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The relative importance of selected factors controlling the oxygen dynamics in the water column of the Baltic Sea

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Abstract

A 1-D biogeochemical/physical model of marine systems has been applied to study the oxygen cycle in four stations of the different sub-basins of the Baltic Sea, namely, in Gotland Deep, Bornholm, Arkona and Fladen. The model consists of biogeochemical model of Neumann et al. (2002) coupled with the 1-D General Ocean Turbulence Model (GOTM). The model has been forced with meteorological data from the ECMWF reanalysis project for the period 1998–2003, producing a 6-year hindcast validated with datasets from the Baltic Environmental Database (BED) for the same period. The vertical profiles of temperature and salinity are relaxed towards both profiles provided by 3-D simulations of General Estuarine Turbulent Model (GETM) and observed profiles from BED. Modifications in the parameterisation of the air/sea oxygen fluxes have led to significant improvement of the model results in the surface and intermediate water levels. The largest mismatch with observation is found in simulating the oxygen dynamics in the Baltic Sea bottom waters. The model results demonstrate the good capability of the model to predict the time-evolution of the physical and biogeochemical variables at all different stations. Comparative analysis of the modelled oxygen concentrations with respect to the observation data is performed to distinguish the relative importance of several factors on the seasonal, interannual and long-term variations of oxygen. It is found that the natural physical factors, like the magnitude of the vertical turbulent mixing, wind speed, the variation in temperature and salinity field are the major factors controlling the oxygen dynamics in the Baltic Sea. The influence of limiting nutrients is less pronounced, at least under the nutrient flux parameterisation assumed in the model.

1 Introduction

The Baltic Sea is a semi-enclosed and brackish sea, which together with other physical as well as socio-economic characteristics makes it very sensitive to anthropogenic pressures (Bonsdorff et al., 2001). Eutrophication remains the most pressing problem in the region, as nitrogen and phosphorous inputs are still high, despite considerable efforts to reduce discharges. Pulses of water streaming in at the bottom through the Danish straits transport salty and oxygen rich water from the North Sea into the Baltic Sea (Omstedt et al., 2004). The strong pulses are driven by special atmospheric forcing conditions, which cause large and long-lasting sea level differences between the Kattegat and the Western Baltic. Since the early 1980s, the Baltic Sea has experienced long-lasting stagnation periods with absence of strong pulses. Only in 1993 and 2003 such major inflows took place (Jakobsen, 1995; Feistel et al., 2003). Inflows from the North Sea are currently the principle source of oxygen in the deep water. The deepwater basins in the Baltic Proper suffer severely from long-term oxygen depletion. Oxygen deficiency has prevailed over very large areas. In the central Baltic Proper oxygen concentrations were less than 2 ml/l at around a depth of 100 m, or even more shallow than that (HELCOM, 2003). At the same time, the area covered by hydrogen sulphide extended from the main eastern Basin of the Gotland Sea towards the Northern Central Basin (Fig. 1). Typically in August, oxygen was depleted in the bottom water of the Bornholm Basin and the western Gotland Basin. In the Arkona Basin the oxygen situation was good in the near-bottom water, although lower compared to the long-term measurements. The oxygen conditions in the bottom waters of the Baltic Proper continued to be bad during 2003–2006 as well (HELCOM, 2007). The dead zones on the seabed with anoxic areas where hydrogen sulphide forms increased both in size and volume. More phosphorous consequently diffused out of the sediments and into the deep waters of the Baltic. This increased the risk of algal blooms during the next few years.

Additional to the above mentioned horizontal advection of oxygen the principal natural physical factors affecting the concentration of oxygen in the marine environment are temperature and salinity. Oxygen concentrations decrease with increasing temperature and salinity (Quinlan 1980). The other major factor controlling oxygen concentrations is biological activity in the water and at the seafloor: photosynthesis producing oxygen and respiration and nitrification consuming oxygen.

Marine ecosystem models, which involve the interaction of physical and biogeochemical processes, are useful tools for assessing and predicting the trends in oxygen variation and for establishing the areas more susceptible to oxygen deficiency. These models should take into account the important biogeochemical processes and the physical control of the ecosystem driven by advection and diffusion. Efficient models of marine systems can simulate the seasonal evolution, inter-annual variability and spatial heterogeneity across the range of coastal and eutrophic situations with little or without re-parameterisation. Although the usual way to develop such models is to couple circulation models with biological models, simplified model systems based on an 1-D water column models e.g. those of Burchard et al., 2006; Kühn and Radach, 1997; Blackford et al., 2004, can be also reliable in studying marine ecosystem dynamics of coastal marine areas.

The present study aims to assess the relative importance of different factors that are controlling the oxygen cycle in the water column of the Baltic Sea by the use of a 1-D water column model. Thus, the relative importance of following factors is investigated in detail:

- the significance of the principal hydrographic situation is studied by comparing several stations with very different hydrographic characteristics;
- the importance of the accuracy of hydrographic characteristics (temperature/salinity structure) – by comparing oxygen simulations using either measured profiles or results from simulations with a 3-D model;
- the effect of the vertical turbulent exchange – by varying parameters of the turbulence model;
- the influence of the atmospheric forcing – by multiplying the wind speed by a factor from the interval [0.5;1.5];

- the importance of the parameterization of the air-sea oxygen exchange – by comparing different available parameterizations;
- the relative importance of limiting nutrients.

The study is organized as follows. In Sect. 2 we describe briefly the 1-D model and characterize the type of the method used to model the system, while in Sect. 3 we provide the model setup and forcing. Section 4 deals with some model improvements. In Sect. 5 are presented the model results at different stations and comparisons between observations and model results. The model sensitivity analysis is presented in Sect. 6. The last section includes a discussion and some conclusions.

2 Model description

We use the coupled 1-D ecosystem model of Burchard et al. (2006) to simulate the oxygen and nitrogen cycles in some selected stations of Baltic Sea. As the physical part of the 1-D ecosystem model the GOTM (General Ocean Turbulence Model, (www.gotm.net) is applied. The turbulence is modelled with a two-equation turbulence model; one equation for the turbulent kinetic energy and one equation for the dissipation rate of the turbulent kinetic energy, and includes a simple parameterization of deepwater mixing. We have found out that from the large number of well-tested turbulence models implemented in GOTM, the $\kappa-\varepsilon$ model is a very appropriate tool to model the dynamical vertical structure and the actual turbulent diffusive vertical transport in selected Baltic Sea stations.

A biogeochemical model of medium complexity (ten state variables) is used in this study (Neumann, 2000; Neumann et al., 2002). This model is of Eulerian-type, so all state variables are expressed as concentrations, no matter whether they are dissolved chemicals (e.g. nutrients, oxygen) or particles (e.g. phytoplankton cells). For example, the ERSEM (European Regional Seas Ecosystem Model, Baretta et al., 1995) is an Eulerian-type model of higher complexity. In the model, the oxygen utilisation and production is connected with nitrogen conversation. The oxygen concentration controls processes as denitrification and nitrification. If the oxygen is depleted, than the nitrate is used to oxidize detritus, and if nitrate vanishes sulphate is reduced to hydrogen sulphide. Hydrogen sulphide is accounted for as negative oxygen concentrations ($2H_2S=O_2$). Reduction of nitrate (denitrification) is counted as a loss of nitrogen in the model.

The model of Neumann et al. (2002) has been recently coupled to the physical model as BIO_IOW module of the GOTM package. The GOTM-BIO_IOW model has been tested by Burchard et al. (2006) for the Gotland station (BY15) with water depth of about 250 m. The comparisons between model results and observation data from COMBINE program (under the umbrella of HELCOM) for the period 1983–1991 show that the hindcasting of interannual variability of nutrients nitrate and phosphate, and phytoplankton is not satisfactory. It is found that the $\kappa-\varepsilon$ model predicts too shallow mixed layers in the Baltic Sea when applied without limitation of turbulent kinetic energy, $k_{\mathrm{min}}[\mathrm{m}^2/\mathrm{s}^2]$. It is illustrated that the parameter k_{min} can act as a tuning parameter of the model (Burchard et al., 1998, 2006). However, more complete' and accurate studies of model sensitivity analysis and/or model skill assessment have not been reported.

The validity of the 1-D approximation in the Baltic Proper is confirmed also by some other model results (Vichi et al., 2004; Omstedt and Axell, 1998; Stigebrandt, 1987). They are mainly related to the periods, when the advection is negligible (so-called stagnant periods). Despite, that a 1-D model exhibits limitations in simulating seasonal and interannual variability of the deep water mixing and the formation of density currents (Axell, 2001), it is a good tool for basic studies, improving the model parameterisation and investigation of some system properties.

