QUALITY INFORMATION DOCUMENT

North West European Shelf Production Centre
NORTHWESTSHELF_REANALYSIS_BIO_004_011

Issue: 4.2

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Approval date by the CMEMS product quality coordination team: 13/05/2019

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	January 2014	All	Creation of the document for V4.0	Sarah Wakelin	Ed Blockley
2.0	December 2014	All	Addition of biological product assessment (BIO_004_011)	Robert McEwan	Ed Blockley
2.1	February 2015	All	Revision after acceptance V5		Ed Blockley
2.2	13/03/2015	I. 2, II	Warning remarks after evidence of 004_011 interannual nutrient drifts		Ed Blockley
2.3	May 1 2015	all	Change format to fit CMEMS graphical rules		L. Crosnier
3.0	21/01/2016	all	Update for V2 (time series extension to 2014 and addition of MLD)	Sarah Wakelin, Jon Tinker	Marina Tonani
3.0	01/04/2016	all	Revision after V2 AR	Marina Tonani	Marina Tonani
4.0	01/09/2018	all	New version for Copernicus V4 (BIO only)	Susan Kay, Robert McEwan, David Ford	Ina Lorkowski
4.1	17/01/2019	all	The reanalysis was extended to December 2017, with no changes in quality.	Susan Kay	Marina Tonani
4.2	19/04/2019	all	The reanalysis was extended to December 2018, with no changes in quality.	Susan Kay	Marina Tonani

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I EXECUTIVE SUMMARY

I.1 Products covered by this document

NORTHWESTSHELF_REANALYSIS_BIO_004_011: The biogeochemical part of a North West European Shelf Reanalysis performed at ~7km resolution, 1998-2018.

I.2 Summary of the results

The quality of the NWS reanalysis simulation NORTHWESTSHELF_REANALYSIS_BIO_004_011 from 01/01/1998 to 31/12/2016 has been assessed by comparison with observations. With the exception of satellite estimates of chlorophyll from ocean colour observations, the observational data is unevenly distributed in time and space, and quantitative estimates of accuracy should be used with caution.

Chlorophyll: the reanalysis reproduces the spatial and temporal variation of surface chlorophyll seen by satellite, though winter values are lower in model outputs than in satellite (Figure 3), giving an overall median bias of -0.12 mg m^{-3} for the continental shelf (Table 3). Model-satellite correlation is above 0.66 for most regions. Comparison to in situ data, at all depths, has a similar correlation but lower bias (Table 4).

Nitrate: Comparison of surface nitrate to climatology shows that the seasonal cycle is well reproduced (Figure 10). The reanalysis shows a positive bias compared to in situ observations, largest in the Southern North Sea and English Channel (Table 5).

Phosphate: Comparison of surface phosphate to climatology shows that the seasonal cycle is well reproduced, but summer values are lower in the model than observations (Figure 12). There is also a negative bias in the reanalysis compared to in situ observations, except for Southern North Sea and the off-shelf area (Table 6).

Oxygen: Compared to a climatology of observations, the reanalysis values are consistently low, but show the same temporal and spatial patterns (Figure 14). The negative biases are associated with a small positive temperature bias. The model-observation correlation is 0.6 or higher in all areas except the English Channel (Table 7).

pCO_2: Sparsity of observational data makes the model quality difficult to assess, but comparison to the available data suggests that the model has some skill, particularly in shallower areas (Table 8).

pH: Fewer observations are available than for other variables, but on the evidence available the model shows some skill in all regions (Table 9).

I.3 Estimated Accuracy Numbers

Surface log-chlorophyll accuracy, based on the match to daily ocean colour satellite values:

Table 1 Estimated accuracy numbers for surface log10-chloropyll, chlorophyll units mg m^{-3}

Region	**Mean bias** (model mean – observation mean)	**Root mean square error**	**Median bias** (model median – observation median)	**Median absolute error**
Continental Shelf	-0.17	0.51	-0.08	0.16
Offshelf	-0.19	0.81	-0.02	0.16
Full domain	-0.18	0.73	-0.04	0.16

The ocean colour data is taken from the CMEMS catalogue, product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098, 1998-2016. The mean bias of the log-transformed data is -0.01 and the root mean square error 0.26 (from the product QUID).

The following table shows estimated median bias (model-observation) and median absolute error for the on-shelf part of the model domain, based on match-ups to in situ observation. **The estimates should be used with caution**: the in situ measurements are not distributed evenly in time or space and their accuracy is not known. Users are advised to consult the tables in section IV for more information about accuracy within each region: there is considerable variation between regions.

Table 2 Estimated accuracy numbers based on comparison to insitu data for chlorophyll (all depths, actual concentration, not log), nitrate, phosphate, oxygen, surface pCO_2 and pH, for the on-shelf part of the model domain.

Variable	**Median bias (model-observation)**	**Median absolute error**	**Spearman correlation**
chlorophyll	-0.05 mg m^{-3}	0.68 mg m^{-3}	0.69
nitrate	4.0 mmol m^{-3}	5.3 mmol m^{-3}	0.39
phosphate	-0.07 mmol m^{-3}	0.23 mmol m^{-3}	0.44
oxygen	-16 mmol m^{-3}	20 mmol m^{-3}	0.68
Surface pCO_2	0.75 Pa	4.4 Pa	0.18
pH	0.001	0.055	0.20

Note that the accuracy measures use robust statistics: median bias, median absolute error and Spearman rank correlation. Robust statistics are independent of the distribution of the dataset, and so are more appropriate for biogeochemical variables, which often have a non-Gaussian distribution and contain outliers that can distort measures such as the mean. See section III for more information about the metrics used.

II PRODUCTION SYSTEM DESCRIPTION

Production centre name: Met Office, UK

Production system name: North West European Shelf Reanalysis biogeochemistry (CMEMS names: NORTHWESTSHELF_REANALYSIS_BIO_004_011)

Description

The North West shelf reanalysis was produced using the Forecasting Ocean Assimilation Model 7km Atlantic Margin model (FOAM AMM7) which is comprised of version 3.6 of the Nucleus for European Modelling of the Ocean (NEMO) ocean model code (Madec et al., 2016) coupled to the European Regional Seas Ecosystem Model (ERSEM 15.06; Butenschön et al. 2016). Surface chlorophyll values, estimated from satellite ocean colour measurements, were assimilated using the 3D-Var NEMOVAR scheme (Skákala et al., 2018; Waters et al., 2015).

The model is located on the European North-West continental Shelf (NWS), from 40°N, 20°W to 65°N, 13°E (boundary region masked), on a regular lat-lon grid with 1/15° latitudinal resolution and 1/9° longitudinal resolution (approximately 7km square). The model domain is shown in Figure 1, partitioned into shallow (on shelf) and deeper (off shelf) waters. Although the domain extends beyond the shelf to include some of the adjacent North-East Atlantic, the focus of this system is on the shelf itself and the deep water is primarily included to ensure there is appropriate cross-shelf exchange. Thus a hybrid s-sigma terrain following coordinate system (following Siddorn and Furner, 2013) with 51 levels is employed in order to retain vertical resolution on the shelf. However, in order to make analysis and visualization easier for users, the products are delivered on 24 geopotential (z-level) vertical levels based upon the ICES standard depths. Gridpoints near to the model boundaries are strongly affected by the model boundary conditions and so products are provided for the interior of the domain only. The outermost 10 gridpoints and points East of 10°E on the Baltic boundary are masked.

For full details of the physical modelling system, its forcing data and product quality please see the Quality Information Document for that system (CMEMS_NWS_QUID_REAN_PHYS_004_009.pdf).

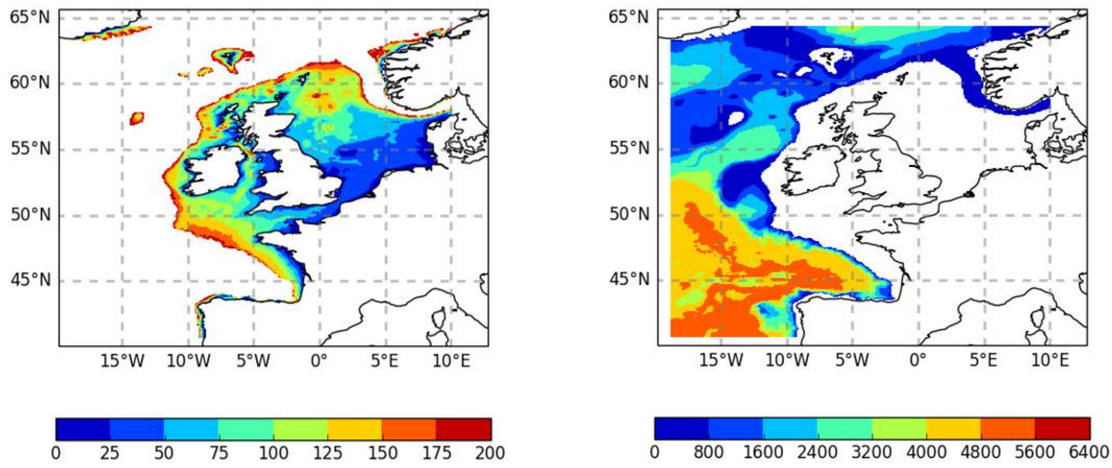


Figure 1 FOAM AMM7 bathymetry showing (left) the domain on the European North West Shelf (defined here as total depth less than 200m) and (right) the domain off the shelf.

