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# Insights on multivariate updates of physical and biogeochemical ocean variables using an Ensemble Kalman Filter and an idealized model of upwelling

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ABSTRACT

Effective data assimilation methods for incorporating observations into marine biogeochemical models are required to improve hindcasts, nowcasts and forecasts of the ocean's biogeochemical state. Recent assimilation efforts have shown that updating model physics alone can degrade biogeochemical fields while only updating biogeochemical variables may not improve a model's predictive skill when the physical fields are inaccurate. Here we systematically investigate whether multivariate updates of physical and biogeochemical model states are superior to only updating either physical or biogeochemical variables. We conducted a series of twin experiments in an idealized ocean channel that experiences wind-driven upwelling. The forecast model was forced with biased wind stress and perturbed biogeochemical model parameters compared to the model run representing the "truth". Taking advantage of the multivariate nature of the deterministic Ensemble Kalman Filter (DEnKF), we assimilated different combinations of synthetic physical (sea surface height, sea surface temperature and temperature profiles) and biogeochemical (surface chlorophyll and nitrate profiles) observations. We show that when biogeochemical and physical properties are highly correlated (e.g., thermocline and nutricline), multivariate updates of both are essential for improving model skill and can be accomplished by assimilating either physical (e.g., temperature profiles) or biogeochemical (e.g., nutrient profiles) observations. In our idealized domain, the improvement is largely due to a better representation of nutrient upwelling, which results in a more accurate nutrient input into the euphotic zone. In contrast, assimilating surface chlorophyll improves the model state only slightly, because surface chlorophyll contains little information about the vertical density structure. We also show that a degradation of the correlation between observed subsurface temperature and nutrient fields, which has been an issue in several previous assimilation studies, can be reduced by multivariate updates of physical and biogeochemical fields.

## 1. Introduction

With the rapid expansion of ocean observing platforms, which now provide a wealth of observations, and growing numerical model capabilities, effective ways of combining observations and dynamic models through data assimilation (DA) are needed. While DA techniques and methodologies are well developed in meteorology and physical oceanography (e.g., Ghil and Malanotte-Rizzoli, 1991; Houtekamer and Mitchell, 1998, 2001; Kalnay, 2003), their applications in marine biogeochemical models are less mature, but actively developing (see reviews of biogeochemical state estimation in Gregg, 2008; Edwards et al., 2015, and state-parameter estimation in Gharamti et al., 2017a, b). Biogeochemical data assimilation falls into two general categories, the optimization of biogeochemical model parameters through minimization of a cost function (e.g., Fennel et al., 2001; Friedrichs et al., 2007; Kuhn et al., 2015) and updates to the biogeochemical model state by incorporating available observations sequentially (e.g., Eknes and Evensen, 2002; Natvik and Evensen, 2003; Ciavatta et al., 2011; Hu et al., 2012; Ford et al., 2012; Mattern et al., 2013; Ford and Barciela, 2017). Recent efforts have shown that model parameters can also be updated sequentially along with the model state variables (e.g., Simon et al., 2015; Gharamti et al., 2017a, b).

For biogeochemical state estimation, efforts have primarily been made in assimilating satellite ocean color observations, predominantly

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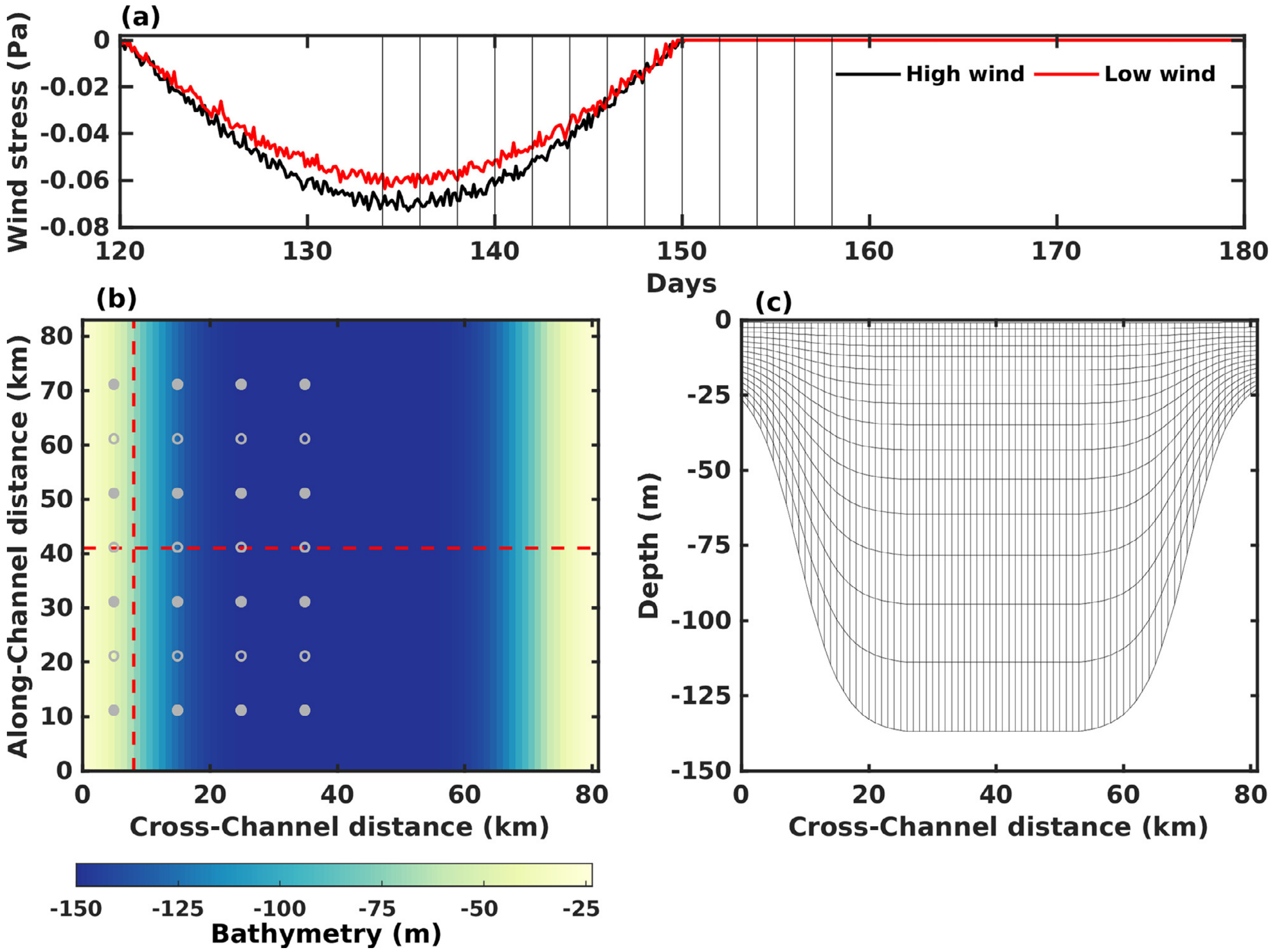


