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An operational, assimilative model system for hydrodynamic and biogeochemical applications for German coastal waters

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The Federal Maritime and Hydrographic Agency (BSH) is introducing a new operational model system for the North and Baltic Sea, focusing on German coastal waters. This model system newly includes a biogeochemical model and a data assimilation component. The data streams are managed carefully to be able to conduct several model runs per day and provide reliable forecast data for internal and external customers. During a pre-qualification phase, model results have been validated with focus on mostly used products. Here we show validation results for tides, temperature and oxygen. The model system is able to simulate the physical and biogeochemical features of the North and Baltic Sea. Nevertheless, BSH is constantly developing the model system to further improve the results and add new components to the system.

operational forecasting | biogeochemical modelling | hydrodynamic modelling | data assimilation | North and Baltic Sea
operationelle Vorhersage | biogeochemische Modellierung | hydrodynamische Modellierung | Datenassimilation | Nord- und Ostsee

Das Bundesamt für Seeschifffahrt und Hydrographie (BSH) führt ein neues operationelles Modellsystem für die Nord- und Ostsee ein, dessen Schwerpunkt auf den deutschen Küstengewässern liegt. Dieses Modellsystem schließt neuerdings ein biogeochemisches Modell und eine Datenassimilationskomponente ein. Die Datenströme werden sorgfältig verwaltet, um mehrere Modellläufe pro Tag durchführen zu können und zuverlässige Vorhersagedaten für interne und externe Kundinnen und Kunden zu liefern. In einer Vorqualifizierungsphase wurden die Modellergebnisse validiert, wobei der Schwerpunkt auf den am häufigsten verwendeten Produkten lag. Wir zeigen Validierungsergebnisse für Gezeiten, Temperatur und Sauerstoff. Das Modellsystem ist in der Lage, die physikalischen und biogeochemischen Eigenschaften der Nord- und Ostsee zu simulieren. Nichtsdestotrotz entwickelt das BSH das Modellsystem ständig weiter, um die Ergebnisse weiter zu verbessern und das System um neue Komponenten zu ergänzen.

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1 Introduction

Germany is connected to the North Sea and the Baltic Sea. Specific physical and biogeochemical processes characterise both regional seas. While the North Sea has a higher salinity and is strongly influenced by tides, which are affecting the German coastline, the Baltic Sea has a lower salinity and can be partly covered by ice in winter, affecting e.g. shipping. German coastal waters and the corresponding coastal zones are subject to many different interests and users. This area is highly impacted by ship traffic, fisheries, offshore wind farming, tourism and other public and economic uses. Therefore, it is of high importance to provide reliable information about the physical and biogeochemical status of the coastal waters. The Federal Maritime and Hydrographic Agency (BSH) is providing short-term forecasts for the most relevant physical parameters since the early 1990s. The forecasts include information about water temperature and salinity, currents, water level and sea ice. For this purpose, BSH is operating a three-dimensional baroclinic circulation model (Dick, Kleine and Müller-Navarra 2001; Dick, Kleine and Janssen 2008; Brüning et al. 2014), downstream drift and dispersion models (Maßmann et al. 2014; Schmolke et al. 2020) and a two-dimensional, barotropic and therefore very efficient variant of the circulation model (the storm surge model) for wind surge forecasting.

With the increasing importance of the Marine Strategy Framework Directive, the impact of eutrophication and the development of oxygen deficiency zones in German coastal areas and in the

North and Baltic Sea in general (e.g. Topcu and Brockmann 2015; Meier et al. 2018), the need for information about the biogeochemical status has become more pronounced during the last years. To be able to provide short-term forecasts about important parameters of the biogeochemical environment as oxygen, chlorophyll and pCO_2 concentration, a biogeochemical model was added to the operational model system at BSH by coupling it to the hydrodynamic circulation model.

The physical and biogeochemical status of the oceans and in particular also the German coastal waters is regularly monitored by collecting in-situ data and via earth observation. These data are gathered and quality controlled by organisations and services such as the Copernicus marine service (CMEMS, marine.copernicus.eu) or EmodNet (emodnet.eu) and are hence a valuable resource to validate and calibrate the model system. Additionally, assimilation of observation data can be used to further improve the quality of model results (Kelley et al. 2002; Losa et al. 2014; Martin et al. 2015; Nerger et al. 2016; Goodliff et al. 2019). We will present the first results of the new operational model framework at BSH including a biogeochemical model and data assimilation.

2 The model system

2.1 Data streams, forcing and setup

Four times a day, BSH is delivering an ocean forecast of physical and biogeochemical parameters to both internal and external customers. The forecast runs start automatically at 0, 6, 12 and 18 UTC, corresponding to the analysis times of the atmospheric forecasts, which are provided by the German Weather Service (DWD) immediately after completion. The ocean forecasting system requires the latest values of the parameters 10 m-wind, air pressure, air humidity, cloud cover and 2 m-air temperature from the atmospheric model ICON (Zängl et al. 2015; Reinert, Frank and Prill 2020) as meteorological input.