ERSEM is a marine biogeochemistry model which simultaneously describes pelagic and benthic ecosystems in terms of phytoplankton, bacteria, zooplankton, zoobenthos and the biogeochemical cycling of C, N, P and Si. ERSEM uses a functional group approach to describe the ecosystem, whereby biota are grouped together according to their trophic level (subdivided according to first size, then trophic role and finally feeding method). Four functional groups of phytoplankton are included, three of zooplankton and one of bacteria. The dynamics of biological functional groups are described by both physiological (ingestion, respiration, excretion and egestion) and population processes (growth and mortality). The differences between the functional groups mainly lie in the rate constants, which are derived from the literature or from allometric considerations and in the food components on the uptake side. Production of the phytoplankton groups is driven by broadband photosynthetically active radiation (PAR), and underwater light field computed with the Beer-Lambert equation of light attenuation.

The version of ERSEM, 15.06, differs from that used in the previous NWS reanalysis in the following key ways:

- It now includes the carbonate system, enabling pCO_2 and pH to be included in the available products.
- The light model has been changed so that the diffuse attenuation coefficient is computed by using broadband absorption and backscattering (i.e. the “Inherent Optical Properties”) of the phytoplankton groups, of water, and of coloured detrital matter and other non-modelled material; the latter is nudged towards climatological satellite data. Suspended particulate matter is not explicitly included in the model.
- The model parameters have been revised and updated; they now match those given by Butenschön et al. (2016).
- ERSEM is now coupled to the NEMO physical model through the Framework for Aquatic Biogeochemical Models (FABM, Bruggeman and Bolding, 2014), which gives greater flexibility. However, this layer is not visible to the end user.

Full information on ERSEM can be found in Butenschön et al. (2016) and references therein.

Remotely sensed ocean colour data are assimilated using the 3D-Var NEMOVAR scheme (Skákala et al., 2018; Waters et al., 2015). Total chlorophyll-a concentration observations are taken from the European Space Agency Climate Change Initiative (ESA CCI) v3.1 daily merged product, CMEMS product OCEANCOLOUR_GLO_CHL_L3_REP_OBSERVATIONS_009_065, and bias corrected following Ciavatta et al. (2016). NEMOVAR is used to calculate increments to the model surface chlorophyll-a concentration, and these increments are split between the four phytoplankton functional types in ERSEM so as to maintain their existing background ratios. Similarly, levels of C, N, P and Si within phytoplanton are updated so that the assimilation does not directly alter the phytoplankton stoichiometry. All increments are applied equally through the mixed layer using incremental analysis update (Bloom et al., 1996). Concentrations of dissolved nutrients are not updated but adjust in response to the changes to phytoplankton. The assimilation configuration is very similar to that described for total chlorophyll by Skákala et al. (2018), except for some minor differences in error specification, and the use of two equally-weighted correlation length scales, equal to the Rossby radius and 100 km, to provide short- and long-scale corrections respectively. The ocean colour product was not continued after 28/10/2018, so for the remaining days of the run a comparable near-real-time product was used: OCEANCOLOUR_ATL_CHL_L3_NRT_OBSERVATIONS_009_036. This might produce a small discontinuity at the end of October 2018; however, this is the winter period, when biogeochemical activity is low, so the effect is minor and the estimated accuracy numbers are not affected.

The ecosystem model used climatologies for the boundary conditions and river inputs: nitrate, phosphate, silicate and oxygen from World Ocean Atlas 2013v2 (WOA, Garcia et al., 2014a,b); alkalinity and dissolved inorganic carbon from GLODAPv2 (Key et al., 2015, and Lauvset at al., 2016) and river nutrient concentrations from a daily climatology as used in the previous NWS reanalysis. Nitrogen deposition at the surface used data from the EMEP project (http://www.emep.int); the last available year is 2015, so the 2015 values were repeated for 2016 and 2018. The ecosystem model is forced by the physical model via an online coupling and is run at the same time step as the physical model (300s).

The reanalysis covers the period 01/01/1998 to 31/12/2018.

Users requiring physical variables for use with the biogeochemical variables provided in this product should use NORTHWESTSHELF_REANALYSIS_PHYS_004_009. This was created using the same physical model, boundary conditions and forcing data as the biogeochemical reanalysis, but with the addition of assimilation of sea surface temperature and profiles of temperature and salinity; the assimilation was found to create some degradation of the biogeochemical outputs and so was not used in this reanalysis. This means that there are some local differences between the physics reanalysis and the physics of the model run reported here, but the biogeochemical outputs are considered to be consistent with either physics set to within their reported level of accuracy. The difference is most likely to be relevant for studies looking at small-scale features and for values close to the mixed layer depth, where greater inaccuracy in the biogeochemical products should be assumed.

III VALIDATION FRAMEWORK

The products assessed are chlorophyll, nitrate, phosphate, oxygen, pCO_2 and pH.

Model surface chlorophyll is compared to daily satellite ocean colour measurements (CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098) to give monthly maps for the whole domain and statistics for sub-regions. This is a different ocean colour product from that assimilated during the reanalysis.

Model nutrients and oxygen are compared to climatological fields from the World Ocean Atlas 2013 (WOA, Garcia et al., 2014a,b) to give monthly maps.

Time series of surface chlorophyll, nutrients and oxygen are compared to in situ measurements from the Western Channel Observatory (point L4; 50°15.0'N, 4°13.0'W, www.westernchannelobservatory.org.uk, Figure 2).

All assessed variables except pCO_2 are compared to in situ measurements from the database of the International Council for the Exploration of the Sea (ICES, 2014), to give statistics summarised in target diagrams. In situ data for surface pCO_2 data is taken from the SOCAT database (Bakker et al., 2016) and the ICES data for pH is supplemented by additional data from GLODAPv2 (Key et al., 2015 and Lauvet et al., 2016).

Robust statistics have been used in all analyses. These are independent of the distribution of the data and so avoid distortion by outliers. Metrics used are:

Number of matched observations (n) All metrics are based on the set of observations and a set of model outputs matched in time and space. In situ (ICES, SOCAT and GLODAPv2) observations were matched to the monthly mean model outputs: a match was considered valid if it was in the same grid cell, within 2 m vertically and 15 days of the observation. Daily ocean colour data was matched to the daily mean surface model outputs for all grid cells where satellite data was available. For the match to the in situ data, where observations are sparse in some areas, the number of matched points is shown in the tables in section IV.

Median Bias: the difference between the median of the model data and the median of the observation (reference) data. This gives an indication of consistent differences between the model and observation, with positive bias meaning the model is higher than observation.

$$Bias = median(x_{model}) - median(x_{reference})$$

Median absolute error (MAE): the median of the absolute difference between the model and observation values at each point. This indicates the average size of the difference between model and observation.

$$MAE = median(abs(x_{model} - x_{reference}))$$

Spearman rank correlation coefficient: this is the Pearson correlation coefficient between the ranked values of the model and observation data: if the model data increases when the observations do, they are positively correlated. It can be interpreted in the same way as the Pearson correlation, i.e. 1 shows perfect correlation and 0 shows no correlation.

Target diagrams: these show the MAE plotted against bias, with both normalised by the interquartile range (IQR) of the observation data, i.e. the difference between the 75th and 25th percentile, a robust measure of the spread of the data. The MAE is unbiased by subtracting the median at each data point for both model and observation dataset. The sign of the x-value is given by the difference between the IQR for the model and reference data. Thus the closer to (0,0) the better the match between model and observation; values to the left of the y-axis show that model has less spread (variability) than observation and negative y-values show that the model values are on average smaller than observations.

x-axis:

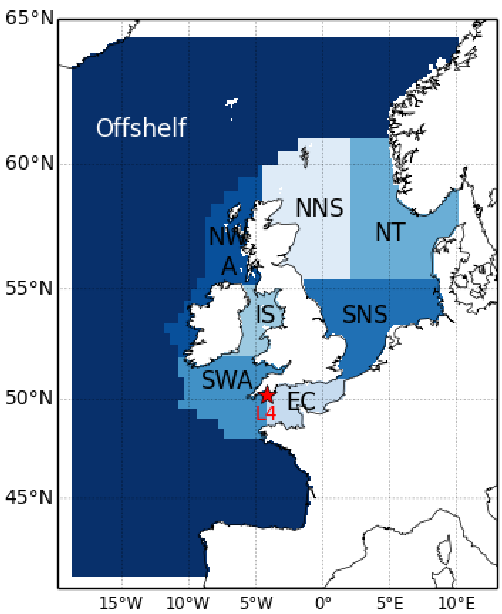
$$sign(IQR_{model} - IQR_{reference}) * \frac{median\left(abs\left(\left(x_{model} - median(x_{model})\right) - \left(x_{reference} - median(x_{reference})\right)\right)\right)}{IQR_{reference}}$$

y-axis:

$$\frac{median(x_{model}) - median(x_{reference})}{IQR_{reference}}$$

In the tables in section IV the bias and MAE are given without normalisation and have the same units as the model; the normalised values used in the target diagram are unitless.

Statistics have been calculated for the whole model domain and for various subregions – see Figure 2 for the location of these regions.



Regions:

EC: English Channel

IS: Irish Sea

NNS: Northern North Sea

NT: Norwegian Trench

NWA: North Western Approaches

SNS: Southern North Sea

SWA: South Western Approaches

The Continental Shelf regions includes all the above, i.e. all regions except Offshelf.

Observation stations:

L4: station L4 of the Western Channel Observatory

Figure 2 Regions and observing stations referred to in this document.