3 Model forcing and setup

The model was run for a 6-year period, from 1 January 1998 to 31 December 2003 and initial profiles were approximated from available oceanographic measurements. This

6-year period includes stagnant (1998–2002) and fluctuant (2003) periods. The only major inflow to the Baltic Sea during the investigated period was in 2003 (Feistel et al., 2003). However, several inflows of less strength occurred during the period (Matthäus and Nausch, 2003).

Depth profiles of temperature and salinity along with surface meteorological data and nutrient components are used to force the model. The meteorological forcing data were taken from the ECMWF (European Centre for Medium Range Weather Forecast, (www.ecmwf.int) data server (ERA-40 re-analysis data). The frequency of meteorological data is six hours. Data sets of temperature, salinity, concentration of oxygen and chlorophyll a for all here studied stations of the Baltic Sea are extracted from the Baltic Environmental Database (BED) via internet based software NEST (http://nest.su.se/bed). The initialization of some initial parameters of the BIO_IOW module is done by the use of BED data, as well. Finish Institute of Marine Research (FIMR) Baltic Sea monitoring data (http://www.fimr.fi/en/tietoa/helcom_seuranta/en_GB/bmp/_data) is also used for model verification. The water transparency of Baltic Sea, measured as Secchi depth, has been thoroughly estimated in the report of Laamanen et al. (2004) and it is assumed to be 5 m in all calculations.

Nutrient fluxes at the air-sea surface have been adjusted in order to parameterise lateral nutrient fluxes which are neglected in the 1-D model. Thus, much higher values than the real ones are used in calculations. In order to highlight the differences between the physical conditions at the studied stations, we fix the surface fluxes and initial concentrations of ammonium, nitrate, and phosphate for all numerical simulations. The estimation of the nutrient values is done on the base of sensitivity analysis. Statistical and graphical techniques are applied to compare quantitatively the multiple executions of the model (Sect. 6.4).

The computed temperature and salinity profiles have been relaxed towards observed profiles (BED data) or profiles calculated with GETM (General Estuarine Turbulence Model) model (www.getm.eu), Stips et al. 2005). The relaxation time is about 5 days. The model is run using a two year repeating cycle of forcing data for 1998 as a “spinup" period in order to achieve a quasi-equilibrium state and obtain reasonable initial conditions.

4 Improvement of the model

We have implemented the model with realistic forcing functions for the station BY15 in the central Gotland Sea (see Sect. 5) for the years 1998–2003. In Fig. 2a, b are shown the surface temperature and oxygen time series, respectively. The model is in a good accordance with the data over the full 6 years' period, especially in describing the seasonal variability. However, it can capture the variation only with lower amplitudes of surface oxygen concentrations during summer (Fig. 2b). The difference between predicted and observed surface concentrations of oxygen is more pronounced during summer of 1999, 2001–2003 when the surface temperature reaches about 23°C (Fig. 2a). This discrepancy is due to an overly simplified computation of the oxygen surface fluxes. So, we have modified the relations for the calculation of the surface oxygen flux in BIO_IOW module.

The oxygen exchange with the atmosphere is usually described by

$$F = V\,(O_{\mathrm{sat}} - O), \tag{1}$$

where F [$g\,\mathrm{O}_2/\mathrm{m}^2\,d$] is the air-sea oxygen flux, V [m/d] is a transfer (piston) velocity, O and O_{sat}[$\mathrm{mmol\,O_2/m^3}$] are surface and saturation oxygen concentrations, respectively. In BIO_IOW module the saturation oxygen concentration is calculated by

$$O_{\mathrm{sat}} = a_1 - a_2 T, \quad V = \mathrm{const}, \tag{2}$$

where T is surface temperature and a_1, a_2 are constants (Neumann et al., 2002; Burchard et al., 2006). Although the annual net flux of oxygen through the air-water interface of the Baltic Sea is quite small, Eq. (2) does not allow predicting a correct evolution of the surface oxygen concentration (Fig. 2b).

In the present study, the transfer velocity is calculated by the model of Liss and Merlivat (1986), which includes three regimes (smooth surface, rough surface and breaking waves) depending on the magnitude of wind speed, w:

$$\begin{array}{lll} \text{at} \quad w < 3.6\,[\mathrm{m/s}]: & V = 1.003\,w/Sc^{0.66} & \\ \text{at} \quad 3.6 \le w \le 13\,[\mathrm{m/s}]: & V = 5.9\,(2.85w - 9.65)/Sc^{0.5} & \\ \text{at} \quad 13 < w\,[\mathrm{m/s}]: & V = 5.9\,(5.9w - 49.3)/Sc^{0.5} & \end{array} \tag{3}$$

The Schmidt number Sc is defined as ratio between the kinematic viscosity and the molecular diffusivity of oxygen. We have applied the following expression for Sc (Stigebrandt, 1991)

$$Sc = 1450 - 71T + 1.1T^2. \tag{4}$$

Equation (4) is valid in the interval 0<T<40 C° and thus, it is applicable in the case of non-freezing sea surface. Instead of linear dependence of O_{sat} on temperature involved in the BIO_IOW module, we have used the formula of Weiss (1970). For comparison, in Fig. 2c is shown the drastically improved surface oxygen evolution of the above described test case at BY15 after running the modified BIO_IOW module.

5 Model results and validation

The strong density stratification in the Baltic Sea suppresses the vertical mixing of the water and the transport of oxygen from the surface to the bottom. Only during very exceptional conditions when the inflow lasts long enough (over two weeks) the saline water from the North Sea can reach far enough into the Baltic Sea. The saline water is only very slowly mixed with Baltic Sea water and it flows through the Arkona and Bornholm basins in about six months, then to the central basin of the Baltic Sea, the Gotland Deep, replacing the old Baltic Sea water, often containing little or no oxygen but some hydrogen sulphide (Feistel et al., 2003). Since one of our purposes is to explore the influence of the principal hydrographic situation on the oxygen cycle in the water column of the Baltic Sea, we simulate the oxygen and nitrogen cycles at several stations with very different hydrographic characteristics. For a detailed presentation, we selected four stations from North to South with a quite different location in the Baltic Sea, namely:

- Gotland (249 m depth), a very deep central station BY15 (20 E, 57.3 N) of Baltic Proper, with limited water exchange, with a well-mixed surface layer and salinity stratified deeper layer;
- Bornholm (91 m depth), a central station BY5 (15.9 E, 55.2 N) of the Bornholm basin, with limited water exchange, with a well-mixed surface layer and salinity stratified deeper layer;
- Arkona (47 m depth), a central station BY1 (14 E, 55 N) of the Arkona basin, a shallow station strongly influenced by the pulses of saline and oxygenated water from the Kattegat;
- Fladen (80 m depth), station BY0 (11.5 E, 57.3 N) of the Kattegat basin, close to the North Sea, with the highest salinity among our selected stations.

Each of the first three stations might be considered as a representative station for the corresponding basin (Reissmann, 2006). The regional characteristics of the salinity, potential temperature and oxygen content are represented well by the hydrographic measurements in the corresponding central stations.

5.1 Water column structure

The annual temperature variation in surface waters of the Baltic Sea is great, having differences of up to 20°C. See for example in Fig. 2a the surface temperature at BY15 station. The surface temperature at BY5 behaves in the same way like that at BY15, while the bottom one is approximately constant (7°C) at both stations (it decreases to

3°C only after the inflow of 2003). At BY5 the surface salinity is about 7.5 PSU (7 PSU at BY15) and the bottom salinity varies slightly between 15 and 17.5 PSU (12 and 13 PSU at BY15) and reaches a peak of 19.2 PSU after the inflow in 2003. A halocline separates the lower saline surface water, 6–9 PSU, from the more saline deep water, 15–20 PSU, (for all stations except for BY0, where the surface salinity varies between 16 and 30 PSU and the bottom one between 33 and 35 PSU) and excludes the deep water from vertical mixing. The halocline begins at a depth of about 10–20 m in the Fladen, 30–40 m in the Arkona basin, 35–50 m in the Bornholm basin, and 60–70 m in the Gotland basin (IOW, 2003; Wasmund et al., 1998).

Figure 3 shows the comparison between the simulated and observed density difference, $\rho_t = \rho_b - \rho_s$ [kg/m^3] (where ρ_b and ρ_s are the bottom and surface density, respectively) at BY5. The model well reproduces the observed strength of the stratification, particularly indicating the less stratified winter period and the presence of more stable conditions in summer (Lass et al., 2003; Mohrholz et al., 2006; Sellschopp et al., 2006). The variability of ρ_t is simulated quite well, because of the applied salinity relaxation.

In summer, a thermocline forms at about 15–20 m depth and the temperature of the intermediate water between thermocline and halocline usually remains the same as during the winter (4–10°C). The thermocline exists until October, then in the autumn the surface water starts cooling and sinking until it reaches the temperature of maximum density. Thermocline and density differences in the upper layer disappear and wave and wind actions mix finally the whole layer above the halocline.