Another required input are the newest surge values at the open model boundary in the northern North Sea and in the English Channel. These are generated internally by the BSH North East Atlantic model (Brüning et al. 2014). In addition, tides based on 19 partial constituents derived from different measurements (e.g. Alcock and Vassie 1977; Cartwright, Zetler and Hamon 1979; Cartwright and Zetler 1985), monthly temperature and salinity-data from Janssen, Schrum and Backhaus (1999) and climatological biogeochemical data from the biogeochemical model ECOHAM (Lorkowski et al. 2012) are used at the open model boundary.

Furthermore, discharge data for the German rivers Rhine, Elbe, Weser, Ems and Oder are obtained hourly via Pegelonline (pegelonline.wsv.de). The discharge of the other rivers in the model area and the concentrations of nitrogen and phosphate are taken from the Swedish Meteorological and Hydrological Institute's E-Hype model (Donnelly, Andersson and Arheimer 2016; Hundecha et al. 2016), delivered to BSH once per day. For the concentrations of all other biogeochemical parameters, climatological values from various sources (Pätsch and Lenhart 2008; Baltic Environment Database – BED, nest.su.se/bed), but also reasonable constant values due to missing sources are used. If no daily updated data is available, the model runs with data from the day before. Only if the supply of current data is unavailable for a longer period of time, long-term mean values of discharge and climatological values of all biogeochemical concentrations are used.

To account for atmospheric deposition of organic and inorganic nitrogen and organic phosphorus the latest available EMEP data on atmospheric deposition (emep.int) is downloaded once a year, interpolated on the model grid and recalculated to daily values. The atmospheric pCO_2 concentration is calculated based on atmospheric pCO_2 measured at Mauna Loa from the year 2017 (esrl.noaa.gov), whereby the pCO_2 content according to esrl.noaa.gov is increased by 2 µatm every year.

Finally, two different sea surface temperature (SST) data sets are used in the current assimilation system: The first choice is the Advanced Very High Resolution Radiometer (AVHRR) SST (Kilpatrick, Podestá and Evans 2001), for which a manual quality control is carried out by the BSH satellite data service. If these data are not available or available too late for the operational procedure, the Copernicus Sentinel-3 SST (Donlon et al. 2012) is used. Usually, both of the satellite images are collected, processed and gridded by the BSH satellite data service twice a day, so that the SST image is assimilated every 12 hours. If none of the data sets is available in time, the forecast continues without the assimilation step.

When all input data is available, the BSH model system starts to calculate on two two-way nested grids. While the coarser grid covers the entire North Sea and Baltic Sea from ca. 4° W to ca. 30° E and ca. 49.5° N to ca. 61° N (North Sea), respectively ca. 53° N to ca. 65.5° N (Baltic Sea) with a horizontal resolution of 3 nautical miles, the finer grid covers the German coastal waters from ca. 6° E to ca. 15° E and ca. 53° N to ca. 56.5° N with a horizontal resolution of half a nautical mile (see Fig. 1). In the vertical there are up to 36 layers in the coarser grid and up to 25 layers in the finer grid, whereas the vertical resolution of both grids is identical and the higher number of layers in the coarser grid is only due to the fact that greater water depths exists in the covered area. The upper 20 m are divided in ten layers of 2 m thickness, followed by five layers of 3 m thickness until a water depth of 35 m and fourteen layers of 5 m thickness until a water depth of

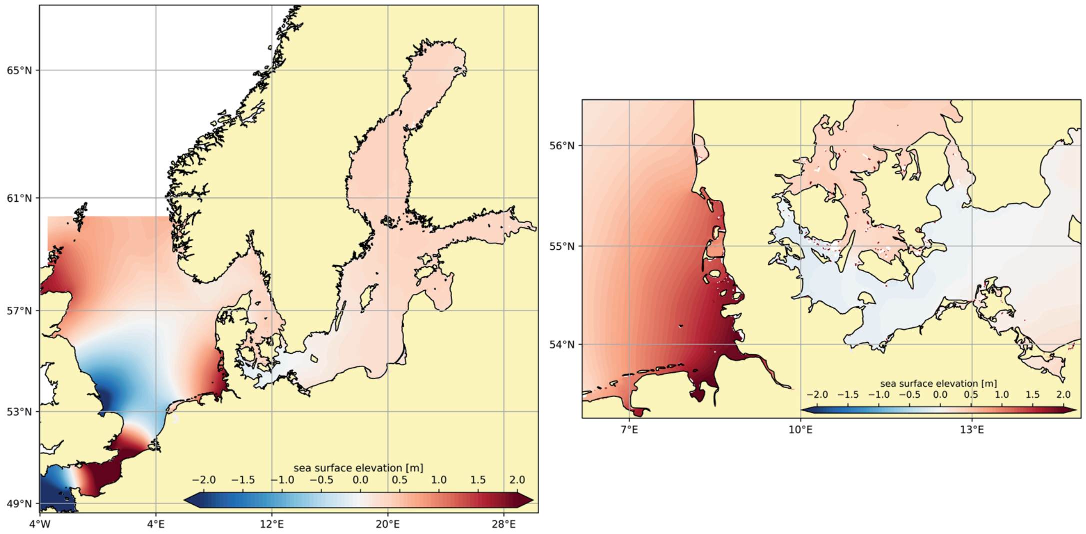

Fig. 1: Modelled sea surface elevation on the coarser grid (left) and on the finer grid (right) on 30 June 2019 at 22:00 UTC. The tidal waves in the North Sea are clearly visible

100 m. In water depths below 100 m, the resolution is relatively coarse with layer thicknesses up to 200 m. Further details of the setup can be found in Brüning et al. (2014) or on the BSH website (bsh.de/DE/THEMEN/Modelle/modelle_node.html).

