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Using satellite-derived optical data to improve simulation of the 3D light field in a biogeochemical model

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Abstract: Satellite images provide a rich data source for environmental modelling. Use of satellite data for calibration or validation of ocean models is now common-place. Satellite observations can also be used more directly to improve model performance - usually through "nudging" of model results towards observed values. We describe a novel approach to satellite data assimilation, applying empirically derived "correction factors" to simulated optical conditions in a process-based, three-dimensional biogeochemical model of a coastal system. The correction factors (which are functions of simulated salinity and suspended solids concentrations) are applied to simulated attenuation and backscattering. The result is improved simulation of optical conditions and a consequent improvement in simulated chlorophyll biomass. This approach has two advantages over traditional nudging: 1) the model retains conservation of mass; 2) the correction factor can be applied beyond the bounds of the satellite observations (e.g. beneath the surface) and can be applied in scenario runs as well as simulations of current or historical conditions. This work also demonstrates the benefits of matching what is modelled to what is observed (in this case, attenuation and backscattering rather than derived optical products).

Keywords: dynamic simulation model, environmental flow, shear stress, benthic plants, nutrient transfer, boundary layer transfers, primary production

1 INTRODUCTION

Complex environmental models are often data-intensive. This can present a problem when *in situ* data collection is difficult or expensive, as is often the case for coastal waters (Robson et al. 2008). Satellite images can provide a rich source of data to fill this gap. MODIS satellites, for instance, provide a wide range of optical products over large areas of the Earth twice daily, with a one-kilometre pixel size (Brando et al. 2006). For Keppel Bay (Queensland, Australia), this has proven an enormously rich data source in comparison with the handful of intensive *in situ* field surveys that have been possible (Brando et al. 2007; Radke et al. 2010).

Satellite observations have their own limitations, among them a) they cannot provide observations beneath the optical surface; and b) higher-level satellite products such as estimated chlorophyll *a* concentrations are themselves the product of an optical model. When using satellite observations to enhance water quality modelling, limitation one implication of (a) is that direct data assimilation techniques can only be applied at the surface, while an implication of (b) is that it is preferable where possible to match the model output to the optical products of the satellite. Cherukuru et al. (2008) demonstrate the development and application of an optical submodel as part of a coupled hydrodynamic and biogeochemical model of the Fitzroy Estuary and Keppel Bay, using local optical data.

2 PREVIOUS MODELLING OF THE FITZROY ESTUARY AND KEPPEL BAY

The Fitzroy Estuary is located just south of the Tropic of Capricorn and is one of the largest rivers feeding into Great Barrier Reef Lagoon (GBRL). Sediment and nutrient loads reaching the GBRL are of concern (Devlin and Brodie 2005; Fabricius 2005; Haynes et al. 2007; Humphrey et al. 2008) so it is important to understand the transport and transformation of sediment and nutrient loads in the estuary and in Keppel Bay, into which the Fitzroy Estuary flows.

Water in Keppel Bay ranges from muddy fresh water near the mouth of the estuary to clear blue sea water in the outer Bay, with both the concentrations and character of suspended particulates and chromatographic dissolved organic matter (CDOM) varying with salinity and time, and lending this region an enormous optical complexity (Brando et al. 2006). Strong temporal variations in water quality and optical properties are associated with a diurnal tidal range of up to 7 m, which forces parcels of water to move up to 30 km within the bay over 6 hours, suspending large quantities of particulate material from the bottom when tidal currents are strong, and depositing much of this material again when the current drops at high- and low-tide (2006).

Previous modelling has resulted in satisfactory simulation of sediment and dissolved nutrient concentrations in Keppel Bay, but poor simulation of chlorophyll (Robson et al. 2008). Increases in phytoplankton production resulting from increased nutrient loads may be responsible for the spread of crown-of-thorns starfish, which directly damage the Reef (Brodie et al. 2005). Improved modelling of chlorophyll will aid management of this threat.

