeochemical models.

Important forcing data consists of salinity, water temperature and shear stress (from HD and SW modules), atmospheric depositions as well as meteorological forcing's such as photosynthetic active solar radiation, together with:

- Model boundaries: Each model require boundary data covering all pelagic state variables.

- Model sources: Weather the model sources are point sources or diffuse source all pelagic state variables need to be specified as source concentrations.

- Initial values: For each state variable initial data needs to be specified, and this is relevant for both the pelagic phase and for the benthic phase (sediments and/or seabed)

In the following the different input data integrated in the biogeochemical models will be described.

[1] The biogeochemical model applied in the regional models include more phytoplankton species groups and hence, silicate becomes a variable for the modelling of diatoms

[2] In the regional model the zooplankton is split into two functional groups, micro-zooplankton and meso-zooplankton

2.1 Model Boundaries

2.1.1 Regional models

Two regional models covering the North Sea and the Inner Danish Waters (IDW) including the Baltic Sea are developed. The North Sea model covers the North Sea and a smaller part of the North Atlantic Ocean and include four open boundaries, three in the North Atlantic Ocean and one in Kattegat, see Figure 2-1. For each of the three boundaries in the North Atlantic Ocean data from ICES (http://ecosystemdata.ices.dk, downloaded July 2019) has been applied. The data in the Atlantic Ocean are sparse, and in order to be able to describe seasonal, spatial and depth variation at the boundaries, the measurements are lumped in space and time. I.e. stations are lumped into three areas (N, W and E), in depth intervals (20, 40, 60, 80, 100, 200, 400, 600, 800, 1000, 2000 and 3000 m) and monthly average values for the period 1990-2016.

With respect to the Kattegat boundary, Swedish observation from the monitoring station Anholt E has been applied (https://www.smhi.se/data/oceanografi/datavardskap-oceanografi-och-marinbiologi/marina-miljoovervakningsdata, downloaded July 2019). Data from Anholt E has been compiled and depth varying boundary data been estimated and applied along the Kattegat boundary.

For all boundaries, observations of chlorophyll-a, inorganic N (NH_4, NO_x), inorganic P (PO_4), total N (TN), total P (TP) and measured concentrations of dissolved oxygen (O_2) have been collected and compiled into the state variables included in the mechanistic model boundaries.

In the IDW model one open boundary is included in Skagerrak, see Figure 2-2. The data applied as boundary data in the IDW model are extracted from the North Sea Model (2D vertical time series), and as the biogeochemical models are similar in the North Sea model and the IDW model all state variables are available for boundary data.