One hydrodynamic model run coupled to the biogeochemical component without data assimilation produces a 120-hour forecast from 0 and 12 UTC and a 78-hour forecast from 6 and 18 UTC. A second hydrodynamic model run with data assimilation (without the biogeochemical component) calculates a 24-hour hindcast and a 6-hour forecast at 0 and 12 UTC.

When the model runs are finished, numerous products for internal and external uses are generated in the form of data and graphics, and the »best estimate« forecast is stored in the archive. Archived data is freely available on request by mail (opmod@bsh.de). BSH provides data from the free run without data assimilation since 2016 and results from the simulation with data assimilation as ensemble mean and standard deviation since 2021. The temporal resolution of the archived data is listed in Table 1. An overview of the complex data streams is displayed in Fig. 2. Hydrodynamic data from older model versions are available since 2000.

2.2 Hydrodynamic model component

The hydrodynamic core of the BSH model system is the HIROMB-BOOS-Model (HBM) (Berg and Poulsen 2012) developed by the BSH together with European partners from the Baltic Sea region with the configuration as described in Brüning et al. (2014). HBM is a computationally very efficient ocean circulation model (Poulsen and Berg 2012a), which was developed with a high emphasis on portability between different computer systems. This is demonstrated by a clean code following ANSI standards (Adams et al. 1997), which also allows massive parallelisation (Poulsen and Berg 2012b; Poulsen, Berg and Raman 2014). Through a series of technical tests, such as the ε-tests (Brüning 2020), the technical status is checked and ensured anew before each code release. With regard to the physical equations, it should be noted in particular that the k-ω turbulence model (Berg 2012) has been extended in recent years by stability and realisability checks. These checks are necessary to ensure that the calculated current data are suitable for the use of operational downstream drift models for oil spill or search-and-rescue applications, especially in extreme situations (Brüning 2020).

	Water level	**Currents**	**Temperature**	**Salinity**	**Sea ice concentration and thickness**	**Oxygen**	**pH**	**Chlorophyll**
Unit	m	m/s	°C	PSU (‰)	1 (conc.) and m (thickn.)	mmol/m^3	1	mg/m^3
Temporal resolution	15 minutes	15 minutes	hourly	hourly	six-hourly	daily (noon)	daily (noon)	daily (noon)
Prognostic/diagnostic	diagnostic	prognostic	prognostic	prognostic	prognostic	prognostic	diagnostic	diagnostic
Ensemble mean and standard deviation	yes	yes	yes	yes	yes	no	no	no

Table 1: Temporal resolution of the data in the BSH model archive. In addition to the deterministic data, the mean and the standard deviation from data assimilation ensemble are also stored in the model archive for some parameters

