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Data assimilation of depth-distributed satellite chlorophyll-α in two Mediterranean contrasting sites

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Abstract

A new approach for processing the remote sensing chlorophyll-α (Chl-α) before assimilating into an ecosystem model is applied in two contrasting, regarding productivity and nutrients availability, Mediterranean sites: the DYFAMED and POSEIDON E1-M3A fixed point open ocean observatories. The new approach derives optically weighted depth-distributed Chl-α profiles from satellite data based on the model simulated Chl-α vertical distribution and light attenuation coefficient. We use the 1D version of the operational ecological 3D POSEIDON model, based on the European Regional Seas Ecosystem Model (ERSEM). The required hydrodynamic properties are obtained (off-line) from the POSEIDON operational 3D hydrodynamic Mediterranean basin scale model. The data assimilation scheme is the Singular Evolutive Interpolated Kalman (SEIK) filter, the ensemble variant of the Singular Evolutive Extended Kalman (SEEK) filter. The performance of the proposed assimilation approach was evaluated against the Chl-α satellite data and the seasonal averages of available in-situ data for nitrate, phosphate and Chl-α. An improvement of the model simulated near-surface and subsurface maximum Chl-α concentrations is obtained, especially at the DYFAMED site. Model nitrate is improved with assimilation, particularly with the new approach assimilating depth-distributed Chl-α, while model phosphate is slightly worse after assimilation. Additional sensitivity experiments were performed, showing a better performance of the new approach under different scenarios of model Chl-α deviation from pseudo-observations of surface Chl-α.
Keywords: data assimilation; ecosystem model; ensemble Kalman filter; Mediterranean Sea; chlorophyll; ocean colour

1. Introduction

The Mediterranean ecosystem exhibits significant complexity, arising from strong air-sea interactions that cause deep and intermediate water mass formations in different areas, enhanced wind-driven thermohaline circulation (Schroeder et al., 2012), nutrient inputs from rivers (Tsiaras et al., 2014) and human activities in coastal areas (Béthoux et al., 2002). The growing awareness of the relation between the dynamics of biochemical properties with the ecosystem functioning has led to several estimates of biogeochemical patterns using in-situ monitoring, satellite earth observations and numerical models (Allen et al., 2002; Marty et al., 2002a; Bosc et al., 2004; Polimene et al., 2007; Socal et al., 2008; D’Ortenzio et al., 2009; Siokou-Frangou et al., 2010; Auger et al., 2011; Reygondeau et al., 2013).

In-situ measurements (Chl-α, dissolved inorganic nutrients, phytoplankton, bacterial and zooplankton biomasses, oxygen concentration, etc) collected by hydrographic surveys and fixed stations may provide enough accurate information to infer a wide range of ecosystem variables in specific areas (Marty et al., 2002a; Manca et al., 2004; Anfuso et al., 2013). During the past years, automated platforms like Bio-Argo floats (Xing et al., 2012; D’Ortenzio et al., 2014) and Bio-gliders (Niewiadowska et al., 2008), equipped with bio-optical and biogeochemical sensors, also demonstrated their potential to monitor biogeochemical properties and assessing the physical-biological functioning in the North-West (NW) Mediterranean. However, in-situ biogeochemical observations are often very limited in time and space, providing little information about inter-annual variability of ecological variables and their coupling with hydrodynamic variables (e.g. temperature, salinity, vertical mixing) on a large scale.

Remotely sensed ocean colour is a unique source of biogeochemical data with high temporal resolution and repeated coverage of the same area, providing essential information about the spatial and time variability of phytoplankton biomass and biological activity. Ocean colour
observations provide a much higher spatial and temporal resolution than the in-situ observations. However, they are based on indirect measurements of the optical properties of the ocean, which are transformed to Chl-α using an appropriate algorithm (O’Reilly et al., 1998; Santoleri et al., 2008; Volpe et al., 2007). In recent years, considerable efforts have been dedicated to studies of the Mediterranean ecosystem functioning through satellite products (D’Ortenzio and D’Alcalà, 2009; Coppini et al., 2012; Volpe et al., 2012). Nonetheless, uncertainty in the chlorophyll retrieval algorithms and cloud coverage may lead to imprecise and sparse observations, especially in coastal areas that are influenced by land inputs of coloured matter and suspended solids (Gregg and Casey, 2004).

Ecosystem models can be used to simulate a broad range of biogeochemical variables, describing their dynamics in relation to the physics of the studied area. A variety of biogeochemical models have been implemented in the Mediterranean Sea (Petihakis et al., 2002, 2009, 2014; Triantafyllou et al., 2003a; Lazzari et al., 2012; Cruzado and Bernardello, 2012; Christodoulaki et al., 2013; Tsiaras et al., 2014). However, model outputs are subjected to uncertainties related to the model structure, parameterization schemes, forcing and initial conditions (Anderson, 2005; Shimoda and Arhonditsis, 2016).

Data assimilation can mitigate for model uncertainties by combining the advantages of the model dynamics and observations. The synthesis of the two can produce estimates of biochemical variables that might not be separately obtained from model simulations and observations. Data assimilation is widely used in numerical weather prediction (Kalnay, 2003) and operational physical oceanography (Cummings et al., 2009). As biological in-situ data sets become more extensive and satellite ocean colour time series reach decadal scales, data assimilation is an emerging field in marine ecology (Gregg et al., 2008; Shulman et al., 2013; Edwards et al., 2015).

The primary goal of data assimilation techniques is to improve the estimates not only of the observed variable, but also of the other model non-observed variables. Assimilation of satellite surface Chl-α was shown to improve the estimates of climatological phosphate concentrations in the Eastern Mediterranean Sea (Triantafyllou et al., 2007), as also those of primary production, nitrogen and zooplankton in global ocean models (Gregg, 2008; Ford et al., 2012). Ciavatta et al. (2011) assimilated satellite Chl-α to improve nutrients, plankton composition and particulate
nitrogen and carbon in a shelf-sea. Nevertheless, assimilation of one variable in a model may introduce biases in some cases to the other model non-observed variables (Nerger and Gregg, 2007; Fontana et al., 2009; Ciavatta et al., 2011). On the other hand, satellite chlorophyll observations that are assimilated into ocean biogeochemical models are often considered to represent the surface Chl-α (Triantafyllou et al., 2007; Ford et al., 2012; Teruzzi et al., 2014). This may also induce significant errors in the inference of other variables of the ecosystem, such as primary production and nutrients (Groom et al., 2005; Siswanto et al., 2005). Based on results of various previous studies as of Prunet and Minster (1996), Triantafyllou et al. (2007) and Fontana et al. (2013), the assimilation of surface Chl-α data only was found not sufficient to constrain the vertical structure of simulated Chl-α and was not able to fully control the trajectory of the considered biogeochemical models. Our idea here is to include more information in the assimilation process to better constrain the ocean subsurface.