Phytoplankton growth depends on light availability, so correctly simulating the optical environment is essential to accurate modelling of chlorophyll concentrations. Given the enormous spatial and temporal optical variability of Keppel Bay, this is difficult to get right. While parallel work aims to improve the simulation of suspended sediments (a major contributor to absorption and backscattering in this environment), the work described here uses satellite data to adjust the optical model and hence "correct" for inaccuracies in simulated concentrations of suspended sediments and other substances. We take a novel approach that allows us to apply a correction factor beyond the extent of the direct satellite observations; e.g. at depth and between clear-sky satellite passes.

3 MODEL DESCRIPTION

The Fitzroy Receiving Waters Model (Robson and Brando 2008) is an application of EMS, an environmental modelling suite with the hydrodynamic model, SHOC (Herzfeld et al. 2005) at its core. SHOC is a three-dimensional, baroclinic, finite difference hydrodynamic model. EMS also includes a sediment dynamic model (Margvelashvili et al. 2006) and an ecology model, consisting of an expanded NPZD model, a mechanistic model that simulates transport and transformations of water-column and sediment nitrogen and phosphorus in various forms as well as primary producers (including phytoplankton) and zooplankton. The model simulates a range of physical and chemical processes including settling and resuspension of particulate materials, degradation and remineralisation of organic nitrogen and phosphorus, nitrification and denitrification, exchanges between water column and sediment pore waters, and growth and mortality of two phytoplankton and two zooplankton groups, separated by size. The ecology model is a descendant of that described by Murray et al. (2000).

The set up and validation of EMS for the Fitzroy Estuary and Keppel Bay is described in detail elsewhere (Herzfeld et al. 2006; Margvelashvili et al. 2006; Robson et al. 2006; Robson and Brando 2008). In summary: the model is forced with estimated daily freshwater flow at the barrage at the upstream end of the model domain, meteorological conditions interpolated from nearby observation stations, temperature, salinity and sea surface height at the outer boundary calculated in a regional-scale hydrodynamic model, within which this model is nested, constant nutrient concentrations at the outer boundary, and chlorophyll and sediment concentrations at the outer boundary obtained from MODIS observations.

The growth of large and small phytoplankton in the model is a function of available nitrogen and phosphorus concentrations, temperature, and light (irradiance).

If nutrients are replete and temperature is constant, growth is a function of the maximum growth rate and light. The growth rate, μ of phytoplankton at depth z is a function of photosynthetically active radiation (PAR) at that depth, I_z, i.e.:

$$\mu = \mu_{\max(N,P,T)} f\left(I_z\right) \tag{1}$$

where $\mu_{\max(N,P,T)}$ is the maximum possible growth rate given the prevailing nutrient concentrations and temperature and $f\left(I_z\right)$ is determined from the size-based formation of Barird (2003). I_z, at the bottom of any given layer of the model, is given as a function of the depth of the layer, d (m), PAR at the top of the layer, I_0, and the attenuation rate of PAR in that layer (k_d, m^{-1}):

$$I_z = I_0 e^{-k_d d} \tag{2}$$

The simple light attenuation sub-model used in earlier work was replaced here with the region-specific optical model described by Cherukuru et al. (2008), using the formulation suggested by Lee et al. (2005). An advantage of this model is that it gives as outputs not only an attenuation rate for photosynthetically active radiation, but also estimates of total attenuation and backscattering, which can be compared directly with the corresponding MODIS products. As calibrated using local optical data, this model gives total attenuation, k_d as:

$$\begin{aligned} k_d &= \left(\text{-0.057+0.482} \cdot \text{at}_{490}\text{0.5 +4.221} \cdot \text{bbt}_{490}\right)\left(1 + 0.09 \times \sin(\theta\text{a})\right) \\ &+\left(0.183 + 0.702 \cdot \text{at}_{490}\text{-2.567} \cdot \text{bbt}_{490}\right)\left(1.465 \text{ -0.667}\times\cos(\theta\text{a})\right)\left(1+z\right)-0.5 \end{aligned} \tag{3}$$