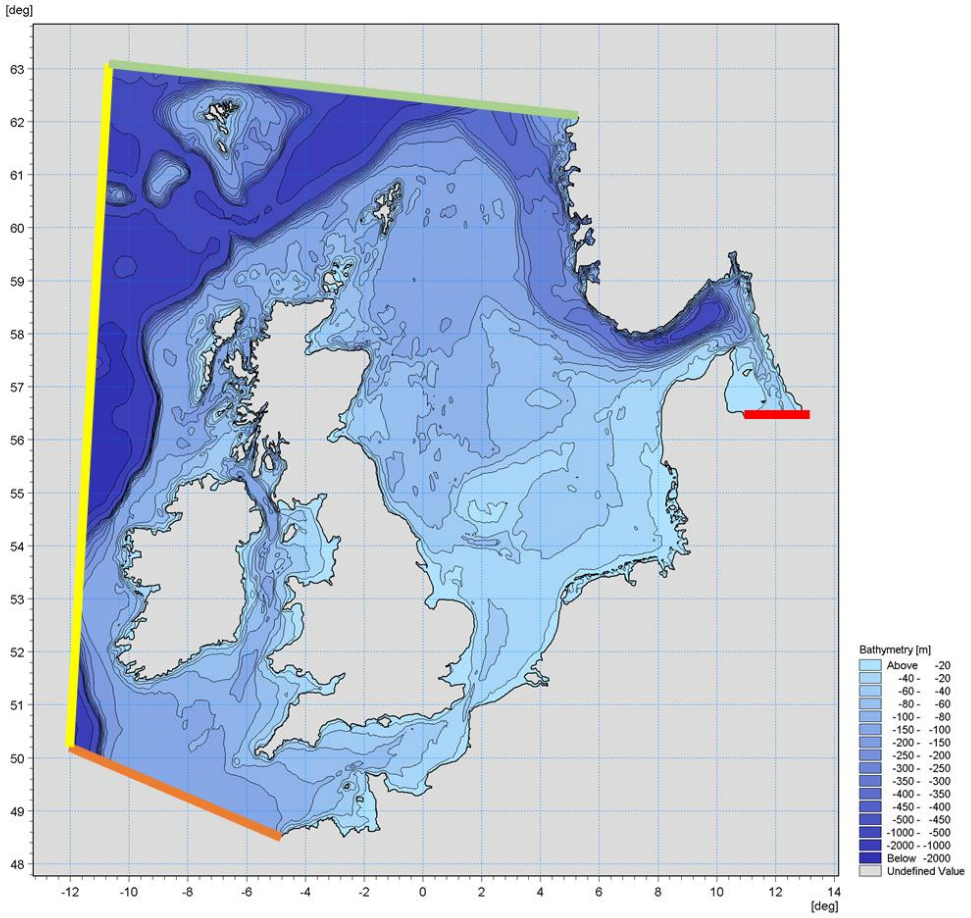

Figure 2-1 Model bathymetry of the North Sea model (UKNS2-HD28). Water depths refer to MSL. The model includes four open boundaries: One in the south-western part of the area (orange line), one west of Ireland (yellow), one just north of the Faroe Islands (green) and one in Kattegat (red).

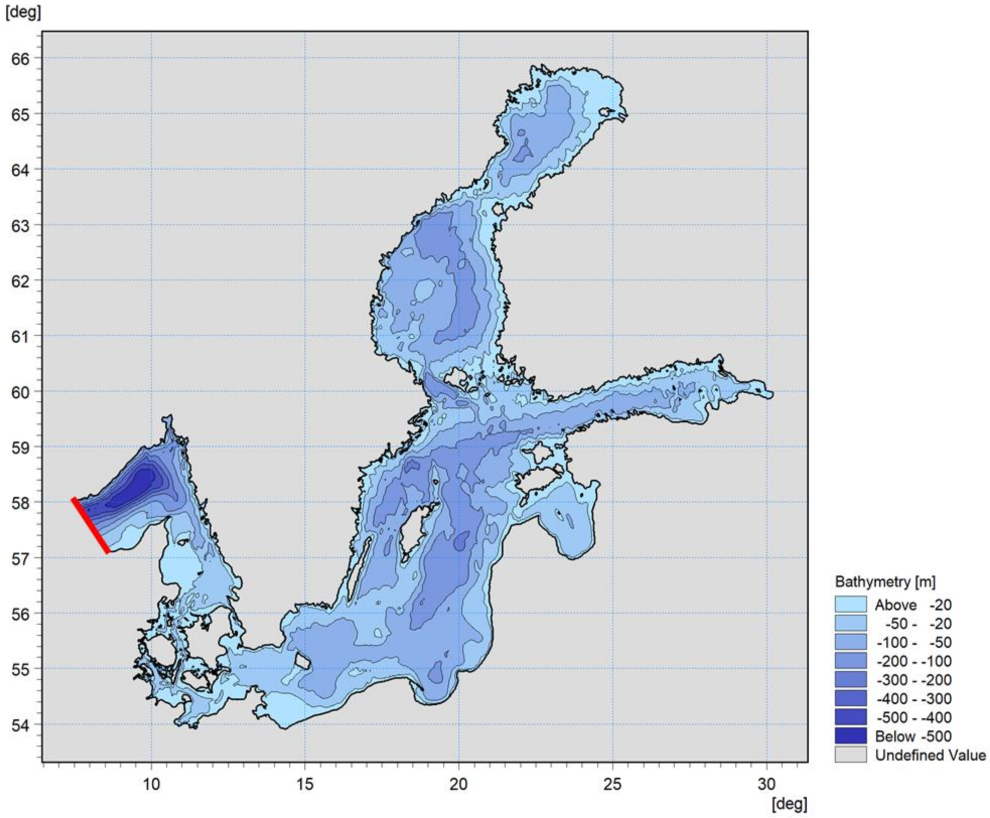

Figure 2-2 Model bathymetry of the Inner Danish Water (IDW) model (DKBS2-HD75). Water depths refer to MSL. The model includes one open boundary located in Skagerrak (red).

2.1.2 Local domain models

Like the IDW model, the three local domain models use modelled data as boundary data. The boundary data for the three local domain models are extracted from the IDW model (2D vertical time series). The specified boundaries shown in Figure 2-3 to Figure 2-5. Notice that boundaries for the different models are shared between models where they have overlapping boundaries.

As described in DHI 2019I the state variables in the IDW model and in the local domain models are not entirely the same. The IDW model has more groups of phytoplankton and two groups of zooplankton. Hence, the specific state variables in the IDW models are summed before applied in the local domain models ensuring mass conservation.