The vertical oxygen distribution at BY5 is shown in Fig. 4 for selected representative days during the year 2001. It is nearly constant in the layer above the halocline except for the summer months. Moreover, the concentration of oxygen is higher in the layer below the thermocline (cold intermediate layer) than in the other water layers. In the halocline the oxygen decreases rapidly, so the halocline acts as a barrier for oxygen penetration into the deep waters.

Thus, one can distinguish three main layers of the sea water column at BY5, as well as at the other three stations:

- surface (mixed) layer, where the temperature, the water salinity and the oxygen concentration are more or less vertically constant;
- intermediate layer (the depths below thermocline till the end of halocline), where the temperature, the water salinity and the oxygen concentration change significantly;
- bottom layer, where the temperature, the water salinity and the oxygen concentration become approximately constant.

In the surface layer, the calculated oxygen concentrations are in a perfect agreement with the measurements. Then, in the intermediate layer the model well predicts the trends in vertical distribution of oxygen. In the bottom layer, the calculated concentrations of oxygen are consistent with observations but do not match them very well. Generally, the vertical structure of oxygen is highly correlated with the measurements in each period of the year.

Correlation coefficient, R, normalised standard deviation, $\tilde{\sigma} = \sigma_m / \sigma_r (\sigma_r$ and σ_m are the standard deviations of the reference and the model field, respectively) and root mean square difference (RMSD) of simulated and measured oxygen concentrations are given in Table 1. The statistics are calculated on the basis of the available measurements of the full water column during the year 1998 at five stations and the corresponding model results. In addition to the statistics for the four studied stations, the statistics for Landsort station, BY31, 440 m depth (see Fig. 1), are also presented to support the model validation. The measured oxygen concentrations of each observation are interpolated on the computational grid of the water column before R, $\tilde{\sigma}$, and RMSD have been calculated (the same procedure have been done for statistics presented in Table 2). It should be noted that the number of observations at each principle station is about 15 and the occurrence of the records in the water column in comparison with the station depth is also similar. So, we can consider the statistics of these stations as equally reliable. The model-data agreement is perfect for BY5, BY15 and BY31 and nearly perfect for the other two stations. The relatively low values of the RMSD in comparison to the variability of data indicate a close match between predicted and observed concentrations. In summary, the statistics confirms the above made conclusions that the model successfully reproduces the water column variability of the oxygen.

5.2 Interannual variability

The model results are analysed at the identified three main water column layers for the period 1998–2003. Figures 5–8 show the modelled time series of oxygen compared with the BED and FIMR (denoted with asterisks in all Figures) data. The time interval between two subsequent major ticks in all time series plots is equal to 2 months. Bottom salinity at BY5 is given in Fig. 6c. At the surface, the modelled oxygen is in near-perfect agreement with the observations (Figs. 5a–8a). In addition, the decreasing and increasing trends are well matched by the model. Such good results indicate that the Eqs. (1), (3) and (4), used to compute the surface oxygen flux, are appropriate for the Baltic Sea, and that the time evolution of surface oxygen is completely determined by the exchange at the surface. Deeper in the water column (in the intermediate layer) at stations BY15 and BY5 (50 m depth in Fig. 5 and 40 m depth in Fig. 6b) the model matches very well the data, too.

However, the model performance in deep water layers, at the bottom, is not really satisfactory. The sediment oxygen demand is only partially taken into account in the model and therefore the simulated bottom oxygen is approximately constant in time at the deep stations BY15 and BY5. The introduction of a real sediment layer is still an ongoing development for this model. Contrary to the surface layer, the horizontal advection of oxygenated water is a very important component of the oxygen dynamics in the bottom layer. This can be clearly seen by sudden increases in bottom oxygen in Figs. 5 and 6, which are also well correlated to increases in salinity (Fig. 6c). The situation is of course even worse at the highly dynamic stations BY1 and BY0, where even more sporadic inflow events occur additional to the effect of seasonal changing temperatures.

The discrepancy between model and observation data is not only due to the omitted horizontal advection because the 3-D circulation model used by Neumann et al. (2002) predicts also too high values of the near bottom oxygen at BY5 and BY15 (stations 213 and 271 in Fig. 13 of Neumann et al., 2002) for the period from 1983 until 1990. Unfortunately the simulation of the horizontal transport of the used 3-D model is too diffusive (see the near bottom salinity in Fig. 5 of Neumann et al. (2002)) so that likely in the simulations no inflowing oxygen rich water arrived in the Gotland Sea. In Neumann et al. (2005) the vertical resolution has been increased, which led to some improvement of the near bottom oxygen concentrations. The calculated time series of near bottom oxygen is passing through the observation data without showing any inflow dynamics. Evidently, the near bottom oxygen dynamics and near bed consumption are not well considered and further adjustments to the model are necessary. However, even the correct accounting of the sediment oxygen demand would not lead to improved simulations here, as we would need to consider advection by applying a 3-D model or at least parameterize the effect of the inflow events on the oxygen concentration for the 1-D runs.

Nevertheless, that the main hydrographic conditions of the Baltic Sea are characterised by the permanent salinity stratification these conditions are not the same for the different regions of the Baltic Sea. The surface temperature varies a lot at all selected stations disregarding their location but the bottom temperature is about constant for the stations of the Baltic Proper and varies seasonally at BY1 and BY0. Also, the variation of bottom salinity is more pronounced at BY1, while the surface salinity changes significantly at BY0. This occurrence is related to the locations of these stations. BY0 is placed in Kattegat, close to the North Sea, where the surface water salinity is affected by the irregular inflows and outflows of salty or brackish water respectively. All water masses exchanging between the North Sea and the central Baltic pass the Arkona Sea. The model predicts the formation of permanent halocline at a mean depth of 30 m at BY1 (Lass et al., 2003, Sellschopp et al., 2006). At the surface and in the intermediate layer, the calculated oxygen evolution for BY1 is in a very good accordance with observation data (Fig. 7). In the bottom layer, however, the seasonal variability is only partially matched by the model, which can capture the variation partly but with a reduced range of amplitudes and with a phase shift of 1–2 months. In particular, the data reaches higher levels of oxygen concentration during winter and lower ones in late summer and behaves similar as at the surface or in the intermediate layer. The rate of oxygen decrease depends on temperature among other things. The correlation coefficient between observed temperature and oxygen fields in the bottom layer is $R(T,O_2)=-0.57$, while that between observed salinity and oxygen is $R(S,O_2)=0.1$. This reveals a close inverse correlation between temperature and oxygen at the bottom.

The halocline sometimes forms at BY0 at nearly 10 m depth. The discrepancy between calculated and observed concentrations of oxygen is the highest at BY0 (Fig. 8). This is expected because the influence of horizontal advection is more pronounced at BY0 than at the other selected stations. Moreover, the values of $R(T,O_2)=-0.82$ and $R(S,O_2)=-0.06$ at BY0 show that the inverse relation of temperature and oxygen at the bottom is even stronger at BY0 than at BY1 and a better parameterisation of oxygen-temperature relations in the bottom layer might be essential.

Summary statistics of the interannual model performance (Table 2) shows a high correlation between the observed and modelled values, the R and $\tilde{\sigma}$ are close to one, the RMSD are relatively small although they are higher than those for the year 1998 (Table 1). The summary statistics are generally less favourable for BY0 and BY1 than for BY5 and BY15 with a lower correlation and the modelled values of oxygen underestimate the measured ones ($\tilde{\sigma}=0.71$ at BY1 and $\tilde{\sigma}=0.65$ at BY0). The low values of the correlation coefficient at BY0 and BY1 are expectable because of the time shift in the bottom oxygen time series (Figs. 7b and 8b). This discrepancy is probably due to a simple modelling of the biological activity and its influence on the oxygen cycle in the water column. Unfortunately, there is not enough observation data to check this

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assumption.

Thus, the statistics presented in Table 2 confirms the information obtained by the time-series plots (Figs. 5–8). It should be noted here that the agreement between modelled and observed oxygen concentrations will be a little better if we exclude the year 2003 from the comparisons. This exclusion could be justified for our 1-D simulations because of the occurrence of the major inflow event in January 2003 (Feistel et al. 2003), which would require the consideration of horizontal oxygen transport.

