# Operational Ecology

**Ecosystem forecast products to enhance marine GMES applications**

**DG SPACE**

Collaborative Project - small or medium-scale focused research project

**Project Number: 283291**

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<td>HCMR</td>
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<td><strong>Author(s):</strong></td>
<td>I Allen, S Arkin, G Cossarini, M Butenschoen, S Ciavatti, A Christensen, S Libralato, B Salihoglu, G Triantafyllou, K Tsiaras, Z. Wan</td>
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OPEC Overview

“OPEC provides an enhanced capability to predict indicators of good environmental status in European regional Seas”

The OPEC project (Operational Ecology) will help develop and evaluate ecosystem forecast tools to help assess and manage the risks posed by human activities on the marine environment, thus improving the ability to predict the “health” of European marine ecosystems. The programme will focus on four European regional seas (North-East Atlantic, Baltic, Mediterranean and Black Seas) and plans to implement a prototype ecological Marine Forecast System, which will include hydrodynamics, lower and higher trophic levels (plankton to fish) and biological data assimilation.

Products and services generated by OPEC will provide tools and information for environmental managers, policymakers and other related industries, laying the foundations for the next generation of operational ecological products and identification of knowledge / data gaps.

OPEC will use the EU’s Global Monitoring for Environment and Security Marine Service as a framework and feed directly into the research and development of innovative global monitoring products or applications. This in turn will advise policies such as the European Marine Strategy Framework Directive and Common Fisheries Policy, as well as the continued monitoring of climate change and assessments of mitigation and adaptation strategies.

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Executive Summary

The aim of this deliverable is the assessment of the reanalysis model systems performance with an emphasis on the non-assimilated variables. Ensemble based data assimilation schemes have been implemented in the OPEC regional model systems (see D2.4). The re-analysis skill is evaluated using the benchmark tool developed in the framework of OPEC and the activities are reported on a regional basis.

The results indicate that while all the model systems demonstrate an increase in the skill of the assimilated variables, the improvement in non-assimilated variables is less clear cut. In some cases data assimilation leads small improvements, in others to a degradation of model performance; the responses depending on the regional and model system in question. This suggests that further work is required before the assimilation systems make a significant impact on the predictive skill.

This deliverable is linked to:
- D3.2 (Assessment of the skill of the REA indicators)
- D3.3 (Report on quantifying model uncertainty and reducing model error)
- D4.2 (Assessment of seasonal predictability for indicators of lower trophic levels in all four regions)
- D4.3 (Assessment of seasonal predictability for indicators of high trophic levels in all four regions)

Relevance to Policy

The target audiences for OPEC research are primarily, decision makers in both the policy and management arenas but also include SME interested in the application of knowledge, the wider marine science research community and the interested public. A particular focus is the Marine Strategy Framework Directive (MSFD) which provides a transparent, legislative framework to apply an ecosystem based approach to the management of human activities in the marine environment. The MSFD aims to achieve ‘Good Environmental Status’ (GES) across Europe’s regional Seas by 2020. The strategies to achieve this must contain a detailed assessment of the state of the environment, a definition of "good environmental status" at regional level and the establishment of clear environmental targets and monitoring programmes. The MSFD also identifies 11 high level descriptors, 5 of which are considered by OPEC (D1 Biodiversity, D3 Commercial Fish, D4 Foodwebs, D5 Eutrophication, and D6 Hydrography). Each descriptor is characterised by a set of indicators which characterise marine ecosystems and requires and understanding of the possible pressures and impacts on them. The diversity in environmental conditions and the issues of scale have implications for the implementation of the descriptors in the assessment of Good Environmental Status (GES). There is no single set of criteria and indicators which can meaningfully be applied to all marine regions/sub-regions, and often not even for a single descriptor within a marine region/sub-region, and this requires a regional approach as used in OPEC. The relationships between OPEC model outputs and descriptors are illustrated in Table 1. This should be viewed as a list of potential data products, with the caveat that the validation of each product is dependent on the available data.
Table 1. Mapping Model Outputs (Characteristics) to Descriptors

<table>
<thead>
<tr>
<th></th>
<th>D1 Biodiversity</th>
<th>D3 Commercial Fish</th>
<th>D4 Foodwebs</th>
<th>D5 Eutrophication</th>
<th>D7 Hydrography</th>
</tr>
</thead>
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<tr>
<td><strong>Physio-chemical</strong></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>X</td>
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<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Salinity</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
<td></td>
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<tr>
<td>Nitrate</td>
<td>X</td>
<td></td>
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<tr>
<td>Phosphate</td>
<td>X</td>
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<tr>
<td>Silicate</td>
<td>X</td>
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<td></td>
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</tr>
<tr>
<td>Oxygen</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>pH</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Biological</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorophyll</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Primary Production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Phytoplankton Biomass</td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Zooplankton Biomass</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Fish Stocks</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Sea Birds</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Community Production</td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes**

**D1 Biodiversity:** Marine biodiversity is the range of life forms in the seas and oceans. This biodiversity may be measured by number of species, genetic resources and functional diversity. This makes assessing biodiversity a difficult process, given the variety of species and their functions in an area or region, as well as the genetic variation between individuals of a species, the structure of plant and animal communities, and their physical environment. The state of an ecosystem and therefore biodiversity is highly dynamic; changes in the state or pressures in one part of the ecosystem can lead to unexpected changes in another part, easily affecting overall biodiversity. This descriptor therefore has a strong inter-relationship with other MSFD descriptors. GES for biological diversity is deemed to be maintained when the quality and occurrence of habitats and the distribution and abundance of species are in line with prevailing physiographic, geographic and climatic conditions. OPEC has developed a number of products that can be used as indicators of biodiversity, particularly in terms of pelagic habitat (e.g. Chlorophyll, oxygen, pH, primary production).
D3 Commercial Fish: The Descriptor 3 definition for GES is: “Populations of all commercially exploited fish and shellfish are within safe biological limits, exhibiting a population age and size distribution that is indicative of a healthy stock.” Key criteria for measuring GES include the level of fishing pressure, the reproductive capacity of the stock and the age and size distribution of the assessed population. A suite of modelling tools has been implemented, each targeting the major exploited fish resources in each of the MSFD regions. A diversity of approaches has been used ranging from foodweb and size structured models to Individual Based (IBM) and multi-species stock assessment models.

D4 Foodwebs: Climate change will exacerbate the impacts of human activity on the structure and function of marine ecosystems, and the services they provide. The combined effects of climate, fishing, nutrient loading and pollution impacts at both organismal and population levels, influencing the competitive ability and dominance of key marine species, which in turn reorganises the structure of marine food webs. The MSFD states that GES is achieved if the integrity of food webs ensures the long-term abundance and reproduction of its species. Coupled physical to ecosystem models allow use to calculate marine foodweb properties in terms of OPEC models e.g. Ecopath with Ecosim, Ecospace allow

D5 Eutrophication: Eutrophication refers to the processes related to discharge of macronutrients in the marine environment that stimulate the rapid growth of microalgae and lead to disruptive effects on the marine environment. The eutrophication descriptor focuses on both anthropogenic and natural causes (i.e. human induced increased river nutrient loads, and coastal nutrient increases due to climate effects), and their direct (increased phytoplankton blooms or decrease in transparency) and indirect (decrease of benthic plants) effects. Eutrophication has broad reaching impacts and can have negative impacts on other descriptors such as biodiversity, non-indigenous species, food webs and commercial fish. OPEC models are able to provide estimates for recent trends and future forecasts for several of the indicators for eutrophication. Although each model has different structures and characteristics, indicators relevant to this descriptor that can be addressed by OPEC biogeochemical models include: nutrient concentration in the water column, chlorophyll concentration, phytoplankton biomass, dissolved oxygen. Additionally some models can provide more detailed information on nutrient ratio and phytoplankton community composition.

D7 Hydrography: Hydrographical conditions are the physical properties of seawater (temperature, salinity, depth, currents, waves, turbulence, turbidity). They play a crucial role in the dynamics of marine ecosystems. In the near shore regions many of these are directly influenced by human activity so can be targeted by policy and management actions. GES assessment and targets are based on quantifying the extent, distribution and severity of permanent alterations in hydrographical properties as a result of human activities.

Introduction

A primary objective of OPEC is to set-up ecological modelling systems for the next generation GMES marine ecological service in European Seas. Each regional model system comprises a core coupled hydrodynamic-plankton model, a HTL component, a representation of the carbon chemistry and a data assimilation system. The model systems are described in detail in D2.5. These have been used to perform 20 yr hindcast of each region and to benchmark model performance (see D2.8). In order to improve hindcast simulations and the initial conditions for Rapid Environment Assessment (WP3) and to assess the predictability of seasonal forecast (WP4) data assimilation is required. Therefore ensemble based assimilation schemes have been implemented in the OPEC regional model systems. This deliverable focuses on assessing the performance of the reanalysis model systems with an emphasis on evaluating the performance of non-assimilated variables. We first present a synthesis of the reanalysis results and lessons learnt for the future implementation of data assimilation. The activities are the reported on a regional basis in greater detail.
1. Regional synthesis and lessons learnt

*Table 1.1. Assimilation effect on nutrients.*

**ME**: good ≥ 0.5, poor ≤ 0; **% MB**: good ≤ 20%, poor ≥ 100%;

**PCC** good > 0.75, poor < 0.20; **RI**: good 0.8-1.2, poor > 2 or <0

### Chlorophyll (mg m$^{-3}$)

<table>
<thead>
<tr>
<th>Region (partner)</th>
<th>ME</th>
<th>% MB</th>
<th>PCC</th>
<th>RMSE</th>
<th>uRMSE</th>
<th>RI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baltic (DMI)</td>
<td>0.04</td>
<td>10</td>
<td>0.23</td>
<td>4.99</td>
<td>4.98</td>
<td>2.01</td>
</tr>
<tr>
<td>NE_Atlantic (PML)*</td>
<td>-0.2</td>
<td>22.2</td>
<td>0.34</td>
<td>2.21</td>
<td>2.17</td>
<td>1.99</td>
</tr>
<tr>
<td>Mediterranean (HCMR)</td>
<td>0.03</td>
<td>-3</td>
<td>0.27</td>
<td>0.33</td>
<td>0.33</td>
<td>1.3</td>
</tr>
<tr>
<td>Mediterranean (OGS)</td>
<td>0.08</td>
<td>-1</td>
<td>0.60</td>
<td>0.08</td>
<td>0.08</td>
<td>1.4</td>
</tr>
<tr>
<td>Black_Sea (METU)</td>
<td>0.24</td>
<td>-40</td>
<td>0.53</td>
<td>1.13</td>
<td>1.10</td>
<td>Inf</td>
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</tbody>
</table>

### Nitrate (mmol m$^{-3}$)

<table>
<thead>
<tr>
<th>Region (partner)</th>
<th>ME</th>
<th>% MB</th>
<th>PCC</th>
<th>RMSE</th>
<th>uRMSE</th>
<th>RI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baltic (DMI)</td>
<td>0.08</td>
<td>14</td>
<td>0.49</td>
<td>4.15</td>
<td>4.11</td>
<td>1.37</td>
</tr>
<tr>
<td>NE_Atlantic (PML)</td>
<td>-1.9</td>
<td>-108.4</td>
<td>0.46</td>
<td>11.12</td>
<td>7.86</td>
<td>2.05</td>
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<tr>
<td>Mediterranean (HCMR)</td>
<td>0.09</td>
<td>20</td>
<td>0.32</td>
<td>1.30</td>
<td>1.29</td>
<td>2.1</td>
</tr>
<tr>
<td>Mediterranean (OGS)</td>
<td>-0.24</td>
<td>-4</td>
<td>0.21</td>
<td>3.18</td>
<td>3.18</td>
<td>2.1</td>
</tr>
<tr>
<td>Black_Sea (METU)</td>
<td>-0.53</td>
<td>48</td>
<td>0.16</td>
<td>6.75</td>
<td>6.61</td>
<td>Inf</td>
</tr>
</tbody>
</table>

*from satellite reference data; * from in situ reference data
Reanalysis simulations were performed for the period 2000-2009 in OPEC regional systems, using a variety of data assimilation methods. In all the model systems except the Baltic Sea, remote sensing Chl-a (SeaWiFS, MODIS, GlobColour) was assimilated. In the Baltic, (DMI) a 3DVAR scheme was implemented to assimilate satellite SST and temperature/salinity in situ profiles, since the satellite chl-a data products have large uncertainty/error in this optically complex region.