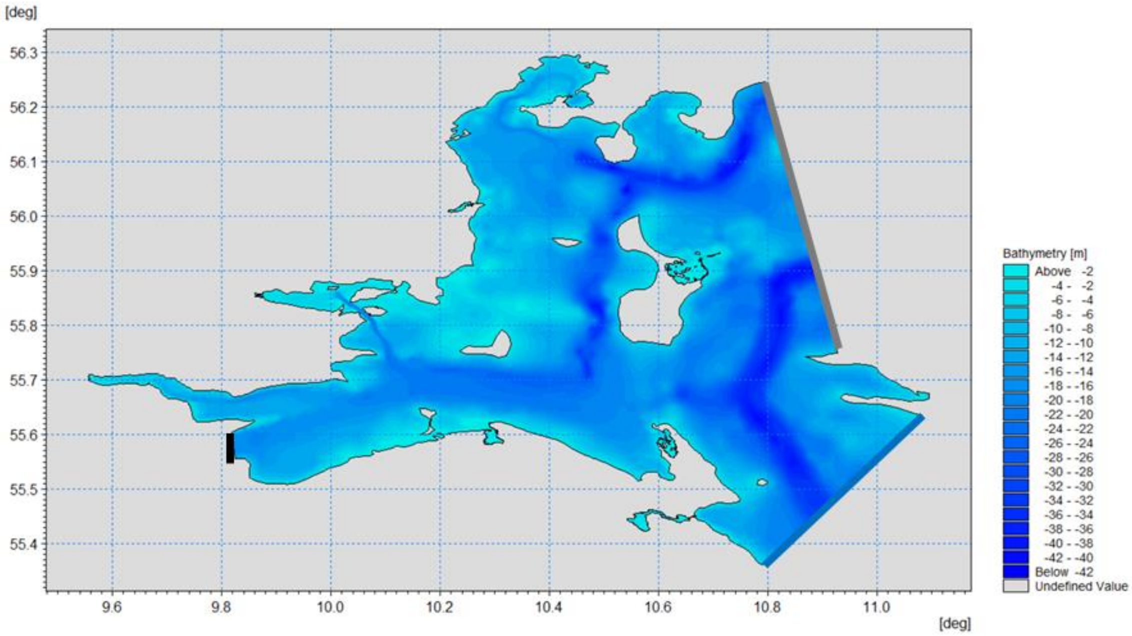

Figure 2-3 Model bathymetry of the Northern Belt Sea model (NBS). Water depths refer to MSL. The model includes three open boundaries marked with gery, black or blue colours. The boundary in Little Belt (black) is shared with the Southern Belt Sea model and the boundary in Great Belt (blue) is shared with the Smaalandsfarvand model.

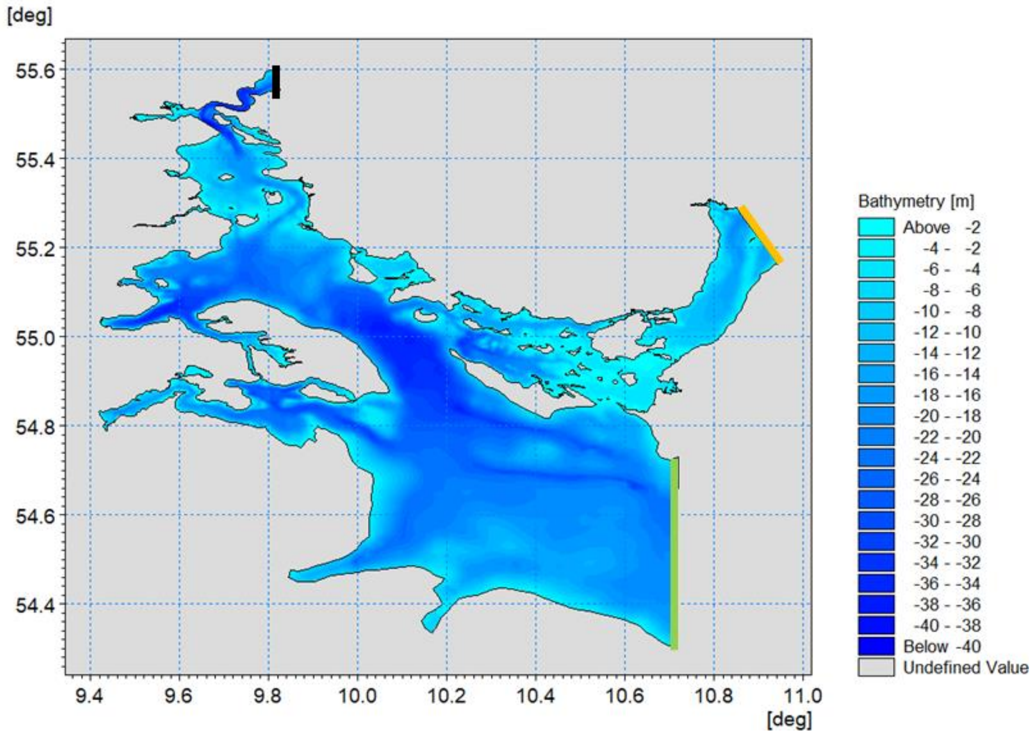

Figure 2-4 Model bathymetry of the Southern Belt Sea model (SBS). Water depths refer to MSL. The model includes three open boundaries marked with black, green and orange colours. The boundary in Little Belt (black) is shared with the Northern Belt Sea model and the boundary South of Langeland (green) and the boundary north of Langeland (orange) are both shared with the Smaalandsfarvand model.