Oceanographic observations suggest that optical properties and optically significant components of seawater often exhibit a considerable vertical variation in the upper ocean (Stramska and Stramski, 2005). A deep chlorophyll maximum (DCM) within the penetration depth, the first optical depth, can influence the values of ocean properties that are retrieved from remote-sensing reflectance and ignoring it may lead to an underestimation of primary production (Sathyendranath and Platt, 1988; Platt et al., 1991; Platt and Sathyendranath, 1993). This vertical inhomogeneity poses a challenge for well understanding the values of ocean properties that are retrieved from remote-sensing reflectance, including the chlorophyll concentration. Shulman et al. (2013) argued that satellite data provide an estimate of the average chlorophyll concentration over the layer between the surface and the first optical depth. Thus, the assimilation of satellite-derived chlorophyll concentrations should not consider the data as just surface values, but rather as averages over attenuation depth values. The interpretation of remotely sensed data as chlorophyll data is therefore not straightforward.

In this study, we proceed a new approach to overcome the limitation of the standard approach of assimilating only surface Chl-α, by assimilating Chl-α profile data. The remotely sensed Chl-α is considered to be a weighted average of the water column Chl-α, taking into account the light penetration. The satellite Chl-α is distributed along the water column, based on the model-simulated light attenuation, providing an estimated Chl-α profile that can be
assimilated by the model. We test the proposed approach in two different Mediterranean locations: the DYFAMED and POSEIDON E1-M3A fixed-point open ocean observatories, located in the western and the eastern Mediterranean Sea, respectively (Fig. 1), with multi-parametric monitoring stations (buoys) providing information of biochemical parameters in the euphotic zone. These locations exhibit different ecosystem behaviour regarding productivity, inorganic nutrient concentrations and DCM. They are representative of the apparent eastward decreasing trend in primary production (Moutin and Raimbault, 2002) and the eastward deepening of DCM (Siokou-Frangou et al., 2010; Lazzari et al., 2012). In this way, the performance of the proposed approach for assimilating satellite-derived Chl-α concentrations was evaluated in two areas with available in-situ biochemical data and significantly different light penetration environments.

The paper is organized as follows: Section 2 describes the biogeochemical model and the data assimilation scheme, along with the observational data. The setup of the assimilation system and the experiments are presented in Section 3. The assimilation results are illustrated and discussed in Section 4. Discussion and conclusions conclude the work in Section 5.

2. Materials and methods

2.1 The model

A 1D version of the operational ecological 3D POSEIDON model (POSEIDON forecasting system; www.poseidon.hcmr.gr) was used to evaluate the proposed assimilation approach. The primary objective was to examine the relevance of the new approach before implementing it with a computationally demanding 3D ecosystem model. This also allows us to evaluate separately the approach behaviour at two representative and ecologically different sites: the DYFAMED and E1-M3A stations.

The biogeochemistry is based on the European Regional Seas Ecosystem Model (ERSEM; Baretta et al., 1995), and the required hydrodynamic properties are obtained (off-line) from the POSEIDON operational 3D hydrodynamic Mediterranean basin-scale model simulation (Korres et al., 2007). Daily profiles of temperature, salinity and vertical diffusivity coefficient, simulated at the two Mediterranean locations (DYFAMED, E1-M3A) provided a multi-annual hydrodynamic forcing that was used to drive the 1D ecosystem model. In the vertical, the model
has 25 levels with a logarithmic resolution approaching the surface.

ERSEM is a generic comprehensive biogeochemical model that has been successfully implemented in a number of coastal and open sea ecosystem studies since 1995, such as the North Sea and the NW European continental shelf (Ruardij and Raaphorst, 1995; Pätsch and Radach, 1997; Proctor et al., 2003; Collingridge, 2012; Elkalay et al., 2012), the Mediterranean Sea (Allen et al., 2002; Petihakis et al., 2012, 2014; Hoteit et al., 2005; Christodoulaki et al., 2013; and the Arabian Seas (Blackford and Burkill, 2002; Triantafyllou, et al., 2014). The 3D version of the model in the present study has been implemented in a series of studies in the Mediterranean Sea (Petihakis et al., 2002; Triantafyllou et al., 2003a; Tsiaras et al., 2012, 2014). The basis of ERSEM consists of state variables based on a functional group approach, where biotic groups are distinguished not by species but by their trophic level (producers, consumers and decomposers), subdivided according to size classes, and/or their trophic links. Although within each trophic level the groups are subjected to the same processes, differentiation is achieved through different parameter values. The model includes the primary physiological (ingestion, respiration excretion and egestion) and population (growth and mortality) processes described by fluxes of carbon and nutrients. The pelagic model food web consists of four phytoplankton groups: diatoms (20-200μm, silicate uptake), nanophytoplankton (2-20μm), picophytoplankton (<2μm) and dinoflagellates (20-200μm), bacteria and three zooplankton groups: heterotrophic nanoflagellates (feeding on bacteria, picophytoplankton and nanophytoplankton), microzooplankton (feeding on nanophytoplankton, heterotrophic nanoflagellates and microzooplankton) and mesozooplankton (feeding on diatoms, dinoflagellates, microzooplankton and heterotrophic nanoflagellates). The chemical dynamics of nitrogen, phosphorus, silicate and oxygen are coupled with the biologically driven carbon dynamics. Benthic processes are described by a simple first-order benthic returns module that includes the settling of organic detritus into the benthos and diffusional nutrients fluxes out of the sediment. A more detailed description of the model can be found in Petihakis et al. (2002).

