Using Satellite Observations to Improve Biogeochemical Modelling Of the Fitzroy River Estuary

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Keywords: *remote sensing, data assimilation, transport, biogeochemical, boundary conditions*

EXTENDED ABSTRACT

Modelling of pollutants as they move through rivers and into the marine environment is often constrained by limited availability of observational data, particularly when the models extend into the coastal ocean, where regular monitoring presents a logistical challenge. Satellite observations provide a way forward: remote sensing data can be used to improve validation of models, improve specification of downstream boundary conditions, or be assimilated directly into models.

Assimilation of ocean colour satellite observations into biogeochemical models is in its infancy; partly due to the lack of adequately developed coastal ocean colour products. Coastal waters show a high spatial and temporal variability in optical properties and how they relate to biogeochemical constituents concentrations.

Both remote sensing applications and a mechanistic model have been developed for the Fitzroy River Estuary and Keppel Bay, in Queensland, Australia. A new region-specific algorithm was developed for the satellite datasets of the MODIS sensors. The algorithm provides spatially explicit estimates of sediment concentrations, chlorophyll *a*, and ocean colour. Simultaneously, a three- dimensional hydrodynamic-sediment dynamic-biogeochemical model was developed for the same area. The model simulates transport and transformations of sediments and nutrients in the system as well as primary production and chlorophyll *a*.

We discuss results of assimilation of ocean colour datasets into the biogeochemical and sediment dynamic model. Use of satellite data to specify boundary conditions for sediment concentrations on chlorophyll *a* had a small impact on simulated sediment and nutrient concentrations, but a dramatic impact on estimated export of pollutants to the ocean.

When forced with constant boundary conditions based on the limited available field observations, the model results indicated that 25 kilotonnes of fine sediment was exported to the Great Barrier Reef Lagoon over the period from January and early October 2004. When the open ocean boundary condition was forced with concentrations of suspended solids derived from satellite observations, the results suggested that 19 kT of fine sediments were imported to Keppel Bay across this boundary: a 176% difference in magnitude and reversal of direction.

When the same technique was applied to chlorophyll a boundary conditions, the effect was less dramatic, but still significant: forcing the boundary with satellite data resulted in a 15% drop in the estimated export of nitrogen in the form of phytoplankton.

These results illustrate how different uses of a model (e.g. simulation of conditions within the model domain versus use of the same model to estimate exports across a boundary) may have different data requirements, highlighting in this instance, the importance of an appropriate ocean boundary condition. Further, the results show that use of remotely sensed observational data to set boundary conditions for biogeochemical and sediment transport models is a promising application of data assimilation, with the potential to improve both the models and our ability to interpret the practical significance of the satellite data.

1. INTRODUCTION

Modelling of pollutants as they move through rivers and into the marine environment is often constrained by limited availability of observational data, particularly when the models extend into the coastal ocean, where regular monitoring presents a logistical challenge. Satellite observations provide a way forward: remote sensing data can be used to improve validation of models, improve specification of downstream boundary conditions, or be assimilated directly into models.

While widely used in meteorology and physical oceanography, the application of data assimilation methods to marine biogeochemical problems is just beginning, and many basic elements still need to be determined (Dickey 2003, Moisan et al 2005). The low accuracy of global ocean colour products in coastal systems has until now made it difficult/inefficient to assimilate (Moisan et al, 2005). Recent algorithm developments enable valid retrieval of Chlorophyll, Suspended Solids, Coloured Dissolved Organic Matter concentration in coastal waters, thus creating new opportunities for combining hydro-biogeochemical models with remote sensing data for coastal systems.