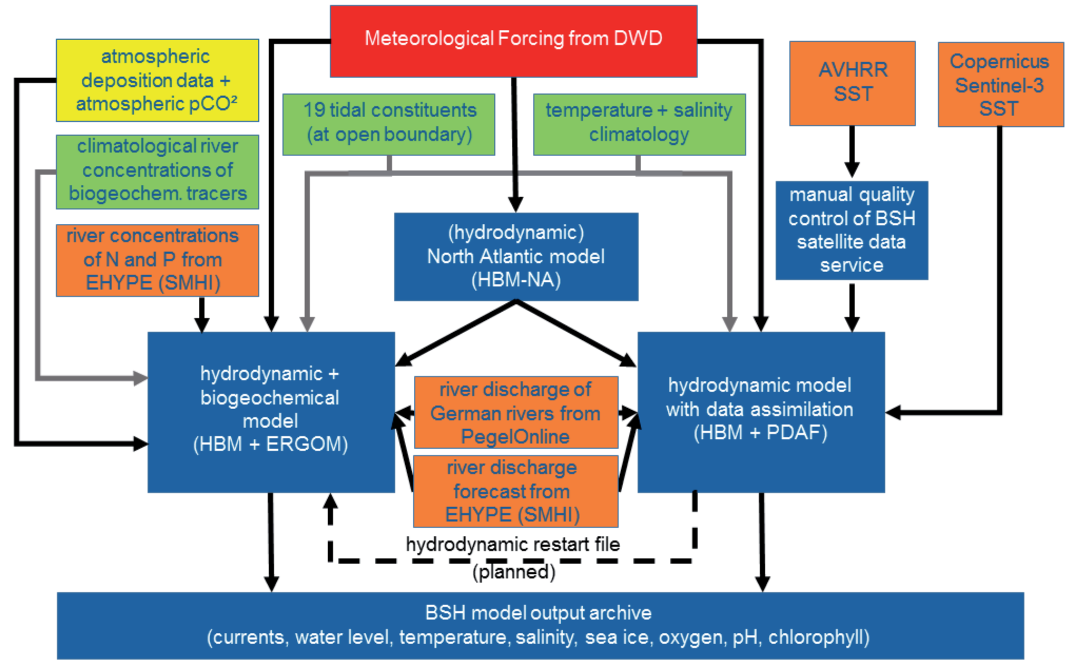

Fig. 2: Data streams for BSH's operational model. Red box: required before each model run (no fall-back position). Orange boxes: required daily, with fall-back positions – both data groups are retrieved automatically. Yellow box: updated manually once a year. Green boxes: climatological data. Blue boxes: model runs/work steps at BSH

2.3 Biogeochemical model component

For the biogeochemical model component, ERGOM (Ecological ReGional Ocean Model) is applied. ERGOM was originally developed for the Baltic Sea (Neumann 2000). It has been adapted to meet the needs for North Sea and Baltic Sea as presented in Maar et al. (2011). The model consists of 15 prognostic state variables for nutrients, plankton, detritus, oxygen, labile dissolved organic nitrogen in the water column (lDON, Neumann, Siegel and Gerth 2015), dissolved inorganic carbon (DIC) and total alkalinity (TA) (DIC and TA according to Schwichtenberg et al. (2020)). Chlorophyll and Secchi depth are calculated diagnostically (Doron et al. 2013; Neumann, Siegel and Gerth 2015), as well as pH and pCO_2 (Zeebe and Wolf-Gladrow 2001). The sediment is not vertically resolved and consists of two nutrient state variables. Fig. 3 provides an overview of the state variables and their interaction. The HBM-ERGOM model system has been applied in different versions in a few previous studies in the North and

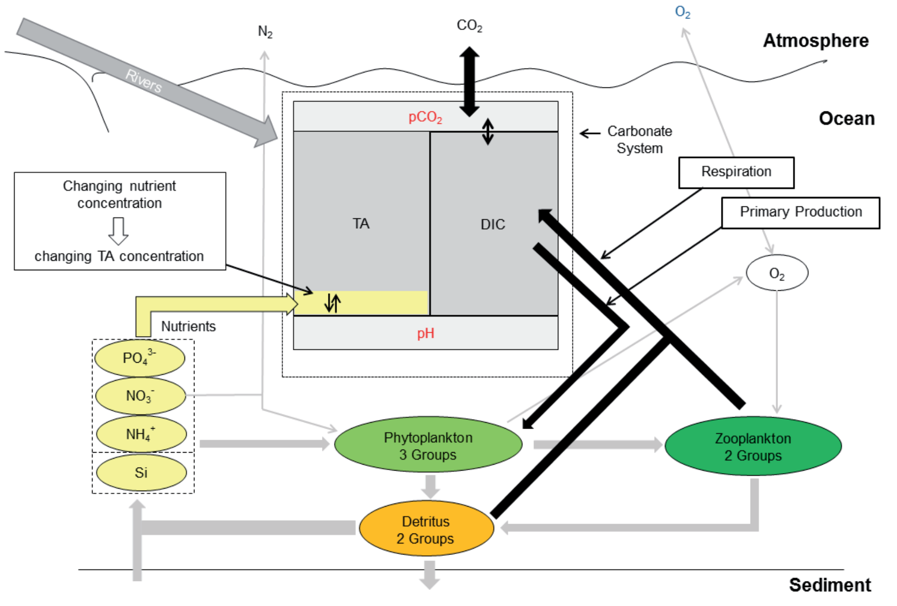

Fig. 3: Overview of state variables and their interaction in ERGOM

Baltic Sea (Maar et al. 2011; Wan et al. 2012) and has been used in several projects at BSH (e.g. Goodliff et al. 2019; Lorkowski and Janssen 2014) as well as in the Copernicus Marine Service (Tuomi et al. 2018) before.

2.4 PDAF

With the aim of improving the forecast skill for the North and Baltic Sea, a data assimilation system has been developed at BSH within the framework of a series of national projects (Losa et al. 2012; Losa et al. 2014; Nerger et al. 2016; Goodliff et al. 2019). For the data assimilation component, we apply the parallel data assimilation framework PDAF (Nerger, Hiller and Schröter 2005; Nerger and Hiller 2013; pdaf.awi.de), which is an open-source framework and simplifies the implementation of ensemble-based Kalman filtering data assimilation method into a numerical model. The Local Error Subspace Kalman Transform Filter (LESKTF) algorithm in PDAF is used in our coupled system. The ESTKF is an efficient formulation of the Ensemble Kalman Filter (Nerger et al. 2012) that has been applied in different studies to assimilate satellite data into different model systems (Tuomi et al. 2018; Androsov et al. 2019; Yang, Liu and Xu 2020; Li et al. 2021).

