QUALITY INFORMATION DOCUMENT

Black Sea Production Centre
BLKSEA_REANALYSIS_BIO_007_005

Issue: 4.1

Contributors: L. Vandenbulcke, A. Capet, M. Grégoire

Approval date by the CMEMS product quality coordination team: 28/04/2020

CHANGE RECORD

When the quality of the products changes, the QuID is updated and a row is added to this table. The third column specifies which sections or sub-sections have been updated. The fourth column should mention the version of the product to which the change applies.

Issue	Date	§	Description of Change	Author	Validated By
1.0	29/08/2016	all	First version of document	L. Vandenbulcke	
	05/09/2016		Final check	L. Vandenbulcke, M. Grégoire, A. Capet.	
	25/10/2016		Revised version	M. Grégoire, L. Vandenbulcke, A. Capet	
2.0	28/01/2017		Version for CMEMS release V3	L. Vandenbulcke, A. Capet, M. Grégoire	
	21/03/2017		Updated EANs (1992-2015)	L. Vandenbulcke, A. Capet, M. Grégoire	
3.0	14/02/2018		Version for CMEMS release V4	L. Vandenbulcke, A. Capet, M. Grégoire	
3.1	10/09/2019		Changing references to dates	L. Vandenbulcke	
4.0	02/04/2020	all	Version for CMEMS V202007	L. Vandenbulcke, A. Capet, M. Grégoire	E. Peneva
4.1	15/01/2021	$1	Update for including interim datasets info	L. Vandenbulcke, A. Capet, M. Grégoire	E. Peneva

TABLE OF CONTENTS

APPLICABLE AND REFERENCE DOCUMENTS

	Ref	Title	Date / Version
[DA1]	CMEMS-BS-PUM-007-005	Black Sea Biogeochemistry Reanalysis Product User Manual	Jan 2021 / 3.1

EXECUTIVE SUMMARY

I.1 Products covered by this document

This document covers BS_REANALYSIS_BIO_007_005, the biogeochemical part of the Black Sea reanalysis product, produced as daily means at ~3km horizontal resolution for the period 1992-2019. Interim datasets (daily and monthly means) are also provided: they consist on operational datasets that will be updated every month M to cover the month M-1 and produced by the BS-BIO MY system, forced by ECMWF ERA5-T. Details on the processing system are provided in [DA1].

The product comprises the 5 following dataset:

- NUTR: phosphate and nitrate;
- PFTC: chlorophyll and phytoplankton biomass;
- BIOL: dissolved oxygen concentration and vertically integrated net primary production;
- CARB: pH, dissolved inorganic carbon (DIC), Total Alkalinity (TA)
- CO2F: partial pressure of CO_2 , air-sea flux of CO_2

The BIOL dataset also includes the bottom dissolved oxygen concentration on the North-Western Black Sea Shelf (NWS), saved as a separate 2D variable.

Interim datasets are also provided: they consist on operational datasets that will be updated every month M to cover the month M-1 and produced by the BS- Biogeochemistry MY system, forced by ECMWF ERA5 atmospheric fields. Details on the processing system are provided in [DA1].

I.2 Summary of the results

The quality of the BLKSEA_REANALYSIS_BIO_007_005 product has been assessed by comparison with in-situ observations collected in the Black Sea since 1992. In the present document, the quality of the product, V202007 (delivery in July 2020) is examined and compared with that of the previous version of the product delivered in 2018, here denoted as V4. This comparison shows some improvements compared to the V4 version, for some variables, whereas other variables are more or less unchanged. A summary of this quality assessment is provided below.

BIOL dataset

Oxygen: The error statistics are very good to excellent. On the North Western Shelf (NWS), the global percentage of bias is small (0.85%), qualifying the model as "excellent", and indicating that it resolves the oxygen dynamics with a very small persistent bias. The standard deviation ratio is close to 1 (i.e. 1.05). The global N-S statistic of 0.88 qualifies the model as "excellent". In the deep sea, interestingly, the new version of the model is able (without any nudging) to simulate the long term rising of the oxycline observed during the recent years. Globally the error statistics are very similar with a higher bias but lower RMS in V202007 while the model is still considered as excellent. The fact that V202007 performs as well as V4 although in V4 a nudging towards oxygen climatologies was imposed, is a striking result.

NUTR dataset

Nitrate.

For nitrate, all the error statistics are improved compared to V4, except r_{σ}, the standard deviation ratio that is closest to 1 in V4, suggesting that the V202007 version simulates a higher variability. For example, on average the model overestimates the nitrate concentration with a bias of 0.35 mmolN.m^{-3} in the open sea while this bias is negligible on the shelf (0.02 mmolN m^{-3}). The standard deviation ratio, Pearson correlation coefficient and RMS, also indicate that the model skills are higher on the shelf than in the open sea: in the open sea, the Pearson correlation is 0.61 (vs 0.68 on the NWS) and the RMS is 1.28 mmol.m^{-3} (vs. 1.16 on the shelf). In both regions, for nitrate, all models skills are higher in V202007 than in V4 (which itself was already higher than in V3).

Phosphate

At V202007, the RMS error is 1.48 mmol.m^{-3} (slightly higher than in V4) with in particular, an underestimation of the concentration below the oxycline. The upper layer and the layers below ~200 m, are well represented. We note a degradation of the model skills from V4 to V202007 which needs to be further investigated. However, the PB and N-S error statistics still qualify the model as "good".

PFTC dataset

Chlorophyll is a diagnostic variable of the BAMHBI model, and is validated by comparison with satellite observations. The model bias is ~0.2 mg/m3 in the open sea and varies between +0.04 and -1.13 mg/m^3 in the shelf and coastal regions. The RMS error is about 0.3 mg/m^3 in the open sea, and varies between 0.5 and 2.0 mg/m^3 in the shelf and coastal regions.

Phytoplankton carbon biomass: no data are available.

Carbonate system dataset

The carbonate system dataset is compared qualitatively to climatology obtained from the literature. It is shown that the model is able to simulate the right range and variability of the variables.

I.3 Estimated Accuracy Numbers

Table 1: Selected Estimated Accuracy Numbers (EANs). We use different statistics in order to assess the performances of the model on different aspects (e.g. variability, accuracy).

metric **V202007**	NOS	PHO	DOX
Bias (mmol m)	**0.20**	**-0.83**	**10.31**
PB		**-46.6**	**7.3**
RMS (mmol m)	**1.22**	**1.48**	**30.5**
r□	**0.86**	**2.56**	**1.03**
□	**0.64**	**0.92**	**0.97**
N – S		**0.37**	**0.94**

II PRODUCTION SYSTEM DESCRIPTION

II.1 Production centre details

a) Production centre name: BS-MFC
b) Production subsystem name: BS-MFC-Biogeochemistry
c) Production Unit:ULiege (MAST)
d) Production centre description for the version covered by this document

The biogeochemical reanalyses for the Black Sea are produced by the MAST / ULiege Production Unit by means of the NEMO 3.6 circulation model online coupled with the BAMHBI biogeochemical model. The workflow runs on the ULiege / CECI "nic4" HPC.

II.2 Description of the NEMO-BAMHBI model system

The Black Sea biogeochemical model (BS-Biogeochemistry) is the Biogeochemical Model for Hypoxic and Benthic Influenced areas (BAMHBI, Gregoire et al., 2008; Grégoire and Soetaert, 2010; Capet et al., 2016b). It describes the foodweb from bacteria to gelatinous carnivores through 24 state variables including three groups of phytoplankton: diatoms, small phototrophic flagellates and dinoflagellates, two zooplankton groups: micro- and mesozooplankton, two groups of gelatinous zooplankton: the omnivorous and carnivorous forms, an explicit representation of the bacterial loop: bacteria, labile and semi-labile dissolved organic matter, particulate organic matter. The model simulates oxygen, nitrogen, silicate and carbon cycling. In addition, an innovation of this model is that it explicitly represents processes in the anoxic layer.
Biogeochemical processes in anaerobic conditions have been represented using an approach similar to that used in the modelling of diagenetic processes in the sediments lumping together all the reduced substances in one state variable. In this way, processes in the upper oxygenated layer are fully coupled with anaerobic processes in the deep waters, allowing performing long term simulations. This fully coupling between aerobic, suboxic and anoxic processes is absolutely necessary for performing the long term reanalysis. Processes typical of low oxygen environments like denitrification, anaerobic ammonium oxidation (ANAMMOX), reduced decomposition efficiency have been explicitly represented (Gregoire et al., 2008). Moreover, the model includes a representation of diagenetic processes (Capet et al., 2016) using an efficient and economic representation as proposed by Soetaert et al., 2000. The incorporation of a benthic module allows to represent the impact of sediment processes on important biogeochemical processes such as sediment oxygen consumption (that is responsible for the generation of hypoxic conditions in summer), the active degradation of organic matter that determines the vigour of the shelf ecosystem (~30 % of the primary production produced in shelf waters is degraded in the sediment) and the intense consumption of nitrate by benthic denitrification that filters a substantial part (~50 %) of the nitrogen brought by the north-western shelf rivers (the Danube being the most important one) and modulates primary production in the deep basin. In addition to a representation of diagenesis, the biogeochemical model represents the transport of sediments by waves. This is an important feature that is necessary in order to sustain the primary production of the deep basin.

At V202007, the BS-Biogeochemistry model is online coupled with the NEMO 3.6 ocean model as for the Near Real Time (NRT) product (i.e. BLKSEA_REANALYSIS_BIO_007_005). The version of NEMO is aligned with that used for the BS-Physics, using a horizontal resolution of ~3km and 31 vertical z-levels.

At the air sea interface, in order to compute the air-sea exchanges of oxygen the BS-biogeochemical model uses the ECMWF ERA-5 hourly surface wind fields. Additionally, in the Black sea, atmospheric nutrients inputs have been found to be comparable to the river inputs and need to be taken into account to close the nitrogen budget at basin scale. They are necessary in order to sustain the primary production in the deep sea. Also, we will use the deposit estimates from Kanakidou et al. (2012) to force the model at the air sea interface (inorganic nitrogen inputs). Rivers nutrients loads data are issued from the SESAME and PERSEUS projects (Ludwig et al., 2009). In the current configuration of the BS-Biogeochemical model, the nutrients loads are gathered into the 6 main river entrances represented in the model domain, which are the Danube, Dniepr, Dniestr, Rioni, Sakarya and Kizilirmak. These river loads consist in annual loads modulated by repeated seasonal distribution. For the forecast, we will use climatological mean values computed over the last 5 years. The Bosporus Strait is open and the boundary condition is described in details in Stanev and Beckers (1999). The Sea of Azov is currently not represented.

II.3 Description of Data Assimilation scheme

The system does not perform any data assimilation nor nudging.

This is different compared to previous version (V4) where temperature, salinity and oxygen were relaxed towards climatology after 2010.

II.4 Upstream data and boundary condition of the NEMO-BAMHBI model

The CMEMS–BS-MFC-Biogeochemistry analysis and forecast system uses the following upstream data:

1. Atmospheric files of air temperature, air dew temperature, total precipitation, cloud coverage, wind velocity and mean sea level pressure, which are obtained from the ECMWF ERA-5 product publically available on the Copernicus Climate Data Store (CDS).
2. River flows and nutrients are based on data generated by the SESAME and PERSEUS EU-funded projects.

No external data are required at the open boundary of the Bosphorus Strait. Indeed, the water and salt fluxes at the Bosphorus are determined in such a way that total sea water and salt are conserved in the domain (Stanev and Beckers, 1999).