2.2 Data assimilation scheme

We use the Singular Evolutive Interpolated Kalman filter (SEIK) (Pham, 2001, Hoteit et al., 2002), which is an ensemble based Kalman filter (KF) that has been successfully implemented in
a number of different physical and ecological ocean applications (Hoteit et al., 2002, 2005, 2007; Triantafyllou et al., 2003b, 2012; Korres et al., 2007, 2012; Nerger and Gregg, 2007; Butler et al., 2012; Mayo et al., 2014). The filter expresses the KF estimate of the system state $X^a(t_k)$ at some time $t_k$ and the corresponding error covariance matrix $P^a(t_k)$ by an ensemble of $N$ (interpolating) states $X^a_1(t_k),...,X^a_N(t_k)$. These are randomly drawn after every assimilation cycle in such a way that their mean and covariance exactly match $X^a(t_k)$ and $P^a(t_k)$, i.e.

$$X^a(t_k) = \frac{1}{N} \sum_{i=1}^{N} X^a_i(t_k)$$

(1)

$$P^a(t_k) = \frac{1}{N} \sum_{i=1}^{N} [X^a_i(t_k) - X^a(t_k)] [X^a_i(t_k) - X^a(t_k)]^T.$$  

(2)

The use of an ensemble of states is very similar to the ensemble Kalman (EnKF) filter of Evensen (2003), but the drawing of the members is constrained to exactly satisfy Eq. (1) and (2), unlike the EnKF which satisfies Eq. (2) only asymptotically (Hoteit et al., 2015). Given such an ensemble, a forecast is produced by integrating the ensemble with the model forward to the time of the next available observation $t_{k+1}$. The forecast state $X^f(t_{k+1})$ and its error covariance matrix $P^f(t_{k+1})$ are then taken as the mean and the covariance of the forecast ensemble. The analysis step is identical to that of the KF, formulated in the reduced-space defined by the ensemble.

The SEIK filter operates as a succession of a forecast step and an analysis step, followed by re-sampling, starting from an initial ensemble $X^a_1(t_o),...,X^a_N(t_o)$. For a detailed description of the algorithm of the SEIK filter the reader is referred to Pham (2001), Hoteit et al., (2002) and Triantafyllou et al., (2003b).

**Forecast step:** One integrates the ensemble forward with the model to obtain the forecast members $X^f_i(t_k)$ as

$$X^f_i(t_k) = M(t_k,t_{k-1})X^a_i(t_{k-1}).$$  

(3)

The forecast state is then
\[ X'(t_k) = \frac{1}{N} \sum_{i=1}^{N} X'_i(t_k) \tag{4} \]

and its error covariance matrix is
\[ P'(t_k) = \frac{1}{r+1} \sum_{i=1}^{r+1} \left( X'_i(t_k) - X'(t_k) \right) \left( X'_i(t_k) - X'(t_k) \right)^T + Q_k. \tag{5} \]

The matrix \( Q_k \) represents the covariance matrix of model uncertainties. \( P'(t_k) \) is then decomposed as
\[ P'(t_k) = L_k \left[ (r+1)T^T T \right]^{-1} L_k^T + Q_k \tag{6} \]

with
\[ L_k = \begin{bmatrix} X'_1(t_k), \ldots, X'_{r+1}(t_k) \end{bmatrix}^T. \tag{7} \]

and the matrix \( T \) is an orthogonal matrix of dimension \((r+1) \times r\) with zero column sums. \( T \) can be chosen as in Hoteit et al., (2002).

**Analysis step:** The observation \( y_k^o \) at time \( t_k \) is used to update the forecast according to
\[ X''(t_k) = X'(t_k) + K_k \left( y_k^o - H_k \left( X'(t_k) \right) \right) \tag{8} \]

where the \( H_k \) is the observational operator. The so-called Kalman gain \( K_k \) is given by
\[ K_k = L_k U_k (HL_k^T R_k^{-1}) \tag{9} \]

with \( R_k \) the observational error covariance matrix, \((HL)_k = [H_k x'_1(t_k), \ldots, H_k x'_{r+1}(t_k)]^T\) and \( U_k \) computed from
\[ U_k^{-1} = \rho \frac{1}{r+1} (T^T T)^{-1} + (HL_k^T R_k^{-1} HL_k)^{-1}. \tag{10} \]

The parameter \( \rho \) is a forgetting factor that is used to account for the model error and other sources of uncertainties in the filter (e.g. low-rank approximation) by inflating the forecast error covariance (Hoteit et al., 2003). The analysis error covariance matrix is then given by
\[ P''(t_k) = L_k U_k L_k^T. \tag{11} \]

**Re-sampling step:** To proceed with the next forecast step, an ensemble is generated after every analysis step based on the so-called 2nd order sampling scheme that exactly matches the
filter estimate and its covariance matrix. More specifically the ensemble members are composed as

$$X^a_i(t_k) = X^a(t_k) + \sqrt{r+1}L_k \left( \Omega_{k,i} C_k^{-1} \right)^T$$  \hspace{1cm} (12)

for $1 \leq i \leq r+1$, where $\Omega_{k,i}$ denotes the $i$th row of a randomly generated matrix $\Omega_k$, and $C_k$ is the square root matrix of $U_k$ that can be computed by Cholesky decomposition. The columns of $\Omega_k$ need to be orthonormal and orthogonal to the vector $[1\ldots1]^T$, so that the $X^a_i(t_k)$ satisfies (1) and (2).

2.3 Observations

2.3.1 In-situ data - Study area

The DYFAMED site (DYnamique des Flux Atmosphériques en MEDiterranée; http://www.obs-vlfr.fr/sodyf/; 2350-m depth; 43°25’N; 7°52’E) is a long-term monitoring station located in the central part of the Ligurian Sea (NW Mediterranean Sea, Fig. 1), 28 nautical miles off continental France. It is surrounded by the permanent geostrophic Ligurian frontal jet flow, associated with the cyclonic circulation of the Northern Current (Millot, 1999). The available times-series of monthly inorganic nutrients (nitrate, phosphate, silicate) and Chl-α profiles used in the present study were obtained from the SeaDataNet database (Pan-European infrastructure for ocean and marine data management, http://www.seadatanet.org), collected between 1991 and 2013. The area of the DYFAMED station is characterized by a spring bloom after the winter deep convection, a summer oligotrophy and a secondary bloom in fall, generated by perturbations caused by the meteorological forcing (Bosc et al., 2004; Morel et al., 1991). Moreover, there is a well-established deep chlorophyll maximum (DCM) at around 40-50m during stratification periods (Marty et al., 2002a). The DYFAMED site is suitable for a 1D modeling study, as this area is not significantly affected by lateral inputs due to the presence of the Ligurian strong horizontal density front (Niewiadomska et al., 2008).

