ARTICLE IN PRESS

[Remote Sensing of Environment xxx \(2016\) xxx](http://dx.doi.org/10.1016/j.rse.2017.03.040)–xxx

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: <www.elsevier.com/locate/rse>

Global marine biogeochemical reanalyses assimilating two different sets of merged ocean colour products

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article info abstract

Article history: Received 23 September 2016 Received in revised form 21 February 2017 Accepted 29 March 2017 Available online xxxx

Keywords: Data assimilation Ocean colour Reanalysis Marine biogeochemistry Carbon cycle

The only observations of marine biogeochemistry with routine global coverage are satellite ocean colour, which provide measurements of ocean bio-optical properties, with coverage still incomplete and limited to the sea surface. Models are therefore required to provide full spatial coverage, and through data assimilation can be combined with observations to create a reanalysis. This can then be used to investigate both observed and nonobserved variables, including those relating to the carbon cycle. As part of the Climate Modelling User Group (CMUG) within the European Space Agency's Climate Change Initiative (CCI) project, two global marine biogeochemical reanalyses have been produced by assimilating ocean colour-derived chlorophyll data into a coupled physical-biogeochemical ocean model over the period September 1997 to July 2012. One reanalysis assimilated CCI products, the other assimilated GlobColour products, with a non-assimilative hindcast run for comparison. Each has been validated against independent in situ observations of chlorophyll, nutrients and carbon cycle variables. The assimilation of either source of ocean colour data was found to improve the model's representation of chlorophyll concentration throughout the water column, including the frequency and positioning of deep chlorophyll maxima. The assimilation also resulted in a slight improvement in nutrient concentrations and surface fugacity of carbon dioxide compared with in situ observations, although the overall impact on mean fields was small. This was found to be due in part to cancelling errors within the model, with the assimilation providing information on model biases, which can be used to inform future climate model development. The reanalyses were also able to reproduce expected seasonal cycles, as well as inter-annual variability related to major climate drivers. This study concludes that both CCI and GlobColour products are suitable for assimilation purposes, and that assimilating ocean colour data is of clear benefit.

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1. Introduction

Reconstructions of the recent past are an important tool for understanding the Earth system. Reanalyses, which combine models and observations through data assimilation, provide consistently-processed gap-free descriptions of the real world. These give information about unobserved quantities, and can be used to help understand responses to observed changes in climate forcings, quantify natural variability, and assess uncertainties in model behaviour. Furthermore, they can be used to provide initial and boundary conditions for other models and forecasts, and to monitor particular variables and processes. Reanalyses can also give insights into model biases and processes, which can be used to inform model development, and can be used as a tool to assess observing systems.

Atmospheric reanalyses (e.g. [Dee et al., 2011](#page--1-0)) are widely used, and reanalyses of the physical ocean state are becoming increasingly mature [\(Stammer et al., 2010](#page--1-0)). The technique is now starting to be applied to

Corresponding author. E-mail address: [david.ford@metof](mailto:david.ford@metoffice.gov.uk)fice.gov.uk (D. Ford). ocean biogeochemistry (e.g. [Fontana et al., 2013; Ciavatta et al., 2016;](#page--1-0) [Ford et al., 2012](#page--1-0)). Of particular interest is information about plankton blooms, primary production, hypoxia, ocean acidification, carbon export, and air-sea exchanges of gases such as carbon dioxide $(CO₂)$, nitrous oxide (N_2O) , methane (CH_4) , and dimethyl sulphide (DMS).

Currently, the only source of observations of ocean biogeochemistry with routine global coverage is remotely sensed ocean colour. From this, products such as sea surface chlorophyll-a concentration (hereafter chlorophyll) can be derived. Following the proof-of-concept Coastal Zone Color Scanner (CZCS) mission, which flew between 1978 and 1986, satellite ocean colour observations have been available, from a number of different instruments, since 1996 ([McClain, 2009](#page--1-0)). The most widely used of these have been the Sea-viewing Wide Field-ofview Sensor (SeaWiFS) on board SeaStar, the Moderate Resolution Imaging Spectroradiometer (MODIS) on board Aqua, and the Medium Resolution Imaging Spectrometer (MERIS) on board Envisat. Together, these have provided a continuous time series of data from 1997 to the present day, and assimilation of these data can be used to generate reanalyses of this period. One challenge in doing so though is that the different sensors cover different time periods and have different error

<http://dx.doi.org/10.1016/j.rse.2017.03.040>

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Please cite this article as: Ford, D., Barciela, R., Global marine biogeochemical reanalyses assimilating two different sets of merged ocean colour products, Remote Sensing of Environment (2016), <http://dx.doi.org/10.1016/j.rse.2017.03.040>

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characteristics and biases, and in order to create a consistent time series these issues must be accounted for in the satellite processing and/or assimilation methodology.