III VALIDATION FRAMEWORK

The quality assessment of the reanalysis simulations (1992-2019) performed with the BS-MFC-Biogeochemistry version V202007 system (described in the previous section) has been done using all the observations available for the Black Sea in existing databases (see the list below, entries 1-7), using various error metrics (see Table 2) and checking as many state variables as possible. A detailed analysis of the vertical and temporal dynamics of oxygen, nitrate, phosphate, ammonium, silicate can be found in Grégoire et al (2008), Capet (2014) and Capet et al., (2013) and is available on request.
Here the skill assessment will be presented for the state variables that are provided to CMEMS and for which observations are available (i.e. dissolved oxygen, nitrate, phosphate and chlorophyll).

Datasets

The datasets used for the computation of the error metrics are given below:

1. From the early 1960s until 1996, many surveys have been organized throughout the basin and have collected physical, chemical and biological data. A large part of these data has been gathered in the Black Sea TU Ocean Base in the frame of the NATO TU-Black Sea project. This database contains data for 116 variables from 271 data sets, including 8,364,731 data values for 26,035 stations (http://sfp1.ims.metu.edu.tr/TU-Black-Sea/inventory).
2. The MEDAR database, see http://medar.ieo.es/
3. The PANGEA database, see http://www.wdc-mare.org
4. The World Ocean data base (WOD)
5. Black Sea Commission data (BSC, 382 data points).
6. The R/V KNORR and R/V Endeavor cruise data (2001-2003-2005)
7. The CMEMS INSITU_BS_NRT_OBSERVATIONS_013_034 product

Details of databases 1-6 are given in Joassin (2011). The CMEMS in-situ biogeochemical database (entry 7 in the list above) starts in the 2010s. Figure 1 shows the distribution of data points per decade, and highlights the fact that after 1995 there are very few observations in the data bases; this complicates the validation of model results.

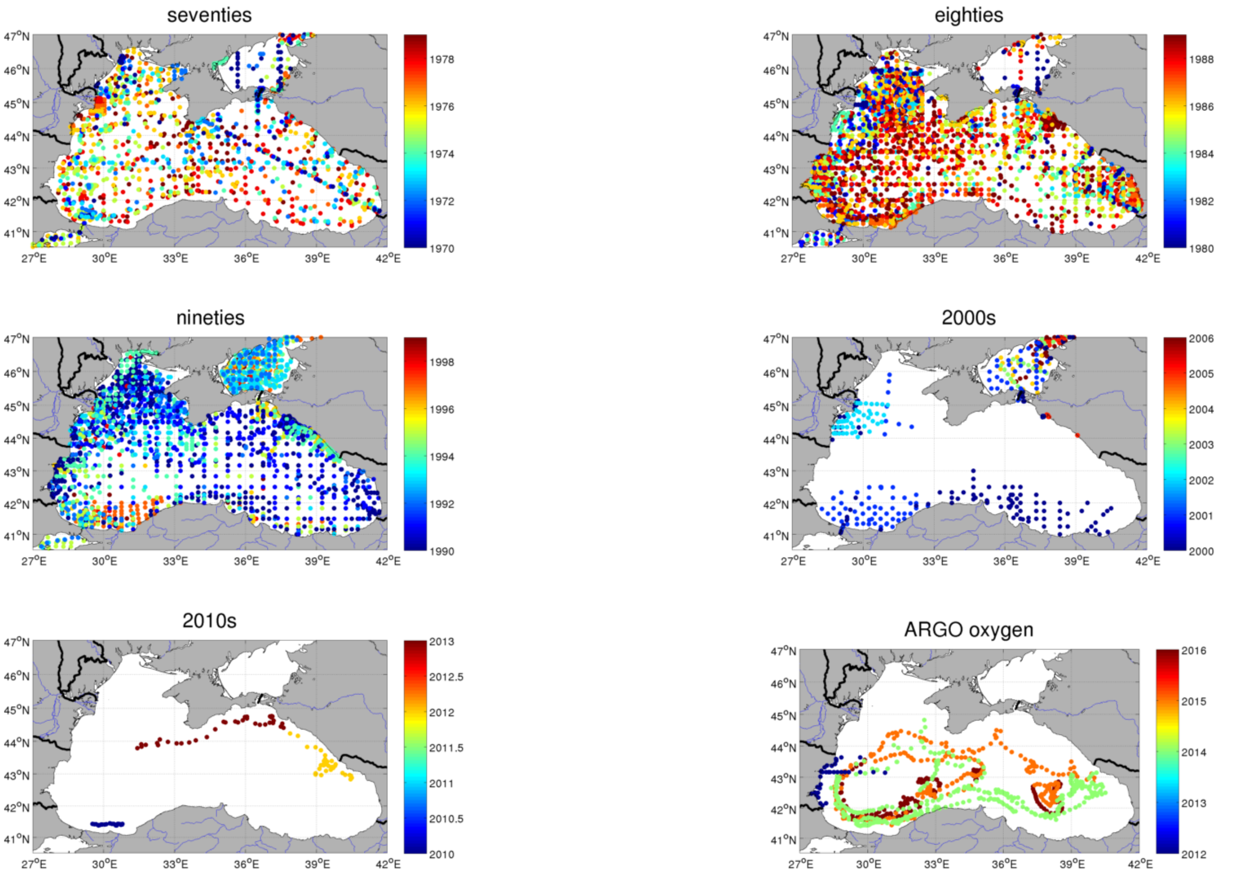


Figure 1: Distribution of data points per decade available in the NATO and WOD data base (the largest data bases in the Black Sea). Only sites where one of the modelled variable (oxygen, NH_4, NO_3/NO_2, POC, PON, Si, TOC, and chlorophyll) has been collected are represented. The last plot shows the position of the Argo floats where oxygen has been collected. The different colors represent the year of sampling. ARGO floats are represented up to 2015 included.

A large part of the Black sea in-situ data is related to oxygen. Indeed, due to the particular Black sea biogeochemical structure, a lot of international programs like US KNORR, Geotraces have collected oxygen and this has been continued with the launch of ARGO floats with oxygen sensors (Figure 1). Figures 2 and 3 show the availability of oxygen data according to the years since 1955 (Fig. 2) as well as their distribution (Fig. 3). Once again, these two figures highlight that after 1995 the amount of data available in international data bases sharply decreased. A substantial part of the validation efforts has been targeted towards the assessment of the ability of the model to simulate oxygen. Oxygen is a variable that integrates various biogeochemical processes like photosynthesis, respiration, chemical reactions, benthic-pelagic coupling and air-sea interface and hence an accurate representation of the oxygen dynamics is required. Moreover, the occurrence of hypoxic events on the Black Sea NWS may compromise the Good Environmental Status of marine waters and it is thus important to check the ability of the model to simulate such events.

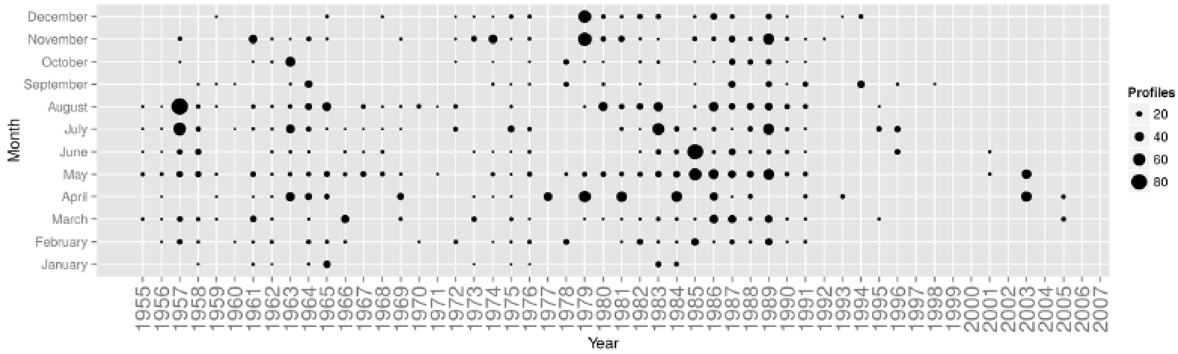


Figure 2: Temporal distribution of the ship-based oxygen profiles merged from the World Ocean Database, R/V *Knorr* 2003 and R/V *Endeavor* 2005 campaigns (Capet et al., 2016a).

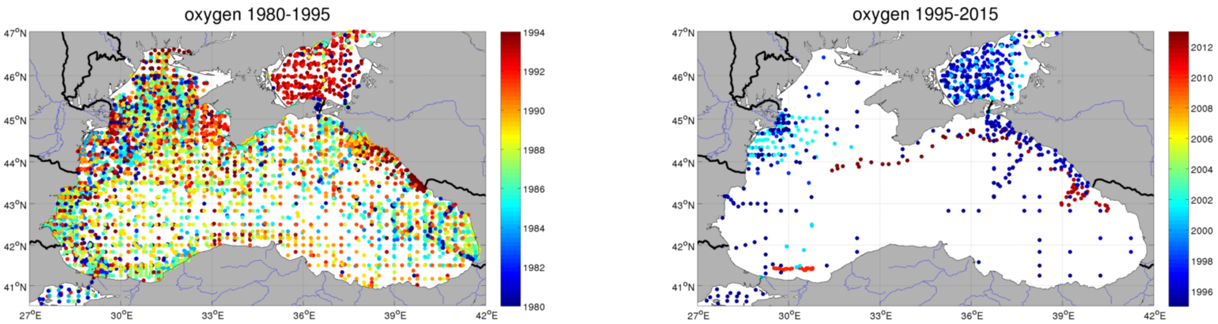


Figure 3: Distribution of oxygen observations during the period 1980-1995; 1995-2015 in the WOD and NATO data bases. (Argo data are not represented in this Figure but their position is shown in Figure 1).

Error Metrics

The quality assessment of model results is done using different errors statistics that allow to quantify model-data mismatches on different aspects. We select statistics that will allow balancing precision estimation ("How well does the model fit each data point?") with trend ("how well the model reproduces the observed seasonal/interannual cycle").

Table 2 presents these statistics (more details can be found in Allen et al., 2007). For the definition of the metrics, "O" represents the observations and "P" is the model output. In addition to these global statistics we assess the ability of the model to simulate the monthly vertical profiles and its temporal variability. The validation exercise is performed at basin scale, for the NWS (shallow region located in the north-western part) and the remainder of the domain (corresponding to the deep basin).

Table 2: List of metrics -- used to assess the model performance. *O* denotes the observation while *P* is the model prediction.

Definition	Meaning	Interpretation
The percentage bias (no units) $PB = \frac{P - O}{O} * 100$	Compares the mean values of *O* and *P*, and expresses the average bias as a percentage value of the *O* average	PB>0: global overestimation PB<0: global underestimation |PB|<10%: excellent skill, 10-20: very good, 20-40: good, > 40 poor (Maréchal, 2004)
Standard deviation ratio (no units) $r_\sigma = \frac{\sigma_O}{\sigma_P}$	Compares the distribution of *O* and *P* around their respective average	>1: larger variability in the observations <1: larger variability in the model
Nash-Sutcliffe efficiency (no units) $N - S = 1 - \frac{\sum(O - P)^2}{\sum(O - \bar{O})^2}$	Relates the model errors to the variability in the observations.	>0.65: excellent >0.5: very good >0.2: good <0.2: poor (Maréchal, 2004)
Pearson correlation coefficient (no units) ρ	Indicates how the variations of *O* and *P* around their respective mean are related	Significant correlations can be concluded for values of ρ above threshold values according to the amount of available data
Chi-squared statistic (no units) $\chi^2 = \frac{1}{n\,\sigma_O^2}\sum(P - O)^2$	Is an estimation of the model cost	The lowest χ^2, the better. This statistic is useful for comparing different versions of the model (model evolution)

IV VALIDATION RESULTS

In the following we will assess the global statistics of the model (computed over the whole model domain), its ability to represent the monthly, seasonal and interannual variability in the deep sea and on the north-western shelf (NWS) as well as the capacity of the model to simulate hypoxic events that seasonally occur on the NWS.