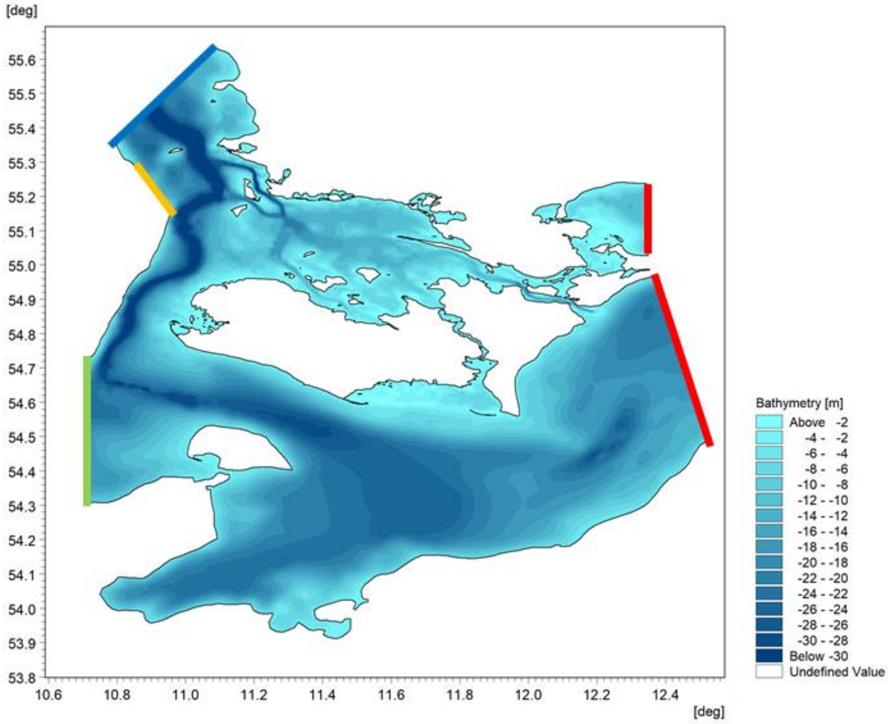

Figure 2-5 Model bathymetry of the Smaalandsfarvand model (SMF). Water depths refer to MSL. The model includes five open boundaries marked with red, blue, organe and green colours. The boundary in Great Belt (blue) is shared with the Northern Belt Sea model and the boundary south of Langeland (green) and north of Langeland (orange) are both shared with the Southern Belt Sea model.

2.1.3 Estuary specific models

As mentioned earlier six estuary specific models have been developed as part of the present project. These six models cover Ringkøbing Fjord, Nissum Fjord, the Limfjord, Mariager Fjord, Odense Fjord and Roskilde Fjord.

Boundary data applied for the estuary specific models origins from NOVANA stations. Hence, for each of the specific models the closest NOVANA station outside the individual estuary have been extracted from http://odaforalle.au.dk and observations are applied for the specific state variables in the model.

In the model period 2002-2016, some monitoring stations have been cancelled, why the boundary data does not necessarily origin from the same monitoring station throughout the entire model period. Monitoring stations applied as boundary data for the individual models are included in Figure 2-6:

- Ringkøbing Fjord: Boundary data are compiled from RKB43 throughout the 15 years of modelling.
- Nissum Fjord: Boundary data are compiled from RKB43 throughout the 15 years of modelling.
- Limfjorden, west: Boundary data are compiled from RKB59 during the years 2002-2010 and from RKB43 for the remaining model period.
- Limfjorden, east: Boundary data are compiled from NOR4410 throughout the 15 years of modelling.

- Mariager Fjord: Boundary data are compiled from NOR4410 throughout the 15 years of modelling.
- Odense Fjord: Boundary data are compiled from FYN6940622 throughout the 15 years of modelling.
- Roskilde Fjord: Boundary data are compiled from VSJ10003 throughout the 15 years of modelling.