Biological activity is another factor controlling oxygen concentrations. The inter-annual variability of simulated and observed average phytoplankton concentrations, shown as average chlorophyll a (Chla) is given in Fig. 9. The time series of calculated Chla concentrations and in situ data of BED and FIMR correspond to the water column average values (from the surface to 20 m depth). Also presented in the figure are the minimum and the maximum monthly mean values taken from satellite images (Environmental Marine Information System (EMIS) database, (http://emis.jrc.ec.europa.eu/). The model predicts a spring bloom mostly composed of diatoms and flagellates in the beginning of March for BY5 (Fig. 9a) and in the beginning of April for BY15 (Fig. 9b). To some extent this result coincides with HELCOM (1996) report stating that the spring bloom of phytoplankton develops earlier at the western part of the Baltic Sea then in its eastern and northern parts. In these areas, a strong spring bloom develops in April/May, followed by a small summer bloom in July/August, and an autumn bloom in October/November. After mild winters, the spring bloom could appear earlier. Also, the regional differences in the timing of the spring blooms are related to the mixing depth (Wasmund et al., 1998). There is a weak evidence of a summer bloom in the model results at BY5 (Fig. 9a), however, it is not simulated for BY15 (Fig. 9b) by the model. Typically, the autumn bloom is predicted to develop in September/October. The autumn peak is well phased and corresponds to all presented observation data. There is a reasonable agreement between the modelled and observed average Chla in 2002 and 2003 at BY5, however, in all other years the model predicts lower bloom peaks than the observed ones at both stations BY5 and BY15. A part of the discrepancy between calculated concentrations of chlorophyll a and observed values could be explained by the simplified parameterisation used for chlorophyll in the model, which is a simple linear function of the N-content (Janssen et al., 2004). Still one has to keep in mind that comparing in situ and model data involves many uncertainties, as the typical random pull of a bucket of water out of a patchy plankton bloom might lead to a drastic over– or underestimation of the real mean Chla concentration in the measurement area. This could be only overcome by rather expensive measurement methods as for example taking about 100 random samples within the comparison region in order to establish confidence intervals for the measurements. Additionally, as depicted in Fig. 9, there is not a good agreement between both measured data types (in situ and satellite data). The satellite data are often missing the spring bloom peak, which might be related to cloud cover during that time. An interesting finding is that the model shows better succession in the phytoplankton content for the years when in situ and satellite data match better. Despite the above mentioned limitations of the model, we can conclude that under the influence of atmospheric forcing and at different hydrographic characteristics the model reproduces the annual and interannual cycles of oxygen typical for the Baltic Sea.

6 Sensitivity analysis

Statistics, such as correlation coefficient, R, normalised standard deviation, $\tilde{\sigma}$, and the normalised “unbiased” root mean squared difference, $\tilde{S}$ (normalised by σ_r) are used to compare the multiple model runs with the reference (observation) data. The difference between RMSD and potential bias is denoted with $\tilde{S}$. The RMSD is a measure of the average magnitude of the difference, while $\tilde{S}$ may be conceptualized as an overall measure of the agreement between the amplitude ($\tilde{\sigma}$) and phase (R) of two temporal patterns. For this reason, R, $\tilde{\sigma}$ and $\tilde{S}$ are referred as “pattern statistics”. The three pattern statistics are related to one another by (Taylor, 2001)

$$\tilde{S} = \sqrt{1 + \tilde{\sigma}^2 - 2\tilde{\sigma}R}. \quad (5)$$

The normalised standard deviation and the correlation coefficient from the model to reference field comparisons may be displayed on a single Taylor diagram (for example, see Fig. 10). The Taylor diagram is a polar coordinate diagram with polar angle proportional to arccos (R) and radial distance from the origin proportional to $\tilde{\sigma}$. Therefore the reference field point has the polar coordinates (1.0, 0). The model to reference comparison points are then assessed by how close they fall to the reference point. This distance is equal to $\tilde{S}$. The relationship (5) makes the Taylor diagram useful because the individual contribution of misfits of amplitude may be compared to misfits in phase to distinguish how they contribute to the normalised unbiased RMSD. The same as for statistics presented in Table 2, all calculations have been done on the basis of all the available measurements of the full water column during the period 1998–2003 and the corresponding model results. It is important to note that the model and reference fields are not log-transformed or averaged in all presented comparisons.

6.1 Effect of vertical turbulent exchange

The results of 10 separate model runs with different values of k_{min} are shown in Fig. 10. It is a Taylor diagram of the sensitivity of the model to the vertical turbulent exchange showing model to reference statistics for the oxygen, phosphorus, ammonium, nitrate and chlorophyll a field during the period 1998–2003 at BY5. The parameter investigated here is the minimum turbulent kinetic energy, k_{min}, which is used in the turbulence model as a parameterization to account for unresolved mixing processes as e.g. internal waves (Burchard et al., 2006). The colour bar represents 10 different values of $k_{\text{min}} \cdot 10^7$ in the interval [5; 30]. Generally, the model performance is the best for oxygen (the highest R values and the smallest $\tilde{S}$ values). Limiting nutrients have intermediate goodness of fit (R values ranging from 0.4 to 0.8 and $\tilde{S}$ values from 0.65 to 1) and the phytoplankton, shown as chlorophyll a, has the highest misfit with observed values. We account for chlorophyll by assuming a classical Redfield ratio of N:C and a constant C: chlorophyll ratio and that may introduce a bias compared to the real system. The spread of comparison points in Fig. 10 demonstrates that k_{min} is an important parameter for predicting all the presented state variables. Since our main interest is more related to the oxygen dynamics we will discuss in detail the sensitivity of oxygen to changes in vertical turbulent mixing. Figure 10 clearly indicates that the model overestimates the interannual cycle at low k_{min} (lower than $7.10^{-7}[\text{m}^2/\text{s}^2]$) and underestimates it at high k_{min} (higher than $15.10^{-7}[\text{m}^2/\text{s}^2]$). The value of $\tilde{\sigma}$ changes rapidly with increasing k_{min}, while the value of R does not. In other words, the vertical turbulent mixing has a higher influence on the amplitude rather than on the phase of the simulated oxygen field. Both minimum of the total RMSD (indicated by "◇") and minimum of the unbiased RMSD are found for $k_{\text{min}}=1.10^{-6}[\text{m}^2/\text{s}^2]$). Thus, the bias between modelled and reference fields has also a minimum at this point. We have found the best fit between the model and reference oxygen fields at BY15 for $k_{\text{min}}=8.10^{-7}[\text{m}^2/\text{s}^2]$), at BY1 for $k_{\text{min}}=25.10^{-7}[\text{m}^2/\text{s}^2]$), at BY0 for $k_{\text{min}}=80.10^{-7}[\text{m}^2/\text{s}^2]$), while at BY31 for $k_{\text{min}}=5.10^{-7}[\text{m}^2/\text{s}^2]$). It appears that k_{min} is an important model parameter and one must decide carefully how to parameterise it when one couples the GOTM-BIO_IOW model with a 3-D circulation model of the Baltic Sea.

There is a trend of decreasing the optimal k_{min} $(80; 25; 10; 8; 5).10^{-7}[\text{m}^2/\text{s}^2])$ with the distance from the entrance of the Baltic Sea, which might reflect the decrease in the effective vertical exchange in the Baltic. The strength of density stratification expressed as the observed mean ρ_t for the period 1998–2003 shows a similar spatial pattern decreasing from South to North: 11.56 at BY0; 8.17 at BY1; 8.63 at BY5; 6.4 at BY15 and 6.41 at BY31.

6.2 Effect of prescribed temperature and salinity profiles

It is worth to note, that the model results depend on the value of the salinity relaxation time scale to observed or calculated by a 3-D model salinity profiles. The shorter is the relaxation time the better is the agreement between model results and observation data. The best fit is found for the relaxation time of 5 days. The model results show that the oxygen dynamics is less sensitive to the temperature relaxation time scale. Nevertheless, we have applied the relaxation time of 5 days for the temperature profiles, too. In this subsection is presented an investigation of how the variability of the salinity and temperature profiles used for relaxation influences the simulated oxygen concentrations. In Fig. 11 are given the normalised pattern statistics of oxygen for the total 6 year period at the four principal stations. Two separate model runs with different profiles used for temperature/salinity (T–S) relaxation are made for each station: with 3-D model profiles (the model points of oxygen are denoted with capital letter “O”) and with observed profiles of BED (denoted with small letter “o”). Also shown on the Taylor diagram are the comparisons of the 3-D model T-S fields to BED data fields (reference). With capital letter “S” are denoted the statistics for salinity and with “T” – for temperature. The colour of all points is altered for each station. Figure 11 indicates that the statistical properties of the 3-D model T–S fields are of good or reasonable quality at all stations. The normalised standard deviation of the T field is in the interval [0.89; 1.08] and $R \geq 0.94$. The 3-D model salinity field is well phased, too ($R \geq 0.88$), however, the model underestimates the observed field. For example, $\tilde{\sigma}=0.45$ at BY15 (marked with a red colour). Despite the misfit, the two comparison points for oxygen at BY15 are very close to each other. The close placement of all pairs of oxygen comparison points shows the close correspondence between model results obtained by the use of 3-D model and observed relaxation data. A related conclusion is that one can utilise 3-D model data for T–S relaxation in all cases when the observation data is scarce or absent.