At BSH, PDAF is implemented with HBM in an online mode, which calls the PDAF library directly in the source code of HBM. With using the online-coupled assimilation system, the time for reading input and writing output is reduced and more efficient for operational forecasting. Currently, the HBM-PDAF system is the only data assimilation system using online mode in the region of the Baltic Sea. We use an ensemble of twelve model states. The state vector includes the sea surface elevation, three-dimensional temperature, salinity and velocities. The initial physical ocean state (i.e. initial ensemble mean) is provided by the operational HBM-run without data assimilation. The ensemble perturbations are generated by mean of the so-called second-order exact sampling method (Pham 2001) with using the model snapshots on both nested model grids of HBM (see chapter 2.1).

3 Validation

3.1 Tides

BSH will provide area-wide tidal predictions for the German EEZ in the North Sea. Due to a lack of observational data in the open North Sea, BSH uses model data as input for these predictions. Modelled water level data of the years 2016 to 2018 were analysed with the harmonic method (e.g. Godín 1972). The analysis followed a two-step procedure with a removal of extreme water level data and non-significant partial tides after the first iteration. A tidal prediction for the year 2019 was calculated and the vertices were identified. The heights and times of high water (HW) and low water (LW) were compared with observational data at six gauges and, for better classification, with the corresponding predictions that were published in the BSH tide tables (BSH 2018). Table 2 shows a summary of the results.

The predictions generated from model data show very good quality. With regard to the peak heights, the results are similar to those of the tide tables. However, the entry times of the peaks still leave room for improvement. While the mean errors are in the same order of magnitude as those of the tide tables, the standard deviation of the model-based forecast is significantly greater. In particular, the standard deviation of the entry time at gauge Fino3 is outstanding, which could be related to the relatively close position of the gauge to an amphidromic point.

3.2 Bottom oxygen saturation

Modelled bottom oxygen saturation is compared against measurement data at three MARNET stations in the North and Baltic Sea (www.bsh.de/DE/THEMEN/Beobachtungssysteme/Messnetz-MARNET/messnetz-marnet_node.html). The position of the stations and a snapshot of the bottom

Tide gauge	**Tide tables**				**HBM model**			
	HW/LW heights		**HW/LW times**		**HW/LW heights**		**HW/LW times**	
	ME [m]	**Std [m]**	**ME [min]**	**Std [min]**	**ME [m]**	**Std [m]**	**ME [min]**	**Std [min]**
Borkum	0.04	0.25	−1.7	11.2	0.06	0.27	2.3	21.3
Cuxhaven	0.05	0.28	−0.7	8.7	0.13	0.33	15.3	14.7
Wittduen	0.03	0.30	−5.5	8.7	0.04	0.31	−3.9	16.3
Helgoland	0.03	0.25	−1.9	6.9	0.05	0.27	3.5	15.2
Fino1					0.03	0.22	−7.7	19.7
Fino3					0.11	0.25	1.2	48.6

Table 2: Mean error (ME) and standard deviation (Std) calculated from the predictions published in the BSH tide tables and predictions based on the HBM model data for the year 2019. For the stations Fino1 and Fino3, no predictions were published in the tide tables

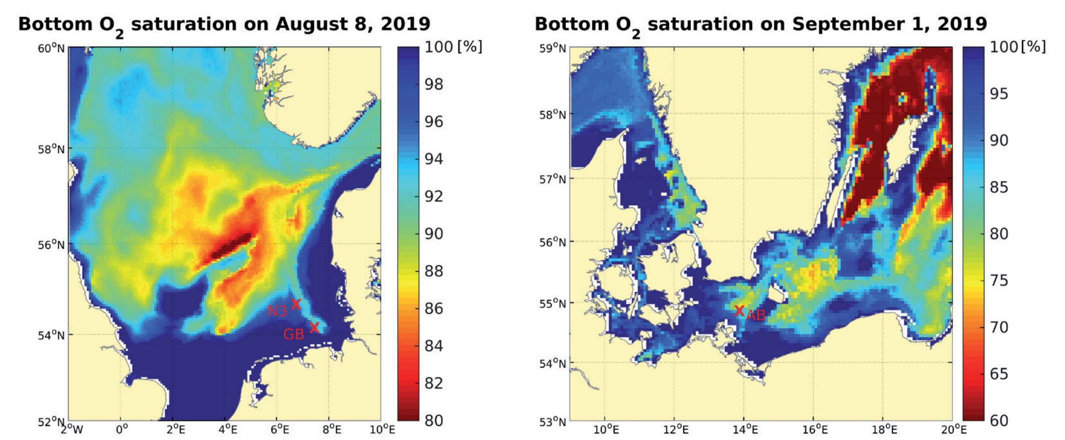

Fig. 4: Bottom oxygen saturation from HBM-ERGOM simulation. Snapshots for North Sea (left) and Danish Straits and Western Baltic Sea (right). Red crosses indicate the position of monitoring stations. (N3: Nordseeboje 3, GB: German Bight, AB: Arkona Basin)

oxygen situation in German coastal waters are displayed in Fig. 4. A seasonal oxygen minimum zone developed in the North Sea, while in the Baltic Sea snapshot, the permanent oxygen deficiency in the Gotland and Arkona Basin and some regional seasonal minima near the coast and around Arkona station occur.