IV VALIDATION RESULTS

IV.1 Chlorophyll

Comparison of monthly mean surface chlorophyll from the reanalysis to ocean colour satellite values (Figure 3, Figure 4, Figure 5, Table 3 and Figure 6) shows that the model reproduces the spatial and temporal variation seen by satellite, though winter values are lower in model outputs than in satellite. This is reflected in the bias figures, which are negative overall because of the low winter values. The model's peak chlorophyll values are higher than satellite in most, but not all, years; however the histogram of log10-chlorophyll (Figure 5) shows that high values are more common in the observations. Since log-chlorophyll is approximately normally distributed it is appropriate to summarise the comparison by the difference between the model and satellite mean, -0.17 for the on-shelf region, and the root mean square difference, 0.51 (see Table 1 for other accuracy statistics for log-chlorophyll). The QUID for the ocean colour product gives its bias as -0.01 and rmsd as 0.26 (using log-transformed values).

For the subregions, the correlation is above 0.66 for most regions (Table 3), reflecting good ability to capture spatial and temporal patterns in these regions. The bias is negative for all regions, but well below the variability of the observations (Figure 6). Accuracy is relatively low (high MAE) in the Southern North Sea and Irish Sea, but the correlation is good for these areas and the MAE in relation to the variability of observations is similar to that of other regions.

It should be remembered that ocean colour data is less reliable for the winter months, when cloud obscures much of the imagery, and in areas strongly influenced by sediment, such as the southern North Sea.

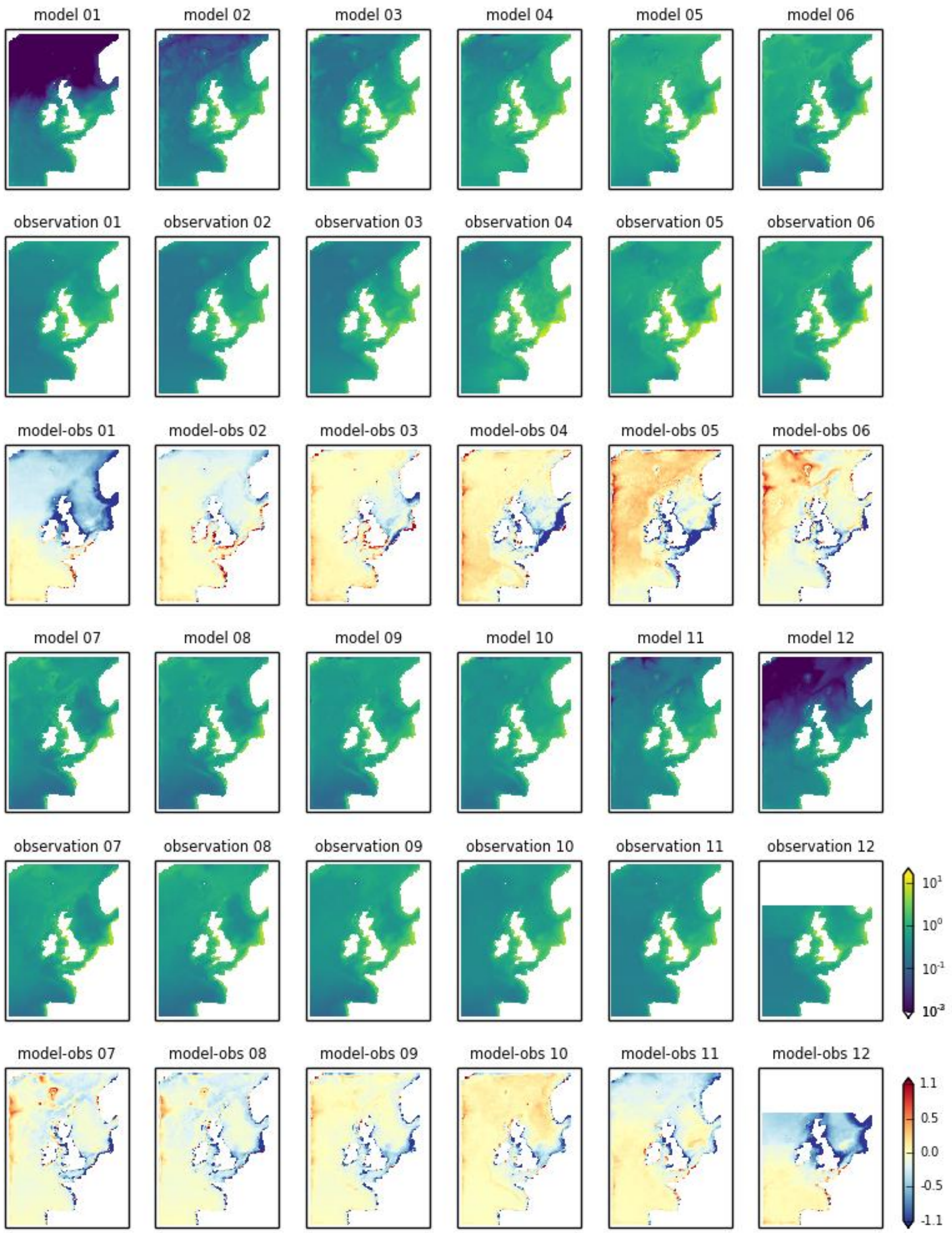


Figure 3 Mean monthly surface chlorophyll concentration from the reanalysis (top row) and ocean color satellite (middle row) and the difference between the mode and ocean colour values (bottom row). All plots show the mean for1998-2016. The ocean colour data comes from CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098, daily values, regridded to match the model.

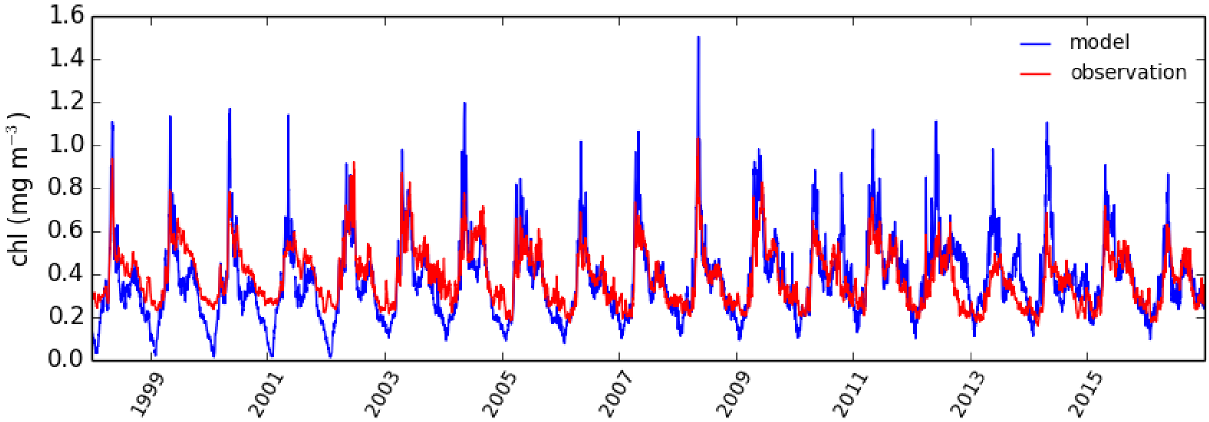


Figure 4 Time series of surface chlorophyll concentration from the model (blue) and ocean colour satellite (red), daily median for the whole domain. The ocean colour data comes from CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098, daily values, regridded to match the model.

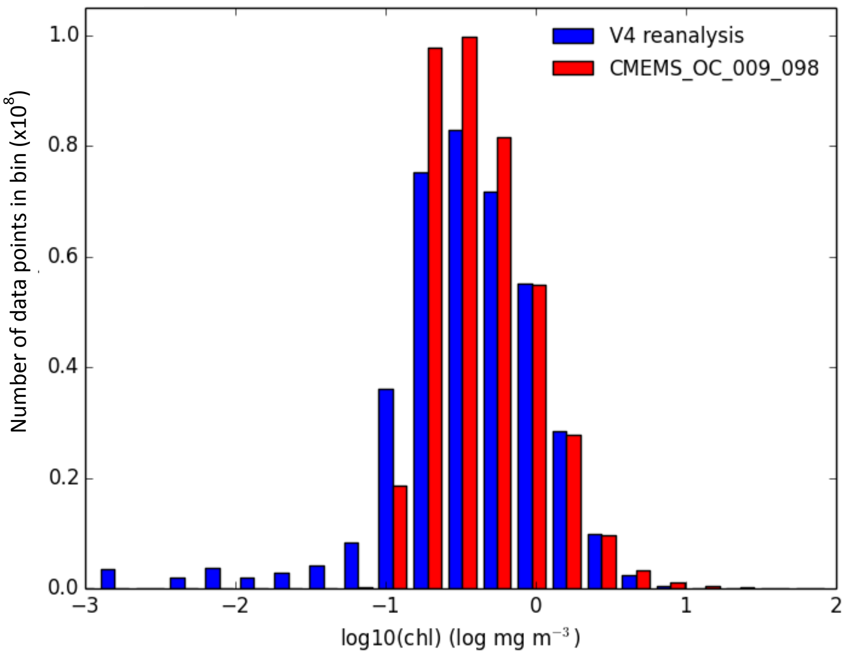


Figure 5 Histogram of surface log10-chlorophyll data from the model and ocean colour satellite (red), daily median for the whole domain, 1998-2016. There is a grid point for each model cell each day, except where satellite data were unavailable due to cloud: these points were omitted from the model data. The ocean colour data comes from CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098, daily values, regridded to match the model.