IV.1 Global statistics

The Global statistics presented in Table 2 are estimated over the whole basin and simulation period.

Table 3 shows the values of the statistics for CMEMS V202007. For comparison purposes, it also shows the CMEMS V4 statistics, which were obtained from the previous QUID version.

For nitrate, all the error statistics are improved compared to V4 except, r_{σ}, the standard deviation ratio that is closest to 1 in V4, suggesting that the V202007 version simulates a higher variability. For phosphate, this is the reverse and this degradation needs to be further investigated. However, the PB and N-S error statistics still qualify the model as "good". Concerning oxygen, globally the statistics are very similar, with a higher bias but lower RMS in V202007 while the the model is still considered as excellent. The fact that V202007 performs as well as V4 although in V4 a nudging towards oxygen climatologies was imposed, is a striking result.

Table 3: Model skill statistics obtained when considering all the observation/model predictions pairs for nitrate (NOS), phosphate (PHO) and oxygen (DOX). Error metrics have been defined in Table 2. The colours are associated to different levels of model performances: light green is excellent, dark green is very good, yellow is good and pink represents poor.

Error statistic	NOS		PHO		DOX	
	V4	**V202007**	V4	**V202007**	V4	**V202007**
Bias	-0.28	**0.20**	-0.72	**-0.83**	7.9	**10.31**
PB	-15.5	**11.33**	-27.5	**-46.6**	6.2	**7.3**
RMS	1.45	**1.22**	1.34	**1.48**	33.2	**30.5**
r_{σ}	0.97	**0.86**	1.24	**2.56**	1.02	**1.03**
ρ	0.41	**0.64**	0.86	**0.92**	0.96	**0.97**
N – S	-0.27	**0.12**	0.62	**0.37**	0.92	**0.94**

The statistics in Table 3 are computed for the whole basin, but additional information appears when analysing separately the open sea and the NWS. Also, in what follows, model performances are analysed regionally.

The regions are shown in Fig. 4. The open sea corresponds to regions 1, 2 and 3 while the north western shelf (NWS) corresponds to regions 4 and 5, and excludes region 7 (in green in Fig. 4) which is considered as the transition region between the NWS and the open sea.

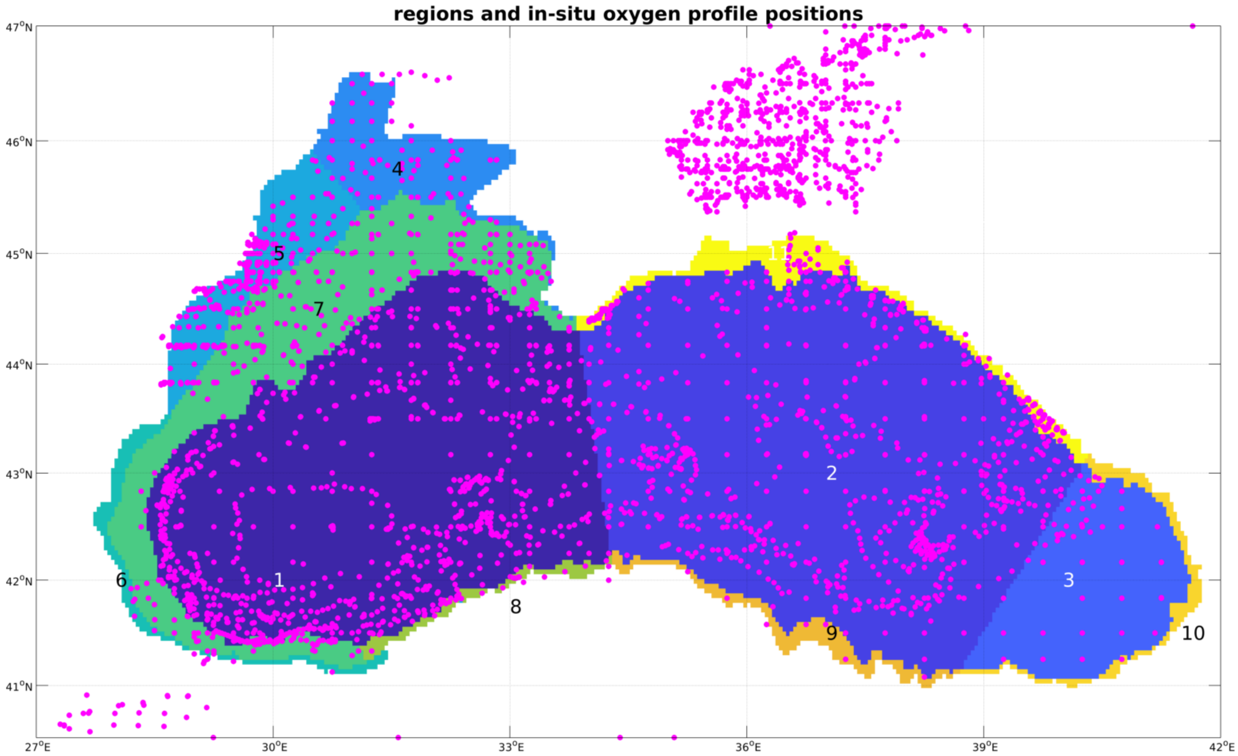


Figure 4. 11 regions of the Black Sea (following Kopelevich et al, 2003) and position of **all** in situ oxygen observations. Regions 4 and 5 on the NWS shelf have depths up to 50m, and region 7 up to 200m. Regions 6, 8, 9 and 11 are bordering the basin anti-clockwise from the Bulgarian coast to the Caucasian coast. Observations outside the modelled area (in the Sea of Azov, the Marmara Sea and around the Dniepr and Dniestr rivers) are discarded.

For example, concerning nitrate, on average the model overestimates the nitrate concentration with a bias of 0.35 mmolN.m^{-3} in the open sea while this bias is negligible on the shelf (0.02 mmolN m^{-3}). The standard deviation ratio, Pearson correlation coefficient and RMS, also indicate that the model skills are higher on the shelf than in the open sea: in the open sea, the Pearson correlation is 0.61 (vs 0.68 on the NWS) and the RMS is 1.28 mmol.m^{-3} (vs. 1.16 on the shelf). In both regions, for nitrate, all models skills are higher in V202007 than in V4 (which itself was already higher than in V3).

Table 4 shows the oxygen error statistics computed in the open sea and on the NWS both for CMEMS 202007 and V4. Let's note that the error statistics in table 4 are an aggregation of the pre-ARGO period (with most data available up to 1996, both in the open sea and the NWS) and the ARGO period (with only oxygen profiles in the open sea (regions 1-2-3), and almost no data on the NWS corresponding to regions 4-5-6-7). For oxygen in particular, the situation changed in between these periods with a shoaling of the oxycline that happened after 2000 and this shoaling was relatively poorly modelled in CMEMS version V2, but is very visible in versions V3 and V4 of the model thanks to nudging. This was the reason why we decided to nudge: to simulate the shoaling of the oxycline evidenced by in-situ data.

Although in the new version V202007, this nudging was removed, the model is able to simulate to progressive shoaling of the oxycline. Compared to V4, the skills of the model are essentially unchanged, with bias slightly increasing, but a lower RMS. In both the NOWS and deep sea, model statistics are still considered as very good or excellent (Table 4).

Table 4: Detailed model skill statistic for oxygen for CMEMS versions 4 (1992-2016) and V202007.

DOX	CMEMS V4			**CMEMS V202007**		
	open sea	NWS	whole basin	**open sea**	**NWS**	**whole basin**
bias	11.7	3.2	7.9	**15.9**	**1.75**	**10.31**
P.B.	11.4	2.1	6.2	**16.0**	**0.85**	**7.3**
RMS	22.6	42.6	33.2	**21.7**	**40.3**	**30.46**
r_σ	0.98	1.04	1.02	**0.98**	**1.05**	**1.03**
ρ	0.98	0.94	0.96	**0.99**	**0.94**	**0.97**
N-S	0.96	0.88	0.92	**0.96**	**0.88**	**0.94**

Here below, we analyse the vertical profiles of biogeochemical variables differentiating the open sea and the NWS.

IV.2 The Open Sea.

IV.2.1 Oxygen

The comparison of modelled and simulated vertical profiles of oxygen in the open sea shows a good representation of the surface dynamics and depth of the subsurface maximum by the model. The depth of the oxycline is quite well simulated in the CMEMS V202007 results (Fig. 5), and generally similar to CMEMS V4 and V3. We note that generally the oxycline is shallower in the observations compared to the model. This was also the case in the previous versions of the system but the differences were larger and increase over the years of simulation. This is the reason why we decided to introduce a nudging in the previous version of the system.

A plot of all observed profiles is presented in Fig. 6, as well as the corresponding model profiles.

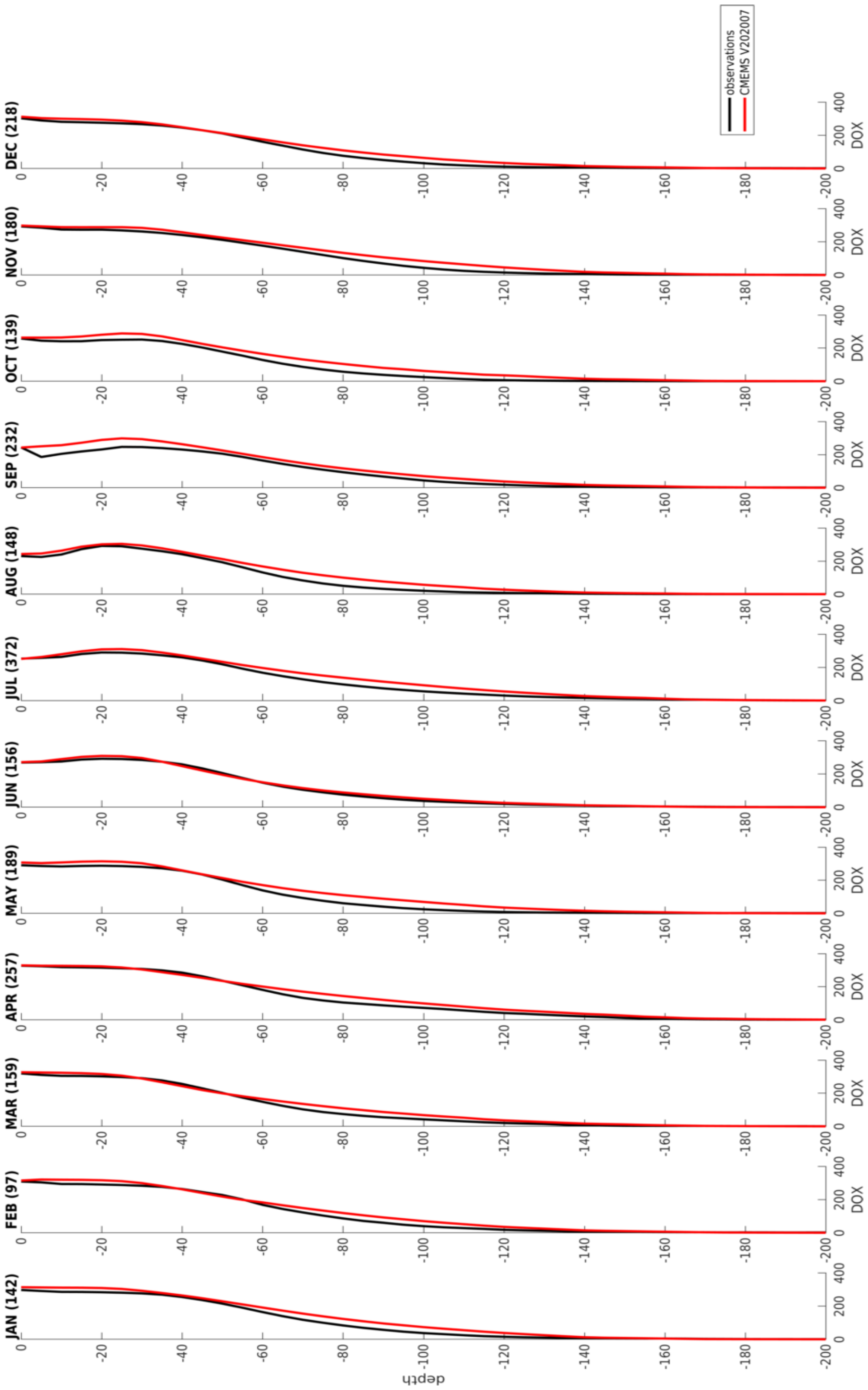


Figure 5: Point to point comparison of monthly vertical oxygen profiles in the open sea: observation (black) and CMEMS V202008 model (red). The number of profiles is indicated in parentheses and concerns the whole period (1992-2019).