6.3 Effect of atmospheric forcing

In order to illustrate the model sensitivity to variations of the atmospheric forcing we present results from five different cases and compare them with the observation data. The normalised pattern statistics of oxygen have been calculated for the period 1998–2003 varying the wind speed by a factor of 0.5, 0.8, 1.0, 1.2, 1.5 (plotted with different colours in Fig. 12). Results for the different stations are denoted with different symbols. The value of k_{min} is fixed to its best fit value which is different for each particular station (see the values of k_{min} already reported in Sect. 6.1). The close grouping of the comparison points for BY15 (circles) indicates that the oxygen dynamics at this deep station is not sensitive to the possible uncertainty in the forcing data. It is obvious, that the oxygen dynamics at all other stations is influenced when the wind speed has been scaled by different factors. A reduction of the wind speed by a factor of 0.5 gives a poorer pattern statistics while the wind speed amplification shows better results. The overall impression given by Fig. 12 is that the increase of the wind speed by a factor of 1.2 has led to a general improvement in the model performance. For the scaling factor of 1.5 the correlation is slightly improved for BY0 and BY1, even though the results for $\tilde{\sigma}$ and $\tilde{S}$ are worse for BY5. Another inference drawn from Fig. 12 can be that the wind speed magnitude of the ERA-40-reanalysis could be possibly underestimated.

6.4 Effect of limiting nutrients

In the model, the nutrient load is taken into account via initial concentrations and surface fluxes of nitrate, phosphate and ammonium. As we have already mentioned in Sect. 3, the nutrient fluxes at the air-sea surface have to be adjusted in order to parameterise lateral nutrient fluxes. In Fig. 13 is drawn a Taylor diagram for testing the model sensitivity to limiting nutrients, showing the model to reference statistics for oxygen (red) and chlorophyll a (green) during the 6 year period at BY5. The results of 150 separate model runs are shown on the diagram and the corresponding intervals from which the initial concentrations and the surface fluxes of nutrients are randomly chosen are given in Table 3. The surface fluxes of nutrients are assumed as constants during one model run. The average values (for the upper 20 m) of chlorophyll a are used for comparisons. It appears that both the oxygen and chlorophyll a are weakly sensitive to the variation in the concentrations of nutrients. Moreover, only the amplitude of the model oxygen field is sensitive, while the phase remains approximately unchanged ($R \cong 0.95$). This is possibly due to the way of the nutrient surface flux parameterisation – as a constant. Typically, the concentrations of nutrients in the Baltic Sea are very low in summer and high in winter. The values of initial concentrations and the surface fluxes of nutrients for which the corresponding RMSDs from oxygen and chlorophyll comparisons reach the minimum are given in Table 3. The comparison points with the minimum RMSD values are indicated by black diamond ("◇") in Fig. 13. It worth to note, that at these points the unbiased RMSDs have also a minimum.

7 Summary and Conclusions

In the present work we have examined the influence of some important physical and geochemical factors on the oxygen concentrations at several regions of the Baltic Sea. For this purpose we used the GOTM-BIO_IOW model. The model has been forced with meteorological data for the 6 year period. Modifications in the parameterisation of the air/sea oxygen fluxes have led to a significant improvement of the model results in the surface and intermediate water levels. Model validation has been done by evaluating the agreement between predicted values of oxygen and observation data from the BED and FIMR data bases. The correlation with observation data is good and consistent for all stations and with low values of the RMSD (Table 1 and 2). Specifically the oxygen dynamics of the surface mixed layer is simulated in close agreement to the observations. The fact that the oxygen dynamics at the surface can be accurately simulated by a 1-D model has been already shown by Vichy et al. (2004) for the BY5 station during the stagnation period 1979–1990. However, it comes certainly at a surprise that even the very dynamic transitional stations BY0 and BY1 in the case when a major inflow event appears (like this in 2003) are very well simulated by the 1-D model, which is ignoring completely the advection of oxygen. Therefore it can be concluded that in the surface layer the dynamic of the mixed layer and the oxygen exchange with the atmosphere are the only parameters controlling the near surface oxygen development.

The largest mismatch with observations is found in simulating the bottom water oxygen dynamics. This is of course not unexpected, as the bottom oxygen concentration in the Baltic Sea is not only determined by the local sediment oxygen demand, but largely influenced by inflowing oxygenated water from the North Sea. As we do not take into account the horizontal advection of oxygen in the used 1-D model we are not able to simulate increasing bottom oxygen during inflow events. Nevertheless it is obvious that the oxygen consumption at the sediment interface demands for an improved parameterisation. But one has to keep in mind, that when incorporating a better sediment oxygen demand parameterization in a 1-D model, the results of the simulation could become worse, because of the high consumption which is not counterbalanced by oxygen transport. The statistical properties of the modelled nutrient and phytoplankton concentrations are also reasonable. This demonstrates the good capability of the model to predict the oxygen dynamics at all selected stations.

The results emphasise the importance of the principal hydrographic situation, the accuracy of the hydrographic characteristics, the variability of the vertical turbulent exchange and atmospheric forcing, the parameterisation of the air-sea oxygen exchange and quantity of the nutrient supplies. It is found that these mechanisms play an important role in the oxygen dynamics in the water column of the Baltic Sea. The model results point out the significant differences between the oxygen cycles in the different regions of the Baltic Sea. For the selected 6 year simulation period the concentration of deepwater oxygen changes seasonally at Fladen and Arkona and has almost no seasonal variability at the two stations of Baltic Proper. Sensitivity analysis has been performed in order to examine the influence of turbulent mixing, forcing functions (salinity and temperature profiles used for relaxation), atmospheric forcing (wind speed), and nutrient loads. The normalised standard deviation, the correlation coefficient and the normalised unbiased RMSD from each model to reference field comparison are displayed on Taylor diagrams. It is found that the natural physical factors, like the magnitude of the vertical turbulent mixing, wind speed, the variation in temperature and salinity are the major factors controlling the oxygen dynamics in the Baltic Sea. The influence of limiting nutrients is less pronounced, at least under the nutrient flux parameterisation assumed in the model.

The interesting fact that the minimum kinetic energy used in the turbulence model giving the best fit of simulations to observations is decreasing with the distance from the entrance of the Baltic Sea, k_{min} = (80; 25; 10; 8; 5)$.10^{-7}$[$\mathrm{m}^2/\mathrm{s}^2$]), could be a hint to increased unresolved mixing due to e.g. breaking internal waves as the strength of the density stratification is increasing in a similar way. Further this clearly underlines the fact that the use of a spatial and temporal constant k_{min} in 3-D applications is inappropriate, an improved parameterization is urgently needed.

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Table 1. Correlation coefficient, R, normalised standard deviation, $\tilde{\sigma}$, and root mean square difference, RMSD [ml O_2/l], of the simulated and measured oxygen concentrations in the full water column for n days of the year 1998.

Year 1998	Fladen	Arkona	Bornholm	Gotland	Landsort
n	16	15	14	15	32
R	0.83	0.83	0.97	0.98	0.99
$\tilde{\sigma}$	0.80	0.94	1.0	0.91	0.94
RMSD	0.61	0.69	0.67	0.95	0.69

Table 2. Correlation coefficient, R, normalised standard deviation, $\tilde{\sigma}$, and root mean square difference, RMSD [ml O_2/l], of the simulated and measured oxygen concentrations in the full water column for n days during the period 1998–2003.

1998-2003	Fladen	Arkona	Bornholm	Gotland
n	96	80	78	77
R	0.79	0.80	0.97	0.96
$\tilde{\sigma}$	0.65	0.71	1.00	0.79
RMSD	0.79	0.88	0.71	1.78

Table 3. Ranges of initial concentrations and surface fluxes of limiting nutrients used in the sensitive analysis. Corresponding values, for which the minimum of the RMSD has been found.