Table 3 Statistics for match-ups between daily model surface chlorophyll outputs and satellite ocean colour chlorophyll (CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	Bias (mg m^{-3})	MAE (mg m^{-3})	Spearman correlation
Full Domain	-0.03	0.14	0.70
Continental shelf	-0.12	0.24	0.67
Offshelf	-0.01	0.11	0.66
Norwegian Trench	-0.10	0.26	0.55
Northern North Sea	-0.10	0.19	0.53
Southern North Sea	-0.23	0.40	0.67
English Channel	-0.13	0.24	0.67
Irish Sea	-0.21	0.44	0.45
South Western Approaches	-0.08	0.14	0.73
North Western Approaches	-0.09	0.24	0.54

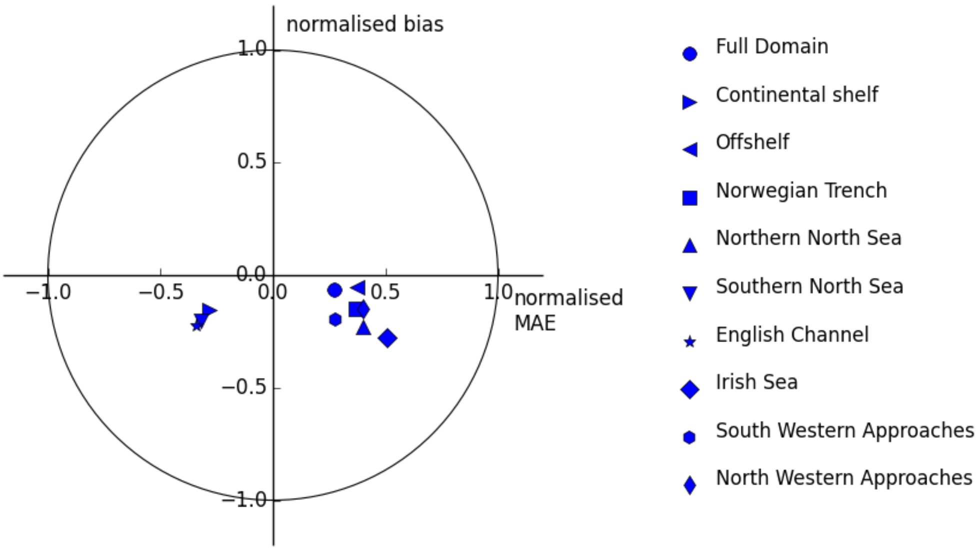


Figure 6 Target diagram for match-ups between daily model surface chlorophyll outputs and satellite ocean colour chlorophyll (CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

Comparison to in situ data is shown in

Figure 77 (time series at observing station L4, surface value, and Figure 8 and Table 4**Erreur ! Source du renvoi introuvable.**, all depths). In this case the bias is not consistently negative and the peaks in chlorophyll observed at station L4 are generally higher than in the model. The timing of blooms is reproduced reasonably well, though noise in the observation data makes this difficult to check (Figure 7). The MAE for match-ups to observations is around 1 mg m-3 for most shallow water regions, lower for deep water areas and 0.675 for the shelf area as a whole. The negative x-values on the target diagram show that the model outputs have lower variability than observation, consistent with Figure 7.

Accuracy figures for the in situ comparison are not the same as those for the comparison to satellite ocean colour chlorophyll, for a number of reasons: the in situ data contains data from all depths, it is based on monthly rather than daily values and the in situ data is less regularly distributed in time and space (note the "n" column in Table 4, which shows the number of observations in each region over the whole time period 1998-2016). Users should assess which comparison is more appropriate for their application of the reanalysis.

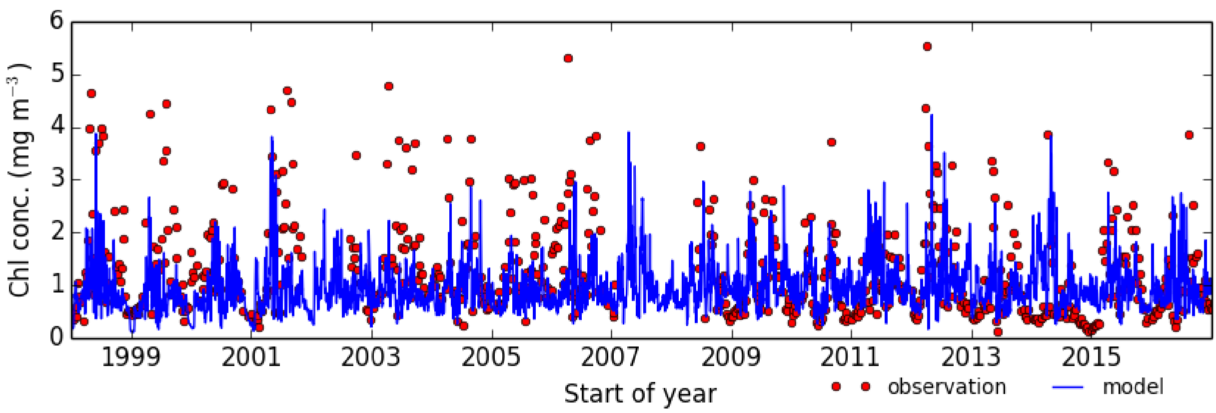


Figure 7 Surface chlorophyll concentration from the reanalysis (blue line) and measurements at station L4 (red circles). See Figure 2 for location of L4; observation data from https://www.westernchannelobservatory.org.uk/l4_chn.php). Please note that a small number of observations higher than 6 mg m^{-3} have been omitted to make the rest of the plot easier to read.

Table 4 Statistics for match-ups between monthly model chlorophyll outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias (mg m^{-3})	MAE (mg m^{-3})	Spearman correlation
Full Domain	44596	0.060	0.598	0.73
Continental shelf	35430	-0.049	0.675	0.69
Offshelf	9166	0.079	0.315	0.80
Norwegian Trench	14904	-0.018	0.484	0.68
Northern North Sea	3606	0.046	0.222	0.72
Southern North Sea	10850	-0.529	1.171	0.64
English Channel	2141	0.230	0.924	0.7
Irish Sea	1521	0.127	1.029	0.34
South Western Approaches	1001	0.114	0.652	0.35
North Western Approaches	1533	-0.624	0.880	0.31

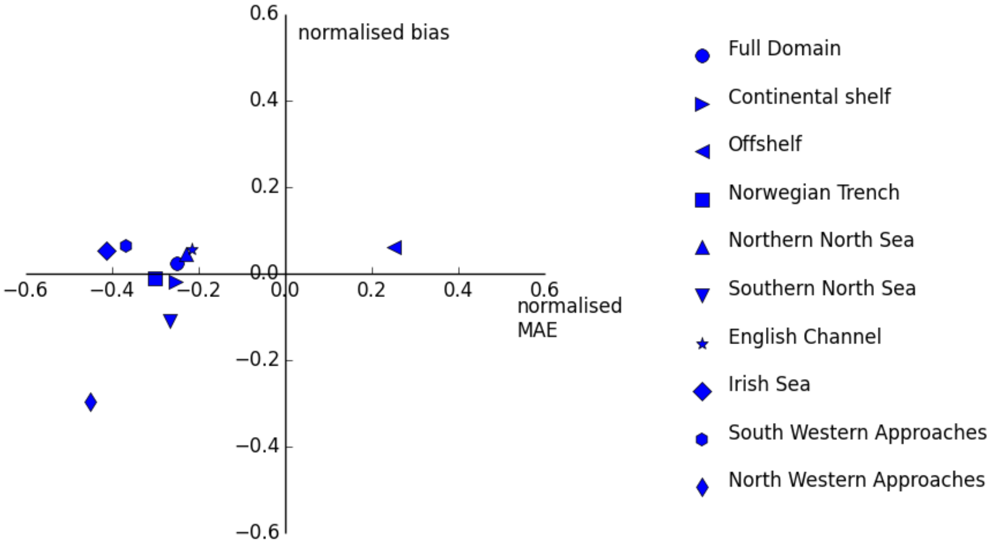


Figure 8 Target diagram for match-ups between monthly model chlorophyll outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

IV.2 Nitrate

Figure 1010 shows the monthly mean surface nitrate concentration compared to the climatology from the World Ocean Atlas (WOA, Garcia et al., 2014a, b). The seasonal cycle is well reproduced. The model underestimates summer nitrate in the northern part of the domain and overestimates in the Norwegian Trench, but otherwise is a good match to the World Ocean Atlas in deep water areas. Nitrate values are generally higher than WOA on the shelf, especially in the east; however WOA is less reliable in coastal areas.

Comparisons of model to in situ data are shown in Figure 9 (time series at observing station L4) and Figure 11 and Table 5 (match-ups to observations in the ICES database). Consistent with the World Ocean Atlas comparison, the bias (model median – observation median) is positive in the shelf areas and highest in the Southern North Sea. The negative bias in the northern deep water area (Figure 10) is not seen in the comparison to ICES database observations (Table 5 and Figure 11), but there are relatively few observations in this area. The MAE is 5 mmol m^{-3} in most regions, but over 10 mmol m^{-3} in the English Channel and Southern North Sea. Model-observation correlation is generally higher in deep water regions than shallower waters. Table 5 shows that in comparison to the variability in observations, the Southern North Sea and English Channel have higher bias and MAE than other regions (Figure 11).