Reviews of ocean biogeochemical data assimilation efforts are given by [Gregg et al. \(2009\)](#page--1-0) and [Dowd et al. \(2014\),](#page--1-0) and the application of such methods to operational forecasting and reanalysis is discussed by [Brasseur et al. \(2009\),](#page--1-0) [Matear and Jones \(2011\)](#page--1-0), [Gehlen et al. \(2015\),](#page--1-0) and [Ford and Barciela \(2015a\)](#page--1-0). Since it provides the largest data source, the majority of ocean biogeochemical data assimilation studies have focussed on assimilating chlorophyll products derived from ocean colour, although the assimilation of other variables has been explored (e.g. [Ourmières et al., 2009; While et al., 2012; Ciavatta et al., 2014; Zhang](#page--1-0) [et al., 2014; Jones et al., 2016\)](#page--1-0). Recent applications of chlorophyll data assimilation for state estimation have used a range of different methods, both univariate and multivariate, and most have been at regional scale (e.g. [Ciavatta et al., 2011; Mattern et al., 2013; Fontana et al., 2013;](#page--1-0) [Teruzzi et al., 2014](#page--1-0)). Only a few studies have assimilated ocean colour data into a global model [\(Nerger and Gregg, 2007, 2008; Gregg, 2008;](#page--1-0) [Ford et al., 2012; Rousseaux and Gregg, 2012, 2015; Gregg and](#page--1-0) [Rousseaux, 2014](#page--1-0)). Such studies have consistently demonstrated the ability of data assimilation to improve the representation of modelled chlorophyll compared to both the assimilated data and independent in situ observations. In general, using chlorophyll assimilation to improve the non-assimilated variables remains a challenge within the community [\(Gehlen et al., 2015\)](#page--1-0), but some studies have begun to show improvements in other model variables. For instance, [Ciavatta et al. \(2011\)](#page--1-0) demonstrated an improved match with a number of non-assimilated variables compared to in situ observations, and [Fontana et al. \(2013\)](#page--1-0) found an improvement in near-surface nitrate. [Ford et al. \(2012\)](#page--1-0) assimilated a merged chlorophyll product using an analysis correction method combined with the multivariate nitrogen balancing scheme of [Hemmings et al. \(2008\).](#page--1-0) This improved surface and sub-surface chlorophyll, whilst other variables were not degraded, with evidence of improvement in some cases. It is the method described in [Ford et al.](#page--1-0) [\(2012\)](#page--1-0) which has been used in this present study.

The work presented here has been performed as part of the Climate Modelling User Group (CMUG; <http://www.esa-cmug-cci.org>/) component of the European Space Agency (ESA)'s Climate Change Initiative (CCI; [Hollmann et al., 2013;](#page--1-0) <http://cci.esa.int>/). For a number of essential climate variables (ECVs), as defined by the Global Climate Observing System [\(GCOS, 2011](#page--1-0)), the CCI aims to produce sets of satellite observation products which are suitable for use as climate data records (CDRs; [National Research Council, 2004\)](#page--1-0). One of these ECVs is ocean colour [\(Sathyendranath et al., 2012; Müller et al., 2015a, 2015b;](#page--1-0) [http://www.](http://www.esa-oceancolour-cci.org) [esa-oceancolour-cci.org/](http://www.esa-oceancolour-cci.org)). In addition to funding the production of CDRs for each ECV, ESA established CMUG to provide assessment of the new data products from a climate modelling perspective, and as a forum linking the earth observation and climate modelling communities.