where the total aborption at 490 nm, at_{490}, is given by:

$$at_{490} = aw_{490} + aph_{490} + anap_{490} + ay_{490} \tag{4}$$

and total backscattering at 490 nm, bbt_{490}, by:

$$bbt_{490} = bbw_{490} + bbp_{490} \tag{5}$$

where the remaining optical variables are obtained from empirical fits of optical measurements to measured chlorophyll concentrations, C, and non-algal particulate concentrations, NAP (both in mg m^{-3}). aph_{490} =0.0331C +0.7574 (N=14, r^2=0.85); anap_{490} = 0.0199NAP-0.0074 (N=8 r^2=0.96), ay_{490} = 0.4173 ay_{440}+0.0027 (N=23, r^2=0.98); bbp_{490}=0.0366 S-0.0312 (N=8 r^2=0.99) and bbw_{490} is backscattering due to water.

EMS was run for the period from December 2003 to June 2004 using MODIS-derived estimates of surface PAR and other inputs as described by Brando and Robson (2007). We will henceforth refer to this first run as the "unconstrained model".

Simulated absorption and backscattering (at_{490} and bbt_{490}) were compared with MODIS estimates of attenuation and backscattering at every surface point in the model domain at every time for which MODIS estimates were available (i.e. during MODIS-Aqua overpasses when cloud cover and surface reflection were low enough to allow a clear view of the water). The ratios between observed and simulated absorption and backscattering were found to be functions of simulated total suspended solids concentrations (TSS, mg m^3) and salinity (S, a unitless value on the practical salinity scale), to a good degree of reliability. These relationships are given as Figure 1.

For the second model run (hereafter, "the constrained model"), we used these empirically derived relationships to "correct" calculated absorption and backscattering, hence:

$$at_{490} = \frac{\left(aw_{490} + aph_{490} + anap_{490} + ay_{490}\right)}{2205TSS + 0.04S} \tag{6}$$

and

$$bbt_{490} = \left(\frac{bbw_{490} + bbp_{490}}{449TSS + 0.03S}\right) \tag{7}$$

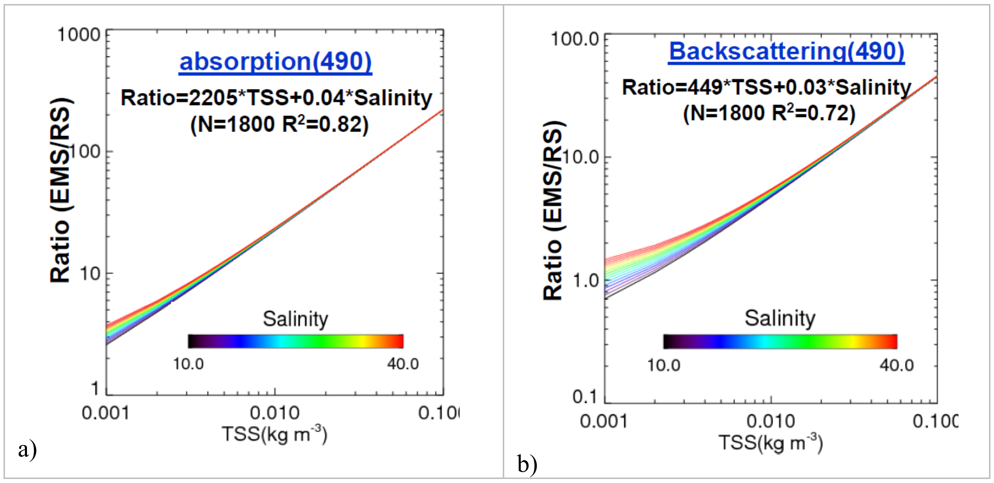

Figure 1 Empirical correction algorithms (a) absorption; (b) backscattering.