At station Arkona (Fig. 5), modelled bottom oxygen is principally higher than observations but the development of the curves during the year are comparable. Fig. 4 shows that modelled oxygen saturation close to the station is lower, indicating a slight spatial displacement resulting from e.g. model bathymetry.

At the two North Sea stations (Fig. 6), bottom oxygen saturation is also higher than observations but the variability at both stations during the year are well represented by the model.

In Fig. 7 modelled bottom oxygen saturation is compared to measured values from the BSH summer cruise conducted from 27.08. to 14.09.2019. The cruise data show an area of low oxygen, which can be seen in the modelled data as well. But, as also visible in the time series plots, modelled oxygen saturation is always higher than observed, still the location of the lowest values match quite well.

3.3 Temperature: effect of data assimilation

SST forecasting skills of both HBM free run and HBM-PDAF runs are validated with the satellite observations, which are used in the assimilation processes. Fig. 8 shows the averaged validation results over the period from July 2019 to June 2020 in the North Sea and the Baltic Sea. The top row displays the centred root-mean-square deviation (cRMSD) of SST forecast when no data assimilation is applied (left) and when the data assimilation with SST satellite is operated (right). The comparison of SST forecasts to satellite observations shows that the HBM free run has difficulties in reproducing SST in the Baltic Sea. In many regions of the Baltic Sea, the cRMSD is larger than 2.5 °C (Fig. 8). Through data assimilation, the SST forecast has significantly improved everywhere in the whole model domain. In the centre of the Baltic Sea and in the Gulf of Bothnia, the cRMSD is more obviously reduced. The bottom

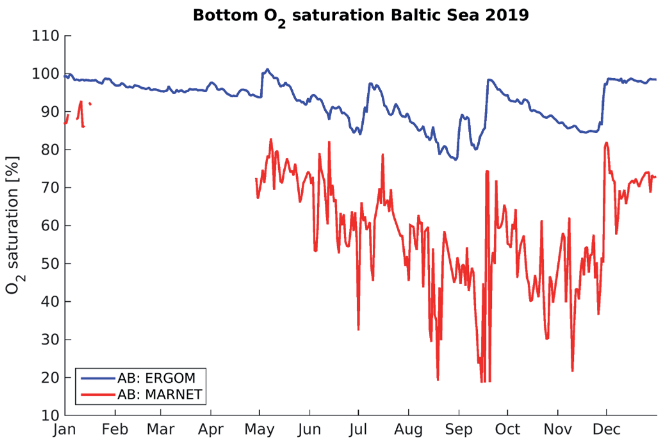

Fig. 5: Bottom oxygen saturation at station Arkona

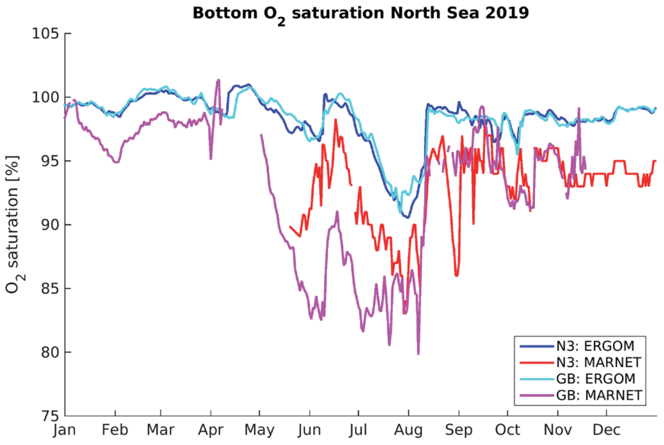

Fig. 6: Bottom oxygen saturation at stations Nordseeboje3 and German Bight

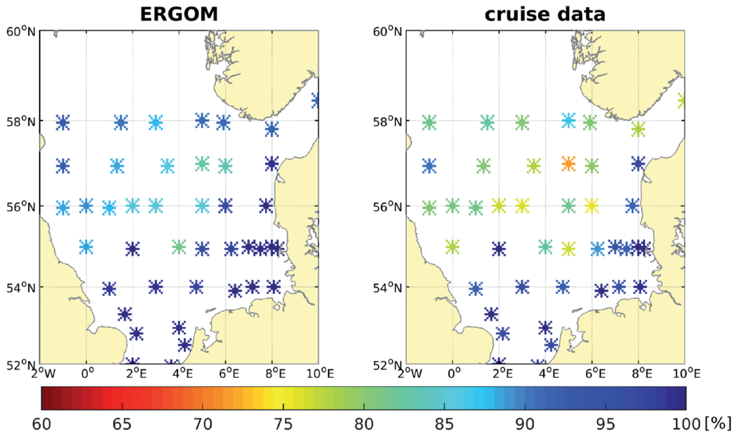

Fig. 7: Comparison of bottom oxygen saturation in the German Bight. ERGOM data on the left are matched up in space and time with data measured during the BSH summer cruise (27.08. to 14.09.2019 with Celtic Explorer)

row of Fig. 8 shows the bias of forecast compared to the satellite observations. The improvement of forecast through ensemble data assimilation is noticed again in both the North Sea and the Baltic Sea. Especially, along the Norwegian trench, along the east coast of England and in the English Channel, the SST bias is strongly reduced by more than 1 °C. Through the assimilation of SST satellite data, the yearly averaged bias is close to zero in the whole model domain. Apparently, with SST observational data assimilation, both model error and bias of SST forecast have been improved.