In the North Atlantic, a localized Ensemble Kalman Filter (EnKF, Evensen, 2003) was implemented, for the monthly assimilation of five-days composites of GlobColour chl-a, taking account of 2-D maps of observation error. In the Mediterranean (OGS), a 3D variational scheme is implemented,
assimilating weekly satellite chl-a by GOS-ISAC-CNR (Mediterranean corrected algorithm) and correcting model phytoplankton concentrations. In the Mediterranean (HCMR), a localized version of the Hybrid-SEIK (combination of singular fixed extended kalman-SFEK and singular extended interpolated kalman-SEIK) filter is implemented, assimilating 8-day SeaWiFS chl-a.

The assimilation performance was evaluated in different systems with emphasis on the non-assimilated variables. Table 1.1 shows hindcast and reanalysis model skill scores for each assimilation system for chl-a, nitrate and phosphate. We should note that the improvement of the assimilated variable (in most cases chl-a) that was achieved in all systems is an important step, indicating the correct implementation of the assimilation scheme. Since the system is constrained by its inherent dynamics, it has the tendency to return to its initial state after the analysis correction. Therefore, a decrease in the model forecast error indicates that the assimilation scheme respects the system dynamics, driving the system closer to the observations in a consistent way. In the North Atlantic (PML), the assimilation resulted in a decrease of the chl-a RMSE (up to -30%) and an increase of correlation (up to +0.25) with satellite chl-a in most areas. In the Mediterranean (OGS), the assimilation results in an increase of the correlation with satellite chl-a from 0.6 in the hindcast to 0.88 in the reanalysis. In the second Mediterranean system (HCMR), the chl-a correlation increases from 0.27 to 0.7, showing an even stronger effect of the assimilation.

The assimilation performance was evaluated by comparing the model-simulated nutrients (nitrate, phosphate, Table 1.1) against available in situ nutrient data which are the most abundant biogeochemical data. Moreover, dissolved inorganic nutrients are those that drive the ecosystem dynamics, particularly in the less productive areas, such as the Mediterranean; in other areas such as the Baltic, light availability may be equally important. Therefore, the effect of assimilation on nutrients is crucial in determining whether the assimilation will drive the simulated ecosystem closer to the reality in an efficient and consistent way (as mentioned above the system has the tendency to return to its initial state after the analysis correction, thus correct nutrient concentrations will significantly contribute to the forecasting capacity of the model between the assimilation periods). The direction of change (increase/decrease) in the nutrient concentrations, following the assimilation of near surface chl-a will depend on the initial model chl-a error (positive/negative) as compared to the satellite and the error covariance matrix that will define whether the correction of nutrients will follow that of chl-a. There is also the case, where the simulated nutrients are in agreement with the observations, although there is a bias in the model chl-a, presumably due to some model parameterization error, in which case the chl-a correction might result in the deterioration of the simulated nutrients. In Table 1.2, the evaluated variables in all systems are shown in different colour, depending on their improvement or deterioration resulting from the assimilation. In the Baltic (DMI) the reanalysis improves the seasonal evolution of the phytoplankton blooms and nutrient concentrations in the surface and can also reproduces the overall features of the vertical profiles. In statistics, the reanalysis performs better than the hindcast for nitrate, in terms of model efficiency (from 0.08 to 0.12) and model bias (from 14% to 11%), and also better for DIP, in terms of model efficiency (from 0.75 to 0.77) and model bias (from -6% to -5%), but a little worse for Chlorophyll a, in terms of model efficiency (from 0.04 tp 0.03) and model bias (from 10% to 9%). In the North-East Atlantic (PML), the effect of the assimilation on the nutrients was stronger in the more productive shelf-sea areas, along the European coast and in the Celtic and Irish Seas. In these areas, the model chl-a was overestimating GlobColour and the assimilation resulted in the decrease of chl-a that triggered an increase of nitrate, due to the negative correlation between phytoplankton and the limiting nutrient, besides to reduce nitrogen assimilation by phytoplankton. As nitrate presented a positive bias in the free run, the assimilation resulted in the deterioration of nitrates. Non-linear impacts of assimilation on the simulated ecosystem processes (e.g. decreased bacterial remineralisation) might have contributed to the improvement of phosphate simulation (i.e. decreased the reference concentrations and bias for this nutrient). In the Mediterranean (HCMR), the model chl-a was underestimated (on average) as compared to SeaWiFS, as well as the nitrate/phosphate concentrations as compared to in situ data. Therefore, the assimilation resulted
in an overall increase of model chl-a and an increase of both phosphate and nitrate due to their positive correlation, as indicated by the error covariance matrix. In the case of phosphate, the negative bias is reduced (from -40% to -22.5%), while for nitrate the moderate underestimation (-20%) turns into a strong overestimation (+165%). This deterioration of nitrates is stronger in areas of the E. Mediterranean where N/P ratios are particularly high (Adriatic, Israel coast, Nile plume) with phosphate being the limiting factor controlling the ecosystem dynamics. In these areas, there seems to be an excess of nitrogen, added in the correction that is not consumed by phytoplankton, which is limited by the available phosphate. Thus, variables (such as nitrates) that are loosely coupled with the assimilated variable (chl-a) are likely to be deteriorated by the assimilation suggesting an additional constraint may be required.

In the other Mediterranean system (OGS), the assimilation result’s in the improvement of simulated nutrients with the exception of a slight increase in the nitrate bias. It is worth noting that the change in the nitrate bias is opposite (from +4% overestimation to -27% underestimation) from the one simulated in the other Mediterranean system (HCMR). This is attributed to the different way that the two assimilation systems have control over the state vector.

With respect to the impact on HTL modelling, RA and HC data from OPATM-BFM (OGS) showed significant changes in the classic food chain and the microbial loop affecting the skill of the EwE extended model on anchovy and sardine biomass estimates. Data assimilation slightly improves the correlation coefficient for both anchovy and sardine, but while the reliability index increased in the reanalysis for anchovy it decreased for the sardine. It is particularly important to understand that any E2E approach requires a good understanding of the HTL predators of the planktonic groups. Data assimilation although might improve the LTL model’s performance, it might result in both positive and negative effects on the skill of the HTL variables.

In summary we draw the following conclusions and recommendations:

1) In all regions the reanalysis simulations demonstrated improved skill for the assimilated variable(s) at the scale of the whole domain.

2) For non-assimilated variables the assimilation improved the skill of some variables and degraded others.

3) There were no common patterns between different regions using similar models (ERSEM/BMF, NE Atlantic, and Mediterranean) but different assimilation schemes. There is a requirement for a data assimilation system inter-comparison experiment (i.e. testing different schemes with the same, hydrodynamic ecosystem model and data sets).

4) The impact of the assimilation schemes was variable across model domains and in part a function of the variability in both models and assimilated variable uncertainty. Further improvement in the quantification of uncertainty in satellite data products is required. Perturbed parameter model ensembles are required to help quantify model uncertainty.

5) The ability to assess assimilation skill is limited by the available independent data. In some cases the data rich areas are in regions where the assimilation has little impact because of large uncertainties. Improved monitoring of key variables is required.

2. Baltic

2.1 Description of the reanalysis experiment

A 10-year (2000-2009) reanalysis simulation of the Baltic Sea has been made using the physical-biogeochemical coupled model HBM-ERGOM. This is the operational model system operated in Danish Meteorological Institute (DMI) which provides operational forecast for the Baltic Sea. The
technical details of the circulation model HBM was reported by Perg and Poulsen (2012). The biogeochemical model ERGOM was developed by Neumann (2000) and Neumann et al. (2002). The adoption of ERGOM into the DMI operational system involved the development of three aspects. Firstly, the parameters were recalibrated. Secondly, the model included an extra parameterization to reflect the impacts of suspended particulate matter (SPM) on light attenuation, which improves spring bloom timing in coastal regions (depth < 50m) (Wan et al., 2013). Thirdly, the model used the varying N/P ratios, which improves spring bloom timing in coastal regions (depth < 50m) (Wan et al., 2014). The model setup for this reanalysis used the 6nmx6nm horizontal grid with 50 vertical layers. The model performance was comprehensively assessed in Wan et al. (2012).

The initial fields for ammonia, nitrate, DIP and DO are extrapolated from the winter means of data (2001~2009) at 16 off-shore long-term monitoring stations from the International Council for the Exploration of the Sea (ICES) website (http://www.ices.dk/indexfla.asp). The initial fields for biological state variables are manipulated through repetitive runs. The open boundary conditions are configured with the data from the World Ocean Atlas 2001 (WOA01, Conkright et al., 2002) for nitrate, phosphate, and DO, and the remaining state variables are set to zero. River loadings and runoffs are derived from outputs of the operational hydrological model. Atmospheric nutrient deposition values are set based on Langner et al. (2009) and Eilola et al. (2009).

Meteorological forcing is described in D2.1. River runoff and nutrient loads are set with the daily averaged data derived from river measurements for 5 German rivers, operational outputs for 43 Baltic catchments by a hydrological model HBV run by the Swedish Meteorological Hydrological Institute (SMHI) (Bergström, 1976 and 1992), and climatology for the remaining rivers.

A 3DVAR method has been applied to assimilate the satellite SST, in situ temperature and salinity profiles into a coupled physical-biogeochemical model in the Baltic Sea.

In general, the basic scheme of 3DVAR is to find the optimal solution of the model state \( x \) which minimizes the following cost function:

\[
J(x) = \frac{1}{2} (x - x_b)^T B^{-1} (x - x_b) + \frac{1}{2} (H(x) - y_o)^T R^{-1} (H(x) - y_o)
\]  

(1)

\( x \) is the model state to be estimated. It usually refers to analysis state vector. \( x_b \) is the background state vector, \( y_o \) is the observation state vector. \( H \) is the non-linear observational operator with which the analysis equivalent of observation \( y = H(x) \) can be obtained to compare with the observation measurements. The superscript \( T \) denotes matrix transpose. In the cost function, the misfit between analysis and background is weighted by the background error covariance \( B \), and the misfit between analysis and observation is weighted by the observational error covariance \( R \). Usually the optimal solution is found by minimizing the cost function \( J(x) \) with respect to \( x \), in which its gradient is also needed for determining the search direction and iteration steps in the minimizing algorithm:

\[
\nabla J(x) = B^{-1} (x - x_b) + \nabla_x H(x)^T R^{-1} (H(x) - y_o) 
\]

(2)

Following an incremental method (Courtie, etc. 1994), Equation (1) is linearized around the background state into the following form:

\[
J(\delta x) = \frac{1}{2} \delta x^T B^{-1} \delta x + \frac{1}{2} (H \delta x - d)^T R^{-1} (H \delta x - d)
\]  

(3)
where \( \mathbf{d} = \mathbf{y}_o - H(\mathbf{x}_s) \) is the innovation vector, \( H \) is the linearized observation operator evaluated at \( \mathbf{x} = \mathbf{x}_s \), and \( \delta \mathbf{x} = \mathbf{x} - \mathbf{x}_s \) is the analysis incremental vector. In this way, the original problem converts into finding an incremental analysis \( \delta \mathbf{x} \). Equation (2) becomes:

\[
\nabla J(\delta \mathbf{x}) = \mathbf{B}^{-1} \delta \mathbf{x} + H^T \mathbf{R}^{-1}(H \delta \mathbf{x} - \mathbf{d})
\]

(4)

In our current scheme, the state vector contains only temperature and salinity model state variables:

\[
\mathbf{x} = \begin{bmatrix} T \\ S \end{bmatrix}
\]

(5)

**Figure 1.** Topography of model domain and locations of 5 observational stations
2.2 Results

Five offshore observational stations (Figure 1 for location) are selected for the point-to-point comparison in the surface. The evolution of RMSE for temperature and salinity is given in Figure 2, where the improvements due to assimilation can be clearly seen. Some comparisons show that chlorophyll and nutrients simulations are improved after the temperature and salinity assimilation (Figure 3). Figures 4-6 indicate that the reanalysis improves the hindcast results, most notably for the periods 2007-2009. The improvement of reanalysis is also displayed through the comprehensive model validation scheme (Wan et al., 2011). The results using the comprehensive model validation scheme are displayed in Figure 7. Table 1 lists the statistic metrics comparing reanalysis and hindcast for Chl, DIN, DIP and Oxygen according to the scheme described in D2.3 (www.marine-
Taylor diagram visually shows the improvement of reanalysis comparing to hindcast for the standard deviation, correlation coefficient, centralised root mean error for Chl, DIN, DIP and Oxygen (Figure 8).