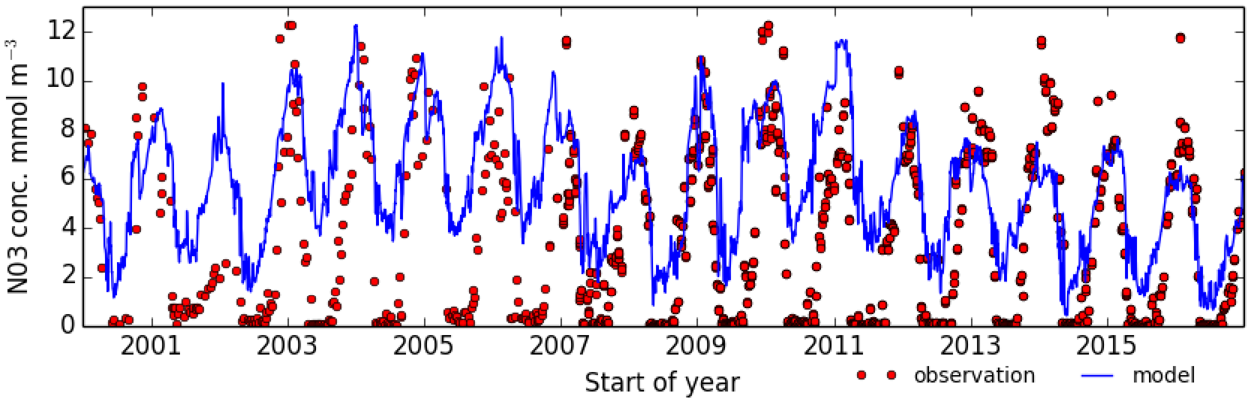


Figure 9 Surface nitrate concentration from the reanalysis (blue line) and measurements at station L4 (red circles). See Figure 22 for location of L4; observation data is from https://www.westernchannelobservatory.org.uk/l4_chn.php.

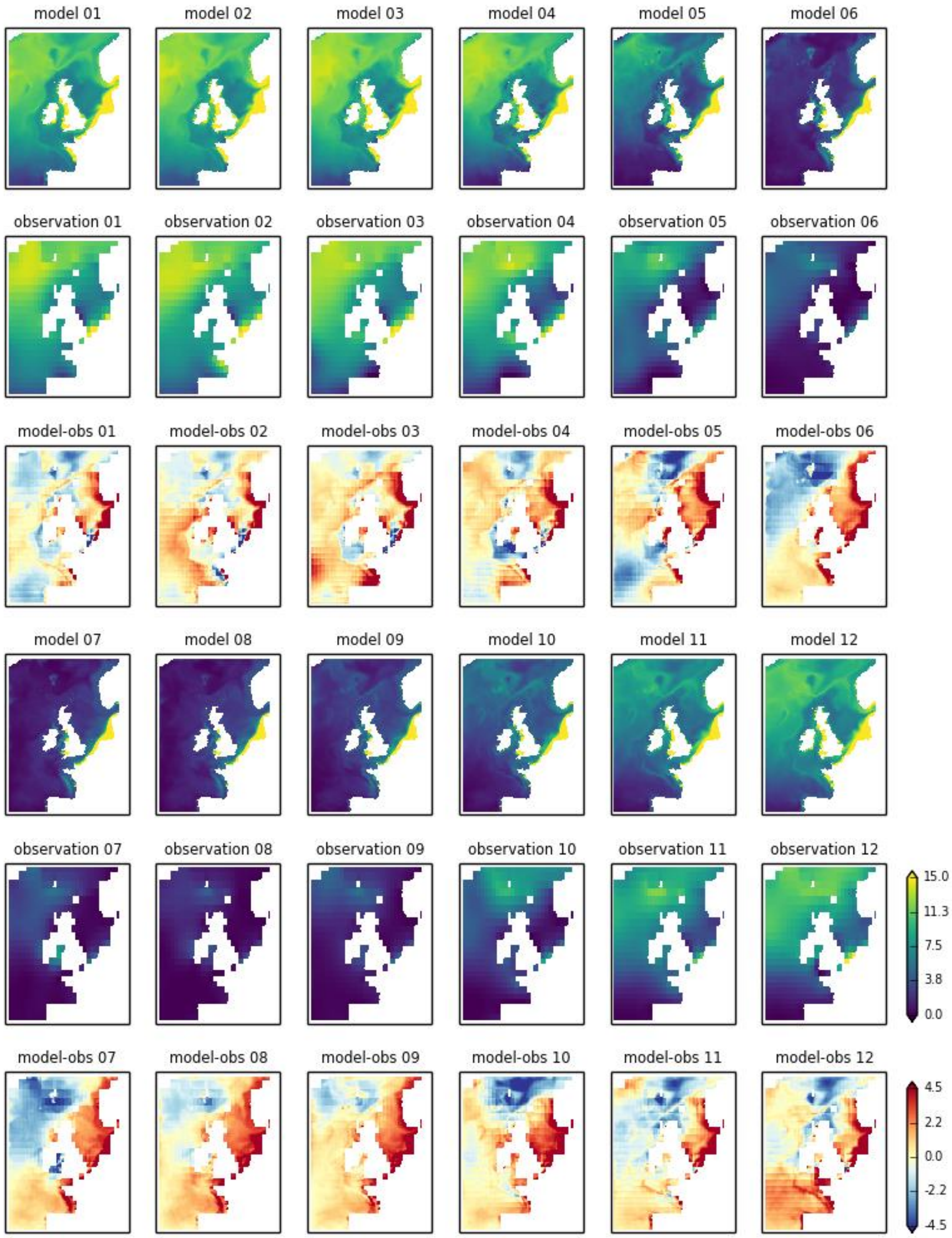


Figure 10 Mean monthly surface nitrate concentration (mmol m^{-3}) from the reanalysis (top row) and the World Ocean Atlas (middle row) and the difference between the model and World Ocean Atlas values (bottom row).

Table 5 Statistics for match-ups between monthly model nitrate outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias (mmol m^{-3})	MAE (mmol m^{-3})	Corr
Full Domain	53893	3.61	4.15	0.42
Continental shelf	44286	4.02	5.27	0.39
Offshelf	9596	0.79	1.42	0.69
Norwegian Trench	19853	4.38	5.30	0.31
Northern North Sea	5034	0.44	1.55	0.61
Southern North Sea	11866	34.13	28.08	0.29
English Channel	1479	10.52	10.66	0.57
Irish Sea	2731	2.81	3.68	0.46
South Western Approaches	1202	0.99	2.17	0.77
North Western Approaches	2194	1.70	1.98	0.64

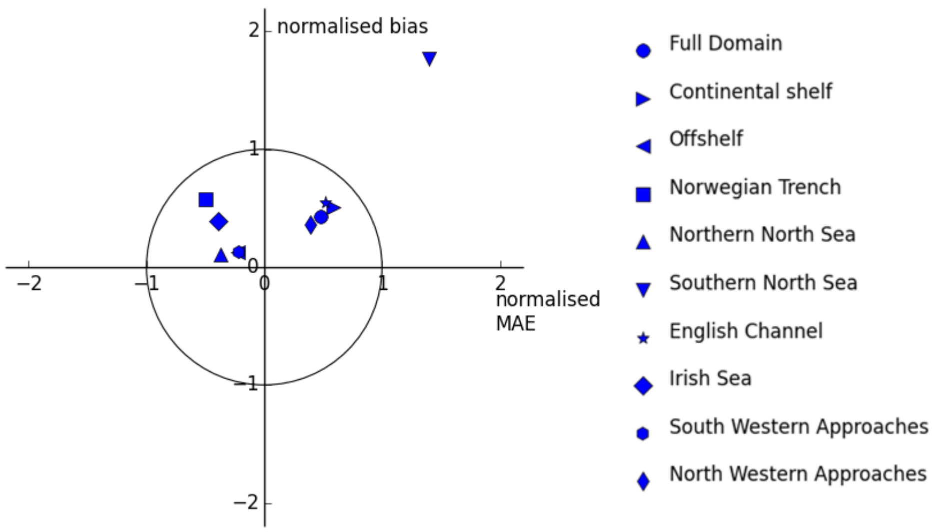


Figure 11 Target diagram for match-ups between monthly model nitrate outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

IV.3 Phosphate

Figure 12 shows the monthly mean surface phosphate concentration compared to the climatology from the World Ocean Atlas (Garcia et al., 2014a, b). The seasonal cycle is well reproduced, but summer values are lower in the model than WOA observations. Model values are higher than WOA at the eastern North Sea coast, but WOA is less reliable in coastal areas.

Comparison to matched in situ data from the ICES database (ICES 2014) is shown in Table 6 and Figure 13. In agreement with the World Ocean Atlas comparison (Figure 12), this shows that the model values are higher than observation in the Southern North Sea and also for the off-shelf area, otherwise model outputs are lower than observation on average. The MAE is 0.1-0.3 mmol m^{-3} for most areas, higher in the Southern North Sea. The correlation is generally highest in the southern part of the domain and the off-shelf area, but again the quality is worst in the Southern North Sea.