To detect the temporal difference between the HBM free run and HBM-PDAF run, SST is further validated with independent in-situ observations at the MARNET stations (positions are shown in Fig. 4). The differences of SST between HBM free run and HBM-PDAF run are approximately up to 1.6 °C at the station Nordseeboje3 and up to 2.1 °C at the station Arkona during the compared period (Fig. 9). These differences change differently with time. Large differences are displayed when temperature rises or drops. For example, after the SST reaches its annual maximum in 2019, the

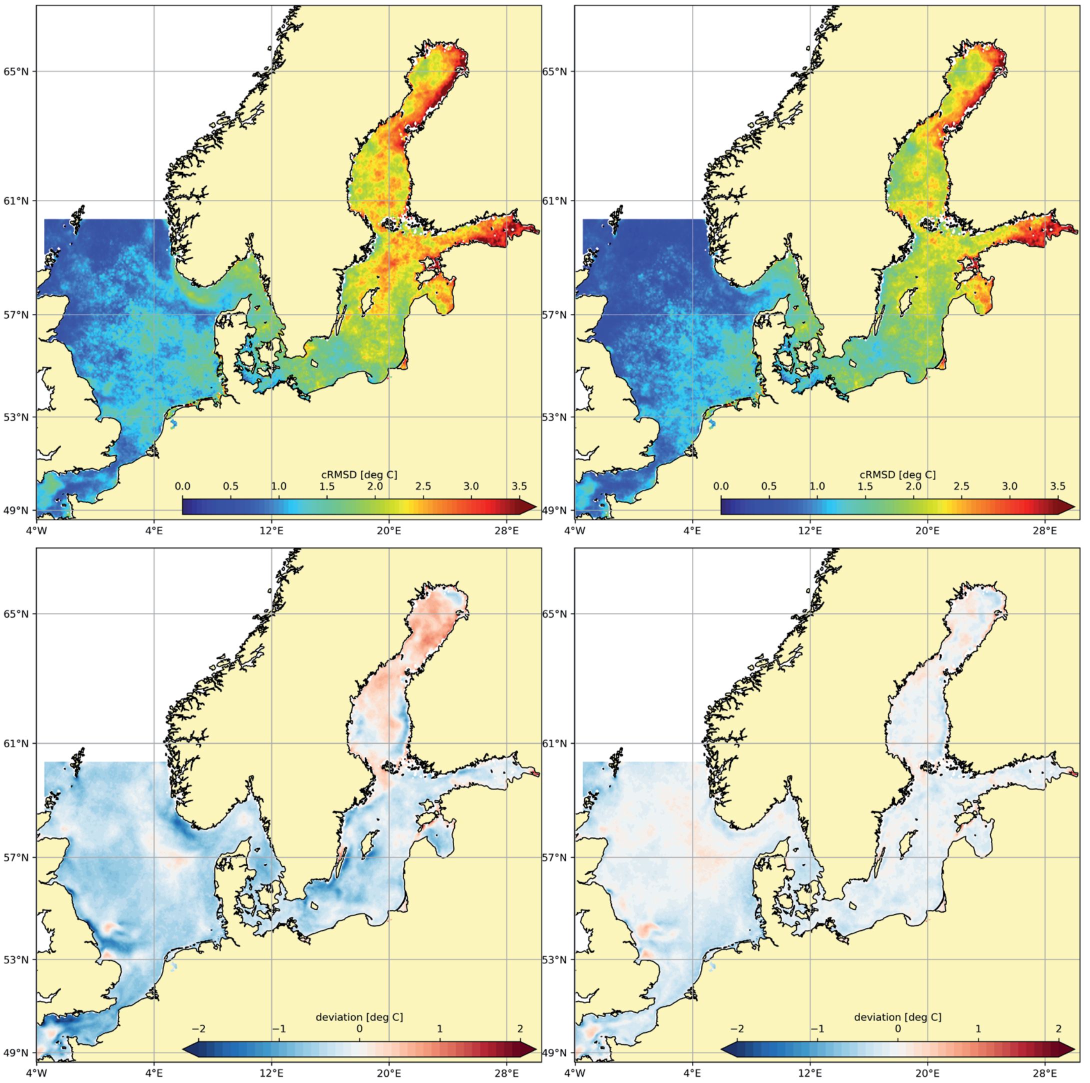

Fig. 8: Spatial distribution of the cRMSD (top) and bias (bottom) from the HBM free run (left) and the HBM-PDAF run (right) in the model domain from July 2019 to June 2020

temperature from HBM free run drops strongly at both stations. The SST from HBM-PDAF run is more close to the observations and decreases slowly. It shows again that the assimilation does a good job of eliminating biases in temperature. During the winter and spring, on the other hand, the temperatures from HBM free run and HBM-PDAF run at these two stations are generally quite close to each other (Fig. 9). One of the reasons might be due to the lack of satellite observations.