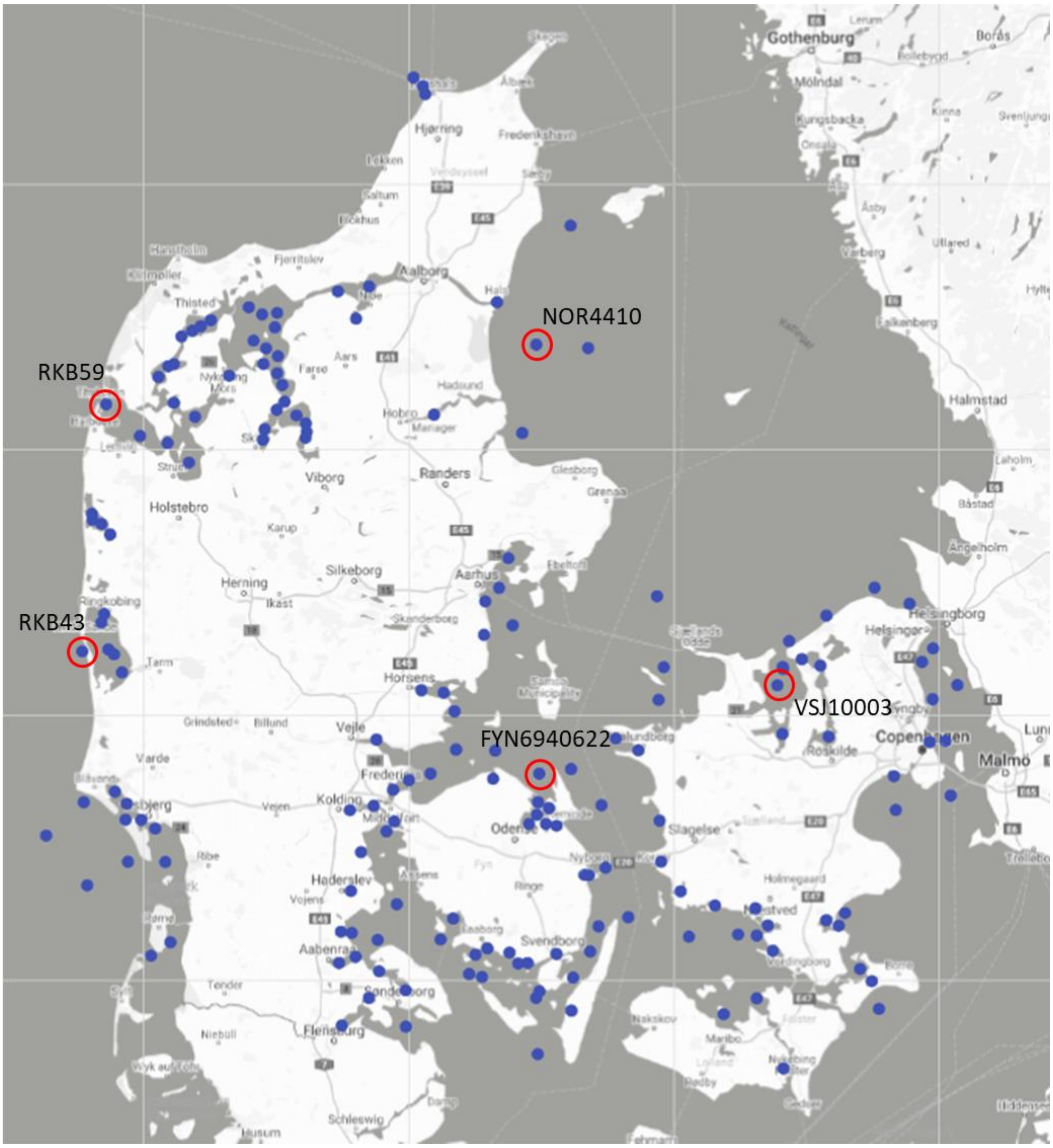

Figure 2-6 Danish NOVANA stations with time series of biogeochemical data during the years 2002-2016. Red circles indicate stations used as boundary data for the estuary specific models. Map and measurement stations are extracted from rbmp2021-2027.dhigroup.com (Google Chrome only).

2.1.4 Reference scenario

One important part of the entire model development is the application of a reference model scenario. The reference model scenario requires considerations of the different input parameters in the different models.

With respect to the boundary data this is handled differently between the different models:

- **The North Sea Model:** The boundaries in the North Atlantic Ocean are assumed to be unchanged even in the reference scenario. Hence, the effects from the reference scenario in the North Sea will be governed by changes in land-based loadings and atmospheric depositions alone (see section 2.2 and section 2.3).

  This is, however, not the case at the Kattegat boundary. During the reference scenario, the Kattegat boundary has been changed according to model results from Baltic Nest Institute (BNI). BNI has modelled the entire period from 1850 to 2006 (HELCOM 2013) and here we apply the modelled relative differences in TN and TP from BNI to the various state variables in the North Sea Model.

- **The IDW model:** As the boundary data included in the IDW model origins from model data extraction from the North Sea model, boundary data from the reference scenario is extracted from the corresponding North Sea model scenario and included in the IDW model.

- **Local domain models:** As the boundary data included in the local domain models origins from model data extraction from the IDW model, all boundary data from the reference IDW model scenario are extracted and included in the local domain models.

- **Estuary specific models:** All estuary specific models utilise measured data as boundaries. To ensure the effect from the reference scenario at the boundaries of those models, the relative differences between the modelled baseline (calibration/validation) and the modelled reference scenario by the IDW mode or North Sea model at the location of the specific stations is calculated. The relative difference is then applied for correction of the measured data and used as reference scenario boundaries in the estuary specific models.

2.2 Land based nutrient loadings

An essential input to the setup of the mechanistic models is the land-based supply of nutrients. Apart from Danish land-based nutrient loadings, the mechanistic models include nutrient input to the Baltic Sea and the North Sea from other countries as well as atmospheric deposition (see section 2.3).