	Phosphorus	Nitrate	Ammonium
Range of initial concentrations [mmol N/m^3]	0.5–0.7	4–9	0.1–0.5
Range of surface fluxes [mmol N/m^3]	0.03–0.1	0.5–1	0.2–0.8
Initial concentrations [mmol N/m^3]	0.6	8.	0.4
with the minimum RMSD for oxygen			
with the minimum RMSD for chlorophyll	0.6	7.	0.3
Surface fluxes [mmol N/m^3]			
with the minimum RMSD for oxygen	0.06	0.7	0.4
with the minimum RMSD for chlorophyll	0.05	0.7	0.7

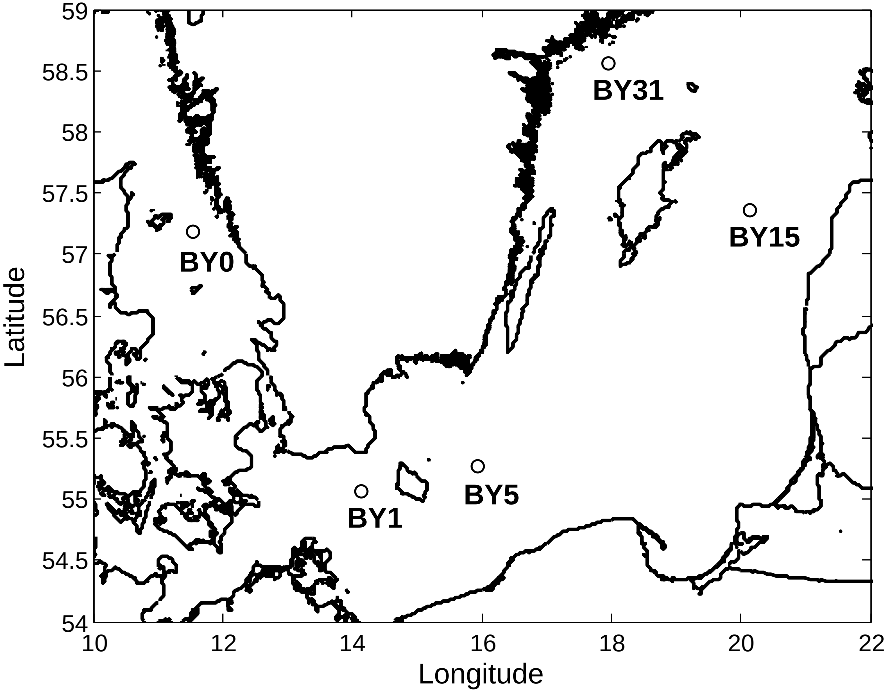

Fig. 1. Map of the Baltic Sea showing the sampling stations: Fladen (BY0), Arkona (BY1), Bornholm (BY5), Gotland (BY15) and Landsort (BY31).

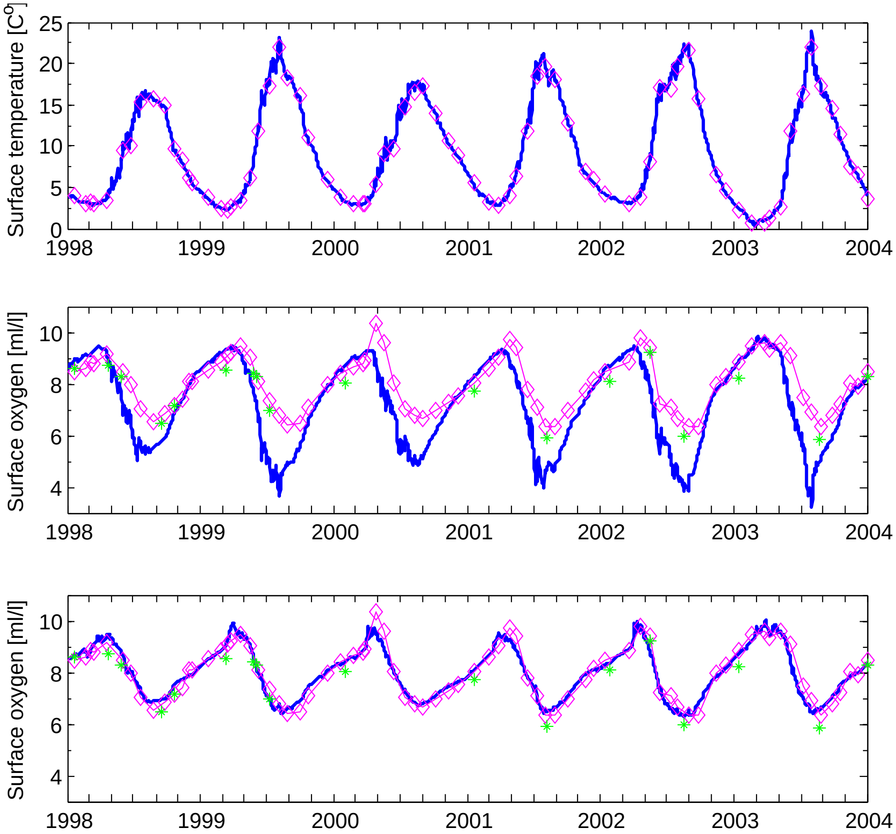

Fig. 2. Modelled (thick solid line) and observed (symbols) values of **(a)** – surface temperature, **(b)** surface oxygen calculated by using GOTM-BIO_IOW and **(c)** surface oxygen is calculated from Eqs. (1), (2), (4), and the formula of Weiss (1970) at BY15. Diamonds represent BED data, while asterisks represent FIMR data.

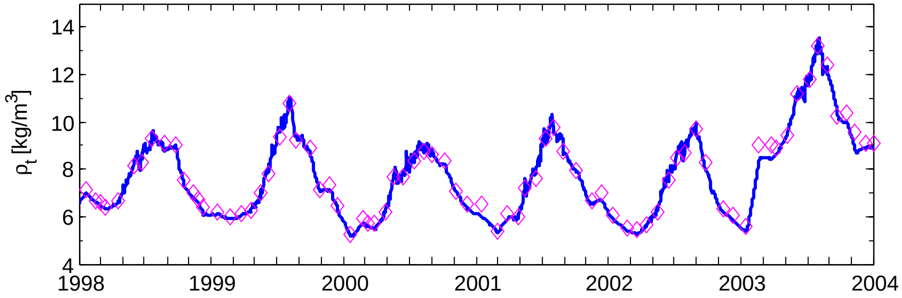

Fig. 3. Modelled (solid line) and observed (symbols) density difference at BY5.

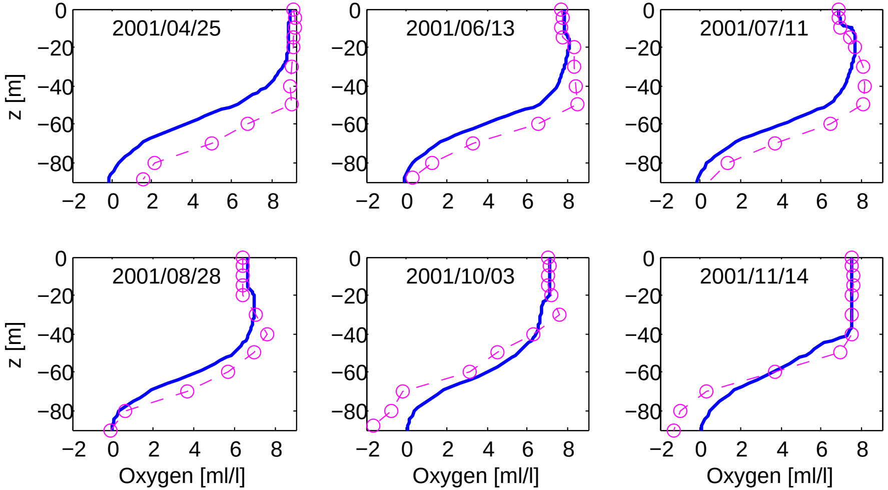

Fig. 4. Vertical oxygen profiles at BY5 in some selected days of 2001. Calculated results are presented with a solid line, while circles connected with a dashed line show the observation data of BED.

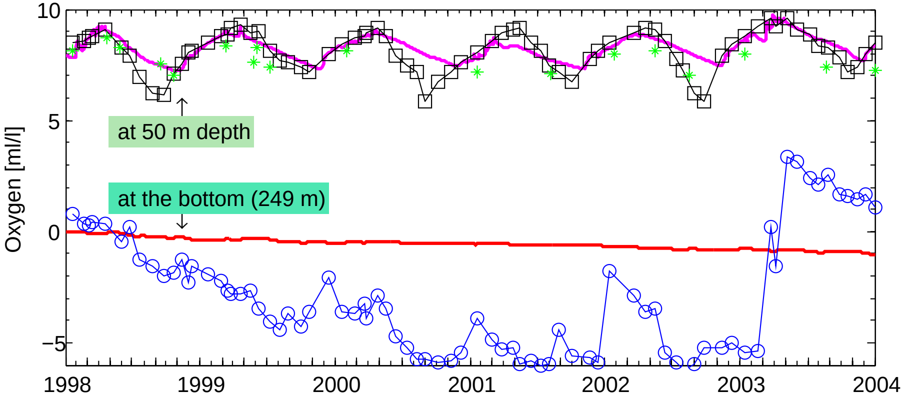

Fig. 5. Oxygen time series at BY15 in 1998–2003. Calculated results are presented with a thick solid line, FIMR data with asterisks, and BED data with squares and circles. Time series are plotted at 50 m depth (magenta line and black squares) and at the bottom (red line and blue circles).