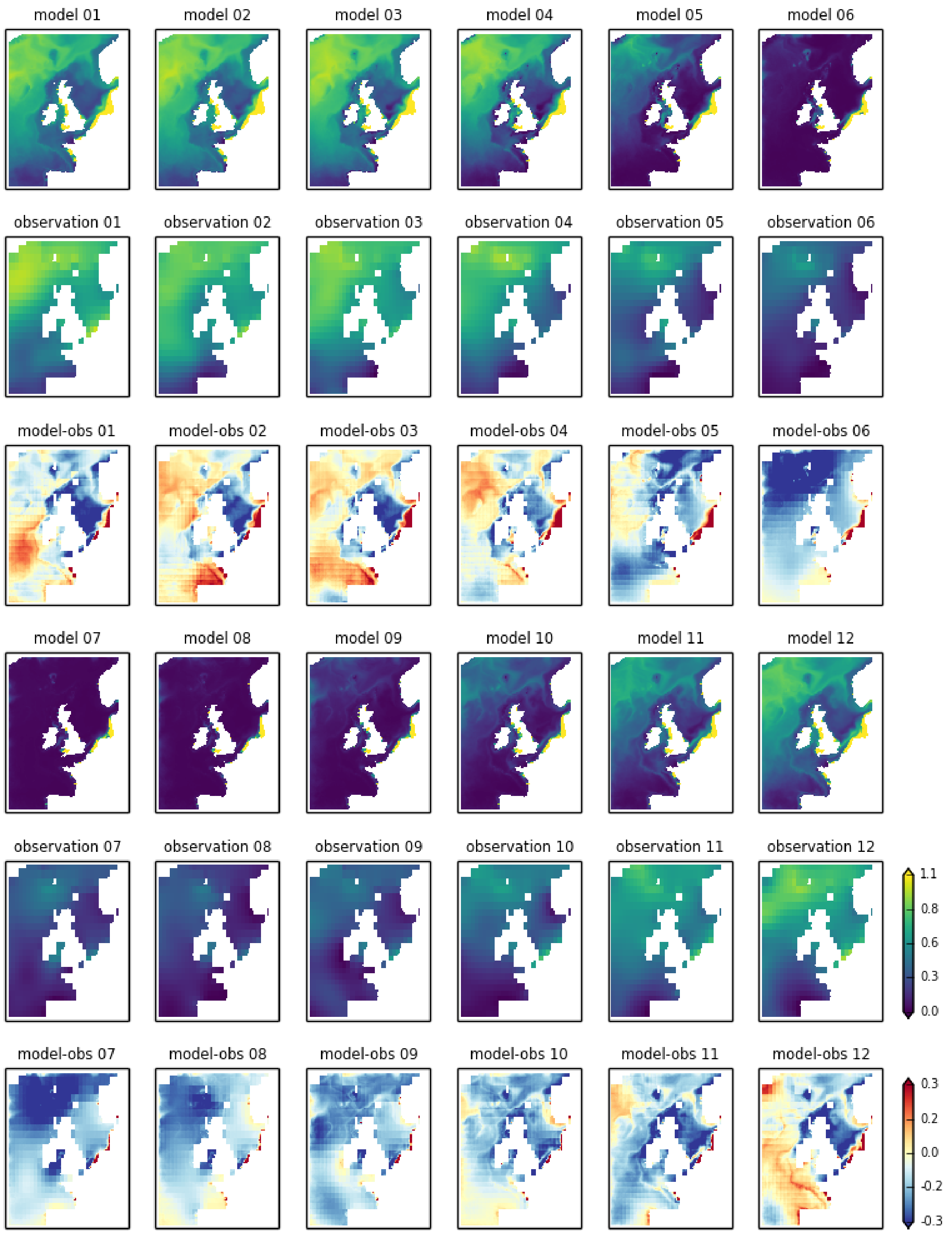


Figure 12 Mean monthly surface phosphate concentration from the reanalysis (top row) and the World Ocean Atlas (middle row) and the difference between the model and World Ocean Atlas values (bottom row).

Table 6 Statistics for match-ups between monthly model phosphate outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias (mmol m^{-3})	MAE (mmol m^{-3})	Spearman correlation
Full Domain	56669	-0.05	0.20	0.51
Continental shelf	46775	-0.07	0.23	0.44
Offshelf	9883	0.12	0.10	0.81
Norwegian Trench	20545	-0.05	0.19	0.41
Northern North Sea	5050	-0.18	0.18	0.51
Southern North Sea	13323	0.62	0.66	0.34
English Channel	1743	-0.24	0.31	0.69
Irish Sea	2799	-0.04	0.13	0.55
South Western Approaches	1334	-0.11	0.11	0.80
North Western Approaches	2054	-0.29	0.24	0.54

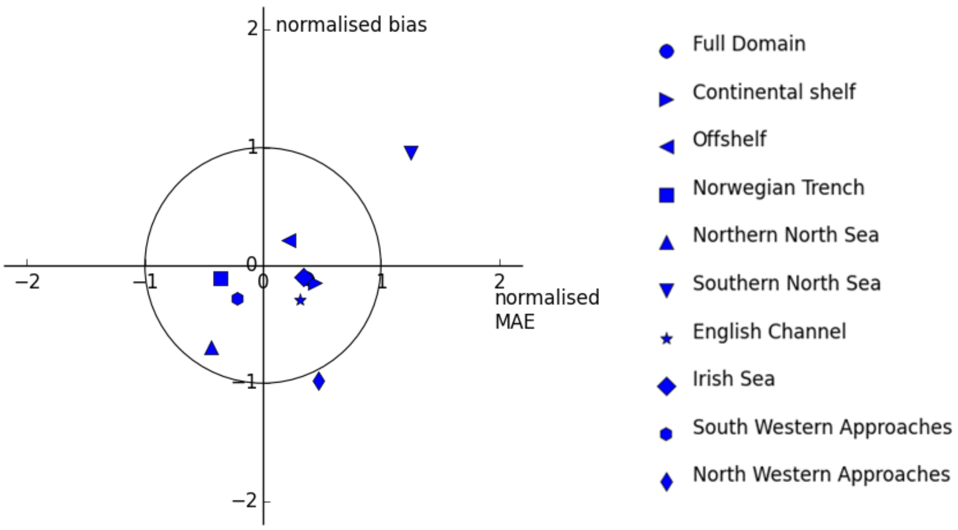


Figure 13 Target diagram for match-ups between monthly model phosphate outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

IV.4 Oxygen

Figure 14 shows the monthly mean surface dissolved oxygen concentration compared to the climatology from the World Ocean Atlas (Garcia et al., 2014a, b). The model values are consistently below WOA values, but show the same temporal and spatial patterns. The negative bias is associated with a slight warm bias in the model outputs (<1°C, see the QUID for the physics product NORTHWESTSHELF_REANALYSIS_PHYS_004_009); the solubility of oxygen is lower in warmer water. In addition it should be noted that the World Ocean Atlas product is based on observations made between the early 1900s and 2012; for much of this period waters were cooler than the reanalysis period, 1998-2016, so the WOA values are likely to be higher than present-day averages.

Comparison to matched in situ data from the ICES database (ICES, 2014) is shown in Table 7 and Figure 15. This also shows the model has consistently lower values than observation, though by a smaller amount: 1-25 mmol m^{-3}, with a lower bias in the off-shelf area. The MAE is 18-22 mmol m^{-3} for most areas, lower offshelf and in the Northern North Sea. The model-observation correlation is 0.6 or higher in all areas except the English Channel.

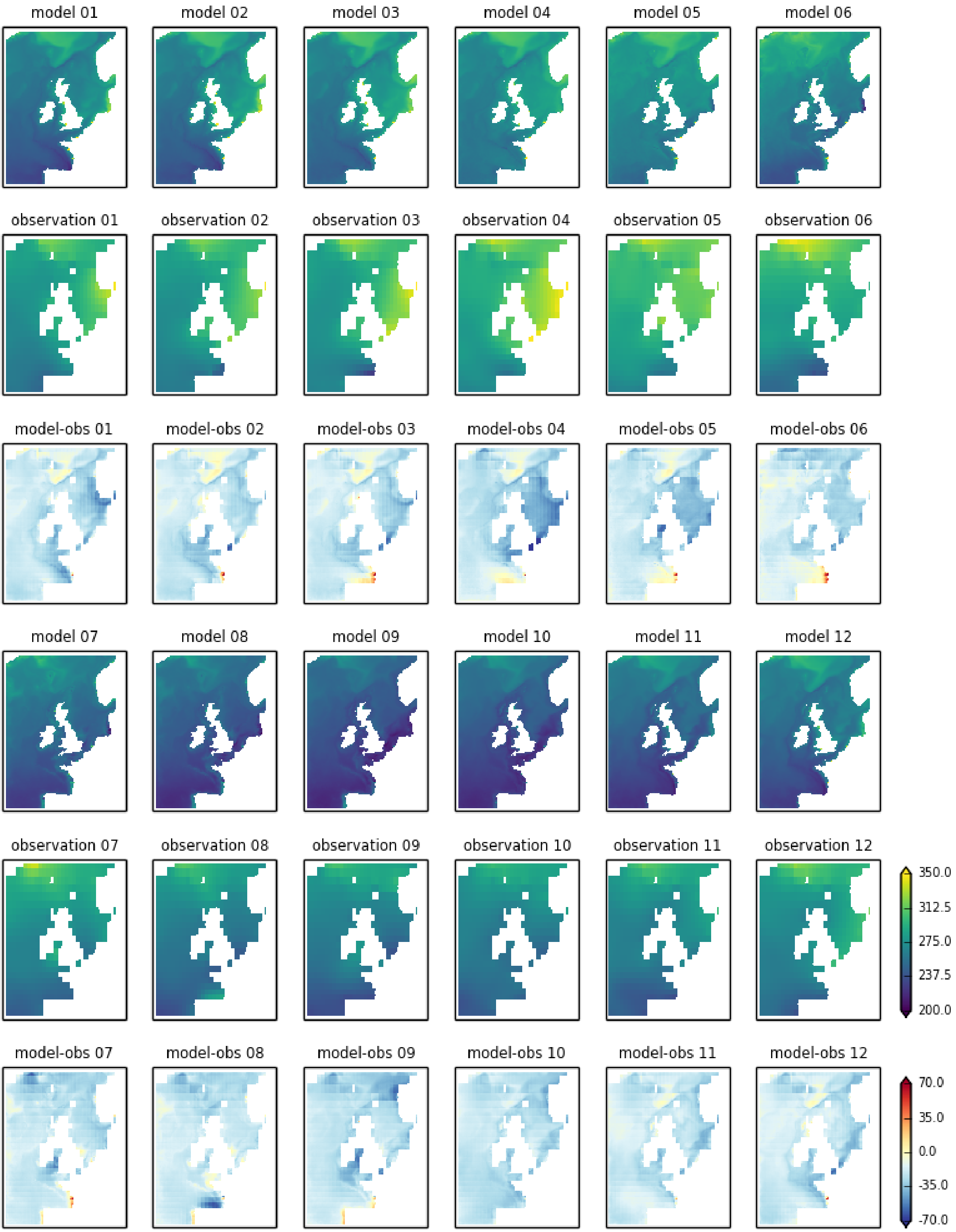


Figure 14 Mean monthly surface dissolved oxygen concentration from the reanalysis (top row) and the World Ocean Atlas (middle row) and the difference between the model and World Ocean Atlas values (bottom row).