This study represents a first attempt to use these new ocean colour products to create a global marine biogeochemical reanalysis, by assimilating them into a coupled physical-biogeochemical ocean model. By way of comparison, a further reanalysis has been created by assimilating ocean colour products from GlobColour ([Fanton d'Andon et al., 2008;](#page--1-0) [Maritorena et al., 2010\)](#page--1-0), which is a previous ESA-funded data product, continued under EU FP7 funding. The objectives of the study were to assess the suitability of each of the satellite data sets for use in reanalyses, and assess the potential of the resulting reanalyses for use in climate studies, and as a tool for the development and improvement of climate models. A particular focus was to assess whether assimilating the products could lead to improved estimates of air-sea $CO₂$ fluxes. This paper details the methodology used to create the reanalyses, and provides an assessment of the impact of assimilating the different data sets, through validation against independent observations. The paper is organised as follows: Section 2 describes the ocean colour data, [Section 3](#page--1-0) describes the model and assimilation, [Section 4](#page--1-0) details the experiments, [Section 5](#page--1-0) presents the results, and [Section 6](#page--1-0) summarises and draws conclusions.

2. Ocean colour observations

This study used two different sets of ocean colour products, available from GlobColour and the ocean colour CCI project (hereafter OC-CCI). Details of each product set are given below, but both provide daily average level three (gridded but not gap-filled) chlorophyll data by merging information from SeaWiFS, MODIS and MERIS. Per-pixel uncertainty estimates are provided in each case. Observations are available globally, but the products are primarily intended for use in case I ([Morel and](#page--1-0) [Prieur, 1977\)](#page--1-0) waters.

In each case the latest available product version at the time the model runs were performed (early 2014) was used. Updated versions of each product have since been made available, but repeating the model runs and assessment with these versions would be computationally prohibitive, so the use of alternative product versions is left for future studies. The versions used are mature product releases widely used by the community, and most of the conclusions drawn apply more generally than to these specific versions.

2.1. GlobColour

The GlobColour project [\(http://www.globcolour.info\)](http://www.globcolour.info) was set up by ESA to provide global merged ocean colour products in support of carbon cycle research and operational oceanography. It ran from 2005 to 2009 in research and prototype mode, and has since transitioned to an operational service, with ACRI-ST delivering on-the-fly ocean colour data and uncertainty estimates together with complete time series. Products are available through the aforementioned website, and continue to be updated in near-real-time.

This study uses the original set of operational GlobColour products (R2008), available at the time the experiments were performed. A detailed description of these products is given in the GlobColour Product User Guide [\(http://hermes.acri.fr](http://hermes.acri.fr) and [http://www.globcolour.info/](http://www.globcolour.info/CDR_Docs/GlobCOLOUR_PUG.pdf) [CDR_Docs/GlobCOLOUR_PUG.pdf](http://www.globcolour.info/CDR_Docs/GlobCOLOUR_PUG.pdf), 19 October 2015). The products were generated on-the-fly from level two radiance data provided by ESA for MERIS, and the National Aeronautics and Space Administration (NASA) for MODIS and SeaWiFS, with different ESA and NASA processings used for different time periods, due to ongoing operational changes. This study uses the global chlorophyll products generated by GlobColour using the Garver, Siegel, Maritorena (GSM) model, as described in [Maritorena et al. \(2010\).](#page--1-0) Chlorophyll is gridded at a resolution of 1/24° (4.63 km at the equator), on an integerised sinusoidal grid. The uncertainty estimates provided are an output of the GSM model ([Maritorena et al., 2010\)](#page--1-0). In contrast to OC-CCI, GlobColour data are not corrected for contingent bias observed between the different sensors, so as not to create a potential false trend due to undetected instrument defects or drift - one objective of GlobColour is to observe and understand the discrepancies between missions and provide feedback to the relevant Space Agencies to ultimately correct for them at source.

The consistency of the processing across the full time series is obviously not permanently ensured in near-real-time, and reprocessing campaigns are regularly performed to realign the time series when Space Agencies deliver updated datasets. Since this study was performed, a major reprocessing (R2014.0) of the GlobColour dataset has been carried out with EU funding (OSS2015, grant 282723), including using consistent ESA and NASA processings for the full time period. The R2014.0 reprocessing was aimed at addressing some of the issues identified in the original product set, including those raised in [Section](#page--1-0) [5.1](#page--1-0) of this paper, and is the version currently available through the GlobColour website.

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