Equations (6) and (7) were applied over the whole three-dimensional model domain, not only at the surface, where MODIS estimates were available. The relationships were assumed to be consistent regardless of depth – this assumption warrants further investigation through analysis of *in situ* optical profiles. Salinity in these formulations effectively acts as a proxy for the optical character of the parcel of water under consideration. Low-salinity water carries recent terrestrial inputs of dissolved and particulate organic matter, which will have a different optical character from the marine water associated with higher salinities. Including TSS in these equations allows a de-facto correction for under- or over-estimation of suspended solids concentrations by the model in different parts of the spatial domain.

4 RESULTS

Application of equations (6) and (7) resulted in markedly improved simulation of the optical environment as represented by total absorption and total attenuation (Figure 1, top and middle) and a consequent improvement in simulated chlorophyll *a* (Figure 1, bottom) in some parts of the model domain throughout the duration of the run. At some other locations, the impact was negligible. The impact on the root mean square error (RMSE) between simulated and MODIS-derived chlorophyll throughout Keppel Bay is illustrated in Figure 3. The mean RMSE over the entire surface dropped from 3.3 to 2.5 mg chl *a* m^{-3}, with the most marked improvements evident near the mouth of the estuary, where suspended sediment concentrations are high.

The introduction of these correction factors had no significant impact on processing times. The CPU demands of this complex, process-spaced and spatially resolved biogeochemical model and others like it are high (in this case, the real time : run time ratio is approximately 30:1), and this is a constraint that limits the application of many automated data-assimilation and calibration techniques.