Table 7 Statistics for match-ups between monthly model dissolved oxygen outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias (mmol m^{-3})	MAE (mmol m^{-3})	Spearman correlation
Full Domain	83953	-13.22	18.82	0.70
Continental shelf	68761	-15.65	20.42	0.68
Offshelf	15192	-1.43	12.59	0.74
Norwegian Trench	31121	-16.04	21.46	0.66
Northern North Sea	4714	-9.07	11.42	0.63
Southern North Sea	26857	-17.97	21.75	0.74
English Channel	2742	-24.67	20.97	0.12
Irish Sea	1648	-13.26	17.97	0.65
South Western Approaches	866	-15.53	18.45	0.62
North Western Approaches	1240	-14.49	18.84	0.66

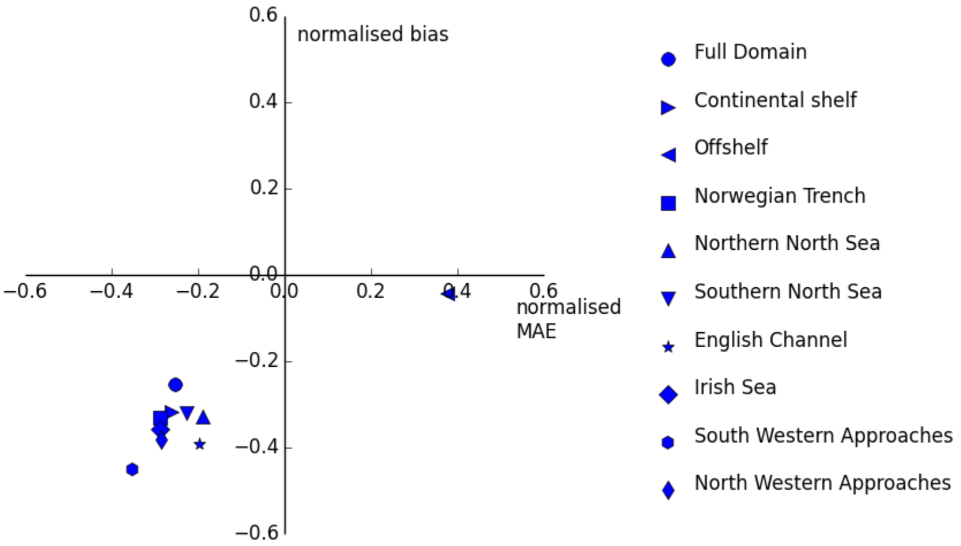


Figure 15 Target diagram for match-ups between monthly model oxygen outputs and in situ observations from the ICES database (ICES, 2014), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

IV.5 pCO_2

Comparison of the modelled surface partial pressure of CO_2 to in situ data from the SOCAT database is shown in

Table 8 and Figure 16. This dataset has a reasonably large number of data points, but they are unevenly spread in space and time (mainly data from cruises) and the statistics should be used with caution; in particular, observations are only available for the surface. The bias is variable in direction and size. MAE is 4-5 Pa; it is lower in the Irish Sea and Northern North Sea but for the Northern North Sea the MAE is quite large in relation to the variability of the observations (Figure 16). Model-observation correlation is low except in the deep water areas; however Figure 16 suggests that model skill in terms of bias and pCO_2 is better in shallow-water areas.

The SOCAT values are for fugacity of CO_2, but the difference between fugacity and partial pressure is small in the conditions of this region.

Table 8 Statistics for match-ups between monthly model pCO_2 outputs and in situ observations from the SOCAT database (Bakker, 2016), for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias (Pa)	MAE (Pa)	Spearman correlation
Full Domain	364428	-0.89	4.67	0.39
Continental shelf	179844	0.75	4.39	0.18
Offshelf	184584	-4.73	5.11	0.58
Norwegian Trench	73494	-0.63	4.29	0.15
Northern North Sea	2591	-1.96	1.35	0.74
Southern North Sea	73741	0.62	4.84	-0.12
English Channel	17633	2.05	4.44	-0.11
Irish Sea	1147	0.63	2.50	0.5
South Western Approaches	18837	-2.18	3.95	0.32
North Western Approaches	1074	4.83	4.35	0.11

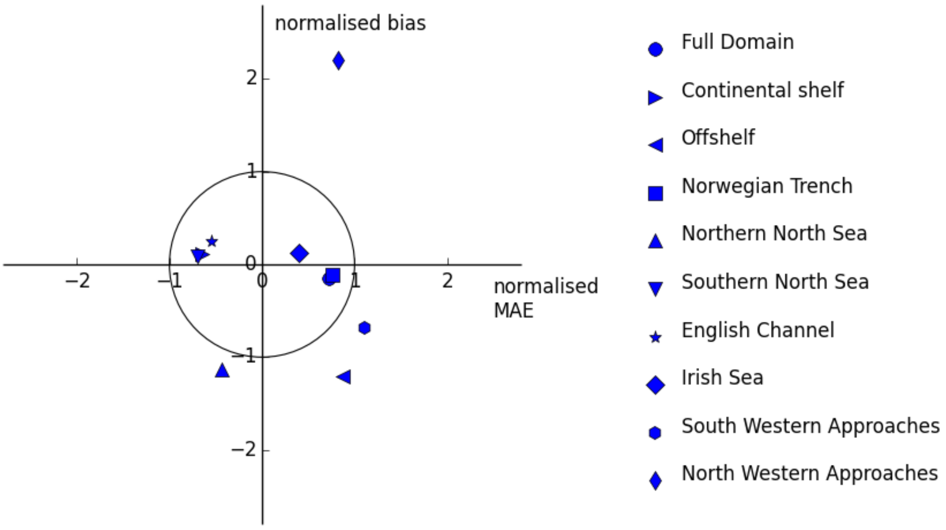


Figure 16 Target diagram for match-ups between monthly model pCO2 outputs and in situ observations from the SOCAT database (Bakker, 2016), for the full domain and sub-regions. See section III for information on how the target diagram is defined.

IV.6 pH

Comparison to in situ data from the GLODAP and ICES databases is shown in Table 9 and Figure 17; note that there are fewer observations available than for other variables. The bias is variable in sign and generally less than 0.02. MAE is 0.05-0.1 in most areas. Model-observation correlation is low except in the deep water areas.

Table 9 Statistics for match-ups between monthly model pH outputs and in situ observations from the GLODAPv2 (Key, 2015, and Lauvset,2016) and ICES (ICES, 2014) databases, for the full domain and sub-regions. See section III for information on the match-up process and statistics provided and the locations of the regions.

Region	n	Bias	MAE	Spearman correlation
Full Domain	16718	0.002	0.053	0.23
Continental shelf	15742	0.001	0.055	0.2
Offshelf	976	-0.001	0.022	0.82
Norwegian Trench	962	-0.020	0.032	0.55
Northern North Sea	695	0.000	0.021	0.69
Southern North Sea	10066	0.003	0.059	0.14
English Channel	1721	-0.034	0.049	0.07
Irish Sea	1143	0.026	0.093	0.24
South Western Approaches	721	-0.019	0.057	0.38
North Western Approaches	528	0.105	0.123	0.38

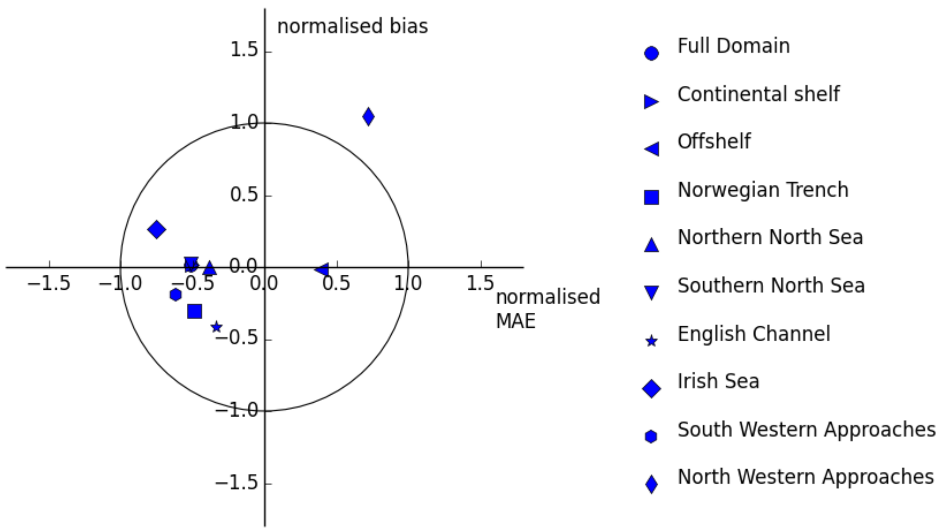


Figure 17 Target diagram for match-ups between monthly model pH outputs and in situ observations from the GLODAPv2 (Key, 2015, and Lauvset,2016) and ICES (ICES, 2014) databases, for the full domain and sub-regions. See section III for information on how the target diagram is defined.