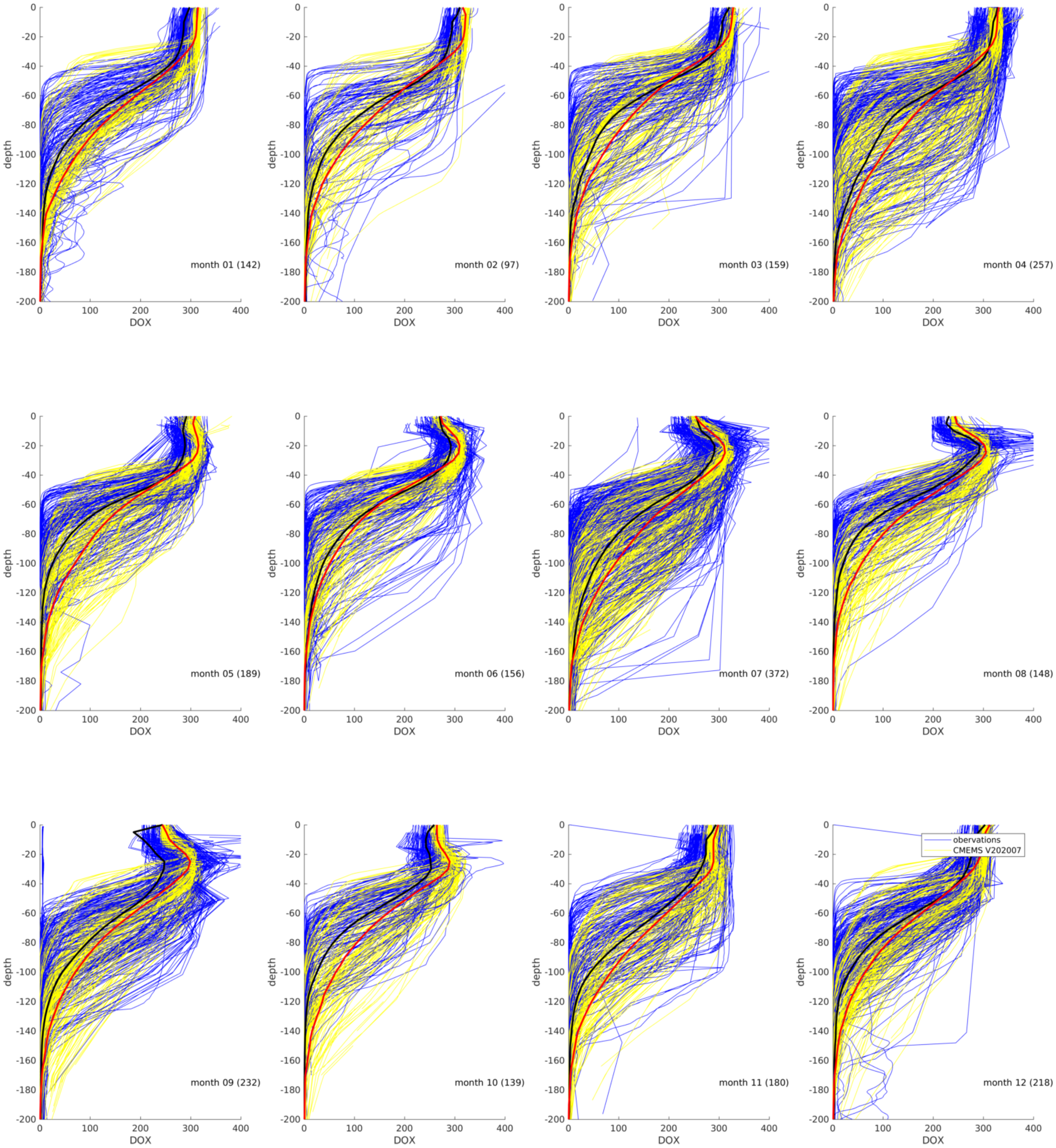


Figure 6. Oxygen profiles in the open sea region during 1992-2019. Individual and monthly mean profiles are represented respectively in blue and black (observations), and yellow and red (CMEMS V202007).

IV.2.2 The oxycline in the open sea

In the last decade, the long-term analysis of oxygen data sets shows that the oxycline has shoaled from 1955 to 2016 (Capet et al, 2016; OSR 2017). This tendency was not well represented by the earlier model versions. In the model versions starting from V3, the model temperature and salinity after 2010 were nudged toward a 2010-2014 “climatology” obtained from all available in situ data (essentially ARGO profiles). Oxygen was also slightly nudged with a longer relaxation time scale. The resulting oxygen profile was well represented by the V3 and V4 versions; the depth of the oxygen maximum and of the oxycline was shallower compared with the V2.2 model.

The V202007 model does not perform any nudging anymore, yet still it is able to represent a shoaling of the oxycline. Figure 7 represents the depth at which, in the model, the oxygen concentration falls below 20 µmol/l, for the profiles corresponding to available observations and represented in Fig. 6.

A linear fit through the points is also plotted, and clearly shows the shoaling over time (about 0.5m/year). This shoaling is studied in more detail, (but based only on observations) in the OSR2017 for the period 1955-present, and the corresponding depth is available as the “Black Sea Oxygen Penetration Depth” OMI on the CMEMS website.

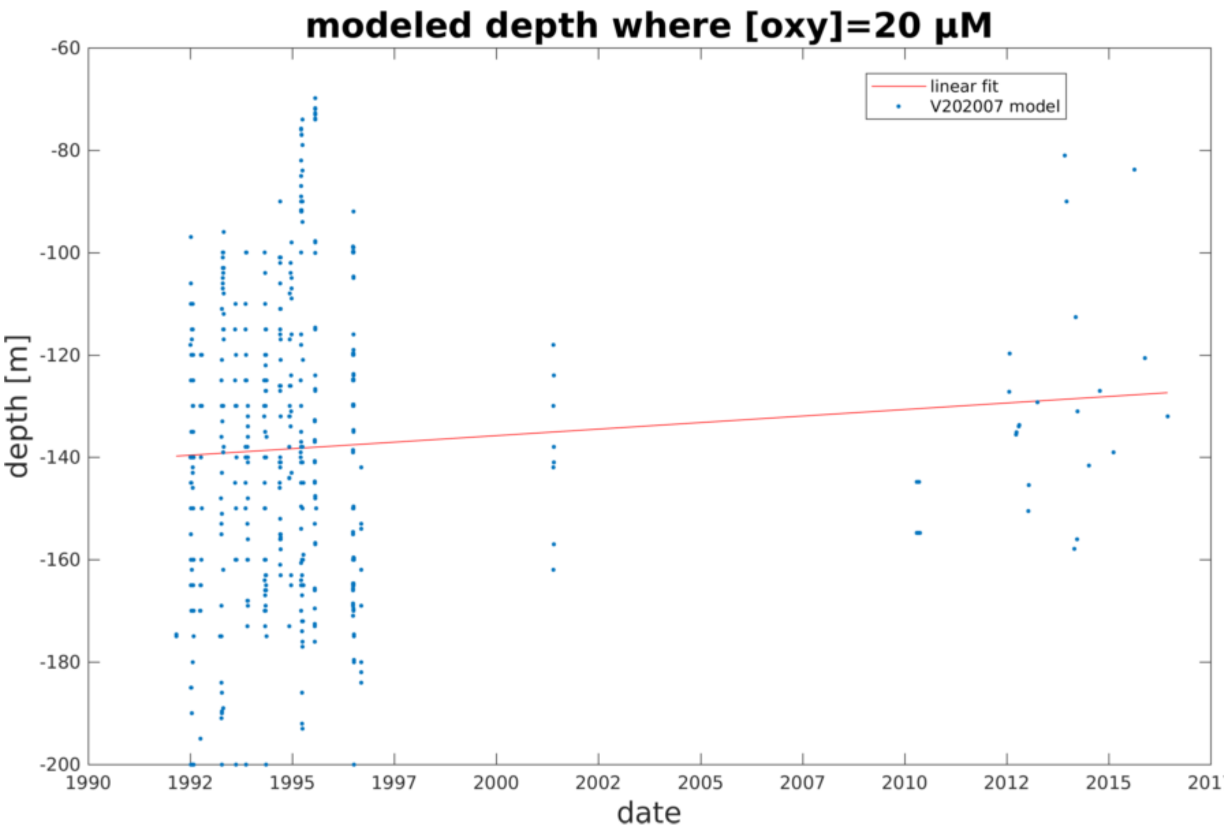


Figure 7. Blue dots: modelled depth at which the oxygen concentration is below 20 mmol/m^3. The depth is computed from the profiles in Fig. 6, corresponding to observed profiles. Red line: linear fit in the cloud of points.

IV.2.3 The nutricline

The V202007 version of the model is able to simulate the order of magnitude of nitrate concentration in the nitracline (~ 3-4 µM) (which was not the case in the previous versions of the model, Figure 8) but overestimates the vertical extension of the nitracline although it simulates quite well the disappearance of nitrates at depths. The fact that the model is able to maintain the nitracline after 20 years of integration reflects the overall good representation of the Black sea nitrogen budget. The input of fixed nitrogen brought by the rivers and the atmosphere roughly compensates the loss by benthic and pelagic denitrification and vertical export to the deep sea.

Phosphate profiles are generally well resolved by the model in the upper layers, but the model strongly underestimates the concentrations below the oxycline and upper anoxic layer. We are investigating this issue.