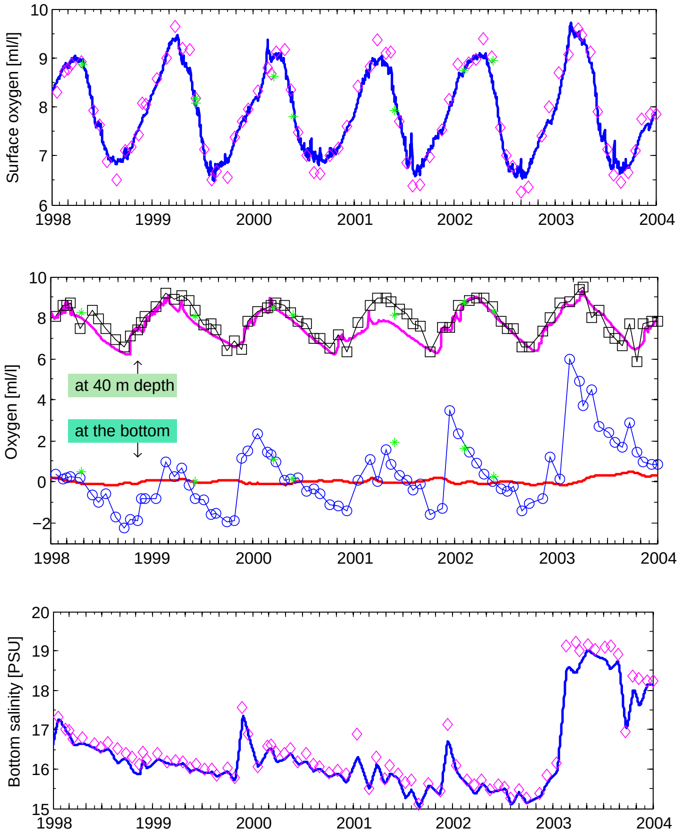

Fig. 6. Time series at BY5 in 1998–2003. Calculated results are presented with a thick solid line and observation data of BED and FIMR with symbols (see capture of Fig. 5 for more details). **(a)** – surface oxygen; **(b)** – oxygen at 40 m depth and at the bottom; **(c)** – bottom salinity.

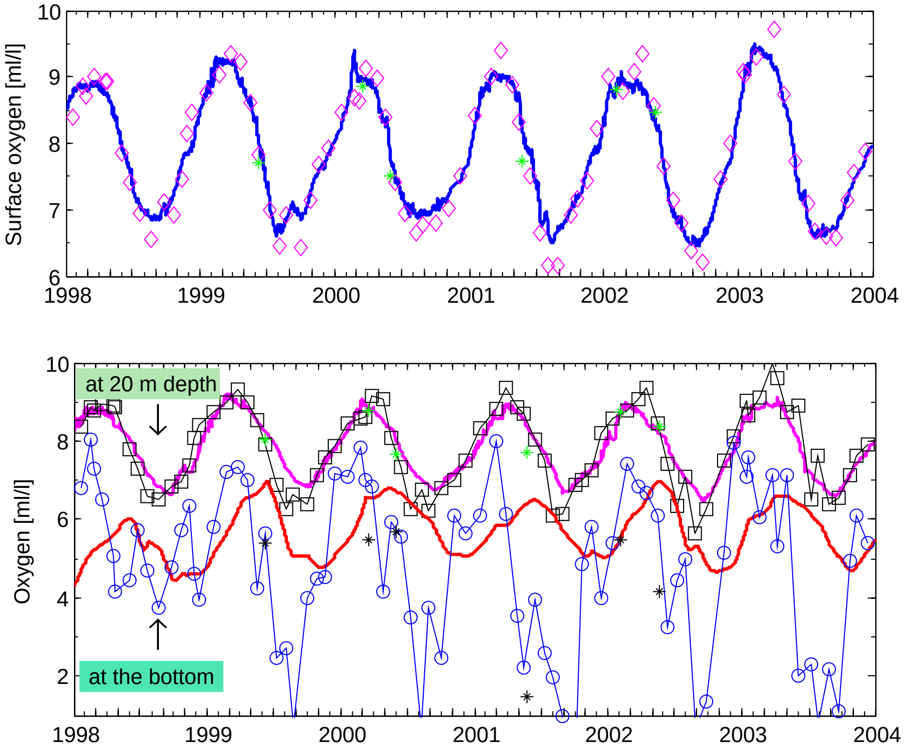

Fig. 7. Oxygen time series at BY1 in 1998–2003. Calculated results are presented with a thick solid line and observation data of BED and FIMR with symbols (see capture of Fig. 5 for more details). **(a)** – surface oxygen; **(b)** – oxygen at 20 m depth and at the bottom.

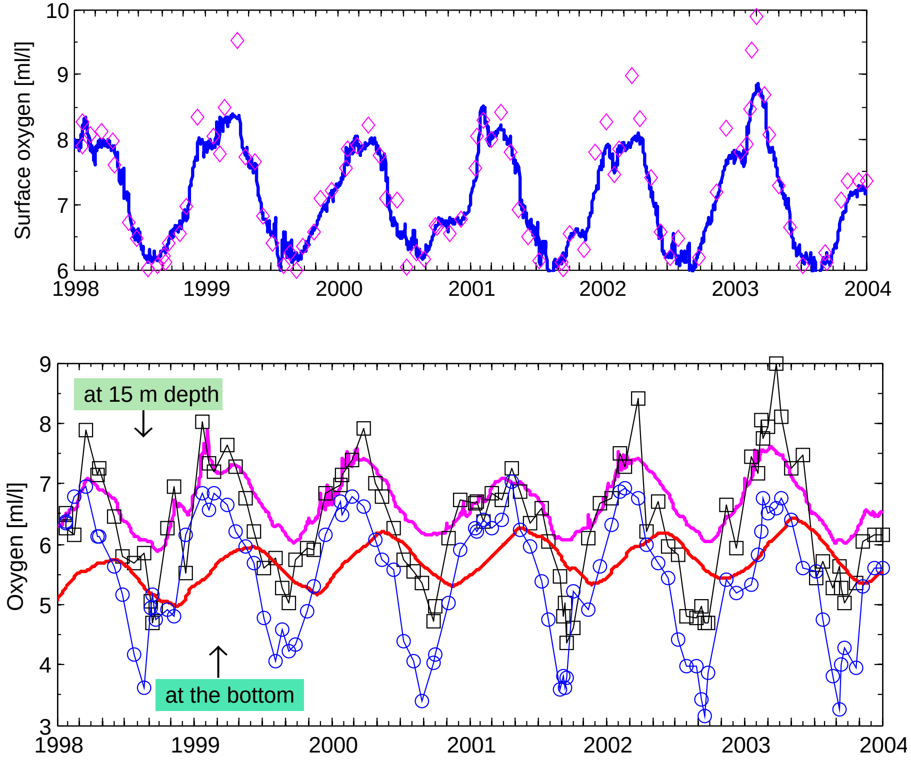

Fig. 8. Oxygen time series at BY0 in 1998–2003. Calculated results are presented with a solid line and observation data of BED with symbols. **(a)** – surface oxygen; **(b)** – oxygen at 40 m depth (magenta line and black squares) and at the bottom (blue circles and red line).

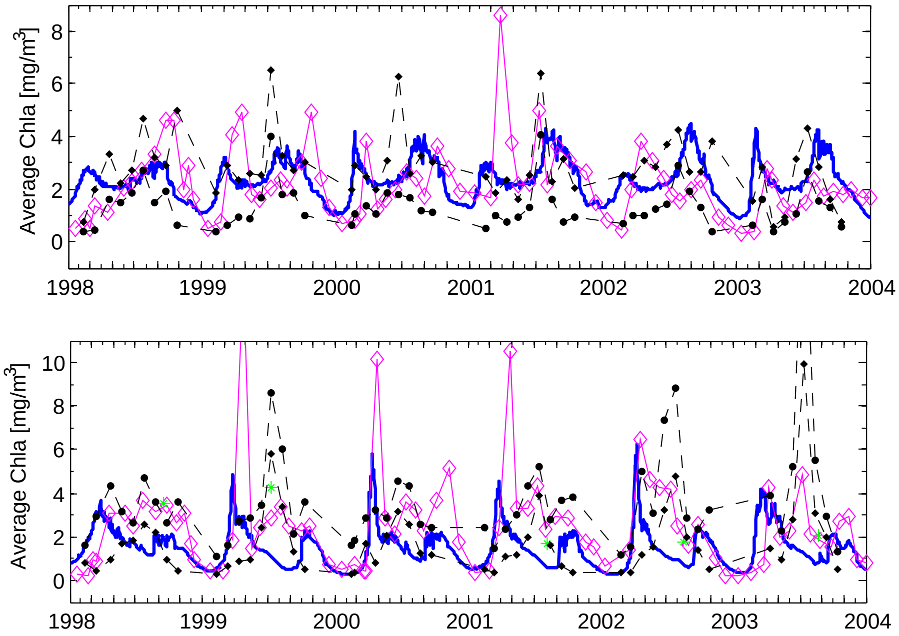

Fig. 9. Modelled (thick solid line) and in situ data (denoted with blank diamonds and asterisks) of average Chla [mg/m^3] at: **(a)** – BY5, **(b)** – BY15. Data from satellite images (EMIS database) is also shown. The filled circles connected with a dash line represent the maximum monthly average concentrations of Chla, while the filled squares represent the minimum ones.