V SYSTEM'S NOTICEABLE EVENTS, OUTAGES OR CHANGES

Date	Change/Event description	System version	other
September 2018	A completely new reanalysis was issued, using an updated biogeochemical model and assimilation of satellite ocean colour chlorophyll data. The model domain was unchanged, with the same resolution as the previous reanalysis.	4.0	
January 2019	At end of 2018, the reanalysis was extended to cover the year 2018. It will continue to be extended on a yearly or 6-monthly basis until it is superseded by a future version of the reanalysis. The quality of the 2017 reanalysis was assessed and was found to be similar to previous years. Further extensions will be assessed in the same way. The statistics in this document refer to the period 1993-2016 and this will only change if the quality of the reanalysis is found to change.	4.1	
April 2019	In April 2019, the reanalysis was extended to cover the year 2018. It will continue to be extended on a yearly or 6-monthly basis until it is superseded by a future version of the reanalysis. The quality of the 2018 reanalysis was assessed and was found to be similar to previous years. The ocean colour product was not continued after 28/10/2018, so for the remaining days of the run a comparable near-real-time product was used: OCEANCOLOUR_ATL_CHL_L3_NRT_OBSERVATIONS_009_036. This might produce a small discontinuity at the end of October 2018; however, this is the winter period, when biogeochemical activity is low, so the effect is minor and the estimated accuracy numbers are not affected. Further extensions will be assessed in the same way. The statistics in this document refer to the period 1993-2016 and this will only change if the quality of the reanalysis is found to change.	4.2	

VI QUALITY CHANGES SINCE PREVIOUS VERSION

The reanalysis (V4) shows more stability in nutrient values than the previous version (V2), which had noticeable drift in nitrate and phosphate and jumps between sections of reanalysis (Figure 18 and Figure 19). V4 has a better match to World Ocean Atlas summer nitrate and phosphate values but higher winter nitrate in some years; both reanalyses underestimate winter phosphate, V4 is lower than V2.

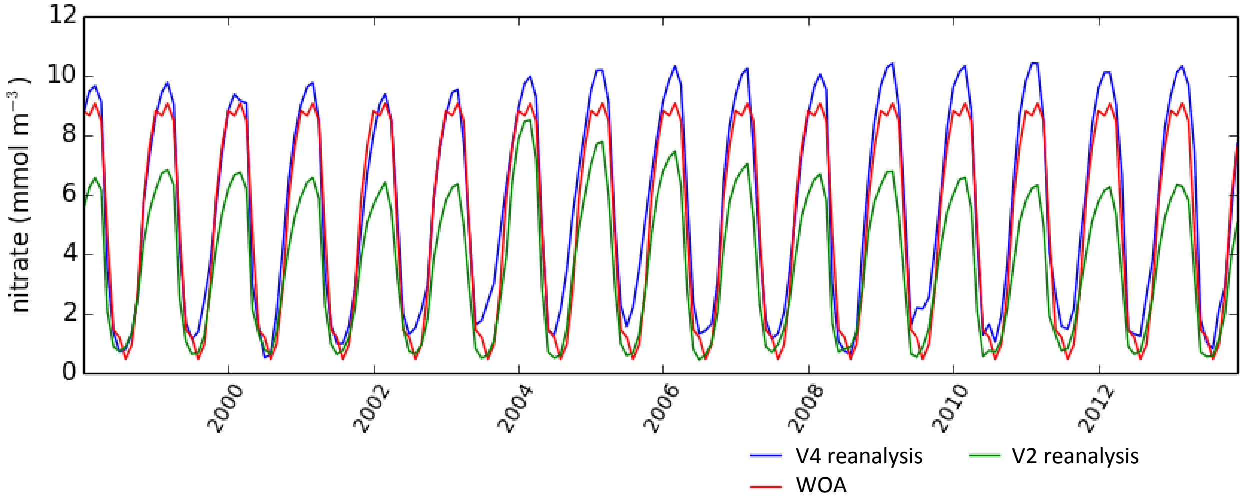


Figure 18 Time series of surface nitrate concentration from the model (blue), World Ocean Atlas climatology (red) and V2 reanalysis (green), monthly median for the whole domain.

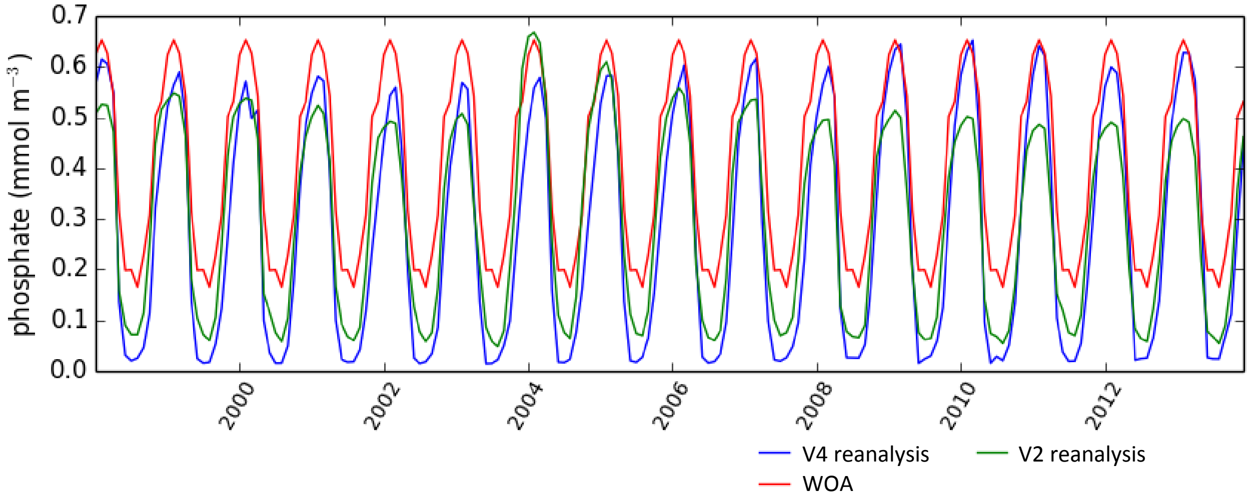


Figure 19 Time series of surface phosphate concentration from the model (blue), World Ocean Atlas climatology (red) and V2 reanalysis (green), monthly median for the whole domain.

The domain median chlorophyll is a better match to satellite ocean colour than V2 in all seasons (Figure 20).

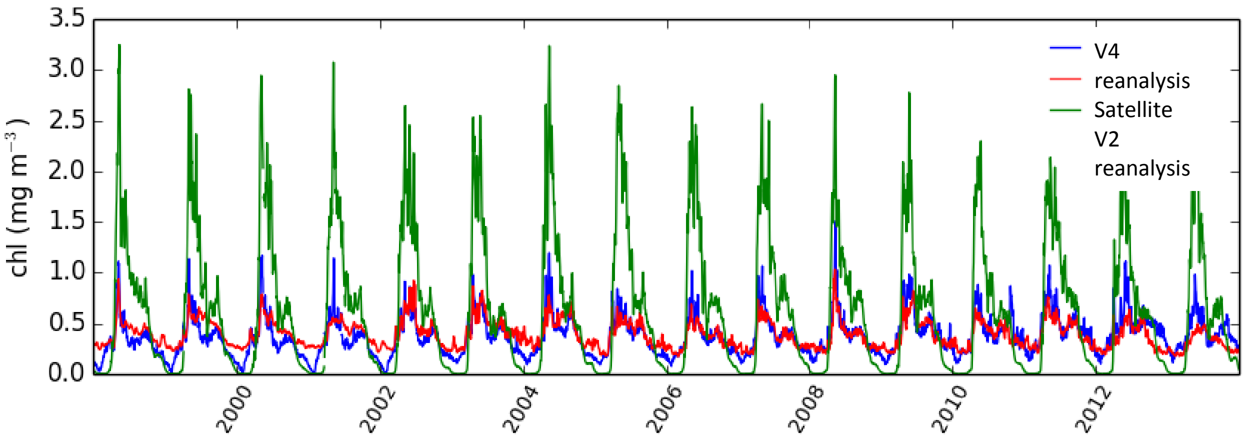


Figure 20 Time series of surface chlorophyll concentration from the model (blue), ocean colour satellite (red) and V2 reanalysis (green), daily median for the whole domain. The ocean colour data comes from CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098, daily values, regridded to match the model.

Regional statistics for the match between reanalysis and ocean colour also shows an improvement between V2 and V4, with higher correlation, lower MAE and comparable bias in all regions (Table 10).

Table 10 Statistics for match-ups between daily model surface chlorophyll outputs (V4 and V2 reanalyses) and satellite ocean colour chlorophyll (CMEMS product OCEANCOLOUR_ATL_CHL_L4_REP_OBSERVATIONS_009_098), for the full domain and sub-regions, 1998-2013. See section III for information on the match-up process and statistics provided and the locations of the regions.

	V4 reanalysis			V2 reanalysis		
Region	**Median bias (mg m^{-3})**	**MAE (mg m^{-3})**	**Spearman correlation coefficient**	**Median bias (mg m^{-3})**	**MAE (mg m^{-3})**	**Spearman correlation coefficient**
Full Domain	-0.04	0.14	0.71	0.08	0.34	0.50
Continental shelf	-0.14	0.25	0.67	-0.10	0.57	0.34
Offshelf	-0.02	0.11	0.66	0.11	0.25	0.58
Norwegian Trench	-0.11	0.27	0.55	-0.11	0.52	0.30
Northern North Sea	-0.11	0.20	0.53	-0.13	0.48	0.31
Southern North Sea	-0.26	0.42	0.67	-0.35	0.87	0.19
English Channel	-0.15	0.24	0.69	-0.09	0.46	0.39
Irish Sea	-0.26	0.45	0.45	-0.53	0.91	0.18
SW Approaches	-0.09	0.14	0.73	0.06	0.48	0.31
NW Approaches	-0.10	0.25	0.54	-0.03	0.51	0.42

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