2. METHOD

2.1. Biogeochemical model of the Fitzroy Estuary and Keppel Bay

EMS (Environmental Modellings System) consists of the hydrodynamic model SHOC (Herzfeld et al., 2005; Margvelashvili et al., 2006) coupled with a sediment transport model (Margvelashvili et al., 2006) and a biogeochemical model descended from the Port Phillip Bay model (Murray and Parslow, 1997). The set-up and application of the biogeochemical model to Fitzroy Estuary and Keppel Bay (FEKB, Figure 1) is described in detail by Robson et al. (2006a; 2006b), while the reasoning behind this choice of model and the steps of the modelling process are discussed by Robson et al. (2007).

Briefly, SHOC is a three-dimensional, baroclinic curvilinear-grid hydrodynamic model, and as part of EMS, simulates transport and mixing of water, heat, salt, and the dissolved and particulate substances represented by the sediment and biogeochemical models.

The sediment model simulates transport of particles in water, settling, resuspension and burial of particles in two sediment layers, and flocculation and disaggregation of cohesive particles. As applied to FEKB, the model was run with three particle size classes, corresponding to sand, silt and clay fractions, plus the particulate components required by the biogeochemical model.

The biogeochemical model simulates concentrations and transformations of nitrogen (N), phosphorus (P) and carbon (C) as dissolved inorganic N and P (DIN and DIP), labile and refractory detrital N, P, and C, and dissolved organic N, P and C in the water column and sediments, as well as three phytoplankton groups (small phytoplankton, large phytoplankton and *Trichodesmium*) plus microphytobenthos, using the mechanistic size-based model for nutrient uptake and phytoplankton growth described by Baird (2003). Processes simulated include mineralisation of particulate and dissolved organic material, denitrification, grazing of phytoplankton by zooplankton, mortality of phytoplankton, microphytobenthos and zooplankton, adsorption and desorption of DIP onto suspended sediments.

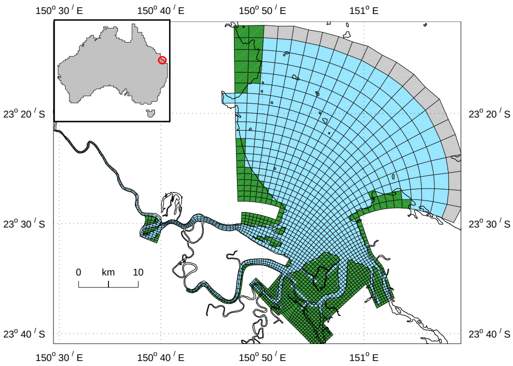

Figure 1. Fitzroy Estuary and Keppel Bay and curvilinear-grid for three-dimensional model

2.2. Observational data and boundary conditions

Three field cruises were conducted in Keppel Bay: two dry-season campaigns (September 2003 and August 2004) and one wet-season campaign (February 2005). These campaigns included intensive sampling of concentrations of nutrients, chlorophyll, and suspended solids (see Radke et al, 2006, for a details), as well as optical properties of the water (Oubelkheir et al., 2006).

The biogeochemical model was initialised with observational data from the September 2006 field trip. Additional input data included meteorological conditions (wind velocity, air temperature, and irradiance), sea surface height at the open boundary (as simulated by a regional-scale hydrodynamic model), flows, nutrient and sediment loads from Fitzroy River (flows determined from a rating curve, and nutrient loads estimated from a previously established relationship between flow and nutrient concentrations (Robson et al. 2006b).

Observational data from the August 2004 and February 2005 field campaigns were used to calibrate the model (Robson et al., 2006b; 2007).

Unfortunately, *in situ* observational data along the open ocean boundary were very limited. For the hydrodynamic model, temperature and salinity at the open boundary were derived from a regional-scale coastal model, while initially, constant boundary concentrations were assumed for nutrients, chlorophyll and total suspended sediments (TSS). Ocean concentrations of 0.2 g TSS m^{-3} as fine sediments, 0 g m^{-3} of coarse sediments, and 0 mg m^{-3} chlorophyll *a* were applied, based on the available observational data from September 2003 and August 2004.