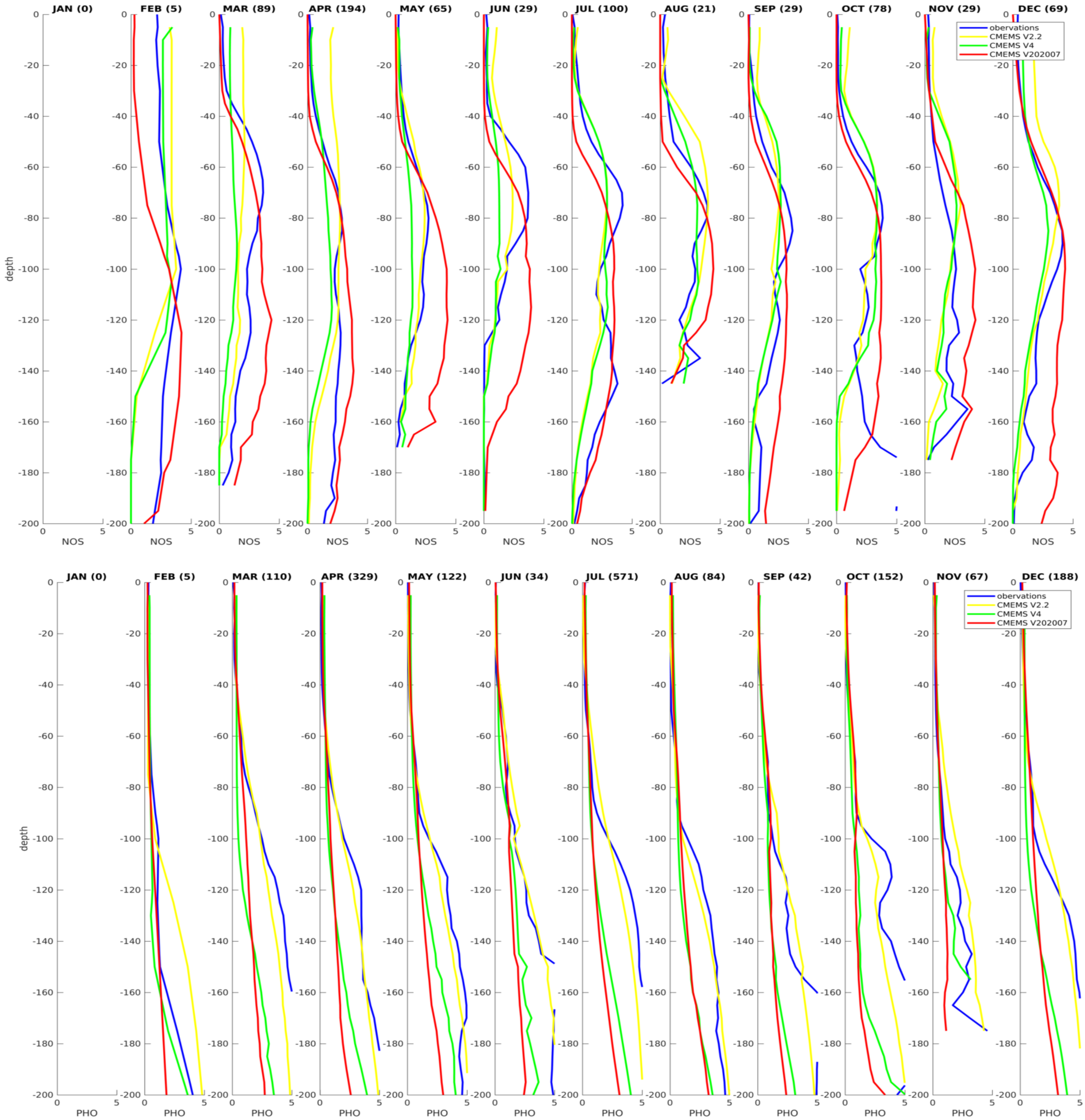


Figure 8. Nitrate (above) and phosphate (bottom) monthly mean profiles for observations (blue), CMEMS V2.2 (yellow), CMEMS V3 (green), CMEMS V202007 (red).

IV.3 The North-western shelf (NWS)

IV.3.1 Oxygen

Global statistics over the NWS

Table 5 shows the model skill statistics for the simulation of dissolved oxygen on the North Western Shelf (NWS). The global percentage of bias is small (0.85%), qualifying the model as “excellent”, and indicating that it resolves the oxygen dynamics with a very small persistent bias over the NWS during the simulated period. The standard deviation ratio is close to 1 (i.e. 1.05) (compared to 1.19 at V4); indicating that the model and observations have similar variability. The global N-S statistic of 0.88 qualifies the model as “excellent”).

Table 5: Model V202007 skill statistics obtained when considering all the observation/model prediction pairs on the NWS. Error metrics are defined in Table 2. The colours are associated to different model performances: light green being excellent, green being very good, yellow being good. The correlations coefficient has been found significant.

Metrics at V202007	Global
P.B. [%]	0.85
ρ	0.94
$N-S$	0.88
r_σ	1.05

The distribution of in situ oxygen observations has already been shown in Fig. 4. However this basin-wide view may be misleading. On the NWS, there are almost no observations during the “observation gap” (2010ies), nor during the ARGO period (2010ies). Hence most observations are available during the first ten years of the simulation. Furthermore, on the NWS, most observations are available in the Danube-influenced region (in front of Romania and in a lesser extent Bulgaria), whereas almost no observations are available in the Ukrainian waters.

Figure 9 shows a heatmap of the amount of observations on the NWS, by bins of 0.3° longitude and latitude.

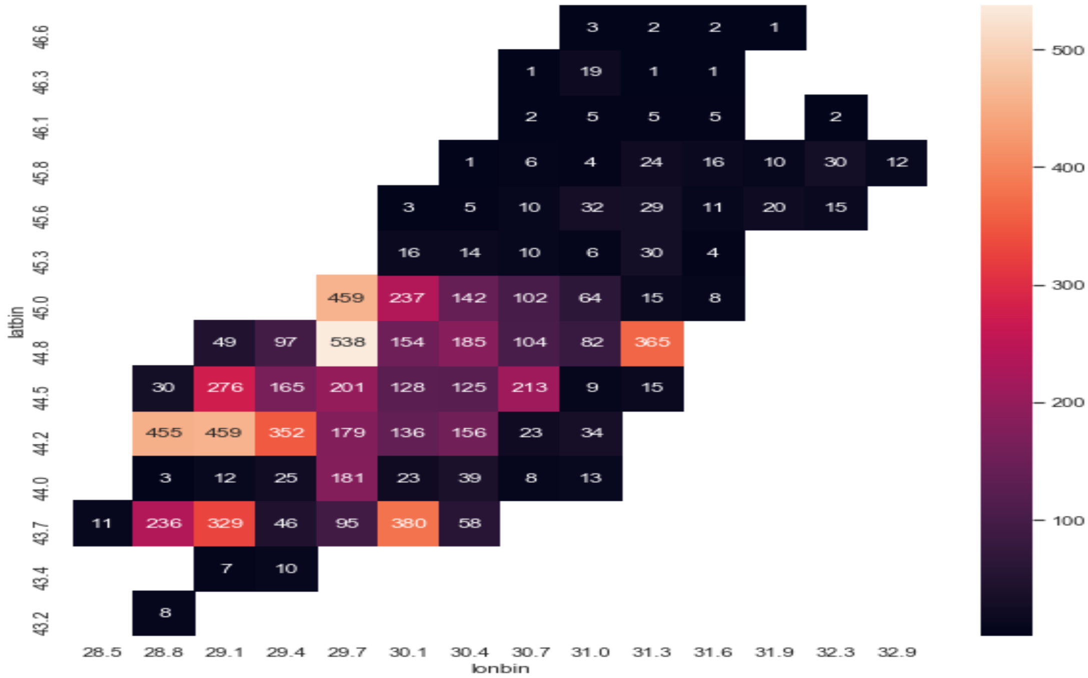


Figure 9. Heatmap representing the amount of oxygen observations on the NWS during 1992-2019

Figure 10 is the equivalent for the NWS of Fig. 5 (open sea), representing the monthly averaged oxygen profile for observations and for the model.

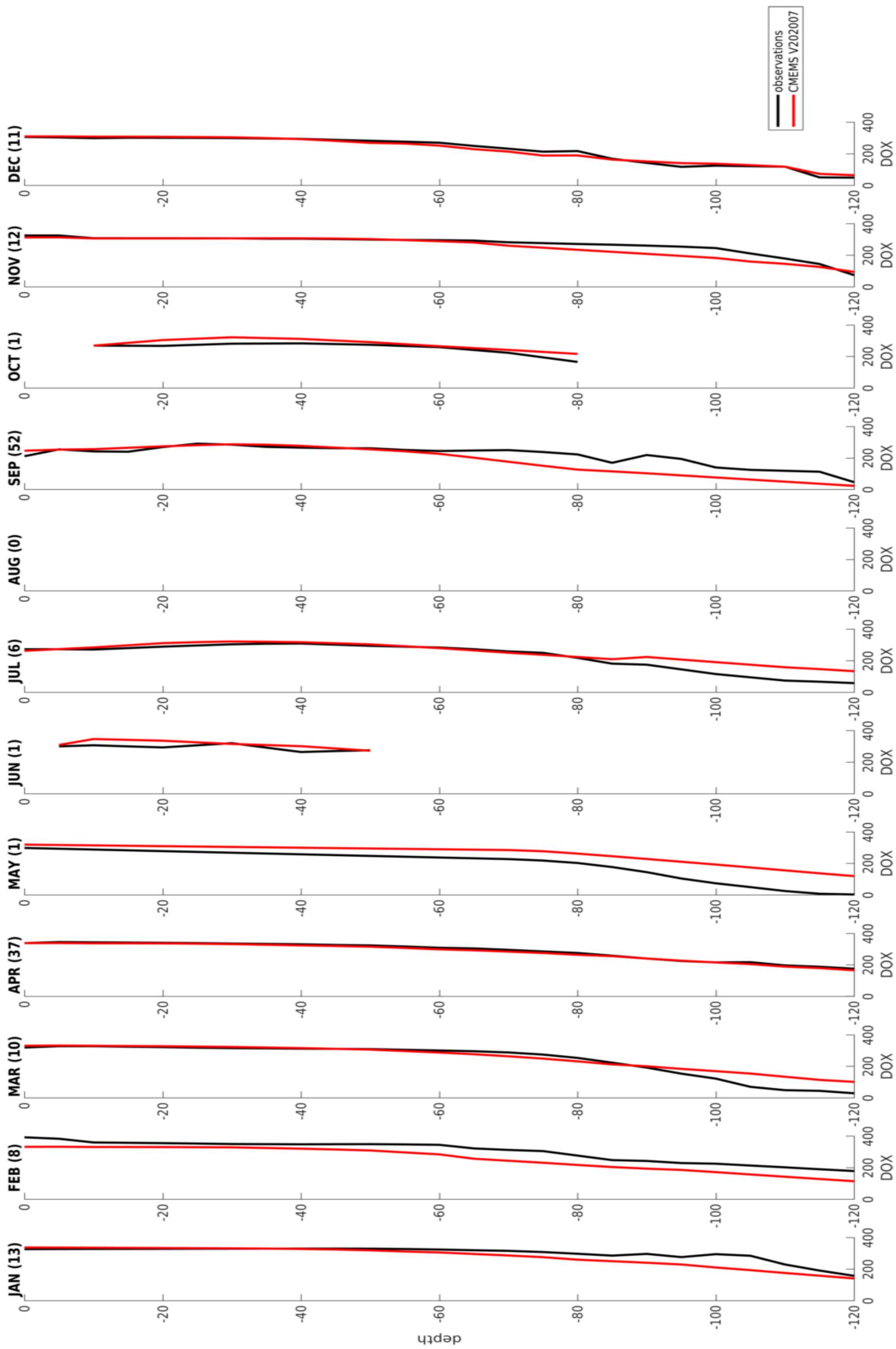


Figure 10. Point to point comparison of monthly vertical oxygen profiles in NWS: observed (black), CMEMS V202007 model (red). The number of profiles is indicated in parentheses.

In Figure 11, the NWS oxygen concentrations at the surface and on the bottom are represented for both the observations and model, again grouped by month. The model is able to represent the seasonal cycle both in the surface and on the bottom.