4 Discussion and next steps

With the presented operational system, BSH is able to provide reliable daily forecast data to external and internal users. The model system uses state-of-the-art techniques to simulate the main physical and biogeochemical features of German coastal waters. The addition of a biogeochemical model to the modelling framework widens the range of data products for different purposes. The inclusion of data assimilation improves the quality of simulated SST. Currently the free run and the run with data assimilation are running in parallel but in the very near future, the hydrodynamic restart file of the forecast with data assimilation should be used for the next forecast run of the model with biogeochemical component with the aim of further improving the forecast skill of the model system.

Nevertheless, there are also weaknesses of the current system, which we aim to improve in the future. As shown, the tides are represented well in terms of water level, but the timing of the peaks should become more accurate. For modelled oxygen saturation, on the other hand, the variability and localisation of low values match quite well, making the model a useful tool to support e.g. measurement campaigns or to filling gaps for monitoring for MSFD and other management plans. However, in all cases shown, the saturation is higher than observed values. Furthermore, the stratification in the model is sometimes too weak (not shown). This affects biogeochemical and physical fields alike.

In order to improve the forecast capability of the model in general, we will massively expand the assimilation of observational data. For example, as requested by customers, the data assimilation of sea ice parameters will be implemented in 2021. Furthermore, the addition of temperature and salinity profiles into the assimilation system should improve stratification, especially in the Baltic Sea, which should also lead to an improvement of biogeochemical model results in deeper model layers (e.g. bottom oxygen). A future step would then be the direct assimilation of biogeochemical data to further improve this model component. Additionally, a new setup with a higher horizontal and vertical grid resolution based on an actual, high-resolution bathymetry data set is being planned. In this setup, the model area will also include large parts of the North-East Atlantic. By moving the open model boundary from the shelf to deep-water areas of the North Atlantic, high-quality data from global tide models can be used as forcing at the open boundaries. This will hopefully lead to significant improvements in the representation of tides in the North Sea and especially in the German Bight. //

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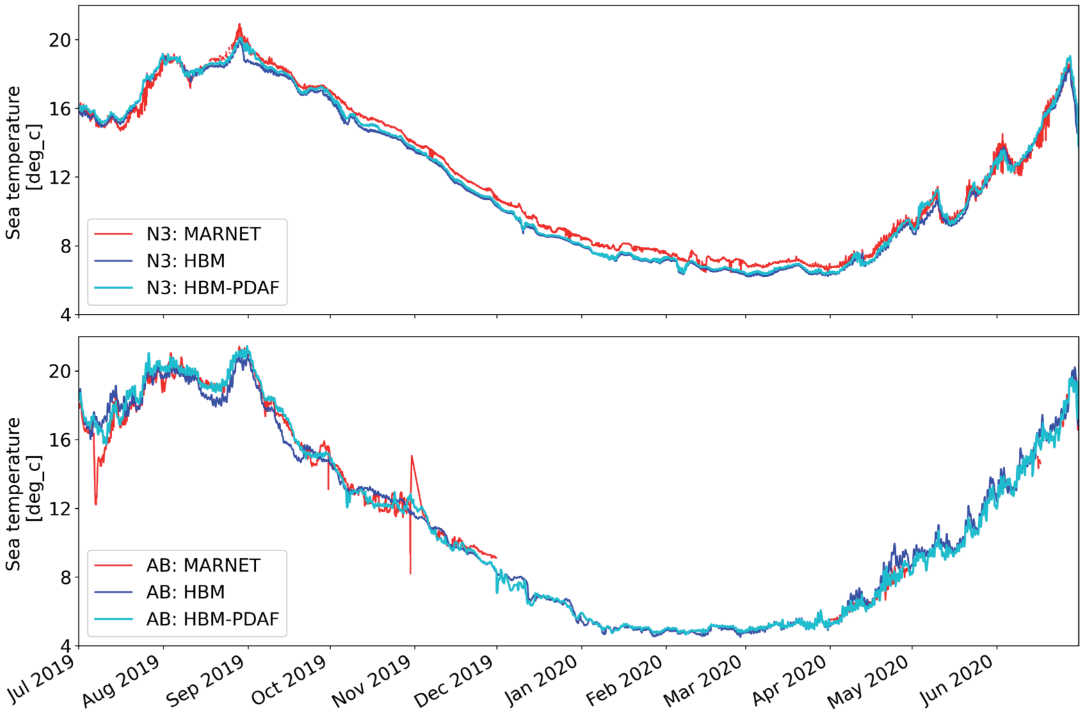

Fig. 9: Comparison of time series of surface temperature from the HBM free run and HBM-PDAF run with in-situ data at station Nordseeboje3 (top) and station Arkona (bottom)

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