The POSEIDON E1-M3A station (35.66N, 24.99E) is located approximately 24 nautical miles north of Heraklion, in the Cretan Sea (Fig. 1) and it is the first multi-parametric station in the Eastern Mediterranean (Nittis et al., 2003; Petihakis et al., 2007). Although the station is
established since 2000, the first efforts focused mainly on the monitoring of the physical parameters, with the exception of automated measurements of fluorescence in a near real time operational mode. In 2010, a monthly in-situ sampling program was established, similar to the one in DYFAMED, with water sampling in standard depths for the analysis of an extensive list of biogeochemical parameters. Because of the lack of long time series of biochemical data at the E1-M3A site, several available datasets spanning different time periods were used to validate the model outputs, from which seasonal means of inorganic nutrients and Chl-α were constructed. These datasets included spatially averaged climatological vertical profiles of inorganic nutrients and Chl-α, downloaded from the OGS data server (Manca et al., 2004). Monthly profiles of nitrate, phosphate and Chl-α, were also available from EU-projects CINCS (Pelagic-Benthic Coupling IN the Oligotrophic Cretan Sea) during 1994-1995, and MATER (Mediterranean Targeted Project II — Mass Transfer and Ecosystem Response) during 1996-1999 (Tselepides et al., 2000; Siokou-Frangou et al., 2002). For the years 2010-2013, in-situ measurements of inorganic nutrients (i.e. phosphate, nitrate) from the monthly sampling program were also available, produced by manual spectrophotometric analysis and Chl-α, derived by fluorometric analysis, from Niskin.

The Cretan Sea has been characterized as one of the most transparent and less productive seas in the global ocean. It is dominated by intense seasonal stratification of the water column and rather transient or recurrent cyclonic and anticyclonic eddies, interconnected by jets without defined time scales (Balopoulos et al., 1999). These feed the euphotic zone with nutrients from the deeper layers, or act as sinks for organic material to the deeper layers, respectively. The open sea character of the location of the E1-M3A site in conjunction with the significant distance from the north coast of Crete ensures no direct influence from the land (e.g. riverine inputs, seawater pollution) on the functioning of the marine ecosystem. However, the significant variability in the circulation patterns, which is strongly coupled with the biological processes (Tselepides et al., 2000), may be difficult to simulate by a 1D model. It is further challenging to validate the proposed assimilation system in a location characterized by very low productivity, as opposed to the DYFAMED site.

To compare with the model outputs against the data, all in-situ data profiles were interpolated at the model depths using bi-linear interpolation.
2.3.2 Satellite data

The assimilating observations consist of SeaWiFS (Sea-viewing Wide Field-of-view Sensor) data of the near surface Chl-α (mg m⁻³), estimated using the Ocean Chlorophyll 4 - version 4 (OC4-v4) algorithm (O’Reilly et al., 1998). The SeaWiFS pre-processed data are global Level-3, 8-day composite products (9X9 km² resolution) available between 1998 and 2007. For the assimilation experiments, time series of Chl-α were extracted at the two specific study areas, the DYFAMED and POSEIDON E1-M3A sites.

2.3.3 Assimilated observations

The proposed approach for processing the satellite data before assimilation describes the dependence of the ocean colour, captured by the satellite sensor, on the exponential decay of the incident light with depth, as this is transmitted through the water column. This exponential decay is given by the Lambert-Beer formulation (Grum and Becherer, 1979):

\[
I = I_o \exp \left( - \int_0^z K(z) dz \right)
\]

where \(I\) is the light radiation reaching depth \(z\), \(I_o\) is the intensity of the incident radiation at the sea surface, and \(K(z)\) is the light attenuation coefficient varying with depth, \(z\). The satellite sensor can capture ocean colour that can be translated into chlorophyll concentration averaged over the upper few meters of the water column. The 90% of the water-leaving electromagnetic radiation, which can be detected by remote optical sensors, originates within a surface layer, called the ‘penetration depth’ (Gordon and McCluney, 1975), at which the downwelling irradiance falls to \(~36.8\%\) of its surface value. The irradiance that reaches depth \(z\) is attenuated by a factor equal to

\[
\exp \left( - \int_0^z K(z) dz \right).
\]

Assuming that the backscattered irradiance would be approximately attenuated in the same way on its return to the surface, a layer of water at depth \(z\) will contribute to the reflectance, diminished by the same factor as in Eq. 14 compared to the surface. Gordon & Clark (1980) suggested that for comparison of remotely-sensed concentrations with surface in-situ
measurements, it is important to estimate the Chl-α concentration that would be ‘seen’ by the satellite. Thereby, based on a proxy for the optical weighted pigment concentration (Clark, 1997; D’Ortenzio et al., 2002) the Chl-α concentration as captured by a remote sensor is the optically weighted average \( (chl_{ave}) \) of the water column Chl-α \( (chl(z)) \) given by:

\[
chl_{ave} = \frac{\int_0^{z_d} chl(z) \exp \left( -2 \int_0^z K(u) \, du \right) \, dz}{\int_0^{z_d} \exp \left( -2 \int_0^z K(u) \, du \right) \, dz}
\]

(15)

where \( z_d \) is the penetration depth, and \( K(u) \) is the depth varying attenuation coefficient simulated by the model. Based on the above expression, the satellite Chl-α \( (chl_{sat}) \) can be approximately distributed in the water column, using the model-simulated Chl-α \( (chl_{lm}(z)) \) and its weighted average \( (chl_{avemodel}) \), which is calculated from Eq.(15), using the model-simulated attenuation coefficient. Hence, the vertically distributed satellite Chl-α is expressed as:

\[
chl_{obs}(z) = \frac{chl_{sat}}{chl_{avemodel}} \cdot chl_{lm}(z)
\]

(16)

which is assumed to follow the vertical distribution of the model-simulated Chl-α, modified by a constant factor \( (chl_{sat}/chl_{avemodel}) \). In this way, the assimilated observations are Chl-α profiles derived from satellite data, weighted by a function taking into consideration that the substance near the surface is optically more important than that at greater depths.

3. Experimental Setup

The initial nutrient profiles (nitrate, phosphate, silicate) for each area were obtained from a winter month (mixing period) of the available in-situ data, by bi-linear interpolation onto the model vertical levels. Initial conditions for biochemical variables other than inorganic nutrients were obtained from simulations of the 3D operational POSEIDON biogeochemical model for the Mediterranean Sea (www.poseidon.hcmr.gr). The state vector is composed of the 38 pelagic model variables.