Figure 4. Seasonal evolution of Chl in the surface. Black cycles for observations, red curves for hindcast and green curves for reanalysis. Unit: mg m\(^{-3}\). A-E for the stations labelled in Figure 1.
Figure 5. Seasonal evolution of DIN in the surface. Black cycles for observations, red curves for hindcast and green curves for reanalysis. Unit: mmol m$^{-3}$. A-E for the stations labelled in Figure 1.
Figure 6. Seasonal evolution of DIP in the surface. Black cycles for observations, red curves for hindcast and green curves for reanalysis. Unit: mmol m$^{-3}$. A-E for the stations labelled in Figure 1.
Figure 7. Comprehensive comparison between simulation (red curves) and reanalysis (green curves) against observations (black cycles). Panels A-C depict the seasonal pattern of model biases for Chl, DIN and DIP, respectively, and Panels D-F show their vertical profiles (vertical axes for depth, unit: m).
Figure 8. Taylor diagram for Chl, DIN, DIP and Oxygen. Filled purple cycles for hindcast, filled blue cycles for reanalysis.

Table 1.1. Model skill for core metrics. Model skill scores are colour coded to give an indication of model skill as follows; Good = green, Moderate = Black, Poor = Red; correlation r good > 0.75, poor < 0.20, ME good = > 0.5, Poor = < 0, Reliability index good 0.8-1.2, poor > 2 or –ve. PBias, good = < 20%, poor = > 100%.

| Hindcast |  |
|---|---|---|---|---|---|---|
| Variable | Unit | Model Efficiency | % Model Bias | Pearson Correlation Coefficient | RMSE | Unbiased RMSE | Reliability Index |
| Chl | mg m$^{-3}$ | 0.04 | 10 | 0.23 | 4.99 | 4.98 | 2.01 |
| DIN | mmol m$^{-3}$ | 0.08 | 14 | 0.49 | 4.15 | 4.11 | 1.37 |
| DIP | mmol m$^{-3}$ | 0.75 | -6 | 0.87 | 0.53 | 0.52 | 0.45 |
| Oxygen | mmol m$^{-3}$ | 0.71 | 7 | 0.86 | 63.21 | 63.11 | 0.95 |

2.3 Summary of reanalysis experiment and lessons learnt

The model results were compared with available data collated from the data from the International Council for the Exploration of the Sea (ICES) (http://www.ices.dk/indexfla.asp). The reanalysis improves the seasonal evolution of phytoplankton blooms and nutrient dynamics in the surface and can also reproduce the overall features of vertical profiles, even though, only temperature and salinity data are assimilated into the model system. Usually, satellite remote sensing Chlorophyll a is the data source used in the data assimilation scheme for biogeochemical models. However, the
satellite remote sensing Chlorophyll a in the Baltic Sea such muddy coastal regions are not reliable. It means the data availability limits the data assimilation scheme directly applying for the biogeochemical model.

2.4 References


3. NE Atlantic

3.1 Description

The North East Atlantic region is represented in figure 9. The data assimilation system for this region is composed by a lower-trophic level ecosystem model (POLCOME-ERSEM) and an assimilation scheme (Ensemble Kalman filter) that were described extensively in a previous deliverable of this project (deliverable D2.4“Description of the coupled model for each region”).

For the benefit of the reader, the ecosystem model describes the hydrodynamics of the North East Atlantic using the Proudman Oceanographic Laboratory Coastal Ocean Modelling System (POLCOMS) (Holt and James, 2001), which is a three-dimensional, baroclinic, finite difference primitive equation model formulated on an Arakawa B-grid. Temperature and salinity are prognostic variables. The hydrodynamic module includes a vertical-turbulence model and calculations of horizontal pressure gradients (Holt and James, 2001).
The marine biogeochemical dynamics are described by the European Regional Seas Ecosystem model (ERSEM) (Baretta et al., 1995), and we refer to Blackford et al. (2004) and Artioli et al. (2012) for an extensive description of the model version used in this work (ERSEM-2004 with carbonate system). The model has 49 biogeochemical state variables and it applies a functional type approach. Primary producers are split into four size-based Phytoplankton Functional Types (PFTs): diatoms, phytoflagellates, picophytoplankton and dinoflagellates. Each of these is defined in terms of its content of chlorophyll, carbon, nitrogen, phosphate, and (for diatoms only) silicate. In the PFTs, the stochiometric ratios of chlorophyll-to-carbon and nutrients-to-carbon ratios are time variable (Geider et al., 1997; Baretta-Bekker et al., 1997). Three functional types of zooplankton, i.e. mesozooplankton, microzooplankton, and heterotrophic nanoflagellates, prey on the different PFTs, as a function of their size. Besides the PFTs, the model describes the dynamics of other optically-active compounds: particulate matter (distinguished in three classes: small, medium and large) and labile and semi-labile dissolved organic matter. The model also includes the dynamics of one bacterial functional group, dissolved inorganic nutrients, oxygen and carbon dioxide. The benthic sub-model is the ERSEM-II benthic model, as proposed and parameterized in Blackford [1997].

The data assimilation scheme for the North East Atlantic system is based on the Ensemble Kalman filter (EnKf; Evensen, 1994; Evensen, 2003), and it was applied following the implementation for shelf-seas described in Ciavatta et al. [2011]. The system uses an ensemble of 100 members, it assimilates surface chlorophyll observations from satellite, and “analyses” (i.e. updates directly) 38 ERSEM variables out of the 49 of the full state vector. The remaining 11 variables are updated through the model equation during the simulation runtime (“forecast” step).

We applied a localized EnKF (Evensen, 2003), i.e. the analysis was carried out grid point by grid point by processing data within a spatial “radius” around the grid point. As in Ciavatta et al. 2011, we applied a spatial variable radius, as a function of the bathymetry of the model domain. In particular, we set a radius of 25 Km for grid points where the bathymetry is lower than 50 m (i.e. in 14% of the points of the model domain), 50 km for bathymetry between 50 – 2000 m (51% of the model domain) and 100 km for bathymetry deeper than 2000 m (35% of the model domain).

State variables and observations were log-transformed prior to the analysis, and afterwards exponentially back-transformed, to guarantee the state corrections are positive [Ciavatta et al, 2011].
Model error is accounted for by applying random perturbations to the incident irradiance field. A Gaussian perturbation with standard deviation equal to 20% of the irradiance value is added during the model forecast step. Furthermore, at the first assimilation step of each year, model error is added to all the variables undergoing the analysis, as white noise drawn from a distribution of pseudo-random fields with error equal to 10% of the value of the variables. The error is lowered to 1% for those variables that have relatively high average values (alkalinity, DIC, ammonia, silicate, small particulate and semi-labile dissolved carbon), to avoid biogeochemically meaningless perturbations.

This set up of the EnKF was applied in the monthly assimilation of remotely sensed chlorophyll data.

### 3.1.2 The assimilated remotely sensed chlorophyll data

GlobColour chlorophyll was assimilated into the North East Atlantic model system.

The GlobColour dataset consists of daily global chlorophyll fields merged between three satellite missions: 1) the Medium Resolution Imaging Spectrometer Instrument (MERIS) aboard ENVISAT, 2) the Moderate Imaging Spectrometer (MODIS) on the Aqua Earth Observing System (EOS) mission, and 3) the Sea-viewing Wide Field of view Sensor (SeaWiFS) on board OrbView-2.

The Version 3.1 of the dataset produced by the GSM semi-analytical merging model (Maritorena et al., 2002) was downloaded from the MyOcean interface, in a binned format at 4km resolution projected on the Integerised SINusoidal projection. For each bin an error is provided, that is computed from uncertainties on the water leaving radiances from each sensor and uncertainties in the retrieval algorithm (Maritorena et al., 2005).

Projection on the North East Atlantic model grid was performed by averaging all bins falling in each model grid cell. The associated error for each grid cell is taken to be the maximum error encountered in the bins used for that particular cell. 5-day composites were computed centred on the first day of each month for the purpose of assimilation.

### 3.1.3 Set-up of the assimilation run

A twelve year-long reanalysis simulation for the years 1998-2009 has been made. A “reference simulation” for the same period was used to compare and assess the performance of the reanalysis simulation. This reference simulation is provided by the last twelve years of the 1991-2009 hindcast simulation, which is described in the Deliverable 2.8 of this Project.

The reanalysis simulation was initialized using the output for December 1997 provided by the above mentioned hindcast simulation. This output was perturbed and resampled to obtain the initial conditions for the ecosystem variables in the 100 ensemble. In the Gaussian perturbation, we sampled distributions of pseudo-random fields with error equal to 10% of the value of the variables. The error was lowered to 1% for those variables that have relatively high average values (alkalinity, DIC, ammonia, silicate, small particulate and semi-labile dissolved carbon, to avoid physically meaningless perturbations.

As in the hindcast, in the reanalysis simulation the atmospheric forcing was given by data from the DMI regional climate model (see Deliverable 2.8 and also Deliverable D2.2: “Meta data for the boundary conditions and forcing functions for each region”). The oceanic conditions at the open boundaries (temperature, salinity, currents and sea surface elevation) were extracted for the years 1998-2009 from the GLORYS reanalysis product (MERCATOR) provided within the MyOcean project. The corresponding conditions for dissolved nutrients and oxygen were extracted from WOA climatology (2005) dissolved inorganic carbon from GLODAP. The rest of the ecosystem variables were solved using no-flux conditions at the open boundaries.

For freshwater fluxes, daily discharge data for 250 rivers in the years 1998-2009 were taken from the Global River Discharge Data Base, and from data prepared by the Centre for Ecology and Hydrology.
River nutrient loading matches that used by Lenhart et al. (2010), with raw data for the UK, Northern Ireland, Ireland, France, Norway, Denmark and the Baltic processed by van Leeuwen (CEFAS, UK) and raw data for Germany and the Netherlands was processed by Pätsch and Lenhart (2004). In addition, Baltic inflow at the belt was represented as river-inflow. Atmospheric input of nutrients was derived from EMEP.

3.1.4 The in situ data

The in situ data used for the skill assessment of the reanalysis and reference simulations is a sub-set of the database used in the benchmarking of the hindcast simulation, described in the Deliverable 2.8 of this Project.

The data was extracted from the International Council for the Exploration of the Sea (ICES) Ecosystem Data Online Warehouse (ICES, 2009) and we carried out a data-quality control to remove data repetitions and biogeochemically meaningless values.

The validation data-set for the reference and reanalysis simulations includes the variables listed in Table 3.1, and values for the period 1998-2009. With respect to the hindcast benchmarking, we did not consider water temperature and salinity for validation, because physical variables are not affected by the biogeochemical assimilation in the NW Atlantic system. We did not include pH and alkalinity neither, as the number of data points available resulted relatively low when applying the validation procedure described in the next section.