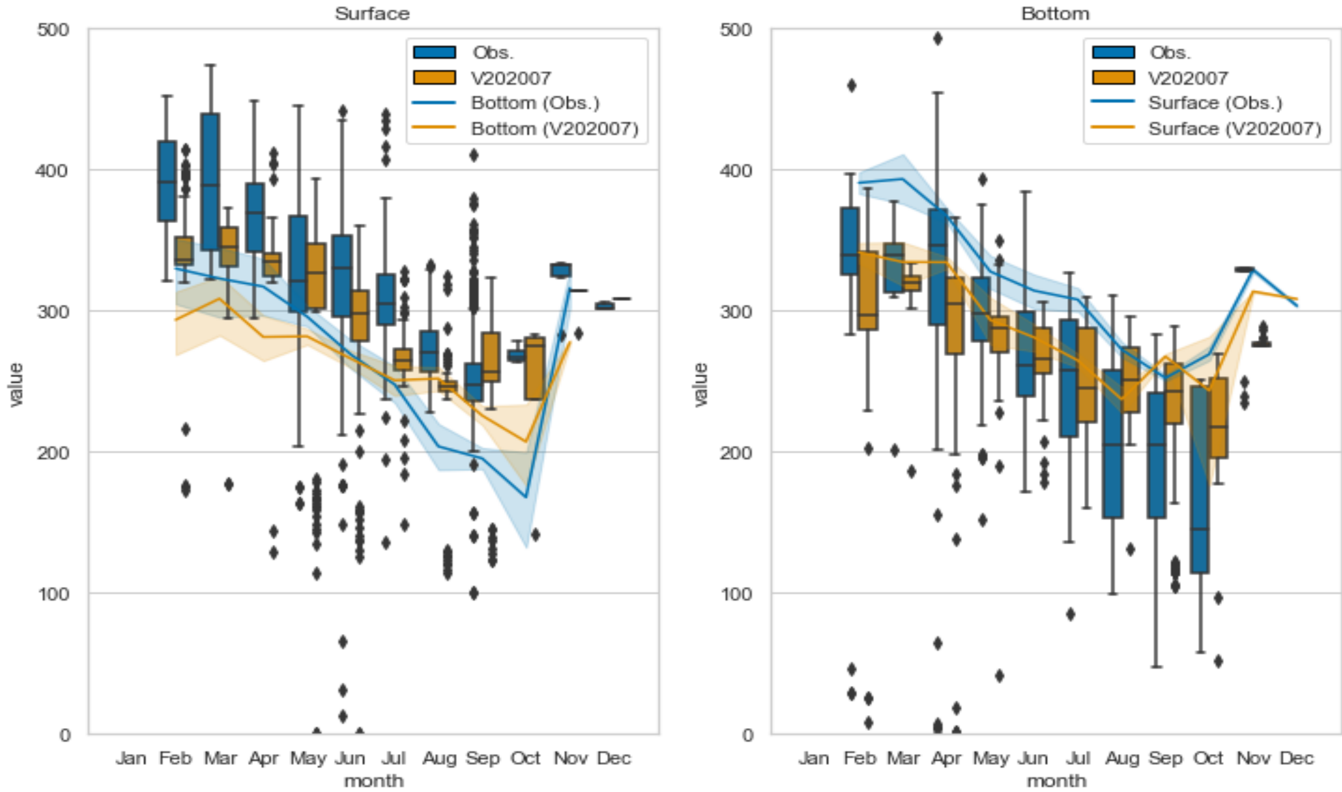


Figure 11. Monthly comparison of oxygen concentrations in NWS: observed (blue) and modelled (CMEMS V202007 - ocre). The boxes represent the median and the 25% percentiles, the bars represent the 95% percentiles. Left panel: surface values. Right panel: bottom values. The curves represent the concentrations of the other panel, so that the bottom and surface concentrations can be compared easily.

IV.3.2 Inorganic nutrients

In general, nitrate profiles are difficult to interpret: high concentrations are observed in spring, but only near the surface and very close to the river mouths. Observed nitrate levels rapidly decrease in May, while this decrease is slower in the model and lasts until August. The decrease seems to be better controlled in the CMEMS V202007 model compared to the previous versions. Finally, winter profiles are well reproduced.

The discrepancy between model simulations and observations for inorganic nutrients are essentially in the region of the Danube's mouth and in spring when the river's discharges are maximum. As concerns the nutrient discharges, the model is forced by annual loads modulated by repeated seasonal distribution for the period 1992-2010 while for 2010-2019 climatological mean values are used due to the lack of observations for these years. It is clear that the value of the inorganic nutrient concentration (NOS, PHO, Silicate, NHS) and organic matter concentration (dissolved and particulate organic nitrogen, carbon) will strongly influence the model solution on the north-western shelf and more specifically in the region of the Danube's mouth. Ideally, the values that are imposed should capture the seasonal cycle and reflect what really reaches the sea. Unfortunately, in the best case, we have annual averaged values (that we modulated with a typical seasonal cycle) and usually the values that we imposed do not take into account the filtering capacity of the Danube's delta. This may explain why the nitrate concentrations in the model are usually higher than in the observations (except in early spring).

Figure 12 is the equivalent on the NWS of Fig. 8 (open sea), showing observed profiles, and modelled profiles (CMEMS V2.2 to CMEMS V202007). As before, concerning nitrate, one can observe that the CMEMS V202007 profiles are the closest to the observed profiles, compared to the CMEMS V2.2 or CMEMS V3 profiles. For phosphates, the model concentration is too low in the deepest parts of the NWS.

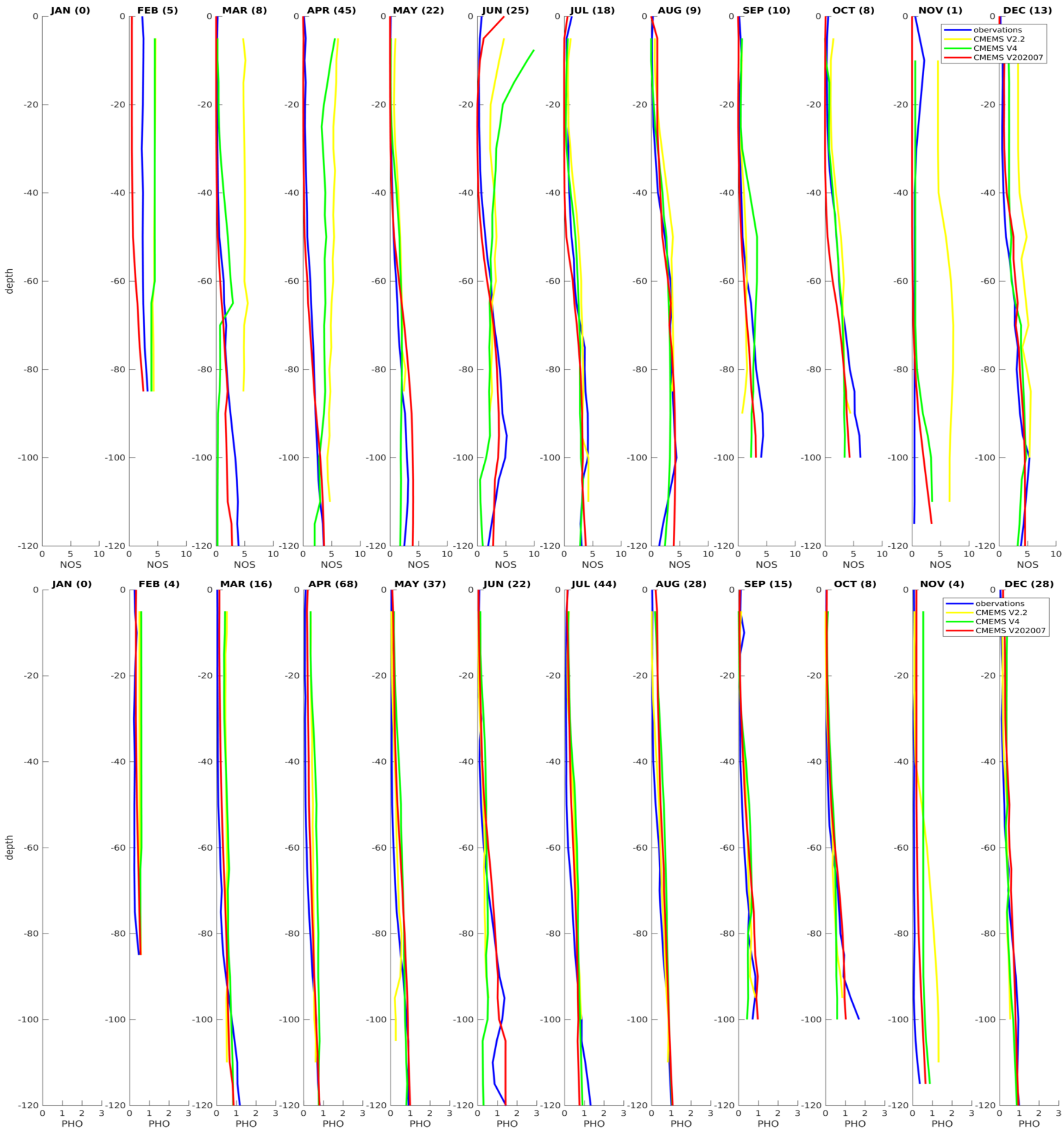


Figure 12: Monthly vertical profiles in the NWS: observed (blue), CMEMS V2.2 model (yellow), CMEMS V4 model (green) and CMEMS V202007 model (red): nitrate (top) and phosphate (bottom). Point to point comparison, the number of profiles is indicated in parentheses.

IV.4 Chlorophyll

In this section, the simulated surface chlorophyll is compared with satellite observations (CMEMS product OCEANCOLOUR_BS_CHL_L3_REP_OBSERVATIONS_009_071); the results are computed for each of the regions (see Fig. 4). Some examples of regional time series are shown in Fig. 13.

It should be reminded here that the model does not assimilate any variables during the 28 simulated years. A detailed study of the capacity of the model to reproduce the contents of the chlorophyll dynamics, as provided by satellite observations, is currently ongoing.

It appears the model surface chlorophyll content is lower than the satellite estimations in the open sea (Fig. 13, first panel), but in the right range on the NWS (Fig. 13, second panel). In front of the Danube, the model chlorophyll variability is too low (Fig. 13, third panel), whereas in other coastal areas, the model performance is good (e.g. shown for region 8 in Fig. 13, fourth panel)

The mean bias is -0.2 mg/m^3 in the open sea, 0.04 mg/m^3 in region 4 (in front of the Dnepr and Dnestr rivers), and negative between -0.1 and -0.34 in the other shelf and coastal regions. The RMS error is between 0.25 and 0.35 mg/m^3 in the open sea regions, and varies between 0.5 and 1.0 mg/m^3 in the shelf and coastal regions, except in region 5 (in front of the Danube) where it reaches 2.0 mg/m^3.

The BGC-ARGO measurements of chlorophyll cover only the last part of BLKSEA_REANALYSIS_BIO_007_005, but cannot be directly used as the Black sea requests the development of a specific algorithm for computing the chlorophyll concentration from the florescence provided by BGC-ARGO (probably due to the presence of anoxic conditions in the Black sea that would delay the degradation of pigments which makes that the classical correction cannot be made). A correction procedure has been developed at ULiege and is currently being implemented for the earlier BGC-Argo years.

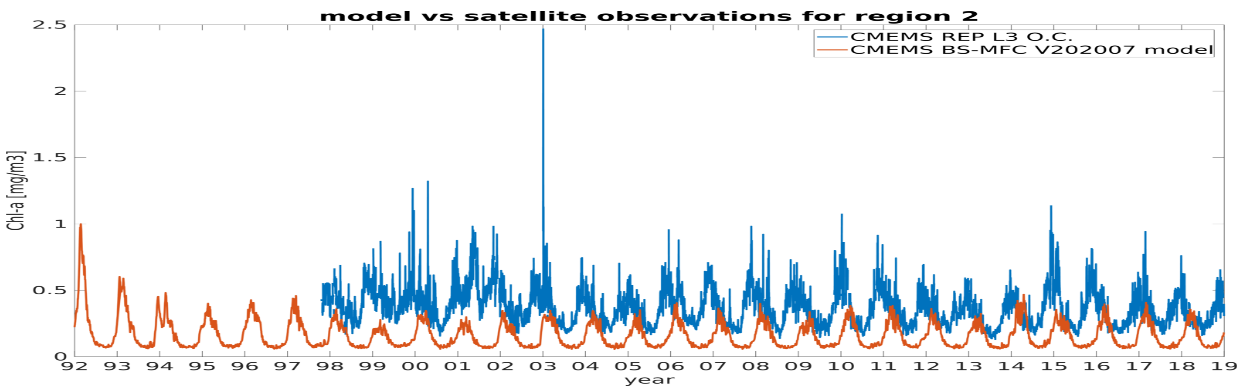


Figure 13: Time-serie of spatial average of surface chlorophyll by regions, obtained from the satellite observations (blue line) and V202007 model (red line). Upper panel: region 2 (central open sea); second panel: region 4 (northern part of the NWS) ; third panel: region 5 (NWS in front of the Romania coastline), lower panel: region 8 (Black Sea southern coastal region) (continues in next page).