For each site, the 1D model simulations were carried out for a chosen period, i.e. from 2001 to 2002, for which both satellite data and the hydrodynamic forcing from the 3D model output were available. We should note that this is an indicative period, as capturing the inter-annual
variability is beyond the scope of this study, given the known limitations of the 1D model. After a spin-up period of 2 years, assimilation experiments were performed with the SEIK filter constraining the model with satellite surface Chl-α data (seikChl-surface run) and satellite depth–distributed profiles of Chl-α (seikChl-profile run).

To initialize the SEIK filter, the model was integrated over a period of 2 years to generate a long sequence of 730 state vectors by storing one state vector every day. A multivariate EOF (Empirical Orthogonal Function; Lorenz, 1956) analysis was then performed on this sequence. The initial ensemble was sampled along the directions of the resulting EOFs as described by Hoteit et al., (2013). The EOF analysis suggests that the first 25 EOFs explain about 99% of the system variability.

Sensitivity assimilation experiments were conducted with different forgetting factor values (ρ, Eq.10), ensemble size, and observational errors variance to determine the values of these parameters achieving the best filter performance regarding the simulated Chl-α and inorganic nutrients. The forgetting factor used in the assimilation runs in both DYFAMED and E1-M3A ecosystems was empirically set to 0.5 after multiple trial and error tests, while the ensemble size was set to 25 members. The ensemble spread follows the seasonal variability of the Chl-α, increasing during the spring bloom period. The observational error covariance matrix (R, Eq. 9) is assumed diagonal, with the diagonal coefficients set as a fraction of the variance of the satellite data at each observed location (Triantafyllou et al., 2007).

The filter performance was assessed by comparing the model analysis surface Chl-α against the satellite Chl-α derived from SeaWiFS. Another important indicator of the assimilation performance is its impact on non-assimilated variables, such as dissolved inorganic nutrients and on the vertical distribution of Chl-α and other variables. Given the limited time coverage of continuous monthly in-situ profiles for inorganic nutrients (i.e. nitrate, phosphate) and Chl-α at all depths over the same years, a seasonal mean ‘climatology’ was constructed from the available observational data set. As mentioned above, capturing the inter-annual variability is beyond the scope of this study, given the limitations of the 1D model. Seasonal averages over 2 years (2001-2002) derived from the model forecast and assimilation experiments were compared against the in-situ ‘climatology’.

To study the overall model skill in the different experiments with and without data
assimilation, the target diagram (Jolliff et al., 2009) was used to compare the seasonal mean simulated profiles with the in-situ data. This graph reports on the x-axis the unbiased root mean square difference (RMSD) between model outputs and reference (in-situ) data. The y-axis indicates the model bias, which is defined as the difference between the means of the two fields. Both axes are normalized by the standard deviation of the in-situ data. Since RMSD is positive, the sign of the x-axis can be used to evaluate whether the model standard deviation is larger (X>0) or smaller (X<0) than the reference field’s standard deviation, in addition to a positive (Y>0) or negative (Y<0) bias. Furthermore, the normalized total root mean square difference (nRMSD), a measure of the average magnitude of the difference between the model results and the reference, is indicated by the distance of a given point from the origin. It is related to the modelling efficiency metric (MEF = 1 – nRMSD², Stow et al., 2009), which provides a measure of the model predictive skill, as compared to an average of the observations. A point plotted at the centre of the target indicates a perfect agreement between model results and the reference data.

To explore the performance of the new Chl-α assimilation approach under different scenarios of model deviation from the ‘true’ trajectory of the observed data, a series of sensitivity experiments with pseudo-observations of satellite Chl-α were performed at the DYFAMED site, where a shallower subsurface chlorophyll maximum is found. The SeaWiFS Chl-α data were thus multiplied by different factors to form pseudo-observation data sets of surface Chl-α that are increased or decreased by 30%, 50% and 70% of the original satellite data. Comparing the pseudo-observations with the free-run, we examined several different scenarios of model Chl-α bias where the free-run overestimates or underestimates the surface Chl-α. The main idea was to study how the data assimilation updates the model forecast depending on the magnitude and sign (underestimation/overestimation) of the model forecast misfit from the pseudo-observations.

It has been found that surface Chl-α measurements can predict the shape of the Chl-α for open-ocean waters (Morel and Berthon, 1989; Uitz et al., 2006) and the total depth-integrated Chl-α concentrations in the coastal ocean (Frolov et al., 2012). These findings suggests that if the model forecast of the Chl-α is accurate enough, it is appropriate to use the above light-attenuation corrected Chl-α adjustment procedure, in order to derive Chl-α profiles. As shown in the seasonal profiles in Fig. 4 and 7, there is a good correlation between the model forecast
(without assimilation) and the in-situ Chl-α profiles. The model forecast is highly correlated with in-situ data (correlation coefficient R>0.9), at DYFAMED station and at M3A station (R=0.8), notwithstanding a smaller correlation (R~0.6) during summer at M3A. Therefore, the model simulated profiles were considered suitable to be used for the vertically distribution of the satellite Chl-α, though some deviation from in-situ data is expected.

4. Assimilation Results

4.1 Assimilation of satellite data

The results of assimilating satellite surface Chl-α and satellite depth – distributed Chl-α profiles at the DYFAMED and E1-M3A sites are presented first. The results of the sensitivity experiments are discussed in the next section.

4.1.1 Assimilation of satellite data at the DYFAMED site

To investigate the performance of the ecosystem model with and without assimilation and to study the benefits of assimilating satellite depth – distributed Chl-α profiles at the DYFAMED and E1-M3A sites are presented first. The results of the sensitivity experiments are discussed in the next section.

Fig. 3 also shows the relative model Chl-α error (\(|\text{Model} - \text{Satellite}|/|\text{Satellite}|\)). The biogeochemical model free-run (Fig. 3, red line) reproduced reasonably well the seasonal cycle of the surface Chl-α, characterized by an intense spring bloom and minimum concentrations during the stratified summer/autumn period. However, it underestimated winter Chl-α, particularly during February, triggered by the increased model vertical mixing that is related to an overestimation of the mixed layer depth (MLD), as compared with the MLD estimated from in-situ data (D’Ortenzio et al., 2005). Moreover, the model surface summer Chl-α was underestimated compared to satellite data. This may be partly attributed to the known limitations of the ocean colour bio-optical algorithms to reproduce very low Chl-α concentrations (<0.15 mg m⁻³; Bricaud et al., 2002; Sancak et al., 2005), which is also supported by the relatively higher satellite Chl-α as compared to the in-situ surface Chl-α during summer (Fig 2).