**Fig. 1.** (a) Wind stress for the high-wind and low-wind model runs. The vertical lines indicate the timing of assimilation steps. (b) Model bathymetry and (c) vertical grid of cross-channel transect. The red dashed lines in (b) show the position of the cross-channel transect and an along-channel section. The circles show the 28 stations where temperature profiles are sampled. The filled circles show the 16 stations where nitrate profiles are sampled. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

satellite-derived chlorophyll, into coupled physical–biogeochemical models (e.g., Natvik and Evensen, 2003; Gregg, 2008; Ciavatta et al., 2011; Hu et al., 2012; Ford et al., 2012; Fontana et al., 2013; Ford and Barciela, 2017). Assimilation of satellite ocean color products other than chlorophyll, such as phytoplankton absorption coefficients (Shulman et al., 2013), diffuse light attenuation coefficients (Ciavatta et al., 2014), and remote-sensing reflectance (Jones et al., 2016) are also being pursued. However, it has long been recognized that deficiencies in biogeochemical fields can arise from deficiencies in the physical state (e.g., Doney, 1999; Oschlies and Garcon, 1999; Doney et al., 2004) because the physics controls both horizontal and vertical transport of nutrients, oxygen, plankton and many other biogeochemical variables. Several studies have investigated the impact of assimilating physical data alone on coupled physical–biogeochemical systems (Berline et al., 2007; Samuelsen et al., 2009; While et al., 2010; El Moussaoui et al., 2011; Fiechter et al., 2011; Raghukumar et al., 2015). One important and perhaps surprising finding drawn from these studies is that, despite the clear improvement in physical model fields, the physical data assimilation alone does not generally improve, but often degrades, simulated biogeochemical fields. For example, While et al. (2010) and El Moussaoui et al. (2011) reported overestimated surface nutrients and chlorophyll concentrations, particularly in equatorial regions, associated with spurious increases in vertical velocities when assimilating physical data in global ocean models. Berline et al. (2007) found large increases in vertical nutrient fluxes in mid-latitudes and sub-tropics that were partly due to the misalignment between physical and biogeochemical fields resulting from updates of the physical fields. Raghukumar et al. (2015) also showed that assimilating physical data leads to elevated production, particularly in oligotrophic regions, and attributed the overestimation to a net upward nutrient flux resulting from high vertical velocity fluctuations due to the "initialization shocks" after updates to the density distribution, and increased nutrient variance on density surfaces due to the adjustment of physical variables in the assimilation step.

Collectively the above studies demonstrate that adjusting only physical or biogeochemical fields is not sufficient to improve the full 3D biogeochemical model state. An obvious next step is the simultaneous updating of physical and biogeochemical fields. Two approaches have emerged to address it. The simpler approach is applying a correction to the nutrient field alongside the physical data assimilation (Shulman et al., 2013; While et al., 2010). The second approach is to jointly assimilate physical and biogeochemical observations into the models. To date, few studies have explored this idea but with encouraging results (Anderson et al., 2000; Ourmières et al., 2009; Song et al., 2016a,b; Mattern et al., 2016). These studies show that assimilating both physical and biogeochemical data can maintain dynamical consistency between the physical and biogeochemical fields and provide better state estimates than only assimilating one or the other. However, one clear drawback of this approach is that the required physical and biogeochemical observations might not always be available concurrently.

Here we propose and test an alternative approach for updating both