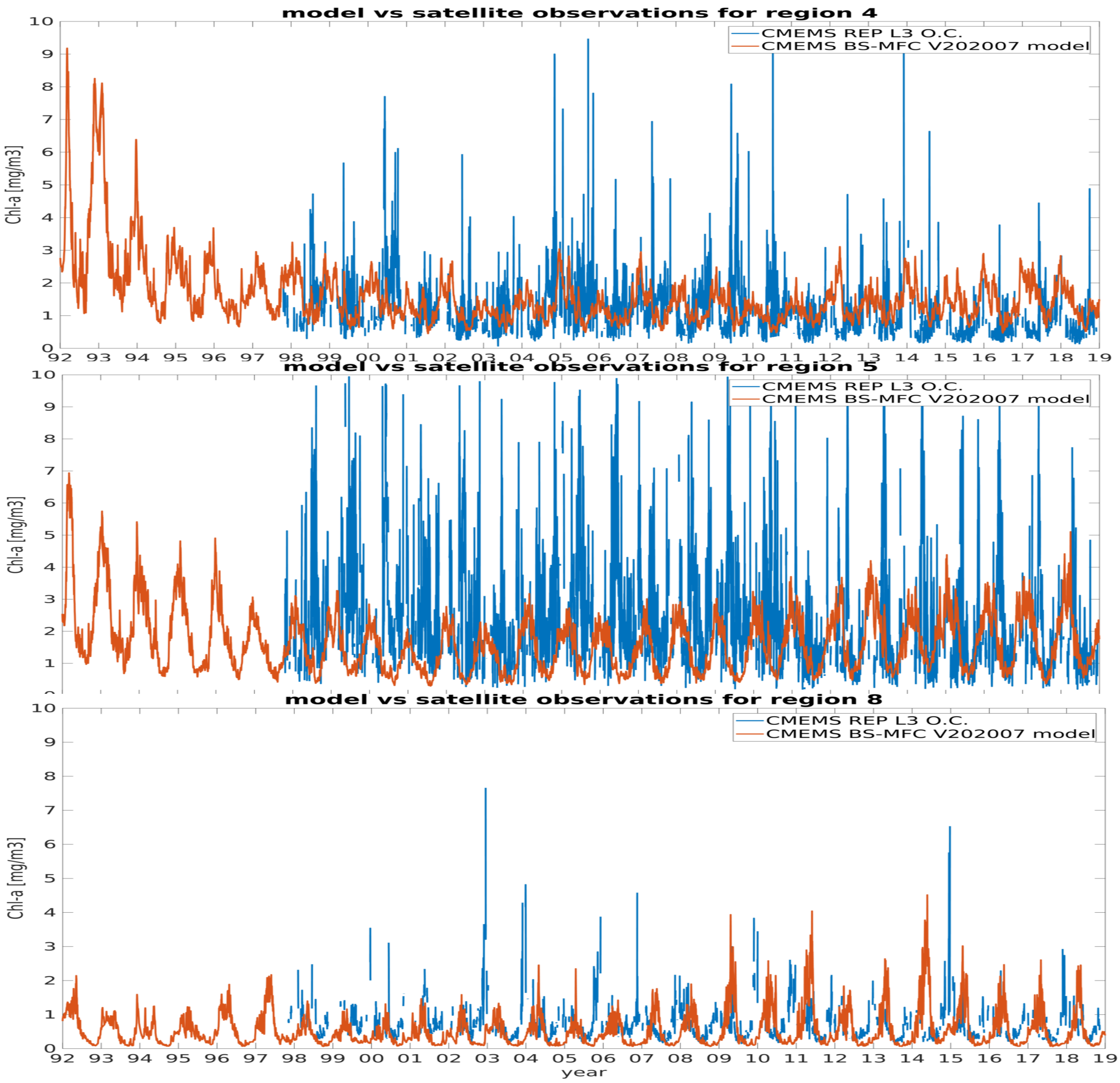


Figure 13: (continued) Time-serie of spatial average of surface chlorophyll by regions, obtained from the satellite observations (blue line) and V202007 model (red line). Upper panel: region 2 (central open sea); second panel: region 4 (northern part of the NWS) ; third panel: region 5 (NWS in front of the Romania coastline), lower panel: region 8 (Black Sea southern coastal region).

IV.5 Carbonate system

The qualitative validation of the carbonate system is realized using KNORR 88 observations described in Goyet et al. (1990), Knorr (2001) data and Sesame 2008 data (Borges, personal communication). In addition, we compared the model with typical profiles collected on a density scale and presented in Moiseenko et al. (2011).

The comparison is not done (as in previous sections) by matching observation and model pairs, but by looking at the general shape of variables (both observations and models) and qualitatively comparing them.

When comparing model values to climatologic measurements, the comparison is best performed as a function of the density anomaly, σ_t [kg.m^{-3}], instead of depth because it is well know that in the Black sea most of biogeochemical variables present particular characteristics at specific density levels. At the surface, σ_t is around 11; it increases to 14-16 in the oxycline zone, and rises up to 16.2 at the starting of the anoxic layer and to 17-17.5 at the bottom.

IV.5.1 Oxygen and nitrate

Oxygen was already quantitatively compared to observations in sections IV.2.1 and IV.3.1. Here, we confirm that the model is able to simulate the disappearance of oxygen at a density of 15.8-16 in agreement with data profiles. Fig. 14 shows the simulated oxygen on a density scale, by plotting points randomly extracted from the model results (random both in time and space). In Fig. 15, the nitracline is clearly visible around σ_t=15.2kg m^{-3} with a maximum nitrate concentration between 4 and 5 mmol.m^{-3}. Surface values are highly time- and space-dependent. In particular, on the NWS, very high values can be found close to river mouths (on the NWS shelf, blue points in the plot).

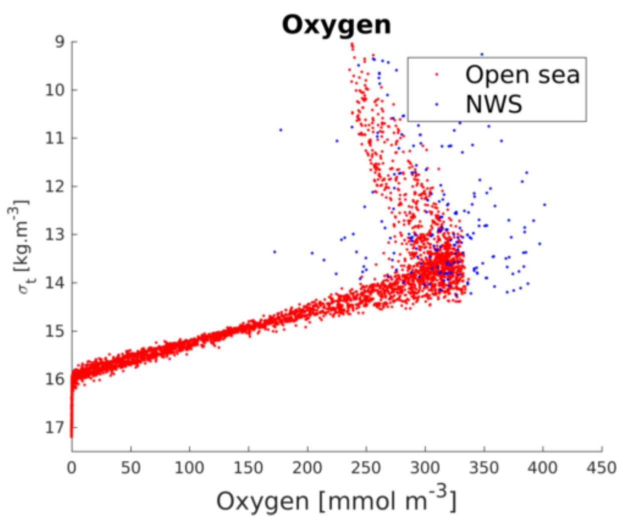


Figure 14. Oxygen as a function of the density anomaly. Vertical profiles are selected randomly in space, and throughout the simulation period (1992-2019), from V202007 model results

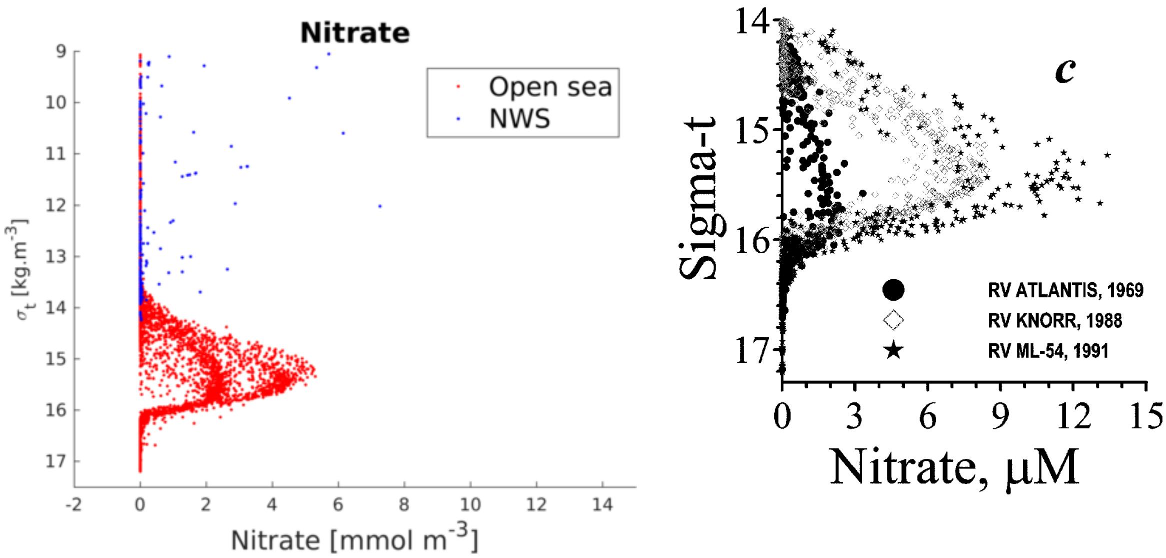


Figure 15. Nitrate as a function of the density anomaly. Left panel: CMEMS BS-MFC V202007 model (1992-2019). Right panel : reprinted from Konovalov and Murray, 2001. It should be noted that after the eutrophication period 1988-1992, it is acknowledged that the value of the nitrate peak has decreased to ~4-6 µM (Borges, 2008, unpublished Sesame data in the deep basin) which is in perfect agreement with the order of magnitude simulated by the model.

IV.5.2 Dissolved Inorganic Carbon

Concerning DIC, it can be seen that the modelled values and the ones from the literature correspond very well (Figure 16).