An upwind advection boundary condition was applied for concentrations at the open ocean boundary. That is, when water flows outwards across the boundary, concentrations from within the model domain are used to calculate fluxes, while the ocean boundary concentrations are used to calculate fluxes when water flows inwards.

2.3. Remote sensing of total suspended solids (TSS), chlorophyll *a* and ocean colour

Analysis of global algorithm products for selected waters in GBR has demonstrated that the global MODIS algorithms may be invalid in inshore FEKB waters (Brando et al., 2006b; Qin et al, submitted). The level of disagreement is at least twofold for concentrations of chlorophyll above 2 µg L-1.

The Adaptive Regional MODIS Algorithm for GBR and Australian Coastal waters (ARMAGNAC) was designed to cope with the significant variability in the specific inherent optical properties of concentration specific light absorption and scattering encountered in these waters (Brando et al., 2006b; Brando et al., 2006a). The algorithm estimates simultaneously the concentration of chlorophyll, total suspended sediment, Coloured Dissolved Organic Matter and the vertical attenuation coefficient, Kd. The principles of this algorithm, which is based on Singular Value Decomposition Matrix Inversion (MIM), have been published for other sensors (Brando and Dekker, 2003; Dekker et al., 2005; Phinn et al., 2005). This algorithm was adapted to MODIS for KEFB waters by Brando et al. (2006b).

2.4. Comparison of model output with remotely sensed data

Quantitative comparison of the model output and the remote sensing data was carried out using two indicators: the anomaly correlations and RMSE. These indicators were computed both as time-series of spatially aggregated indicators and as maps of temporally aggregated indicators. In order to compare the model output of Chlorophyll and Total Suspended Matter with the remote sensing data, we adopted a common spatial and temporal resolution. The model state was output to match the nominal overpass time of the MODIS and AQUA sensors to minimise any difference due to tidal dynamic and resuspension. The model output was regridded from the curvilinear grid (which had grid-cells of a little over 1 km^2 in the outer Bay) to the 1km remote sensing data grid.

2.5. Use of remotely sensed data to force model boundary conditions

Satellite observations indicated that chlorophyll *a* concentrations over most of the open boundary were low, in accordance with the assumed boundary condition applied in the original model. Near the coast, however (i.e. at the northern and southern extremes of the boundary), pulses of elevated chlorophyll *a* were observed (Figure 2), which appeared to be associated with coastal currents and did not appear to originate within the Keppel Bay model domain.

In order to capture this variability, we applied remotely sensed TSS and chlorophyll *a* observations. For each date for which satellite observations were available and of sufficient quality to derive estimates of TSS and chlorophyll *a* concentrations at the open boundary of the model (including 67 occasions between January and October 2004), these observations at 1 km intervals were used to define a spatially-varying concentration field on the ocean side of the open boundary. Where there were gaps in the satellite data, these were filled by simple linear interpolation in space (Figure 2). Daily ocean boundary conditions were then estimated by linear interpolation in time. Again, an upwind advection boundary was applied.

2.6. Calculation of exports to the Great Barrier Reef Lagoon

Fluxes of TSS, total nitrogen, and chlorophyll *a* across a boundary defined one cell in from the open boundary at each time-step were averaged over one-day intervals and tracked for the duration of the simulation.

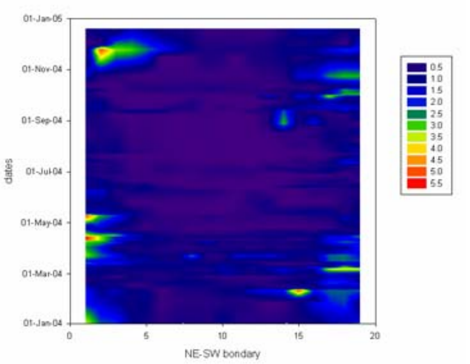

Figure 2. Remote sensing-derived chlorophyll *a* concentrations at the open boundary of the model. Original boundary conditions were set to 0.1μg/L

3. RESULTS

3.1. Validation of the model

Margvelashvili (2006) and Robson (2006b) describe, respectively, the calibration and validation of the suspended sediment and biogeochemical models of Fitzroy Estuary and Keppel Bay. The effectiveness of the biogeochemical model is also discussed briefly by Robson (2007), with conclusions summarised here.