The assimilation improved the model Chl-α, which is in a better agreement with the SeaWiFS data than the free-run, except for a short period of the spring bloom (March) of 2002, when an overestimation is observed, which was triggered by the above mentioned overestimated
vertical mixing. As the timing and magnitude of the spring bloom are mainly controlled by vertical processes, such as the entrainment of deep water nutrients or the dilution of phytoplankton (Behrenfeld, 2010) by vertical mixing. We should note that horizontal processes (advection, diffusion) that are present in a 3D model might effectively reduce the effect of vertical mixing, smoothing properties between different areas. Additionally, given the strong variability of the vertical processes during the spring bloom, the assimilation window of eight days may not be adequate to guide the model towards the ‘true’ trajectory during that period. A sensitivity experiment was performed, adopting a 1-day assimilation window (with linear interpolation between the 8-day Chl-α records), suggests the model can be much better constrained during the spring bloom period (not shown). Nonetheless, the Chl-α assimilation improved the model surface Chl-α after the spring bloom, with the seikChl-profile run showing better performance with a smaller relative estimation error, as compared to the seikChl-surface run.

In Fig.4, the seasonal mean profiles of simulated Chl-α were plotted against the in-situ data. The model free run reproduces the depth of the observed DCM at ~40-50m during the spring bloom and stratification periods, although with lower concentrations, compared to those of the in-situ measurements, but still within the observed ranges. The model Chl-α is significantly improved with the assimilation, particularly in the area around the DCM. Noticing the differences between the SeaWiFS derived Chl-α and the in-situ data (Fig. 2), and given that the assimilation brings the model close to the satellite data, the model near-surface Chl-α is expected to have some bias compared to the in-situ data, such as the underestimation during winter/spring and the overestimation during summer/autumn periods. However, the assimilation and particularly the seikChl-profile run reduced the deviation of model subsurface maximum concentrations Chl-α from in-situ data, except for the summer period.

Seasonal mean vertical profiles of simulated inorganic nutrients against ‘climatological’ seasonal mean in-situ data are also presented in Fig.4. The model free-run, with few exceptions, reproduced reasonably well the observed nutrient vertical distributions and their variability within the observed data ranges in the upper 40m, notwithstanding a general underestimation of nitrate, particularly in the deeper layers. It is worthwhile mentioning here that in the 1D model implementation, horizontal effects, such as the horizontal transport of the pelagic biochemical
functional groups, are not accounted for, which limits the model skills. The assimilation, particularly of the depth-distributed profiles of Chl-α, generally improved the model nitrates, slightly reducing their deviation from in-situ data, despite an overestimation during autumn in the upper 40m. In all periods except summer, the near-surface phosphate was overestimated in the free run that is slightly increased in the assimilation runs, as those were forced to follow the relatively higher satellite Chl-α. During summer, the seikChl-profile phosphate was closely following the in-situ data in the upper 40m.

The overall model skill for the seasonal estimation of the vertical distribution of nitrate, phosphate and Chl-α is graphically summarized in the target diagram in Fig. 5. The free-run and the assimilation runs are inside the unitary circle (nRMSD<1), suggesting a good agreement with the observations, with a MEF close to 1. The assimilation of depth-distributed satellite Chl-α reduced the model bias for nitrate and Chl-α, while it slightly increased the bias for phosphate. The two assimilation runs exhibit a similar negative variability (negative unbiased RMSD) for nitrate and Chl-α, indicating a lower standard deviation, as compared to that of the in-situ data, while seikChl-profile phosphate was found more variable compared to the in-situ data.

The effects of the new assimilation approach upon other non-observed model variables were investigated by comparing model results to published data. The 0-100m integrated annual model primary production was found 138 g C m$^{-2}$ yr$^{-1}$, which was slightly below the mean observed values (180 C m$^{-2}$ yr$^{-1}$, Tusseau et al., 1997; 86-232 g C m$^{-2}$ yr$^{-1}$, mean=156 g C m$^{-2}$ yr$^{-1}$, Marty and Chiaverini, 2002b) and the estimated values from SeaWiFS data (188-213 g C m$^{-2}$ yr$^{-1}$, calculated mean= 200.5 g C m$^{-2}$ yr$^{-1}$, Bosc et al., 2004). The new assimilation approach decreased the deviation from the observed values in the upper 100m by 18% (163 g C m$^{-2}$ yr$^{-1}$), more than the assimilation of surface Chl-α (158 g C m$^{-2}$ yr$^{-1}$). The seikChl-profile run was found also beneficial for the annual mean 0-100m integrated bacterial production, which was increased (9.8 mmol C m$^{-2}$ d$^{-1}$) compared to that of the free run (7.3 mmol C m$^{-2}$ d$^{-1}$ ) and the seikChl-surface (7.6 mmol C m$^{-2}$ d$^{-1}$ ), approaching the observed values of 9.7 mmol C m$^{-2}$ d$^{-1}$ (calculated from Lemée et al., 2002).

4.1.2 Assimilation of satellite data at the E1-M3A site

The assimilation of satellite-derived Chl-α profiles was also tested at the POSEIDON E1-
M3A site in the Cretan Sea (Eastern Mediterranean Sea). Figure 6 shows the time evolution of the surface model-simulated Chl-α against the satellite data and the corresponding model Chl-α error. The assimilation of satellite-derived profiles of Chl-α resulted in a better agreement with the satellite data, as also indicated by the lower model relative error. Although the model follows the observed Chl-α seasonal variability, it underestimates the surface Chl-α, except during the spring bloom (March) period. The free-run departed from the satellite Chl-α after the summer period and was not able to follow its gradual increase in the autumn that is presumably related to the nutrient enrichment due to the erosion of the thermocline and horizontal transport. Assimilation of satellite-derived Chl-α profiles significantly reduced this negative bias. Moreover, the model significantly underestimated the surface Chl-α during February, before to the spring bloom. This behaviour is related to the model time-lagged winter vertical mixing, which results in the deep dispersion of phytoplankton, reducing the phytoplankton biomass in the surface-layer. To mitigate this, the assimilation of satellite data ramped up Chl-α values during spring bloom.