Table 3.1. Name, unit and representative symbols of the variables considered in the assessment of the reanalysis output.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Model symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>chlorophyll</td>
<td>mg m$^{-3}$</td>
<td>Chl</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td>mmol m$^{-3}$</td>
<td>O2o</td>
</tr>
<tr>
<td>Nitrate</td>
<td>mmol m$^{-3}$</td>
<td>N3n</td>
</tr>
<tr>
<td>Ammonia</td>
<td>mmol m$^{-3}$</td>
<td>N4n</td>
</tr>
<tr>
<td>Phosphate</td>
<td>mmol m$^{-3}$</td>
<td>N1p</td>
</tr>
<tr>
<td>Silicate</td>
<td>mmol m$^{-3}$</td>
<td>N5s</td>
</tr>
</tbody>
</table>

3.1.5 Procedure for the assessment of the reanalysis output

The aim of the assessment procedure was to evaluate the skill of the reanalysis simulation, focusing on the impact on the not-assimilated variables. Skill and impacts were assessed with respect to the reference simulation, i.e. the model hindcast re-assessed for just the years 1998-2009.

To this aim, three types of analysis were performed. We:

1. computed maps of changes in skill metrics (RMSE and correlation) for the assimilated satellite chlorophyll.
2. computed maps of changes in the estimates of the average annual distributions of the assimilated and not-assimilated variables listed in Table 2.1
3. computed and compared metrics of the reanalysis and reference skill in estimating the not-assimilated ICES database, using Tables, Taylor and Target diagrams.
The computation of the metrics and diagrams in the above point 3) follows, in general, the benchmarking procedure for the hindcast simulation (see Deliverable 2.8), exploiting the OPEC benchmarking tool (see Deliverable 2.3 “Target variables and benchmarking metrics: Technical Specification of Benchmarking Tool v1”).

In this procedure, the data-to-model match-ups are obtained by setting maximal temporal distances equal to fifteen days and vertical spatial steps equal to 2.5 m. Match-ups nearby the borders of the model domain (i.e. within 0.5° from the limits, in latitude or longitude) are discarded to avoid effects of the boundary conditions. Furthermore, we excluded the match-ups from the Skagerrak/Kattegat area (i.e. the Danish area East of 9° Longitude), where the model is affected negatively by the Baltic boundary condition (see e.g. Artioli et al., 2012).

Outlier’s in the data were excluded from the analysis. The thresholds to define high-value outliers were set by exploiting the results from the hindcast simulation (see Deliverable 2.8); the threshold values are reported in Table 3.2.

The skill analysis at the above point 3 was performed considering the whole set of points resulting from the above matchup procedure.

However, the skill analysis was repeated also for a subset of matchups where the impact of assimilation was particularly evident. This subset included the matchups where the difference between assimilation and reference values was larger than 10% of the reference value. By this way, we evaluated if assimilation had positive or negative effects in those areas and months where the assimilation impacts where the stronger.

Table 3.2. The table lists the lower and upper threshold values we applied to define the outliers in the model and in situ data. Upper values correspond to the 95th percentiles of the ICES data distributions estimated in the benchmarking of the hindcast simulation in the years 1991-2009 (see Deliverable 2.8).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Lower Threshold</th>
<th>Upper Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorophyll</td>
<td>mg m⁻³</td>
<td>1E⁻⁷</td>
<td>10.27</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td>mmol m⁻³</td>
<td>100.</td>
<td>335</td>
</tr>
<tr>
<td>Nitrate</td>
<td>mmol m⁻³</td>
<td>1E⁻⁷</td>
<td>36.</td>
</tr>
<tr>
<td>Ammonia</td>
<td>mmol m⁻³</td>
<td>1E⁻⁷</td>
<td>8.3</td>
</tr>
<tr>
<td>Phosphate</td>
<td>mmol m⁻³</td>
<td>1E⁻⁷</td>
<td>1.24</td>
</tr>
<tr>
<td>Silicate</td>
<td>mmol m⁻³</td>
<td>1E⁻⁷</td>
<td>17.3</td>
</tr>
</tbody>
</table>

3.2 Results and discussion

3.2.1 Skill in the estimation of the assimilated chlorophyll data

The average distributions of chlorophyll from satellite, the reference and reanalysis outputs are compared in Figure 10. A qualitative comparison suggests that both the reference and reanalysis simulations reproduced, in general, the coastal-offshore gradients of the concentrations and the higher concentrations in the North part of the spatial domain. The reference overestimated the observations, in particular in the Norwegian Trench, English Channel, Irish Sea and Armorica Shelf,
while data were underestimated in the Dutch and German coastal areas. Assimilation smoothed the reference bias in all the above-mentioned areas.

Figure 10. Maps of the average distributions of chlorophyll concentration in the years 1998-2009 computed from the assimilated GlobColour data and from the reanalysis and reference outputs. The differences between analysis and reference distributions are also shown.

The quantitative skill assessment confirms that the reanalysis simulation provided better estimates of the chlorophyll concentrations in the North East Atlantic in the years 1998-2009, when compared with the reference simulation. Assimilation decreased the root mean square error and increased the correlation with the assimilated satellite data in the largest part of the model domain. This is highlighted in Figure 11, which shows the maps of the Root Mean Square Error (RMSE) and correlation obtained by comparing the time series of monthly satellite data and monthly assimilation output (analysis) in the years 1998-2009, at each point of the model domain. The graphs on the right side of figure 11 show the differences in the RMSE and correlation with respect to the reference output. Table 3.3 enumerates the grid points where the two metrics were improved, deteriorated or left substantially unchanged with respect to the reference. As one can see, remarkable improvements of the metrics where obtained in large parts of the model domain. The most evident improvement in the metrics (decreases of RMSE up to -30% and increase of the correlation up to 0.25, Figure 11) were obtained in the areas mentioned above where the reference overestimation of chlorophyll was most evident (see Figure 10). We note that the improvement in the RMSE and
correlation were obtained also in the Norwegian Trench, despite correlation with the satellite data remained substantially poor in that area.

**Figure 11.** Maps of the RMSE and correlations between assimilated chlorophyll data and assimilation output (“analysis”) in the years 1998-2009 (panels on the left). On the right, maps of the differences in the metric values computed from the assimilation output (left panels) and reference outputs.

**Table 3.3.** The table lists the fraction of grid points of the model domain where the root Mean Square Error (RMSE) and the correlation of the analysis with the assimilated chlorophyll data were improved (green font), deteriorated (red) or substantially comparable (yellow) with respect to the metrics obtained for the reference run. The metrics were defined “comparable” when the differences between analysis and reference were smaller than 1% for RMSE, and smaller than 0.01 for correlation, in absolute values.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Improved</th>
<th>Deteriorated</th>
<th>Comparable</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE</td>
<td>93%</td>
<td>7%</td>
<td>0.1%</td>
</tr>
<tr>
<td>Correlation</td>
<td>58%</td>
<td>8%</td>
<td>34%</td>
</tr>
</tbody>
</table>

Besides improvements in the analysis, the assimilation run also improved the monthly model forecasts of the chlorophyll distributions (here we remind that “forecasts” are the model estimates before the assimilation step, see Section 2.1). As one can see in Figure 12 and Table 3.4, the RMSE of
the chlorophyll forecasts decreased in a large part of the model domain (75%), while the correlation remained substantially unchanged.

The improvements in the metrics for the assimilated chlorophyll data were expectable for the output of the EnKF analysis. This result indicates essentially that the assimilation scheme was correctly implemented and properly tuned in the North East Atlantic region [Triantafyllou et al., 2007; Gregg et al., 2009; Ciavatta et al., 2011]. The improved metrics for the forecast output were less obvious. They indicate that the monthly EnKF re-initialization of the state vector impacted the simulation of the ecosystem evolution, leading to improved estimates of the phytoplankton distribution after 30 days from the assimilation steps.

**Table 3.4.** The table lists the fraction of grid points of the model domain where the root Mean Square Error (RMSE) and the correlation of the forecasts with the assimilated chlorophyll data were improved (green font), deteriorated (red) or substantially comparable (yellow) with respect to the metrics obtained for the reference run. The metrics were defined “comparable” when the differences between analysis and reference were smaller than 1% for RMSE, and smaller than 0.01 for correlation, in absolute values.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Improved</th>
<th>Deteriorated</th>
<th>Comparable</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE</td>
<td>74%</td>
<td>26%</td>
<td>0.3%</td>
</tr>
<tr>
<td>Correlation</td>
<td>20%</td>
<td>13%</td>
<td>68%</td>
</tr>
</tbody>
</table>
3.2.2 Skill in the estimation of the independent in situ data

Assimilation of GloBColour chlorophyll impacted the estimates of unassimilated biogeochemical data in the North East Atlantic model.

This is illustrated in figure 13, which shows the average annual distributions obtained in the reanalysis simulation, and the difference of these distributions from the reference ones. Differences up to 10% are evident for all the variables, with the exception of dissolved oxygen, for which differences were in the order of 1%. We note that the chlorophyll distribution in Figure 13a differ from the one shown in Figure 10, since the former was computed from the monthly averages of the reanalysis and reference output, rather than from the instantaneous output at the assimilation steps as in figure 10.

As one can see from figure 13, the assimilation impacts on unassimilated variables were highly heterogeneous in space. Impacts were in general more relevant in the more productive shelf-sea areas, along the European coast and in the Celtic and Irish seas. In all these areas, the general trends of change were a decrease of the chlorophyll concentration, which triggered an increase of nitrogen (both ammonium and nitrate) and decrease of phosphate and silicate concentrations (but for the latter nutrient we note also an increase in the southern North Sea).

Assimilation impacts were less evident in the western oceanic waters as well as in the central and northern part of the North Sea.

Due to the spatial heterogeneity of the assimilation impact, as well as to the spatial distribution of the ICES data, one obtains different assessments of the assimilation effects on the model skill, depending if the bulk ICES dataset is analysed, or just a subset of matchups selected in the regions where assimilation had the major impacts.

Assimilation and reference skill in hindcasting the in situ data are comparable when the outputs are assessed against the bulk of the ICES data set. This is shown in Table 3.5, which compares the values of the skill metrics for the reanalysis and references output, computed using the OPEC benchmarking tool and the whole set of matchups. In this case, the differences between the metrics are low for most of the variables. The strongest impact was recorded for ammonium and nitrate, for which the RMSE increased by ~8% after chlorophyll assimilation.

However, both the reanalysis and reference simulations had a moderate skill in representing the dissolved oxygen dynamic, for which the Model Efficiency scored +0.4, the reliability index was close to 1, and the correlation reached ~0.7. Correlations with the data were not negligible (higher than 0.5) also for silicate. On the other hand, performance was rather poor for nitrate and ammonia. Notably, all the nutrients had relatively high percentage bias, with negative values, indicating that both the model and the reanalysis tended to overestimate the data measured in the North East Atlantic region in the years 1998-2009. The results are coherent with those obtained in the benchmarking of the hindcast simulation for the whole period 1991-2009 (see Deliverable 2.8).
Figure 13.a Impacts of satellite chlorophyll assimilation on the simulation of chlorophyll, oxygen and nitrate. The panels on the left show the average annual distribution computed from the reanalysis output in the years 1998-2009. The panels on the right show the differences between the average annual distributions computed from the reanalysis and reference output.
Figure 13.b Impacts of satellite chlorophyll assimilation on the simulation of the unassimilated variable ammonium, phosphate and silicate. The panels on the left show the average annual distribution computed from the reanalysis output in the years 1998-2009. The panels on the right show the differences between the average annual distributions computed from the reanalysis and reference output.

Table 3.5. Core skill metrics for the reference and reanalysis simulation in the North-West Atlantic, in the years 2008-2009, when using the bulk ICES dataset. The last section of the table lists the absolute differences between reanalysis and reference values (for % model bias and correlation), or the percentage difference (i.e. the difference divided by the reference value, for RMSE and unbiased RMSE). Model skill scores are colour coded to give an indication of model skill as follows; Good = green, Moderate = Black, Poor = Red; correlation r good > 0.75, poor < 0.20, ME good = > 0.5, Poor = < 0, Reliability index good 0.8-1.2, poor > 2 or -ve. PBias, good = < 20%, poor = > 100%.