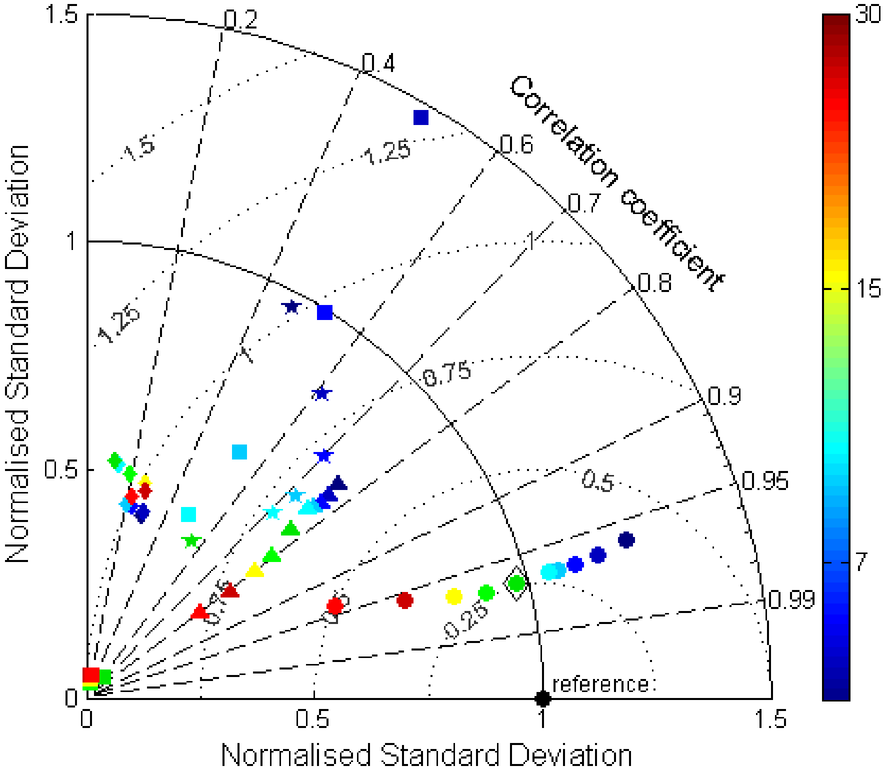

Fig. 10. Taylor diagram for the model sensitivity to the vertical turbulent exchange parameterization (different values of k_{min} are used) showing model to reference statistics for the oxygen (denoted with circles "•"), phosphorus (denoted with triangles "△"), ammonium (asterisks "∗"), nitrate (diamonds "◇") and chlorophyll a (squares "□") field for the period 1998–2003 at BY5. The colour bar represents 10 different values of $k_{min}.10^7$ in the interval [5;30]. The minimum value of the RMSD for oxygen is indicated by black diamond ("◇").

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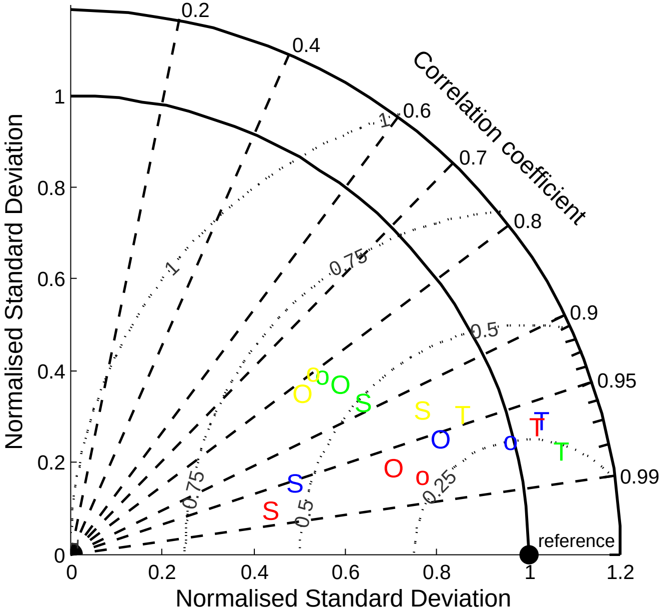

Fig. 11. Comparison between the normalised pattern statistics of oxygen calculated for the period 1998–2003 from two separate model executions with different profiles used for temperature/salinity relaxation. With capital "O" are denoted the statistics obtained by using model 3-D temperature/salinity fields for relaxation and with small "o" those obtained by using observation data of BED (reference). Also shown on the Taylor diagram is the comparison of 3-D model temperature/salinity fields to BED data fields (reference). With capital letter "S" are denoted the statistics for salinity and with "*T*" – for temperature. The statistics for different stations are presented with different colours: Bornholm – blue; Gotland – red, Arkona - green; Fladen – yellow.

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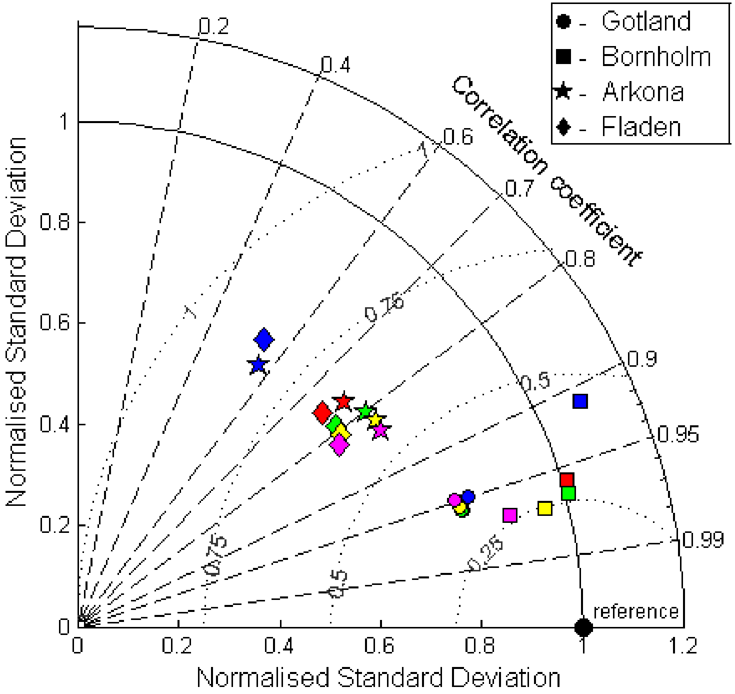

Fig. 12. Normalised pattern statistics of oxygen at the principal stations for the period 1998–2003. Different colours represent model executions with different wind speed scaling: 0.5 – blue; 0.8 – red; 1.0 – green; 1.2 – yellow; 1.5 – magenta.

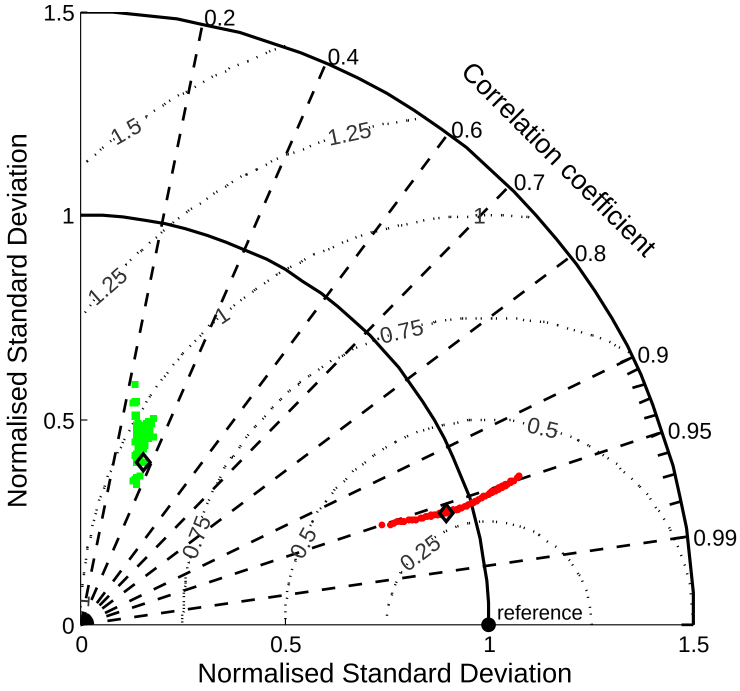

Fig. 13. Taylor diagram for model sensitivity to limiting nutrients showing model to reference statistics for the oxygen (red) and the chlorophyll a (green) field for the period 1998–2003 at BY5. The comparison points with the minimum RMSD values are indicated by black diamond ("◇"). The ranges of the intervals in which vary the initial concentrations and surface fluxes of nutrients are given in Table 3.