2.2.1 Danish land-based nutrient loadings

Data on Danish land-based nutrient loadings were provided by Danish EPA via DCE/AU, Department of Bioscience. The data are part of the national inventory elaborated by AU every year (method described in Windolf et al. 2011 and data presented in Thodsen et al 2019), which is similar to the reporting to HELCOM[3]. However, an important difference between the national data and the data adopted by AU for the mechanistic modelling is the resolution in time. Whereas the national data are reported on an annual basis, the data used for the modelling were provided on a daily basis, both for water discharges and nutrient loadings.

The data covered the period from 1990 to 2016 and were distributed into 4th order marine waters, which are even more detailed than the 114 Danish marine water bodies. The mechanistic modelling applied data for the period 2002-2016, with distribution of the loadings into approximately 340 Danish freshwater and nutrient sources.

[3] Data applied was delivered by AU to DHI in January 2020

The loadings were estimated as discharges of total nitrogen (TN) and total phosphorus (TP). Since the mechanistic models differentiate between the different chemical forms (inorganic/organic, dissolved/particulate, nitrogen and phosphorous species), the data were subsequently divided into nutrient forms required by the modelling. Through an assessment of available observations on nutrients in water discharged from Danish catchments, monthly relations between inorganic and organic nutrients were developed and applied to divide TN and TP into an inorganic and an organic fraction. By combining TOC and COD/BOD observations, the organic part was further split to separate the organic nutrients into the three forms adopted in the modelling process.

2.2.2 Baltic Sea land-based nutrient loadings (HELCOM)

Data on loadings (other countries than Denmark) of TN and TP to the Baltic Sea are based on a combination of modelled data (https://hypeweb.smhi.se/explore-water/historical-data/europe-time-series/) and loadings extracted from HELCOM's Baltic Sea Pollution Load Compilation (PLC-6) (HELCOM 2018).

The HELCOM data corresponds to the official data around the Baltic Sea, but as is the case for the Danish land-based loadings the model development requires data with a higher spatial and temporal resolution than reported in HELCOM 2018 (or similar PLC's). Hence, we have combined modelled data from SMHI (https://hypeweb.smhi.se/explore-water/historical-data/europe-time-series/) with HELCOM data, using the daily variation in Q, TN and TP from the model but ensuring the summed data year-by-year (2002-2016) corresponds to the annual data in HELCOM 2018.

The spatial resolution in the data (https://hypeweb.smhi.se/explore-water/historical-data/europe-time-series/) is higher than the data used in the IDW model. The SMHI data have been aggregated to account for all catchments around the Baltic Sea but represented by 51 rivers/point sources in the Baltic Sea (besides Danish rivers/streams) and combined by HELCOM data on basin-scale. The distribution of the rivers in the Baltic Sea is shown in Figure 2-7.