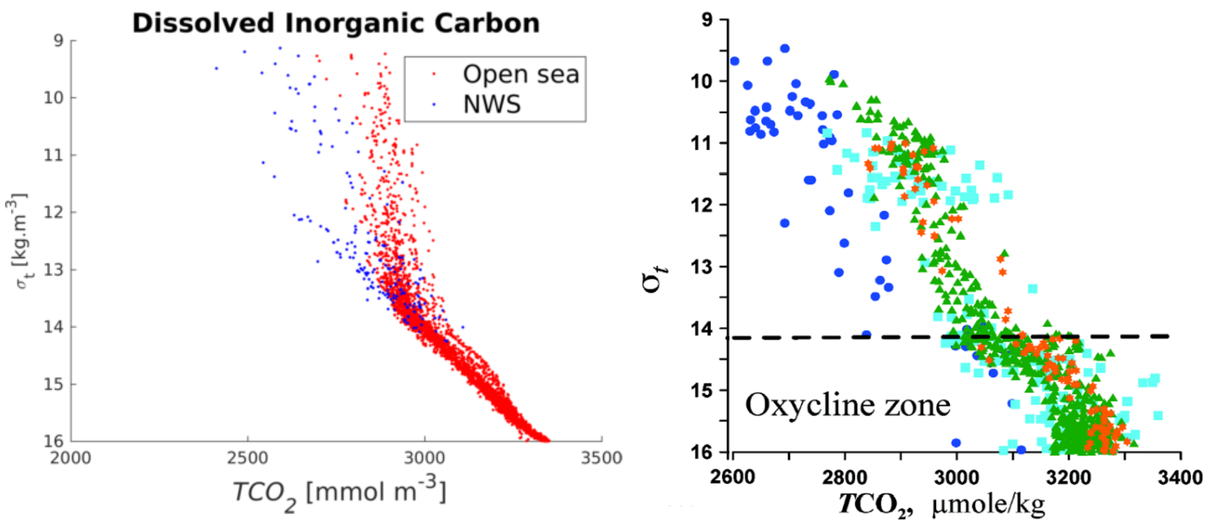
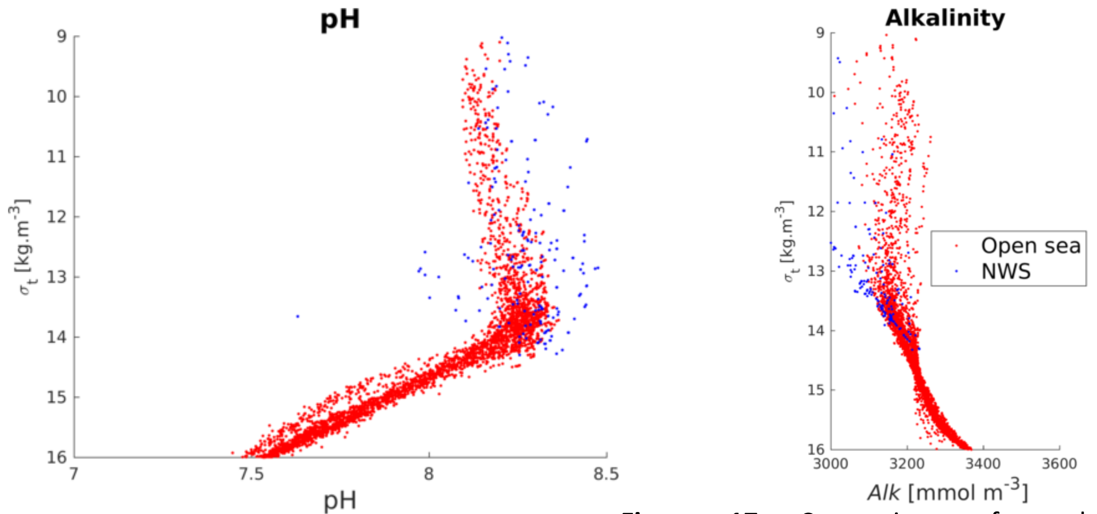


Figure 16. Dissolved Inorganic Carbon as a function of the density anomaly. Left panel: CMEMS BS-MFC V202007 model (1992-2019). Right panel: reprinted from Moiseenko et al, 2011

IV.5.3 pH and Total Alkalinity

As for DIC, values for pH and alkalinity, from the model and from the literature, are compared qualitatively. Figure 17 shows that the shape of the model profiles in function of density, as well as magnitudes of the variables, correspond very well with the climatology of observations (red stars corresponding to the 90ies)



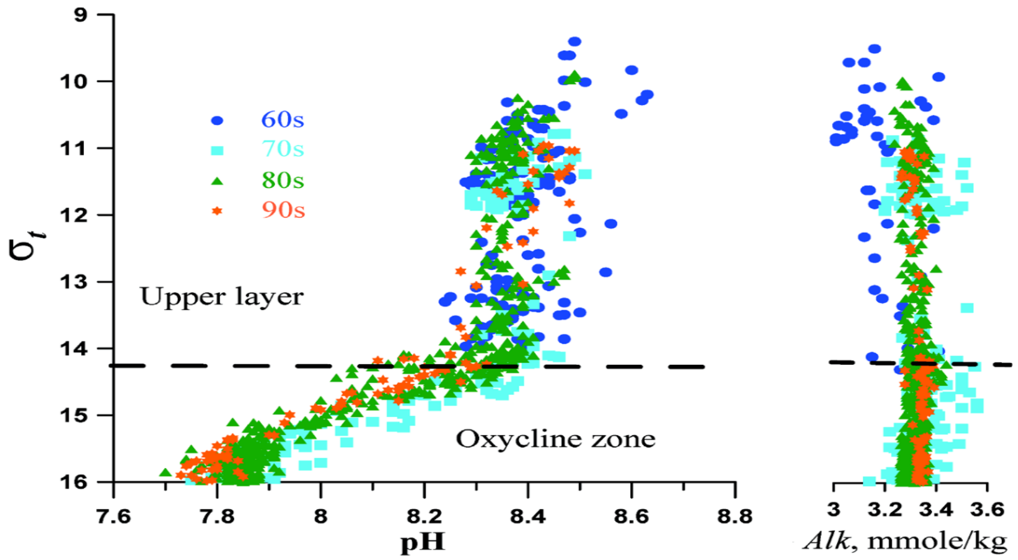


Figure 17. Comparison of model and observations of pH (left) and Alkalinity (right) as a function of the density anomaly. Top panels: CMEMS BS-MFC V202007 model (1992-2019). Lower panels: reprinted from Moiseenko et al. (2011).

IV.5.4 pC02

For the pCO2 variable, one can again see qualitatively from Fig. 18 that model and literature are in good agreement. The right panel shows a tendency of increasing values during the recent decades, the red stars corresponding to the 90ies. The pCO2 continued to increase in the 2000's and 2010s. The modeled values (left panel) correspond indeed to the upper range of the right panel.

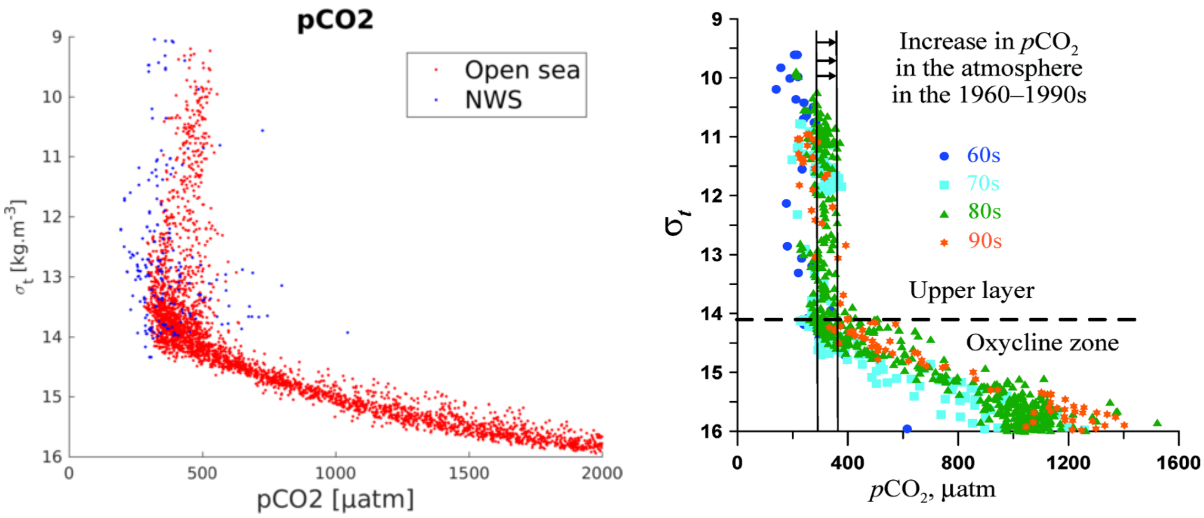


Figure 18. Comparison of model and observations of pCO2 as a function of the density anomaly. Left panel: CMEMS BS-MFC V202007 model (1992-2019). Right panel: observations, reprinted from Moiseenko et al. (2011).

V SYSTEM'S NOTICEABLE EVENTS, OUTAGES OR CHANGES

The Black Sea biogeochemistry MYP product at V202007 underwent major changes compared to previous versions:

- The physical forcing model was changed from GHER to NEMO 3.6. It is now aligned with the Black Sea physical products, and is exactly similar to the Black sea near-real time products. The horizontal resolution is aligned with the other products (~3 km), i.e. it increased compared to previous versions (~ 5 km).
- The atmospheric forcing fields are obtained from ECMWF ERA5 (previous versions used ERA-Interim).
- A carbonate system module was added to the BAMHBI biogeochemical model, allowing to deliver 2 new datasets.
- The nudging was completely removed.

Interim datasets will be operationally produced since May 2021.

VI QUALITY CHANGES SINCE PREVIOUS VERSION

Compared to previous versions, version V202007 underwent major changes listed in the previous section. There is a large beneficial impact on the quality of the chlorophyll variable. The quality of the other variables remained essentially unchanged, with some variables slightly improved and others slightly degraded.

VI.1 Details about the Interim dataset

Regarding the new Interim dataset, there are no significant changes in quality with respect to the overall timeseries as described in the document.

VII REFERENCES

	Ref	Title	Date / Version
DA 1	CMEMS-PQ-MGT	CMEMS Product Quality Management Plan	Not detailed yet
	Allen et al., 2007	Allen, J. I., Somerfeld, P., Gilbert, F., 2007. Quantifying uncertainty in high-resolution coupled hydrodynamic-ecosystem models. *Journal of Marine Systems,* 64 (1-4), 3(14), contributions from Advances in Marine Ecosystem Modelling Research, 27-29 June, 2005, Plymouth, UK, AMEMR.	
	Capet et al., 2016a	Decline of the Black Sea oxygen inventory. Biogeosciences 2016	
	Capet et al., 2016b	Integrating sediment biogeochemistry into 3D oceanic models: A study of benthic-pelagic coupling in the Black Sea. Ocean Modelling, 2016	
	Capet et al., 2013.	Capet, A., Beckers, J.-M., & Grégoire, M. (2013). Drivers, mechanisms and long-term variability of seasonal hypoxia on the Black Sea northwestern shelf – is there any recovery after eutrophication? Biogeosciences, 10, 3943-3962	
	Capet, 2014	Study of the multi-decadal evolution of the Black Sea hydrodynamics and biogeochemistry using mathematical modelling. PhD Thesis, Université de Liège, 2014	
	Gregoire et al., 2008.	Grégoire, M., Raick, C., & Soetaert, K. (2008). Numerical modeling of the deep Black Sea ecosystem functioning during the late 80's (eutrophication phase). Progress in Oceanography, 76(9), 286-333.	
	Gregoire and Soetaert, 2010.	Grégoire, M., and Soetaert, K. (2010). Carbon, nitrogen, oxygen and sulfide budgets in the Black Sea: A biogeochemical model of the whole water column coupling the oxic and anoxic parts. Ecological Modelling, 15.	
	Kopolevich et al., 2003	Kopelevich O. V., S.V. Sheberstov, I.V. Sahling, S.V. Vazyulya, V.I. Burenkov (2013). Bio-optical characteristics of the Russian Seas from satellite ocean color data of 1998-2012. Proceedings of the VII International Conference "Current problems in Optics of Natural Waters (ONW 2013)", St.-Petersburg (Russia), September 10-14, 2013.	
	Joassin, 2011	Joassin, P., 2011. Mathematical modeling of biogeochemical processes associated to a coccolithophorid (emiliania huxleyi) bloom - study of the seasonal and long-term variability of biogeochemical properties in the Black Sea using a data interpolating variational analysis (DIVA). Ph.D. thesis, Université de Liège.	
	Maréchal, 2004.	Maréchal, D., 2004. A soil-based approach to rainfall-runoff modelling in ungauged catchments for England and Wales. PhD thesis, Cranfield University. 157 pp.	
	Stanev and Beckers, 1999	Numerical simulations of seasonal and interannual variability of the Black sea thermohaline circulation. Journal of Marine Systems 22	
	Vandenbulcke, 2015	The seamod.ro operational stochastic Black Sea forecasting system. Ocean Modelling, 2015	