Region: NE Atlantic  
Model: POLCOMS-ERSEM  
Met forcing: DMI regional hindcasat  
Hindcast time period: 1991-2009  
Reference time period: 2008-2009  
Reanalysis time period: 2008-2009  
Contact: S Ciavatta (avab@pml.ac.uk)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Model Efficiency</th>
<th>% Model Bias</th>
<th>Pearson Correlation Coefficient</th>
<th>RMSE</th>
<th>Unbiased RMSE</th>
<th>Reliability Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chl</td>
<td>mg/m^3</td>
<td>-0.2</td>
<td>23.2</td>
<td>0.343</td>
<td>2.21</td>
<td>2.17</td>
<td>1.99</td>
</tr>
<tr>
<td>O2o</td>
<td>mmol/m^3</td>
<td>0.4</td>
<td>4.1</td>
<td>0.682</td>
<td>27.66</td>
<td>25.44</td>
<td>1.05</td>
</tr>
<tr>
<td>N3n</td>
<td>mmol/m^3</td>
<td>-2.2</td>
<td>-116.0</td>
<td>0.449</td>
<td>11.63</td>
<td>8.02</td>
<td>2.08</td>
</tr>
<tr>
<td>N4n</td>
<td>mmol/m^3</td>
<td>-2.4</td>
<td>-85.4</td>
<td>0.277</td>
<td>2.93</td>
<td>2.64</td>
<td>2.19</td>
</tr>
<tr>
<td>N1p</td>
<td>mmol/m^3</td>
<td>-2.5</td>
<td>-67.9</td>
<td>0.314</td>
<td>0.51</td>
<td>0.42</td>
<td>1.63</td>
</tr>
<tr>
<td>N5s</td>
<td>mmol/m^3</td>
<td>-2.9</td>
<td>-84.8</td>
<td>0.556</td>
<td>5.87</td>
<td>4.96</td>
<td>1.72</td>
</tr>
</tbody>
</table>

Reference
More insights on the assimilation performance can be achieved if the skill assessment focuses on a selected subset of matchups, where the assimilation impact was particularly strong.

In those areas and months where data assimilation had the strongest impact on the reference simulation, this impact improved noticeably the estimates of in situ chlorophyll and phosphate data, but also deteriorated nitrogen and silicate estimates.

This can be seen in Table 3.6, which lists the values of the metrics computed using matchups where the differences between reanalysis and reference outputs were higher than 10% (see Section 2.1.5). The values of these metrics are represented also in the Taylor and target diagrams in Figures 14 and 15. Reanalysis chlorophyll is closer than reference to the optimal point in both the Taylor diagram (Figure 14) and target diagram (Figure 15) as a consequence, respectively, of a higher correlation and lower RMSE with respect to the in situ chlorophyll data (Table 3.6).

Similarly, Reanalysis phosphate is closer than the reference to the optimal point in the Target diagram (Figure 15), thanks to the lower bias and RMSE (Table 3.6). The decreased RMSE moved reanalysis closer to the optimal point in the Taylor diagram (Figure 14), despite the slight decrease of the correlation (Table 3.6).

Differently, reanalysis nitrate, ammonium and silicate are farer than reference from the optimal points in both the Taylor and Target diagrams, as a consequence of a general worsening of the metric values.

An evident feature in the Target diagram of nitrate (Figure 15) is the shift of the representative point from the II quadrant (reference) to the first. This indicates that the assimilation increased the simulated variability of nitrate, up to overestimate the variability observed in situ. However, this latest overestimation was negligible, since the nitrogen point fells close to the radius-1 circle in the Taylor diagram (Figure 14). Also the variability of ammonium and silicate was further overestimated.

### Percentage and absolute differences

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Model Efficiency</th>
<th>% Bias</th>
<th>Model Correlation Coefficient</th>
<th>RMSE</th>
<th>Unbiased RMSE</th>
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after assimilation of satellite chlorophyll, as indicated by the increased distances from the radius-1 circle in the Taylor diagrams (Figure 14).

The reanalysis deterioration of the nitrate estimates can be considered a drawback of the improved estimation of chlorophyll, and a consequence of the model overestimation of nutrients. This can be argued by adopting the conceptual model suggested by Gregg et al. (2009) to explain the impact of chlorophyll assimilation on the balance of plankton-to-limiting nutrients.

In our application, the reference run overestimated both satellite chlorophyll (Figure 10) as well as nitrate (Table 2.5). Assimilation led to a general decrease of the chlorophyll estimates (Figure 10 and 13), closer the remotely sensed observations (Figure 11 and 12). The decrease of chlorophyll triggered a decrease of the total phytoplankton biomass (not shown). This will in general decrease the phytoplankton uptake of nitrogen, leading to higher nitrogen concentrations in the water column, when compared to the reference simulation. This would explain the higher percentage bias of the nitrogen forms in Table 2.6.

Analogous negative impacts of chlorophyll assimilation on the estimation of unassimilated nutrient concentrations have been previously observed by, e.g., Fontana et al. 2009; Nerger and Gregg 2007, 2008; Gregg, 2008.

**Table 2.6.** Core skill metrics for the reference and reanalysis simulation in the North-East Atlantic, in the years 2008-2009, when using matchups selected in those areas and months where the difference between reanalysis and reference estimates were higher than 10%. The last section of the table lists the absolute differences between reanalysis and reference values (for % model bias and correlation), or the percentage difference (i.e. the difference divided by the reference value, for RMSE and unbiased RMSE). Model skill scores are colour coded to give an indication of model skill as follows; Good = green, Moderate = Black, Poor = Red; correlation r good > 0.75, poor < 0.20, ME good = > 0.5, Poor = < 0, Reliability index good 0.8-1.2, poor > 2 or –ve. PBias, good = < 20%, poor = > 100%.

Region: NE Atlantic  
Model: POLCOMS-ERSEM  
Met forcing: DMI regional hindcast  
Hindcast time period: 1991-2009  
Reference time period: 2008-2009  
Reanalysis time period: 2008-2009  
Contact: S Ciavatta ([avab@pml.ac.uk](mailto:avab@pml.ac.uk))

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### Percentage and absolute differences

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### Variable Reanalysis Reference

#### Chlorophyll

#### Nitrate
Figure 14. Taylor and Target diagrams visualizing the reanalysis skill in hindcasting surface in situ data of chlorophyll, dissolved oxygen and nitrate concentrations.

<table>
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<td><img src="image" alt="Diagram" /></td>
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3.2.3 Discussion
The performance of the reanalysis simulation was negatively impacted by the relatively high errors and number of missing values in the assimilated chlorophyll data. Indeed, where assimilated data have high errors (compared to the model error) or the data are missing, the EnKF localized assimilation scheme carries out relatively small corrections, if any, to the model forecasts (Evensen, 2003).

Figure 15. Target diagrams visualizing the reanalysis and reference skill in hindcasting surface in situ data of ammonium, phosphate and silicate.
The number of assimilated monthly data and their average percentage error in the years 1998-2009 are shown in Figure 16. As one can see, at none of the grid points was available the whole set of 144 monthly data in the 12 years of reanalysis simulation, and less than half of the data were actually available at high latitudes, above 55°N. Composites from December till February were typically not-available or extremely sparse due to the high latitude, low solar angle and cloud cover in the study region. The percentage errors of the data were higher in the shelf-area and in particular in the Central and North - North Sea.

Importantly, the combination of high errors and sparse data in the North Sea explains, at least in part, why the impact of assimilation was relatively low in this region (see Figures 10, 11, 12, 13). Furthermore, if one considers that a large part of the in situ data used for model validation comes from the Central and North - North Sea (see e.g. Figure 17), it results also explained the low impact of assimilation on the reference skill metrics, when the bulk of the ICES data in the region is considered (see Table 2.5).

Figure 16 Number of monthly assimilated chlorophyll data in the years 1998-2009 and average values of the percentage errors of the data.

Neglecting the areas of low assimilation impact (due to high satellite errors, missing data or other factors) leads to a reduction in the number and coverage of the in situ data used for the reanalysis assessment in Table 3.6 and Figures 14 and 15.

This is exemplified in Figure 17, which compares the sampling sites of the nitrogen data in the bulk ICES database, and the subset of sites where the differences among reanalysis and reference estimates of nitrogen where higher than 10%. These were the sites used for the assessment in Table 3.6 and Figure 14 and 15. Similarly, Figure 18 compares the monthly distribution of the total number of ICES nitrogen data, versus the subset applied in the reanalysis-to-reference comparison.

The comparison of the two maps in Figure 17 confirms that assimilation impacts were low in the regions were the errors of the satellite data were higher (e.g. Central and North North Sea). Figure 18 confirms that impacts where comparatively higher in spring-summer than in winter-autumn, when chlorophyll data were more often unavailable for assimilation.

Figure 17 and 18 also highlight that the assessments of the reanalysis and reference performance in Table 3.6 and Figure 14 and 15 focused on shelf region and the productive months, i.e. in the most challenging areas and seasons for a marine ecosystem model. This explains why the metrics in Table 3.6 tend to be less satisfactory than the ones computed on the bulk of the ICES data (Table 3.5).
Finally, we note in Figure 16 that not even the bulk ICES sampling sites covers areas of were assimilation has the strongest impact on the reference estimates of nitrogen, such as the shelf-break South East of Ireland (see Figure 13a). Analogous considerations hold for the other validation variables. The poor sampling in areas where assimilation had strong impacts contributes to explain the relatively low changes of the metrics values in Table 2.6.

Figure 17. Sampling sites of the bulk of ICES nitrogen data in the years 1998-2009 (left) and subset of samples used in the assimilation and reference skill analysis in Table 2.6 (right).

Figure 18. Number of nitrogen data in the whole ICES database for years 1998-2009 (left) subset of samples used in the assimilation and reference skill analysis in Table 2.6 (right).

3.3 Summary and lessons learnt

The reanalysis simulation in the North East Atlantic region improved markedly the estimates of the assimilated chlorophyll GlobColour data in the years 1998-2009.

Both the estimates provided by the monthly EnKF “analysis” and by the model 30-day “forecasts” had better skill (higher correlation and lower root mean square error) in reproducing the spatial-temporal patterns of the assimilated data.

The results for the EnKF analysis indicate essentially that the assimilation scheme was correctly implemented and properly tuned in the North East Atlantic region [Triantafyllou et al., 2007; Gregg et al., 2009; Ciavatta et al., 2011].

The results of the 30-days “forecasts” indicate that a monthly frequency of assimilation was adequate to improve the simulation of the chlorophyll patterns observed from satellite.

The reanalysis simulation demonstrated some skill in reproducing the spatial-temporal patterns of oxygen, nitrate and silicate, as resulted from the comparison of the output with the bulk of the un-assimilated in situ data available in the North East Atlantic. However, nutrients were overestimated by the reanalysis, as well as by the reference simulation. This outcome is coherent with the general model overestimation of nutrients in the North East Atlantic region observed in the hindcast simulation for years 1991-2009 (see OPEC Deliverable 2.8).
Assimilation of GlobColour data improved, in general, the simulation of in situ data of chlorophyll and phosphate, but increased the bias of nitrogen and silicate estimates. This was evident when a subset of the in-situ data was used to compare reanalysis and reference performance, while the changes were less evident when the whole data-set was exploited for the comparison.

Here we remark that assimilation can often lead to the deteriorations for the unassimilated data, in particular for those variables that have biased reference estimates (see e.g. Fontana et al. 2009; Nerger and Gregg 2007, 2008; Gregg, 2008; Ciavatta et al., 2011; Ford et al., 2012). In our application, the model was overestimating both GlobColour chlorophyll and nitrogen concentration in large parts of the model domain. Thus, the assimilation decrease of chlorophyll exacerbated the overestimation of nitrogen, according to the balancing effect of assimilation on phytoplankton/limiting nutrient concentration described by Gregg et al (2009). Future improvements in the model simulation of the nutrient concentrations (e.g. through the refinement of the initial conditions, improvements of the parameterization of the phytoplankton functional types) could likely support data assimilation in further improving the biogeochemical reanalysis in the North East Atlantic.