A quantitative estimate of overall model performance can be obtained by comparing model predictions with field observations interpolated to the same grid for both the wet-season and dry-season campaigns. Arhonditsis and Brett (2004) reviewed the performance of 153 published mechanistic aquatic biogeochemical modelling studies. For the purposes of the current discussion, "reasonable performance" will be defined as a coefficient of determination (r^2) better than the 40th percentile of these studies. By this measure, the Fitzroy/Keppel Bay model achieved reasonable spatial agreement for concentrations of dissolved nitrogen and phosphorus (achieving r^2=0.49 for DIN and 0.37 for DIP; Robson, 2007).

The level of agreement between model simulations and observations for particulate materials appeared less satisfactory, with an r^2 of 0.37 for TN (with a 35% relative error) and an r^2 of 0.19 for TP (with an 83% relative error). Arhonditsis and Brett (2004) do not provide statistics for comparisons for TN or TP. This result is not surprising given the extreme variability of concentrations of particulate materials in the field. Total suspended solids concentrations at some sites in Keppel Bay were observed to vary by two orders of magnitude within the space of a few hours, due to tidal advection and resuspension (Margvelashvili et al., 2006), and the hydrodynamic model indicates that parcels of water in parts of Keppel Bay move by up to 20 km between low and high tide (i.e. the tidal excursion in some parts of Keppel Bay is around 20 km) during spring tide events. Hence, there are large uncertainties in the *in situ* field data as well as the model with regard to concentrations of suspended particulates.

The suspended sediment model itself was calibrated primarily against more intensive data obtained at three sites. As reported by Magvelashvili (2006), the model predicts the correct range of variability (approx. 0.03-300 g L^{-1}) of the sediment concentrations between neap and spring tides and the correct range of intratidal variability during high and declining spring tide, but overestimates sediment concentrations at the beginning of the spring tide.

3.2. Validation of remote sensing algorithms for chloropyll *a* concentrations

For validation purposes the only data set available that was independently available from the remote sensing algorithm development is the GBRMPA "long term in situ chlorophyll data set", which includes measurements going back as far as 1992.

Table 1 presents the summary of the comparison of chlorophyll retrieval from MODIS AQUA data with the CHL_Carder and ARMAGNAC algorithm for 2003-2004 with the long term in situ chlorophyll data. The number of pixels that are available for the comparison with *in situ* data is lower for the CHL_ARMAGNAC (20 pixels) than for CHL_Carder retrieval (70 pixels). The ARMAGNAC implementation suffers from an "over-cautious" flagging that limits the number of processed pixels. This is probably due to the necessity of ARMAGNAC to use all the available MODIS bands for the inversion (Brando et al 2006b).

Table 1. Root Mean Square Error of chlorophyll (in μg l^{-1}) retrieval from MODIS AQUA data using CHL_Carder and ARMAGNAC algorithms for the MODIS validation 2003-2004 and the biogeochemical modelling data.

	No of points	RMSE
CHL_ARMAGNAC	20	1.55
CHL_Carder all points	70	2.22
CHL_Carder same points as MIM	20	2.00
CHL_BGCM same as ARMAGNAC	20	2.87

3.3. Initial comparison of model output with remotely sensed data

The quantitative comparison of the model output and the remote sensing data was carried out using two indicators: the anomaly correlations and relative RMSE. These indicators were computed both as time-series of spatially aggregated indicators (only when at least 100 observations were present, Figure 3) and as maps of temporally aggregated indicators (Figure 4).