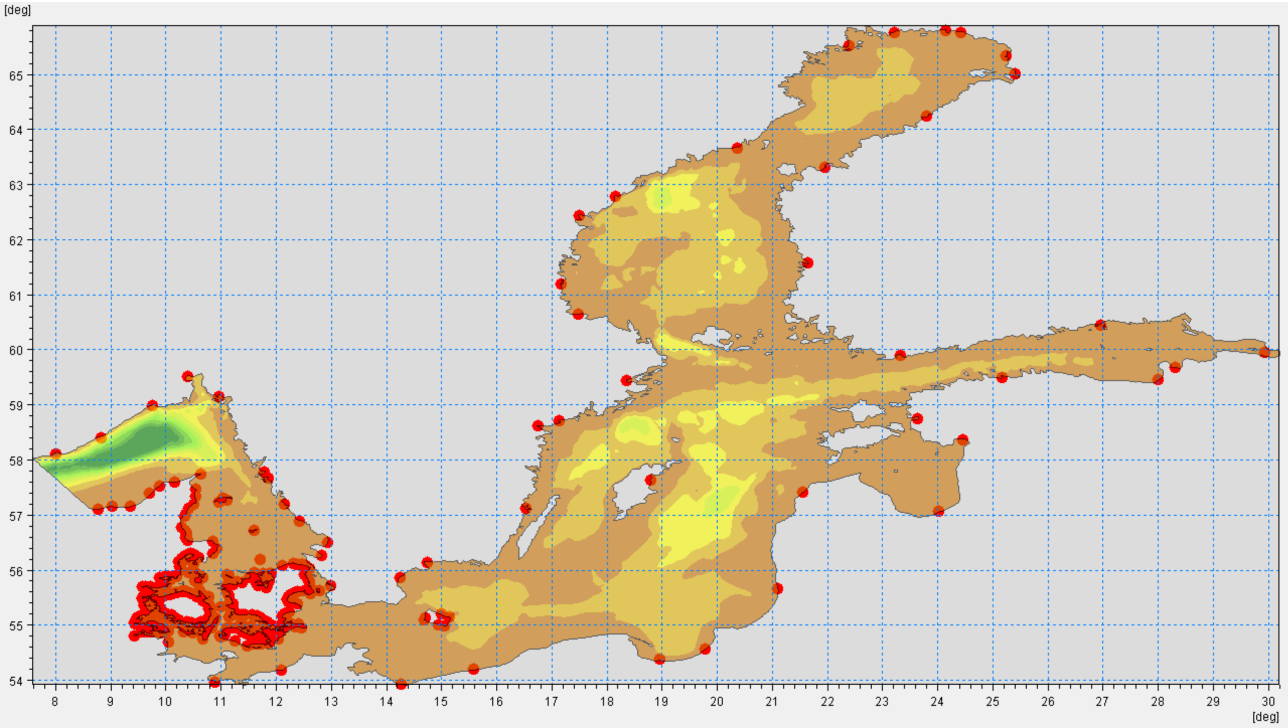

Figure 2-7 Illustration of the location of freshwater sources in the IDW model. The sources represent the main rivers in the Baltic Sea but are scaled to include all local run-off from land to sea. In Denmark, 4th order area run-off distributed to main rivers and streams are applied.

Differentiation of TN and TP loadings was done according to Stepanauskas et al. (2002) as also described in Erichsen & Timmermann 2017.

2.2.3 North Sea land-based nutrient loadings (OSPAR)

The loadings to the North Sea consist of two data sets. For the German and Dutch rivers measured data were applied (German data delivered by German authorities (https://www.nlwkn.niedersachsen.de/startseite/) and https://waterinfo.rws.nl). These data cover both discharge data (Q) as well as measured data of inorganic and organic nutrients. Hence, the governing loadings to the German Bight is based on measured data.

Data used for United Kingdom, Ireland and France are based on the SMHI model data (https://hypeweb.smhi.se/explore-water/historical-data/europe-time-series/).

No regional nutrient budgets are available from OSPAR why we have applied the modelled data directly for those countries but have used measured data for the governing rivers.

2.2.4 Reference scenario

With respect to the reference scenario the Water Framework Directive (WFD) prescribe that *"the values of the biological quality elements for the surface water body reflect those normally associated with that type under undisturbed conditions, and show no, or only very minor, evidence of distortion"* (EU 2000). Hence, during the reference scenarios we have applied background concentrations of TN and TP in all rivers.

The data behind those background concentrations are described in Bøgestrand et al. (2008) and Bøgestrand et al. (2014) and delivered to DHI from the EPA. TN concentrations are similar to the concentrations used in Erichsen & Timmermann 2017 whereas some updates have been made with respect to TP.

For the reference loadings to the Baltic Sea, we have applied a similar approach as described in Erichsen & Timmermann 2017. As desceibed above, the model development is based on HELCOM's Baltic Sea Pollution Load Compilation (HELCOM 2018), but this data set does not include reference loadings. Instead the Baltic Sea nutrient loadings from 1850-2006 reconstructed by Gustafsson et al. (2012) and Savchuk et al. (2012) and combined with the HELCOM loadings covering 2007-2016 (HELCOM 2018) were used relatively together with the HELCOM (2018) data. The relative difference within the different sub-basins defined in Gustafsson et al. (2012) and Savchuk et al. (2012) between the present day (average 2002-2016) and historical (average 1890-1910) data from the reconstruction were inflicted on the HELCOM (2018) data to provide a reference loading dataset applicable in the mechanistic model.

In the North Sea only few information was available for an assessment of reference loadings. In Gadegast & Venohr (2015) they report concentrations of TN and TP from a number of German and Dutch rivers around year 1880 and year 2005. Hence, we have used the relative difference between the two sets of concentrations and applied to all rivers in the North Sea.

2.3 Atmospheric deposition

In addition to the land-based loadings of N and P, the mechanistic models require input of atmospheric deposition of N, which is an important additional source of nitrogen to marine ecosystems. Data on atmospheric N deposition are provided by AU, Department of Environmental Science. The data form part of the national inventory elaborated annually by AU (Geels et al. 2012; Ellermann et al. 2012) and prepared using deposition modelling covering the period 2002-2016.

2.3.1 Baltic Sea (HELCOM)

In the HELCOM load compilations (PLC-6) (HELCOM 2018) atmospheric depositions is also estimated, and as for the land-based loadings, we scale the modelled data (Geels et al. 2012; Ellermann et al. 2012) to match the year-by-year depositions reported in HELCOM 2018.

2.3.2 North Sea (OSPAR)

OSPAR does not estimate the yearly depositions as does HELCOM, why we use the modelled data provided by AU unchanged for the North Sea model.