Finally, we note that the performance and assessment of the reanalysis simulation was impacted by errors and missing values in the assimilated data, as well as by the spatial distribution of the in situ data used for the computation of the skill metrics.

In particular, assimilated satellite data were relatively poor in quality and quantity in the North Sea, leading to small impacts of assimilations in this area. However a large part of the in situ validation data comes from this area, explaining why here assimilation did not impact noticeably the reference skill. To this regard, we note that the use of future satellite products with lower error and higher spatial coverage, e.g. the ESA CCI Ocean Colour products (Sathyendranath et al., 2012), could advantage the application of ocean colour assimilation for biogeochemical reanalysis in the European seas.

On the other hand, relevant impacts of assimilation were observed in areas where in situ data for validation where not available, such as the shelf-break located South West of Ireland. We hope for an increased sampling and monitoring in this area, which is critical also for carbon budgeting in the North East Atlantic (Wakelin et al., 2012).

3.4 References


4. Mediterranean (HCMR)

4.1 Description

The Mediterranean coupled hydrodynamic/biogeochemical model (POM-ERSEM) along with the model setup (initial conditions, river inputs, open boundary conditions) are described in deliverable D2.4 (www.marine-opec.eu/downloads/OPEC_D2.4.pdf). The atmospheric forcing for the hindcast simulation was obtained from the regional climate model HIRHAM5 simulation, provided by DMI (see D2.2 www.marine-opec.eu/documents/deliverables/D2.2.pdf). In the re-analysis run, 8-day average remote sensing Chl-a data (SeaWiFS) are assimilated.

The data assimilation scheme is based on the SEEK (Singular Evolutive Extended Kalman) filter approach. The reanalysis described here uses the Singular Fixed Extended Kalman (SFEK) filter, assuming persistence of the error sub-space with time, and its Ensemble version and the Singular Extended Interpolated Kalman (SEIK) filter, in which the linearization used in the SEEK filter is replaced by linear interpolation (Triantafyllou et al., 2003). Moreover, following (Nerger et al., 2006) a localized analysis algorithm was used to filter out noisy, and possibly spurious, long-range correlations in the analysis phase of the SEIK filter. The idea is based on the assumption that observations have negligible influence for the analysis update of a certain grid point if they correspond to a location that has a large distance to that grid point. In this case, only observations within a certain distance from the grid point need to be taken into account for the analysis of the state of this location. The local analysis is advantageous since the localization increases the degrees of freedom in the update of the state estimate. More details may be found in deliverable D2.4 (www.marine-opec.eu/downloads/OPEC_D2.4.pdf). In an attempt to further improve the performance of the assimilation system, a new algorithm was developed (the Hybrid SEIK filter), combining the analysis of SEIK and SFEK. The main idea that has been introduced by Hoteit et al. (2002) is to evolve a small number of ensemble members, while keeping the rest of the basis fixed. The main difference in the present Hybrid filter from that in Hoteit et al (2002) is that the evolving members are those contributing the least to the error filter representation, while in Hoteit et al. (2002) it is the opposite. In this framework, the flow-dependent covariance tracks changes in the ecosystem dynamics, while the invariant covariance helps mitigating the inbreeding of the ensemble, and also acts as an inflator imitating the role of the model errors covariance.

4.2 Results

4.2.1 Comparison against SeaWiFS Chl-a (assimilated variable)

The re-analysis skill was evaluated using the benchmark tool and the methodology (Target and Taylor diagrams, model efficiency etc.) described in the deliverable D2.3 (www.marine-opec.eu/downloads/D2.3_tech.v1.pdf).
Figure 19. Seasonal mean Chl-a Relative RMSE (RRMSE=(model-SeaWiFS)/data*100), averaged over 2002-2008 period for Free run (left) and assimilation (Hybrid-SEIK filter) run (right).

As shown in Figure 19, the Chl-a Relative RMSE (RRMSE) is significantly reduced in the assimilation run, as compared to the free run. In the latter, an overestimation is found in the Levantine basin (Eastern Mediterranean) with a maximum during the winter-spring period. Furthermore, an underestimation is observed in the Adriatic and N. Aegean Seas, as well as in the Western Mediterranean, particularly during summer and during spring in the G. of Lions dense-water formation site. Overall, the assimilation scheme presents a very good performance in terms of Chl-a relative error, particularly during the spring period. However, there are a few areas, such as the Egyptian and Israeli coast and the Alboran Sea, where there appears to be an increased error after the analysis step.
Figure 20. SeaWiFS (top-left) and model simulated near-surface Chl-a without assimilation (top-right) and with the Hybrid-SEIK (bottom-left) and SFEK (bottom-right) assimilation filters, averaged over 12-19/07/2002. The colored boxes indicate the western and eastern Mediterranean basins, the Adriatic Sea (green), the N. Aegean Sea (red) and the Gulf of Lions (blue), where Figures 21 and 22 refer.

An example of the assimilation results is shown in Figure 20, demonstrating the model simulated 8-day Chl-a average against SeaWiFS for July 2002. The free run (without assimilation) underestimates Chl-a, particularly in the western basin, as well as in the Adriatic and Aegean Seas. In the runs with assimilation (SFEK, Hybrid-SEIK), it is clear that the Chl-a model error is reduced. The Hybrid-SEIK filter appears to better depict Chl-a local maxima in the western basin (Adriatic, G. Lions, Alboran Sea) and has an overall better performance as discussed below.

In Figures 21 and 22, the model simulated Chl-a seasonal multi-year variability is shown against SeaWiFS, averaged over different areas (W. Mediterranean, E. Mediterranean, N. Aegean, Adriatic, G. Lions). Again, it may be seen that the Hybrid-SEIK Chl-a closely follows the SeaWiFS variability, while SFEK is also performing well and presents significant improvement compared to the free run. More specifically, the Hybrid-SEIK filter appears to better reproduce the winter-spring Chl-a peaks in the Western Mediterranean that are mostly related to deep convection events in G. Lions (shown in the same Figure). In the Eastern Mediterranean, the Chl-a overestimation that is found in the free run during winter-spring period appears reduced in SFEK and even further in Hybrid-SEIK runs. Examining the N. Aegean and Adriatic areas, it can also be noticed that the runs with assimilation and particularly the Hybrid-SEIK better reproduce the Chl-a inter-annual variability that is present in the SeaWiFS. This inter-annual variability is probably related to the variability of river and BSW inputs that is not described in the free run (river input data are only available up to 2000, average 1995-2000 inputs are used in 2000-2009 run).
Figure 21. Near-surface model Chl-a, simulated by the free run (blue line) and the runs with assimilation (red=Hybrid-SEIK, black=SFEK), against SeaWiFS (green line), averaged over western (middle), eastern (bottom) and the entire Mediterranean (top).

Figure 22. Near-surface model Chl-a, simulated by the free run (blue line) and the runs with assimilation (red=Hybrid-SEIK, black=SFEK), against SeaWiFS (green line), averaged over the N. Aegean (top), the Adriatic Sea (middle) and the Gulf of Lions (bottom), indicated in Figure 20.
Figure 23. Average Chl-a relative error (RMSD/||SeaWiFS||) for the free run (blue line) and the runs with assimilation (red=Hybrid-SEIK, black=SFEK).

In Figure 23, the Chl-a relative error (RMSD/||SeaWiFS||) for the free run and the runs with assimilation is presented. The Hybrid-SEIK has the better performance, showing the lower relative error, followed by SFEK. It deserves noting that in all runs the error is minimum during spring and maximum during summer-autumn period.

In Figure 24, the Taylor and target diagrams are shown for the three runs (Free run, Hybrid-SEIK, SFEK) against SeaWiFS. The model-data correlation is increased from 0.25 in the free run to 0.4 in SFEK and 0.6 in the Hybrid-SEIK run. The runs with assimilation exhibit a smaller RMS error (Hybrid-SEIK=0.8std, SFEK=0.92std, Free=0.97std) and a standard deviation (Hybrid-SEIK=0.5std, SFEK=0.37std, Free=0.32std) that is closer to that of SeaWiFS. Similarly, in the target diagram, the Hybrid-SEIK and SFEK show a slightly reduced (negative) bias and a better total RMSD score (reasonable), as compared to the free run. The level of variation for all three runs is typically smaller than the SeaWiFS. As mentioned above, the Hybrid-SEIK has an overall better skill as compared to SFEK and the Free run. We should note that in all the above Figures, the 8-day average model results are compared against SeaWiFS. This comparison is more representative, since it includes the model forecast period prior and after the analysis that occurs in the middle of the 8-day period. Finally, in Figures 25, 26 the density plot, target and taylor diagrams created with the benchmark tool, are shown for model simulated (Free run and Hybrid-SEIK) against SeaWiFS Chl-a.

Figure 24. Taylor (left) and target (right) diagrams, comparing the SeaWiFS Chl-a with model Chl-a simulated by the Free run (without assimilation), the Hybrid-SEIK and SFEK assimilation runs.
Figure 25. Density plot of SeaWiFS Chl-a against model Chl-a simulated by the Free run (left) and the Hybrid-SEIK (right) assimilation run.

Figure 26. Taylor (bottom) and target (top) diagrams (benchmark tool), comparing the SeaWiFS Chl-a with model Chl-a simulated by the Free run (left) and the Hybrid-SEIK (right) assimilation run.
4.2.2 Comparison against in-situ data

4.2.2.1 DYFAMED

In an attempt to assess the skill of the assimilation in the entire water column, the simulated nutrient vertical profiles are compared against the DYFAMED data (Figure 27) that is the most comprehensive dataset in the Mediterranean. It may be seen that both nitrate and phosphate in the assimilation run (Hybrid-SEIK) are increased approaching the in situ data concentrations. This can be verified by the target diagrams (Figure 28), showing a decreasing bias and RMS error in the case of the assimilation run.

![Figure 27. Evolution of phosphate (left) and nitrate (right) profiles at DYFAMED (top) against model simulated (bottom) with the free run and the one with assimilation (SEIK).]
4.2.2.2. SeaDatanet in situ data (1990-2000)

In Figures 29-32, target and Taylor diagrams are shown for phosphates, nitrates, silicates and chl respectively, for the free run and the assimilation run (Hybrid-SEIK) against in situ data collated from the SeaDatanet database for 1990-1999 period, since data in 2000-2009 period are very limited. So, the model output in the re-analysis period is essentially validated against a “climatology” constructed by 1990-1999 dataset. In the case of phosphates, a slight improvement may be seen in the re-analysis run (Figure 29, Table 4.1), in terms mostly of bias (decreased) and standard deviation (increased). In the case of nitrates and silicates, the assimilation in the re-analysis run appears to be poor having a negative effect particularly in terms of bias as shown in Table 4.1 (not shown in Figure 29, since the score is outside the target/Taylor diagrams). An important improvement can be seen for (in-situ) Chl-a (Figure 32), where the correlation is increased from 0.33 to 0.47, the PBIAS is decreased from -20% to +5% and ME is increased from 0.08 to 0.19 (Table 4.1). The standard deviation is increased from 0.33 to 0.46 (mg/m³), approaching the variability of the observations (0.75 mg/m³). The negative effect of the assimilation on nitrates and silicates is most probably

Figure 28. Target diagrams (benchmark tool) for model phosphates (top), nitrates (middle) and silicates (bottom) profiles, simulated without assimilation (left) and with the Hybrid-SEIK assimilation filter (right), against DYFAMED data.
related to the fact that the ecosystem dynamics are controlled by the phosphate, which is the limiting factor, particularly in the E. Mediterranean. As shown in Figure 33, the fractional change in phosphate (assimilation with regard to the free run) is similar to that of Chl-a. However, the assimilation run increases the nitrate in the E. Mediterranean areas, where N/P is particularly high (e.g. Adriatic, Nile plume, Israel coast etc.). In those areas, there seems to be excess nitrogen that is not “consumed” by phytoplankton, which is limited by the available phosphate. Therefore, while in the case of phosphate, an error in the analysis correction is not propagated, since the phosphate concentration is directly controlled by phytoplankton, an error in the nitrate correction caused by inconsistency in the EOFs calculation may be accumulated. An additional assimilation run was performed for 2000, where a constraint was imposed on the simulated N/P and Si/P ratios in order to prevent from the nitrates and silicates deviation. Model results show an improvement decreasing the simulated bias (nitrates PBIAS is decreased from -165% to -125%). However, some additional effort is required for a better customization of the assimilation system.