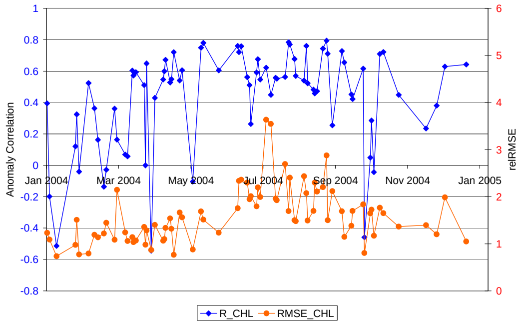

Figure 3. Comparison of chlorophyll *a* concentrations from the original model output and the remote sensing data. Time-series of spatially aggregated Anomaly correlation (left axis) and Relative RMSE (right axis)

The chlorophyll *a* concentrations as estimated with the original model output and the remote sensing data were overall in good agreement along all of the simulation period with an anomaly correlation of ~0.60-0.80 for the April 2004 to December 2004 period and a relative RMSE of ~ 1-1.5 (Figure 3). The original model output and the remote sensing data were in good agreement across all the model domain as a whole, with a relative RMSE of ~ 1 (Figure 4b), but showed poor correlation in the eastern portion of the domain where most of the sediment flow occurs.

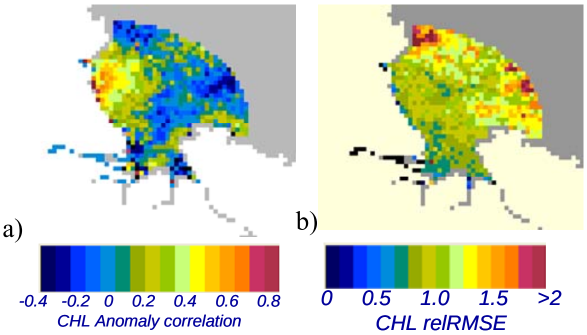

Figure 4. Comparison of chlorophyll *a* concentrations from the original model output and the remote sensing data. Maps of (a) temporally aggregated Anomaly correlation and (b) Relative RMSE.

3.4. Effect on simulated concentrations of suspended solids and chlorophyll *a* of forcing boundary conditions using satellite data

The spatially-varying concentration field of chlorophyll *a* concentrations on the ocean side of the open boundary (Figure 2) showed several pulses of concentrations higher than those set for original boundary conditions (0.1 μg/L). These pulses were mostly located at the NE and SW ends of the boundary as a result of coastal currents and in some cases were associated with local runoff events, and were where the original model output and the remote sensing showed the poorest agreement (relative RMSE of > 1.5, Figure 4b).

The effect of variation of the boundary conditions on the simulated concentration of chlorophyll *a* was small. Hence to evaluate the effect of these new open boundary conditions the comparison between the two fields was performed using log transformed fields (Figure 5 and 6).

The new forcing led to a minor improvement of the anomaly correlation (Figure 5a) while the relative RMSE_log for the model output using the statellite estimates was lower than the original model run along all of the simulation period (Figure 5b) and at the portion of the domain closer to the boundary (Figure 6).

3.5. Effects on simulated fluxes across the boundary

When forced with constant boundary conditions based on the limited available field observations, the model results indicated that that 25 kilotonnes of fine sediment was exported to the Great Barrier Reef Lagoon over the period from January and early October 2004. When the open ocean boundary condition was forced with concentrations of suspended solids derived from satellite observations, the results suggested that 19 kT of fine sediments were imported to Keppel Bay across this boundary: a 176% difference in magnitude and reversal of direction.