Seasonal mean vertical profiles of simulated Chl-α, nitrate and phosphate against ‘climatological’ seasonal mean in-situ data are displayed in Fig. 7. The model closely reproduces the main features of the observed nutrient and Chl-α vertical distributions in the E1-M3A site. The assimilation of satellite-derived Chl-α profiles improved the simulated nitrate and Chl-α, as compared to the in-situ data. It also improved the simulated phosphate in the upper layer (0-20m), while an overestimation of phosphate was found in all runs, below 50m. As mentioned above, the Cretan Sea is characterized by the presence of semi-permanent mesoscale eddies and aperiodic water masses (Cretan Intermediate Water (CIW), Transient Mediterranean Water (TMW), Souvermezoglou et al., 1999) penetrating the area and significantly affecting the biogeochemical dynamics. This information is missing in the 1D model, in which horizontal processes are omitted. We should also note that the surface in-situ phosphate appears greater than the simulated, except for winter, which could possibly be attributed to atmospheric deposition that is not included in the model. A recent study about the atmospheric deposition of inorganic nutrients suggested that those might have a major impact on the marine ecosystem (Christodoulaki et al., 2013). Finally, even though the concentration of the well marked in-situ summer DCM at ~100m is underestimated by the model, both in free and assimilation runs, the
model Chl-α in all cases was found close to the in-situ data ranges.

Figure 8 shows the overall model skill for the seasonal estimation of the vertical distribution of nitrate, phosphate and Chl-α, summarized in target diagrams. All the runs fall inside or close to the unitary circle for nitrate and Chl-α, suggesting a MEF close to 1. Nitrate seasonal estimations are inside the R=0.7 marker, showing an even higher correlation with the reference data. The seikChl-profile run reduced the model bias for Chl-α, while all the runs exhibited a similar bias for nitrate. A quite similar negative unbiased RMSD for nitrate and Chl-α is observed for all the runs, suggesting a lower variability than the in-situ data. Finally, seikChl-profile phosphate estimations were found more biased than the other runs estimations with an increased variability in comparison with in-situ data.

The 0-100m integrated annual model simulated primary production was found 61 g C m⁻² yr⁻¹, which is very close to the observed mean values (30-80 g C m⁻² yr⁻¹, mean=59 g C m⁻² yr⁻¹, Psarra et al., 2000). The assimilation runs increased the annual primary production to 64.5 g C m⁻² yr⁻¹ assimilating surface Chl-α, and to 68 g C m⁻² yr⁻¹ assimilating depth-distributed Chl-α, slightly deviating from the observed mean value, although they remain within the observed data range. However, the annual depth-integrated model bacterial production slightly increased after assimilation (free run: 10.6 g C m⁻² yr⁻¹, seikChl-surface run: 11. mg C m⁻² yr⁻¹, seikChl-profile run: 11.5 g C m⁻² yr⁻¹) approaching the observed value of 13.14 g C m⁻² yr⁻¹ (Van Wambeke et al., 2001).

4.2 Sensitivity experiments

Fig. 9 plots the time evolution of the model near surface Chl-α relative error, as it results from the free-run and the assimilation of the pseudo-observations (see section 3), using both assimilation approaches. The relative error of the seikChl-profile run was generally smaller compared to that of the seikChl-surface run and the free-run. In all cases where the free-run overestimates or underestimates the observed Chl-α, the seikChl-profile run dealt better with the deviation of the model simulated Chl-α from the pseudo-observations. However, both assimilation runs did not work well during the January-February period of increased positive model Chl-α bias, (‘pseudo-observations’ - model Chl-α > 0) during the increased vertical mixing winter period results in the enrichment of the euphotic zone with deep-water nutrients.
To further analyze the sensitivity results, those were summarized in a simple bar graph, shown in Fig. 10. Each bar represents the percentage difference of the relative model Chl-α error of each assimilation run in the different sensitivity experiments. The middle bar illustrates this difference as obtained from the assimilation of the real satellite Chl-α data. One may see that the sensitivity assimilating pseudo-observations generated by a decrease of 70% of the SeaWiFS data, presents the larger difference. When the deviation of the simulated model Chl-α from the observations is increased, the seikChl-profile approach imposes a stronger update on the forecast, as compared to that of the seikChl-surface run. Overall, the assimilation of satellite-derived profiles of Chl-α increases the observational information and enhances the efficiency of the assimilation to update the forecast bringing the surface Chl-α closer to the observations.

5 Discussion and conclusions

This work proposes and tests a new approach for processing satellite Chl-α data, distributing those in the vertical, before assimilation into an ecosystem model. The new approach derives satellite depth-distributed Chl-α profiles, based on the model simulated Chl-α vertical distribution and light attenuation coefficient. We considered two contrasting, regarding biological productivity, Mediterranean sites: the DYFAMED and POSEIDON E1-M3A fixed-point open ocean observatories, located in the western and the eastern Mediterranean Sea, respectively. Our goal was to evaluate the above approach in two different ecological regimes. The POSEIDON E1-M3A site is characterised by significant circulation variability, coupled with the biological processes and is more oligotrophic and transparent, as compared to the DYFAMED site. On the other hand, the DYFAMED site is richer in nutrients and phytoplankton biomass and presents a shallower DCM.

Free-run model simulation (without assimilation) and assimilation experiments were performed with the SEIK filter, assimilating satellite surface Chl-α data (seikChl-surface run) and satellite depth-distributed profiles of Chl-α (seikChl-profile run) over a two-year window. The model and filter solutions were evaluated against remotely sensed Chl-α and seasonal profiles of available in-situ data for nitrate, phosphate and Chl-α, showing good agreement with the data and reproducing reasonably well the ecosystem functioning at the DYFAMED and POSEIDON-E1-M3A stations. However, some weaknesses were also observed, especially
during winter in both areas, related to the overestimated model-simulated winter vertical mixing that resulted in the Chl-α decrease due to dilution of the water column and a slight overestimation during the spring bloom period. As has been stressed throughout this paper, horizontal processes were not accounted for in our 1D model implementation, which strongly limits the model capabilities. Additionally, the assimilation 8-day window was not found sufficient to constrain the model during the fast varying spring bloom period at the DYFAMED station, suggesting the need for assimilating data more frequently.