2.3.3 Reference scenario

Model data on atmospheric nitrogen deposition under reference conditions are provided by AU, Department of Environmental Science. The year reference simulation is conducted with an atmospheric model describing transport, chemical reactions and deposition of various chemical species including NO_X and NH_4 (Geels et al, 2012). The atmospheric model is forced with historical emissions provided by IIASA, "Representative Concentration Pathways" (RCPs; from http://tntcat.iiasa.ac.at:8787/RcpDb/dsd?Action=htmlpage&page=welcome) while the meteorological forcing corresponds to present days (2002-2016). Hence, the latter is coherent with the mechanistic modelling meteorological forcings. The resulting N deposition data is provided as monthly means (from a 10-year simulation) with a spatial resolution of 5 × 5 km^2 and used without any post processing in the marine mechanistic models. More detailed descriptions can be found in Geels et al. (2012) and Ellermann et al. (2013).

2.4 Initial values in the pelagic phase

2.4.1 Regional models

Initial values for all state variables applied in the North Sea model were estimated based on measurements within the North Sea. The estimated values were applied as constants all over the model domain and the model repeated for four subsequent years – hence, year 2002 was run four times before used for the calibration/validation.

Due to the retention time in the Baltic Sea (approximately 30 years) a similar approach was not applicable in the IDW model. Here estimated initial values were developed using measurements scattered around the Baltic Sea. This was, however, not done as a part of the present project but initial values were reused from previous model work (Erichsen & Timmermann 2017).

2.4.2 Local domain models

Initial values in the local domain models are based on extracted initial values from the IDW model.

2.4.3 Estuary specific models

Initial values applied in the estuary specific model are based on measurements and some subsequent years (1-2 years) of re-runs.

2.4.4 Reference scenario

During the reference scenario modelling initial values have not been changed except for the IDW model. As the retention time is large in the Baltic Sea, we have applied a reduction in C, N and P state variables corresponding to the relative changes observed in BNIs 1850-2006 model results (HELCOM 2013). The BNI model results from HELCOM (2013) are included in the estimated nutrient targets to the entire Baltic Sea.

The relative differences in the modelled results between 1900 and 2006 is applied basin by basin to the different state variables

2.5 Sediment data

Pools of organic and inorganic nutrients in the sediments play a vital role in many of the Danish water bodies. Hence, it is important to create 2D maps of a range of parameters (Organic C, N, P and Si and inorganic sediment and porosity).

The methodology differs between the regional models and the local and estuary specific models

2.5.1 Regional models

The initial pools on seabed substrate are based on data on mud content from EMODNET (http://www.emodnet-geology.eu/data-products/). The mud content was converted to organic carbon content according to Leipe et al. (2011). The content on nitrogen, phosphorus and silicate was estimated according to Redfield ratios.

2.5.2 Local and estuary specific models

Sediment maps are based on the seabed type. Seabed types can be divided in erosion-, transport and deposition area. The maps are calculated by current speed and shear stress, hence the physical energy that determines the morphology of the seabed. Next to seabed type a database of 125 sediment profiles measured around Denmark was compiled and used to make empirical relationships between sediment profiles and model state variables. Measured profiles were grouped by geographical area, type and depth. Based on this a map was calculated with empirically estimated sediment maps.

2.5.3 Reference scenario

In a reference scenario the sediments are assumed to be different compared to present day sediment maps. To account for changes in the sediments we have applied the relative differences between present day sediment maps and historic sediment maps estimated by BNI (HELCOM 2013). The BNI model includes pools of C, N and P in the sediment s and we have applied the relative difference basin by basin to the sediments in the IDW model.

The BNI model does not cover estuary specific model domains, but we have assumed similar sediment changes as reported in HELCOM 2013 in the basin covering the Danish Straights.

In the North Sea model, we have not implemented any sediment changes and allow the model to find a new equilibrium in the sediments.

2.6 Benthic vegetation

Benthic vegetation (Ephemeral and Perennial macroalgae, Eelgrass and Benthic diatoms) was calculated by running MIKE ECO Lab model for 3 years starting with constant initial values over the whole domain. After the 3 year run, biomasses for benthic variables have stabilized based on death and production. Areas with low light and unsuitable conditions lose biomass over time and die out while areas suitable conditions will gain biomass. These maps were used for model calibration.

2.6.1 Reference Scenario

In the reference scenario we apply updated eelgrass biomass maps. Here we assume a linear increasing biomass between 0.5m and 2m and a linear declining biomass between 2m and the reference depth limit.

2.7 Model forcings

Beside the hydrodynamic model some external forcings are needed.

2.7.1 Solar radiation

Solar radiation is calculated by global radiation and STORMGEO clearness percentage for period 2002-2004 and CSFR clearness from 2005-2016.

2.7.2 Waves/Share stress

As re-suspension is included as an important parameter when modelling the light regime in the biogeochemical model (DHI 2019l) we have included significant wave heights and wave period and mean wave direction in the model. The wave parameters are extracted from MIKE Spectral Wave (SW) model (DHI 2017) and together with the current from the hydrodynamic models used to estimate the actual shear stress at the seabed. For the estimation of shear stress, we apply the Soulsby & Clarke (2004) and Soulsby (2006).

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