Figure 29. Target (top) and taylor (bottom) diagrams for model surface phosphates simulated without assimilation (left) and with the Hybrid-SEIK assimilation filter (right) over 2000-2009 period, against SeaDatanet in situ data over 1990-1999 period.
Figure 30. Target (top) and taylor (bottom) diagrams for model surface nitrates simulated without assimilation (left) and with the Hybrid-SEIK assimilation filter (right) over 2000-2009 period, against SeaDatanet in situ data over 1990-1999 period.
Figure 31. Target (top) and taylor (bottom) diagrams for model surface silicates simulated without assimilation (left) and with the Hybrid-SEIK assimilation filter (right) over 2000-2009 period, against SeaDatanet in situ data over 1990-1999 period.

Figure 32. Target (top) and taylor (bottom) diagrams for model surface Chl-a simulated without assimilation (left) and with the Hybrid-SEIK assimilation filter (right) over 2000-2009 period, against SeaDatanet in situ data over 1990-1999 period.
Figure 33. Average fractional change (Assim/Free-1) of the assimilation run with regard to the free run for chl-a, phosphates and nitrates.

Table 4.1 Model skill scores are colour coded to give an indication of model skill as follows; Good = green, Moderate = Black, Poor = Red; Correlation r good > 0.75, poor < 0.20, ME good = > 0.5, Poor = < 0, Reliability index good 0.8-1.2, poor > 2 or –ve. PBias, good = < 20%, poor = > 100%.

Region: Mediterranean (HCMR)
Model: POM-ERSEM, Anchovy IBM
Met forcing: DMI regional hindcasat
Hindcast time period: 1990-2009
Reanalysis time period: 2000-2009
Contact: ktsiaras@hcmr.gr (Kostas Tsiaras), gt@hcmr.gr (George Triantafyllou)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Hindcast</th>
<th>Reanalysis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Model Efficiency</td>
<td>% Model Bias</td>
<td>Pearson Correlation Coefficient</td>
</tr>
<tr>
<td>Nitrate</td>
<td>Mmol m⁻³</td>
<td>0.086</td>
<td>20.30</td>
</tr>
<tr>
<td>Phosphate</td>
<td>Mmol m⁻³</td>
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</tr>
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<td>Silicate</td>
<td>Mmol m⁻³</td>
<td>-0.29</td>
<td>19.34</td>
</tr>
<tr>
<td>Chl</td>
<td>Mg m⁻³</td>
<td>0.08</td>
<td>20.9</td>
</tr>
<tr>
<td>Chl/SeaWiFS</td>
<td>Mg m⁻³</td>
<td>0.03</td>
<td>-3.2</td>
</tr>
</tbody>
</table>
4.3 Summary of reanalysis experiment and lessons learnt

The skill of the assimilation system (POM-ERSEM) was evaluated against in situ (SeaDatanet, DYFAMED) and remote sensing (SeaWiFS) data. The assimilation significantly reduced the Chl-a error, exhibiting a good performance on the Chl-a analysis. Among the non-assimilated variables, phosphates that are the main limiting factor in the Mediterranean were improved in the re-analysis run. However, the filter failed to reduce the error of nitrates and silicates. Therefore, some additional effort is required for a better customization and tuning of the assimilation system.

4.4 References


5. Mediterranean (OGS)

5.1 Description

The OGS Mediterranean model system, described in deliverable D2.4, consists of the following components:

- LTL: transport-biogeochemical model (OPATM-BFM) which is coupled with a carbonate system module; the spatial resolution of Mediterranean Sea domain is 1/8° x 1/8° in horizontal and 72 vertical levels;
- DA: 3D-variational scheme with assimilation of SeaWiFS and MODIS weekly averaged chlorophyll maps;
- HTL: Ecopath with Ecosim for the Adriatic Sea sub-region.

Atmospheric and physical forcing for the hindcast simulation are derived from the MyOcean Mediterranean Forecast System (MFS) which is based on the NEMO model managed and run by INGV (Italy). The data assimilation consists of a 3D variational scheme that uses weekly averaged satellite chlorophyll maps provided by GOS-ISAC-CNR (Italy) within the MyOcean project. The coupling of LTL and HTL models is provided with an off-line integration in agree with the scheme presented in Libralato and Solidoro (2009). Details of the implementation of the model system components as well as of the boundary and initial conditions are provided in the deliverables D2.4.

The aim of the present deliverable is to compare two simulations: the hindcast run (HC) and the reanalysis run (RA) which differs from the previous by the assimilation of surface chlorophyll. Results of the hindcast simulation are present in the deliverable D2.8, the present deliverable focuses on showing the improvements in the skill performance of the model that uses the assimilation scheme.

The two simulations were carried out at the CINECA supercomputer facility (Italy) with the following computational features:

- for the hindcast run: 2048 cores on IBM BG/Q “FERMI” (performance: 10 years simulated in around 27 hours).
- for the reanalysis run: 96 cores on IBM PLX (performance: 6 months simulated in 24 hours).
5.2 Comparison for the assimilated variable: surface chlorophyll

The comparison of HC and RA results shows that RA improves the simulation skill of surface chlorophyll (the assimilated variable). The time series of the monthly mean concentrations of chlorophyll (Fig. 34) produced by RA are closer to the satellite observations than those of the HC run for all the sub-regions (see D2.8 for their definition).

The Taylor diagram and the target diagram (Fig. 35) resume the skill improvement of the RA. In the target diagram (Fig. 35a) the RA point is closer to the reference point than the HC point, the correlation coefficient is higher (0.88 for RA and 0.59 for HC), and unbiased RMSD of RA is much lower.

As shown in Table 5.1, the bias of RA (-0.003 mg chl m\(^{-3}\)) is worse than bias of HC (0.001 mg chl m\(^{-3}\)), though such numbers remain very low. This is because the model summer underestimates and winter overestimates balance each other, meaning that the bias computed on the annual cycle is not appropriate to evaluate model skill. Bias should be applied to sub-regions and specific seasons. Density plots (Fig. 36) show that the underestimation of the data of the HC run is not present in the RA run.

The main statistics obtained by means of the benchmarking tool are resumed in Table 5.1, showing a general improvement for all indexes.

![Figure 34. Time series of the monthly mean surface chlorophyll concentration for satellite, and HC and RA runs.](chart)
Seasonal maps of RMSD are computed by comparing the monthly maps of the SeaWiFS dataset with those of the model simulations. HC simulation shows the highest values of RMSD in the Gulf of Lions, Alboran Sea and northern part of Aegean Sea (Fig. 37, left column). Higher errors are in winter and spring seasons.

The relative reduction of the RMSD obtained by the RA run (right column of Figure 37) is computed for each grid point of the domain by applying the following equation:

\[
\frac{(\text{RMSD}_{\text{HC}} - \text{RMSD}_{\text{RA}})}{\text{RMSD}_{\text{HC}}}
\]

The figure shows that the largest relative reduction of the RMSD are reported for the eastern sub-regions (reduction higher than 60% in all seasons), however these regions are those characterized by the lowest RMSD, therefore in absolute terms the reduction of uncertainty is lower than that of the western sub-regions.

In the western sub-regions significant reduction are registered in the Tyrrhenian Sea and South Western Mediterranean region. Further, the reduction of 45%-75% of the RMDS in the North-Western Mediterranean sub-regions in winter and spring correspond to a significant reduction of the absolute error.
<table>
<thead>
<tr>
<th>Season</th>
<th>RMSD of Hindcast</th>
<th>Reduction of RMSD</th>
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<tr>
<td>Winter</td>
<td><img src="image1" alt="Winter RMSD" /></td>
<td><img src="image2" alt="Winter Reduction" /></td>
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<tr>
<td>Spring</td>
<td><img src="image3" alt="Spring RMSD" /></td>
<td><img src="image4" alt="Spring Reduction" /></td>
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<tr>
<td>Summer</td>
<td><img src="image5" alt="Summer RMSD" /></td>
<td><img src="image6" alt="Summer Reduction" /></td>
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<tr>
<td>Autumn</td>
<td><img src="image7" alt="Autumn RMSD" /></td>
<td><img src="image8" alt="Autumn Reduction" /></td>
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</table>
Figure 37. Map of RMSD of surface chlorophyll for the hindcast simulation (left), map of relative reduction of the RMSD between reanalysis and hindcast simulations. Maps are computed considering off-shore area (gridpoints with water column larger than 200m).

5.3 Comparison for non-assimilated variables: Nutrients and dissolved oxygen

The statistics obtained by the benchmark tool have been compared in Figures 38-39 and resumed in Table 5.1.

The correlation coefficient is higher in RA for all the nutrients and for oxygen, even if improvements are quite small. The RMSE and the BIAS are improved in the RA run for almost all variables, with differences more relevant for silicate. The BIAS of RA nitrate changes sign and slightly increases, highlighting that, in the RA simulation, the model overestimates nitrate observations. However, an evident reduction of RMSE is observed in both upper and deeper layers.

Generally, the model efficiency of the reanalysis improves for all the variables: slightly increases are registered for oxygen, nitrate, and silicate, while for phosphorus no change is observed for both upper and deeper layers.

Dissolved oxygen data set is the poorest in terms of match-ups: the data set includes only two cruises (one for October 2001 and one for April 2011). The improvement of RA simulation with respect to HC is slightly evident both in the upper and in the deeper layer in both target and Taylor diagrams.
PHOSP upper

PHOSP deeper

SLCA upper

SLCA deeper

OXY upper
Figure 38. Taylor diagrams for the upper layer and for the deeper layer for nitrate, phosphate, silicate and oxygen. Comparison between HC simulation (left) and RA simulation (right).

<table>
<thead>
<tr>
<th>TARGET DIAGRAM</th>
<th>HC</th>
<th>RA</th>
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<tr>
<td>NTRA upper</td>
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<tr>
<td>NTRA deeper</td>
<td><img src="image3" alt="Diagram" /></td>
<td><img src="image4" alt="Diagram" /></td>
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<tr>
<td>PHOSP upper</td>
<td><img src="image5" alt="Diagram" /></td>
<td><img src="image6" alt="Diagram" /></td>
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</table>
Figure 39. Target diagrams for the upper layer and for the deeper layer for nitrate, phosphate, silicate and oxygen. Comparison between HC simulation (left) and RA simulation (right).

Table 5.1. Skill assessment statistics for hindcast and reanalysis simulations. Skill assessment computation of all variables, but chlorophyll, is performed for two layers: upper layer (0-200) and deeper layer (200m-bottom of water column). Skill assessment of Chlorophyll is performed for surface layer only.