The filter successfully improved the near-surface model Chl-α. The assimilation of satellite-derived Chl-α profiles resulted in a better model agreement with the satellite data in both areas and improved the consistency between the model and in-situ Chl-α subsurface maximum concentrations. This agreement was more pronounced at the DYFAMED site. The Chl-α at ~50m depth, where the DCM is found at the DYFAMED site, is not “visible” by the satellite, weakly contributing (<1%) to the backscattered radiation reaching the satellite sensor. However, the subsurface Chl-α within the first optical depth (~25m) can be significantly different from the surface Chl-α during stratification periods and therefore might significantly affect the backscattered radiation, as captured by the satellite. In the case of DYFAMED, the difference between the Chl-α weighted average (Eq.15) and surface Chl-α is ~7% during summer/autumn period (Fig. 11), which is above the 5% threshold used by Stramska and Stramski (2005) in the backscattered light difference to classify the effect from DCM as significant. The impact of the proposed approach is more pronounced at DYFAMED, where the difference between the surface Chl-α and its weighted average in the vertical is higher (Fig. 11).

The data assimilation of satellite Chl-α resulted in a slight deterioration of the model-data fit in some cases, mostly for phosphate. One should have in mind, however, that the change in the nutrient concentrations after assimilation is determined by the model Chl-α estimation error. Therefore, one should also consider the case, where the simulated nutrients are in agreement with the observations, while the model Chl-α may be biased, in which case the Chl-α update by the data after assimilation might deteriorate the model nutrients. This is the case with nitrate in the upper 50m during autumn at DYFAMED and M3A for example, where the assimilation results in the slight overestimation of the model. This happens because the model near surface Chl-α is lower than the satellite and the assimilation tries to correct that, forcing an increase of inorganic
nutrients.

Annual primary and bacterial productions were improved with the new assimilation approach, notwithstanding an overestimation of the M3A annual primary production. It would be of course ideal if data assimilation could correct every aspect of the model, but this is unfortunately not possible, given the limited coverage of the observations and the important model limitations. A more modest goal would be, therefore, to consider the assimilation system to be successful when the model Chl-α is efficiently improved and forecasted, as phytoplankton is an essential part of the biogeochemical model, hoping that the model dynamics are good enough to properly propagate the Chl-α information to all model variables, or otherwise without significantly deteriorating some of the model variables.

Our results suggest that overall the assimilation of depth-distributed satellite data instead of just surface Chl-α enhance the assimilation results. Sensitivity experiments have also shown that the new assimilation approach suggests a better performance under different scenarios of model deviation from surface observations. The results obtained so far are promising, and encourage us to test the new approach in the 3D POSEIDON ecological model to develop in the future a more efficient tool for assimilation of satellite data.

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References


Figure captions

Figure 1. Average SeaWiFS Chl-α (mg/m3) for 2000-2003.

Figure 2. Monthly climatology of in-situ surface Chl-α and SeaWiFS Chl-α at DYFAMED and M3A stations. January and February are missing from the figure because of the lack of data.

Figure 3. Time evolution of the near-surface model Chl-α concentrations and the relative error, simulated by the free-run (red line) and the assimilation runs (green line = seikChl-profile run, black line = seikChl-surface run), against the 8-day SeaWiFS Chl-α data (blue dotted line) at the DYFAMED station for 2001-2002.

Figure 4. Seasonal average profiles of the Chl-α, nitrate and phosphate concentrations simulated by the free-run (red line) and the assimilation runs (green line = seikChl-profile run, black line = seikChl-surface run), against in-situ seasonal average profiles at the DYFAMED station for 2001-2002.

Figure 5. Normalized target diagram for the seasonal average of nitrate (×), phosphate (■) and Chl-α (♦) concentrations, simulated by the free-run (red colour), the seikChl-profile run (green colour) and the seikChl-surface run (black colour), against seasonal average profiles at DYFAMED site. The axes are normalized by the reference field standard deviation. The thick line corresponds to a normalized total nRMSD of 1.0. The dashed line corresponds to a positive correlation (R) between model and observations of 0.7 (refer to Jolliff et al., 2009 for definition) for which all points between it and the origin are greater than R.

Figure 6. Time evolution of the near-surface model Chl-α concentrations and its relative error, simulated by the free-run (red line) and the assimilation runs (green line = seikChl-profile run, black line = seikChl-surface run), against SeaWiFS Chl-α data (blue dotted line) at the E1-M3A station for 2001-2002.

Figure 7. Seasonal average profiles of the Chl-α, nitrate and phosphate concentrations simulated by the free-run (red line) and the assimilation runs (green line = seikChl-profile run, black line = seikChl-surface run), against in-situ seasonal average profiles at M3A station for 2001-2002.

Figure 8. Normalized target diagram for the seasonal average of nitrate (×), phosphate (■) and Chl-α (♦) concentrations, simulated by the free-run (red colour), the seikChl-profile run (green colour) and the seikChl-surface run (black colour), against seasonal average profiles at E1-M3A site. More details can be found in Fig. 5.
Figure 9. Time evolution of the near-surface Chl-α relative error (\(|\text{Model-Satellite}|/|\text{Satellite}|\)) at DYFAMED, simulated by the free-run (red line) and the assimilation runs (green line = seikChl-profile run, black line = seikChl-surface run) for the sensitivity experiments. The assimilated ‘pseudo-observations’ were generated by a 30 %, a 50 % and a 70 % reduction and increase of the SeaWiFS Chl-α over 2001.

Figure 10. Percentage difference between the seikChl-surface and the seikChl-profile annual average relative errors (\(|\text{Model} - \text{Satellite}|/|\text{Satellite}|\)), for each sensitivity experiment (see Fig.9).

Figure 11: Fractional change \([(\text{Chlavemodel} - \text{Chlsurf})/\text{Chlsurf}]\) of Chl-α weighted average in the vertical (Eq.15), over the surface Chl-α at DYFAMED and M3A stations.
Figure 1
Figure 2
Figure 3
Figure 4
Figure 5
Figure 6
Figure 7

M3A Seasonal Average 2001–2002

Figure 7
Figure 8
Relative Error Chl−a 2001

Figure 9
Figure 10

[seikChl-profile - seikChl-surface] of Relative Error
surface Chl-a 2001
Figure 11
Highlights

1. Ecosystem modeling in two contrasting areas in the Mediterranean Sea.
2. Data assimilation of optically weighted depth-distributed satellite chlorophyll-α data.
3. Assimilation of depth-distributed satellite chlorophyll-α data improves model DCM.