When the same technique was applied to chlorophyll *a* boundary conditions, the effect was less dramatic, but still significant: forcing the boundary with satellite data resulted in a 15% drop in the estimated export of nitrogen in the form of phytoplankton

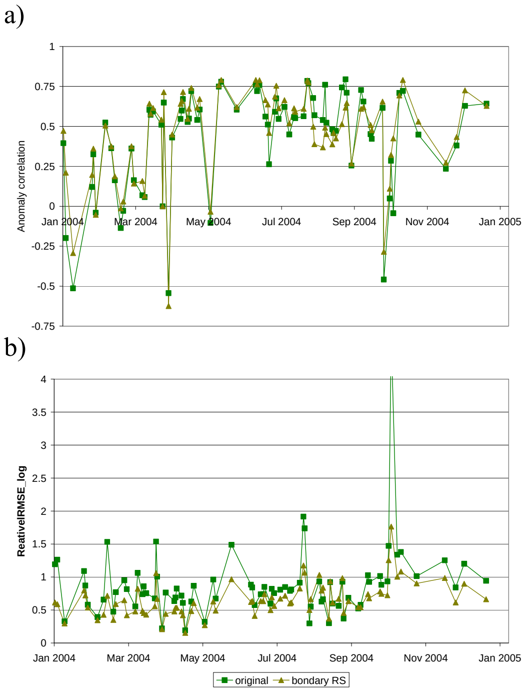

Figure 5. Comparison of chlorophyll *a* concentrations from the model output using boundary conditions and the remote sensing data. a) Time-series of spatially aggregated anomaly correlation and (b) Relative RMSE_log.

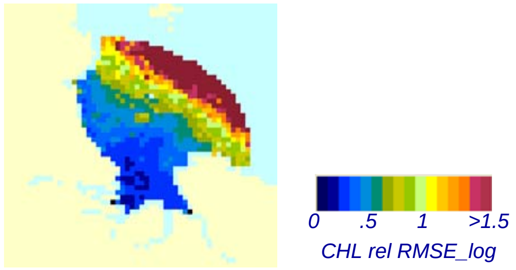

Figure 6. Comparison of Chlorophyll a concentrations from the model output using boundary conditions and the remote sensing data. Map of temporally aggregated Relative RMSE_log.

4. DISCUSSION

These results illustrate how different uses of a model (e.g. simulation of conditions within the model domain versus use of the same model to estimate exports across a boundary) may have different data requirements, highlighting in this instance, the importance of an appropriate ocean boundary condition.

While it is not clear to what extent the estimated sediment and nitrogen exports calculated by either the original method or with the assimilation of remotely sensed data near the outer boundary are accurate, it is clear that there is a high degree of uncertainty in these estimates. Despite this, the model facilitates estimation of materials fluxes at a time-scale not amenable to simple data-based methods, and can be used in conjunction with exports calculated on longer timescales through data-based methods to provide a more complete overall picture of how the system functions (Webster et al., 2006).

More generally, the results show that use of remotely sensed observational data to set boundary conditions for biogeochemical and sediment transport models is a promising approach, with the potential to improve both the models and our ability to interpret the practical significance of the satellite data.

Linear interpolation in time of satellite-observed concentrations at the model boundary, as applied here, does not take into account the large tidal movements of water in Keppel Bay. In future work, this may be addressed by combining satellite data with a hydrodynamic model at a larger spatial scale to set boundary conditions for the estuary-scale coupled model.

In a continuation of the work described in this paper, we are currently exploring with colleagues other avenues for assimilation of satellite observational data with the biogeochemical model and the sediment transport model. One avenue is the use of local optical measurements and remotely sensed light attenuation estimates to develop an improved model for light attenuation based on the specific optical characteristics of dissolved and particulate substances in Keppel Bay. A second is the use of satellite observations to supplement *in situ* data to improve calibration and parameterisation of the sediment model. A third approach is the direct assimilation of observational data, where available, across the model domain.

Assimilation of satellite observations with mechanistic models is likely to become increasingly important in the near future, as it combines the merits of both tools. While the satellite observations may provide reliable spatially resolved and temporally dense estimates of conditions in the field, well-designed models may offer a better picture of what is happening beneath the surface of the water, allow a more complete analysis of the importance of various different physical, biological and chemical processes in driving the system, and have the potential to be used in a predictive mode. Neither tool alone can fulfil all these functions, but used together, each may support the other.

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