<table>
<thead>
<tr>
<th>Region: Mediterranean (OGS)</th>
<th>Model: OPATM-BFM-EwE</th>
<th>Met/Circulation forcing: ECMWF/MyOcean V3 Reanalysis</th>
<th>Hindcast time period: 1999-2011</th>
<th>Reanalysis time period: 1999-2011</th>
<th>Contact: <a href="mailto:gcossarini@ogs.trieste.it">gcossarini@ogs.trieste.it</a> (Gianpiero Cossarini), <a href="mailto:slibratalo@ogs.trieste.it">slibratalo@ogs.trieste.it</a> (Simone Libralato)</th>
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<tr>
<td><strong>Variable</strong></td>
<td><strong>Unit</strong></td>
<td><strong>Hindcast</strong></td>
<td><strong>Reanalysis</strong></td>
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<td></td>
<td></td>
<td><strong>Model Efficiency</strong></td>
<td><strong>% Model Bias</strong></td>
<td><strong>Pearson Correlation Coefficient</strong></td>
<td><strong>RMSE</strong></td>
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<td></td>
<td></td>
<td><strong>MH</strong></td>
<td><strong>HC</strong></td>
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<td>CHL</td>
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<tr>
<td>DOXY deeper</td>
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<td>0.68</td>
<td>0.29</td>
<td>20.49</td>
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<td>NTRA upper</td>
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<td>0.21</td>
<td>3.18</td>
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<tr>
<td>NTRA deeper</td>
<td>mmolN m⁻³</td>
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<td>2.62</td>
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<tr>
<td>PHOS upper</td>
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<tr>
<td>PHOS deeper</td>
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<td>0.50</td>
<td>0.14</td>
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<tr>
<td>SLCA upper</td>
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<td>0.21</td>
<td>4.05</td>
</tr>
<tr>
<td>SLCA</td>
<td>mmolSi m⁻³</td>
<td>-0.08</td>
<td>-38.36</td>
<td>0.69</td>
<td>3.25</td>
</tr>
</tbody>
</table>
5.4 Comparison of HTL variables: hindcast and reanalysis

No assimilation was performed on HTL variables; nevertheless the aim of the comparison between hindcast (HC) and reanalysis (RA) simulation is to highlight a) effects of modified LTL on the HTL dynamics and b) the changes in skill of the model.

In order to do so, the same approach implemented for the HTL hindcast simulation (see Deliverable D2.8) was performed for the reanalysis, thus using the same fishing effort and fishing mortality time series. As a difference between HC and RA, the data assimilation of chlorophyll on OPATM-BFM reanalysis run, resulted in different productivity changes over time for phytoplankton, picoplankton and bacterioplankton. These plus the anomaly function representing an estimation of input/output of phosphate in the system were the forcing that distinguished between the HC and RA run for the extended EwE model.

This led to a reanalysis simulation for the EwE extended that was compared with the corresponding hindcast simulation: comparison restricted to the HTL outputs, and in particular to target variables, i.e. anchovy and sardine.

Although the reanalysis assimilated chlorophyll only in the OPTM-BFM, this had quite substantial impacts on the production rates for phytoplankton, picoplankton and bacteria, that are used to force the extended EwE model. Namely, as shown in figure 40 the OPATM-BFM reanalysis simulation showed a slight reduction of productivity for large phytoplankton groups both during the spring bloom and in the summer period with respect to HC. On the other side both picoplankton and bacteria showed an increase in productivity over the RA period (1999-2010) with respect to HC.

In EwE extended model these productivity forcings implies a general increase of the microbial loop in the RA with respect to HC, with negative effects in terms of biomass cascading up in the food web. In fact, most of the HTL variables show a reduction in biomass in RA simulation compared with HC, as can be seen in figure 41.
Figure 40. Monthly productivity ratios over time, relative to initial conditions, taken from the OPATM-BFM simulations for the HC (black line) and RA (red line) and used to force the Extended EwE model. Relative productivity ratio over time for phytoplankton (upper panel), picoplankton (middle panel) and bacteria (lower panel).

Figure 41. Average biomass ratio (and SD) between variables of the Extended EwE in the HC and RA simulation (period analysed 1999-2010). These synthetic results showed remarkable relative biomass change for many groups of the HTL model, due to the relative reduction of importance of grazing food chain with respect to microbial loop.
The skill of the EwE extended model results for reanalysis and hindcast are evaluated for anchovy and sardine biomass estimates using the OPEC benchmark tool presented in deliverable D2.3. As reported in Table 5.1, above, the effect of data assimilation on the OPATM-BFM (reanalysis) produce a slight improve of correlation coefficient for both anchovy and sardine, but while the reliability index increased in reanalysis for anchovy, it decreased for sardine. As a general insight the reanalysis produced an improvement for anchovy representation but a reduction of some skill parameters for sardine.

Minor skill modifications from the EwE extended model are highlighted by figures 42 and 43, respectively for anchovy and sardine. Despite these minor changes in model skill, the total biomass in RA was 25% and 18% lower than in HC for the period 1999-2010 (the assimilated period in the OPATM-BFM) thus highlighting the relevance of assimilation on HTL dynamics.

Figure 42. Target and Taylor diagrams for anchovy biomass for HC (left) and RA (right).
5.5 Summary of reanalysis experiment and lessons learnt

The assimilation of biogeochemical data produced an improvement of all skill indexes for all variables. The improvement is much more significant for assimilated variables, while changes in not assimilated variables (nutrients and oxygen) are smaller. Assimilation improves nitrate and silicate by slightly correcting the model overestimation of the surface data. Surface correction is then propagated to the deeper layer. Assimilation improves oxygen, reducing the model underestimation of surface. For phosphate the changes are almost negligible.

Overall the comparison between HC and RA HTL simulation showed the propagating effects up to the food web of potential changes in the classic food chain and microbial loop. This general result suggests that any end-to-end approach need a better knowledge of HTL predators of planktonic groups. It also highlight that data assimilation improvements for LTL might result in both positive and negative effects on the skill of HTL variables.
6. Black Sea

6.1 Description of the reanalysis experiments

The physical model used for the Black Sea is an implementation of the Princeton Ocean Model (POM). The model was forced using DMI reanalysis atmospheric fields and river discharge rates obtained from the Black Sea database. The model was initialized using World Ocean Atlas fields, spun up for five years and then the hindcast simulation was performed for the period 1990-2009. The resulting physical fields were stored daily in order to force the LTL model.

The LTL model contains thirty state variables that include four phytoplankton types, four zooplankton types, oxygen, hydrogen sulphide, inorganic nutrients, detritus as well as the carbonate system variables. The model was initialized using typical winter profiles and spun up for five years. The hindcast simulation was performed for the period 1990-2009.

Another LTL model run was performed for the reanalysis period 2000-2009. A data assimilation scheme based on the Singular Fixed Extended Kalman (SFEK) filter was implemented in order to sequentially assimilate remotely observed 8-day composites of surface chlorophyll-a concentrations, which were obtained from the GlobColour product. SFEK is a simplified version of the Singular Evolutive Kalman (SEEK) Filter and proceeds in two steps:

1. **Forecast Step:** The state is integrated forward in time using

   \[ x_\alpha(t_k) = M(t_{k-1}, t_k) x_\alpha(t_{k-1}), \]

   where \( x_\alpha(t_k) \) is the value of the model forecast at time \( t_k \) and \( M(t_{k-1}, t_k) \) is the model operator. In both the SFEK and the SEEK Filters, the covariance matrix \( P(t_k) \) is approximated by a rank-\( r \) matrix \( P^r(t_k) \) which can be decomposed using

   \[ P^r(t_k) \approx L_k U_k L_k^T, \]

   where \( L_k \) is a unitary matrix containing the error subspace directions and \( U_k \) is a symmetric, positive definite matrix. In the SEEK Filter, the error subspace directions \( L_k \) are also propagated forward in time using the model operator during every forecast step, however in the SFEK filter, they are kept fixed (i.e. \( L_k = L_0 \) for all \( k > 0 \)). This relies on the observation that the estimation errors in numerical experiments are often reduced after the first correction step and it significantly reduces the computation time of the filter since the propagation of error space directions requires \( r + 1 \) integrations of the model at every time step. Besides time considerations, our choice of the SFEK Filter stemmed from the fact that it is a stepping stone toward the SEEK filter, which we plan to implement in the near future.

2. **Correction Step:** Whenever observational data are available, the filter updates the matrix \( U_k \) and the state \( x_\alpha(t_k) \) using

   \[ U_k^{-1} = \rho U_{k-1}^{-1} + (H_k L_0)^T R^{-1} (H_k L_0), \]

   \[ x_\alpha(t_k) = x_f(t_k) + L_0 U_k L_0^T H^T R^{-1} (Y_k - H_k x_f(t_k)) \]

   where \( x_f(t_k) \) is the model forecast for time \( t_k \), \( x_\alpha(t_k) \) is the corrected state at time \( t_k \) that will serve as the initial condition of the next time step, \( R \) is the observation covariance matrix, \( H_k \) is the observation operator, \( Y_k \) is the vector containing the observations for time \( t_k \) and \( \rho \) is the forgetting factor.
The error subspace directions \( \mathbf{L}_e \) were obtained by first spinning up the model for 5 years in order for the solutions to reach a statistically steady state and doing another 2-year run in which the state is recorded every 3 days. The mean of the sequence of recorded states was used as the initial state of the filter while the error subspace directions were obtained by computing the multivariate Empirical Orthogonal Functions (EOFs) of the recorded states using Singular Value Decomposition (SVD).

Suitable choices for the error subspace dimension and the forgetting factor were obtained through twin-experiments in which a reference run of the model was performed to create a sequence of pseudo-observations every 8 days. The pseudo-observations of surface chlorophyll were perturbed with white noise (standard deviation of 0.5 mg m\(^{-3}\)) and assimilated into the model to assess the performance of the assimilation scheme and determine the values of the error subspace dimension and the forgetting factor that result in the highest reduction in the Relative Root Mean Squared Error (RRMSE) for most of the variables. For each state variable, RRMSE can be defined through

\[
RRMSE = \frac{\| \mathbf{x}_{\text{ref}}(t_k) - \mathbf{x}_{\text{ref}}(t_k) \|}{\| \mathbf{x}_{\text{ref}}(t_k) - \overline{X} \|}
\]

where \( \mathbf{x}_{\text{ref}}(t_k) \) is the value of the state variable in the reference run and \( \overline{X} \) is the mean state of the sample computed during filter initialization.

The hindcast run of the physical model was validated using a database that was collated using data from IMS-METU cruises as well as fields form the Black Sea Ocean Database. The validated physical variables are temperature, salinity and the density derived variables, potential energy anomaly and mixed layer depth. The validated LTL variables are nitrate, phosphate, ammonium, dissolved oxygen, hydrogen sulphide as well as in-situ chlorophyll. The hindcast run was further validated for the reanalysis period 2000-2009 for a direct comparison of the hindcast and reanalysis runs to be possible.

### 6.2 Results

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<th></th>
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<th></th>
</tr>
</thead>
<tbody>
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<td>Hindcast Efficiency</td>
<td>% Model Bias</td>
<td>Pearson Correlation Coefficient</td>
<td>RMSE</td>
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<td>Temperature</td>
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<td>Mean 4</td>
</tr>
<tr>
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<td>------------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>Nitrate</td>
<td>mmol m⁻³</td>
<td>-0.531</td>
<td>47.6117</td>
<td>0.1567</td>
<td>6.7533</td>
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<tr>
<td>Phosphate</td>
<td>mmol m⁻³</td>
<td>0.0404</td>
<td>79.6059</td>
<td>0.5572</td>
<td>1.5939</td>
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<tr>
<td>Ammonium</td>
<td>mmol m⁻³</td>
<td>-1.8438</td>
<td>0.2769</td>
<td>0.5168</td>
<td>5.7347</td>
</tr>
<tr>
<td>Dissolved Oxygen</td>
<td>mmol m⁻³</td>
<td>0.3705</td>
<td>22.5354</td>
<td>0.7638</td>
<td>95.8554</td>
</tr>
<tr>
<td>Hydrogen Sulfide</td>
<td>mmol m⁻³</td>
<td>0.3176</td>
<td>-27.9064</td>
<td>0.715</td>
<td>10.1167</td>
</tr>
<tr>
<td>Chlorophyll</td>
<td>mg m⁻³</td>
<td>0.2439</td>
<td>-40.3049</td>
<td>0.5314</td>
<td>1.1279</td>
</tr>
</tbody>
</table>

### 6.3 Summary of reanalysis experiment and lessons learnt

Despite all the efforts put into the development of the assimilations scheme, the twin experiments reveal that the assimilation scheme is incapable of achieving the desired reduction in RRMSE and the convergence of the model fields to (pseudo-)observations. As a result, the assimilation runs for the 2000-2009 could not be performed. Efforts are being put into resolving this issue through consultations with the OPEC partners in HCMR. Once the issue is resolved, this document will be updated accordingly.