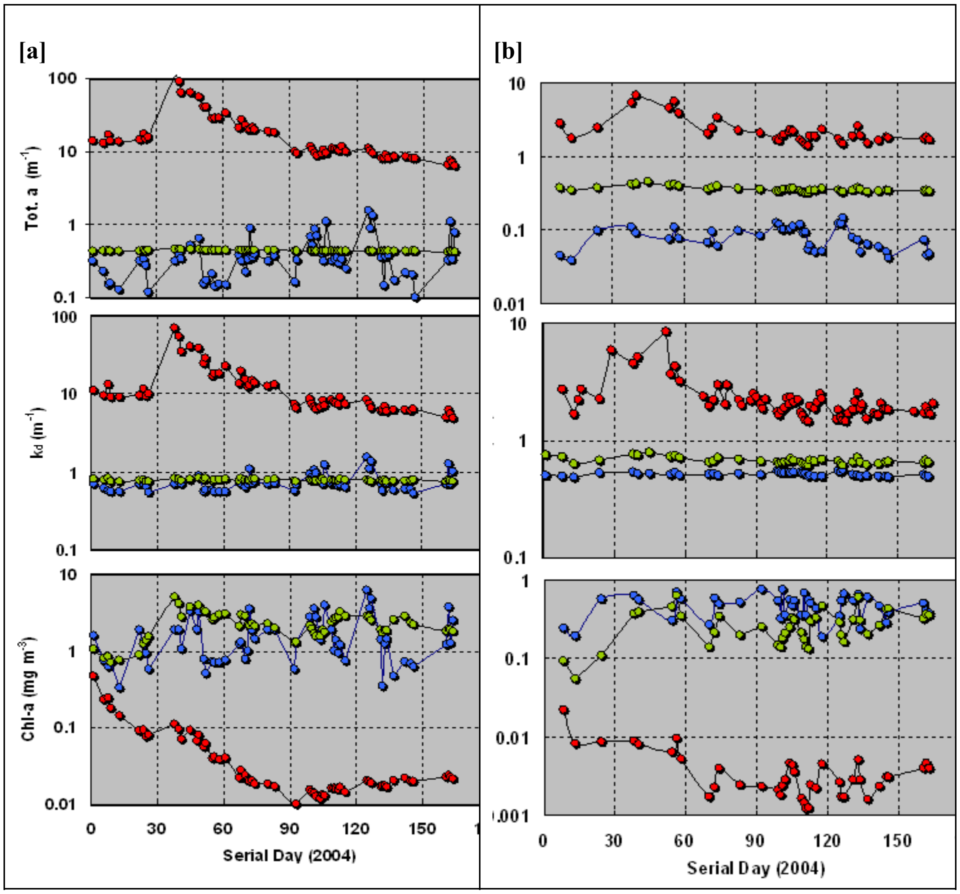

Figure 2 Time series comparison plots of total absorption (top), diffuse attenuation (middle) and chlorophyll (bottom) at two stations in Keppel Bay (a) a coastal station and (b) in clear water approximately 30 km from the coast. Key: MODIS estimates (blue), model reference run (red), and constrained model run (green).

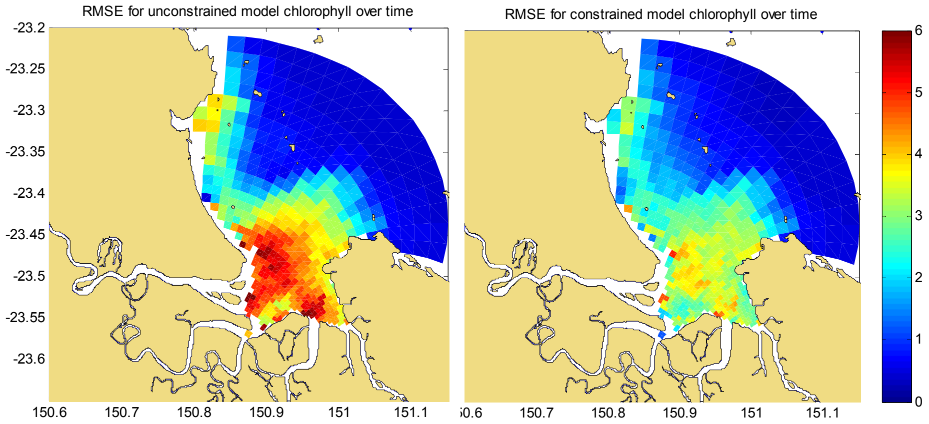

Figure 3 Root mean square error (RMSE) obtained by comparing time-series of model output and MODIS estimates of chlorophyll *a* during a three-month model run. Left: unconstrained model. Right: with empirical correction factors applied to calculated attenuation and backscattering. White areas are either beyond the domain of the model (outer bay) or beyond the domain within which the MODIS algorithm can be used to estimate chlorophyll (estuary and tidal creeks).

5 CONCLUSIONS

We have demonstrated a new approach to the use of satellite observations to improve simulation results from an aquatic biogeochemical model. Empirical correction factors obtained by comparing output from a reference model run with MODIS products were applied to calculated absorption and backscattering in subsequent model runs. This resulted in an incremental, but still useful, improvement in simulated chlorophyll *a*, with a marked improvement in some parts of the model domain.

The approach that we have described has distinct advantages over simple nudging of a modelled suspended sediments and chlorophyll towards observed concentrations, especially when applied in the context of a biogeochemical model. The model retains conservation of mass as well as the underlying process-based relationships between phytoplankton growth, light and nutrients. This approach also provides the capacity to apply a correction factor beyond what the satellite can see (i.e. at depth and over time).

The approach allows us to (speculatively) use what we've learnt about the relationships between simulated salinity, TSS and the model's optical performance below the surface and beyond the timeframe of satellite observations. Once calibrated for a particular environment, the correction factor can be applied even for speculative scenario simulations, such as simulating the impact of reductions in nutrient loads that are expected to result from planned improvements in catchment management.

There is a need for continued work to improve the model separately, through improved process representation and further calibration against satellite and *in situ* observations. Such work is ongoing in the Fitzroy Estuary and Keppel Bay. The use, where appropriate, of empirical correction factors such as those demonstrated here provides a tool to improve simulation results in the meantime. The calculated correction factors can be updated whenever the model itself is improved, to further improve predictions.

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