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Evaluating the eReefs Great Barrier Reef marine model against observed emergent properties

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Abstract: The eReefs marine models simulate hydrodynamics, sediment dynamics, biogeochemistry and optical conditions in three dimensions on 1 km and 4 km grid scales across the whole Great Barrier Reef (GBR) Lagoon. The models are designed to support management of the Great Barrier Reef through operational provision of near real-time hydrodynamic, water quality and optical conditions over the reef, as well as supporting prognostic scenarios to facilitate catchment management policy. During development, the hydrodynamic and biogeochemical models were calibrated and validated against remotely sensed temperature, *in situ* measured physical properties, and *in situ* sampled dissolved and particulate nutrient species at sparsely distributed monitoring sites, most of which are located in near-shore waters along the length of the GBR Lagoon. A range of evaluation metrics provided a baseline degree of confidence in the model results. An additional level of confidence can be achieved by evaluating the model's performance in reproducing a range of system-scale *emergent properties*. These are large-scale patterns and relationships that are neither directly coded into the model nor used in model calibration – ideally, relationships that are not obvious from an inspection of the model algorithms, but arise from the complex system that these algorithms combine to create. This paper describes the evaluation of the 4 km grid-scale eReefs marine models against a range of emergent properties. Properties used in this evaluation included (a) the relationship between chlorophyll *a* concentrations and phytoplankton community size-structure; (b) the relationship between river discharge and annual mean photic depth on the mid- and outer-shelf; and (c) the relationship between flood-plume optical class and water quality. The results show good agreement across all three sets of emergent properties, enhancing confidence that the eReefs suite of process-based models is producing "the right results for the right reasons," correctly simulating a complex range of physical and biogeochemical processes across the Great Barrier Reef.

Keywords: *Model evaluation, emergent properties, Great Barrier Reef, phytoplankton community structure, photic depth*

1. INTRODUCTION

The eReefs marine models are a suite of three-dimensional hydrodynamic, sediment dynamic, optical and biogeochemical process models that provide near-real time and hindcast simulations of the 300,000 km^2 Great Barrier Reef Lagoon in three dimensions. The models and their evaluation against routine observational monitoring data and remote sensing observations have been described in detail by Herzfeld et al. (2016) and Baird et al. (2016a) The overall vision for eReefs was described by Chen et al. (2011) and the information architecture supporting the model and other data products have been described by Car (2013) and Yu et al. (2016). The modelling builds on earlier work that was confined to Keppel Bay (Margvelashvili et al., 2003, Robson et al., 2006, Webster et al., 2006, Webster et al., 2003), and includes significant model enhancements. The seagrass submodel is described by Baird et al. (2016b), the optical submodel by Baird et al. (2016c) and the *Trichodesmium* submodel, by Robson et al. (2013). Calibration of the sediment transport model is described by Margvelashvili et al. (2016). Application of the biogeochemical model to a study of ocean acidification in the Great Barrier Reef has been discussed by Mongin et al. (2016). Application of the optical model to detection of flood plumes is described by Baird et al. (submitted).

The models are increasingly being used as a tool by both scientists and managers of the Great Barrier Reef to facilitate better understanding of the system and reporting of conditions in the water. There is also work underway to use the models within a policy framework, to guide the setting of improved water quality targets (The State of Queensland, 2017) and to understand the likely impacts of improvements in catchment management on water quality and reef health. In the context of a critical decline in coral cover and reef health in recent years (Ainsworth et al., 2016, De'ath et al., 2012, Great Barrier Reef Marine Park Authority, 2017) and the enormous social, economic and conservation value of the Great Barrier Reef (O'Mahoney et al., 2017), it is essential to hold the models we use in managing this asset to the highest possible standard of evaluation, to fully understand the strengths and limitations of these models. The eReefs models have already been evaluated carefully against a range of traditional performance metrics calculated against time-series of *in situ* observational monitoring and remote sensing data, as well as *ad hoc* comparison of vertical and horizontal glider profiles (Herzfeld et al., 2016), but additional evaluation measures can build confidence that the models are not only matching historical observations, but also correctly representing the underlying processes.

A major advantage of process-based models such as those used in eReefs is that they should be able to predict not only features against which the model has been calibrated or trained, but also the process rates behind those features and emergent properties of complex system function (Robson, 2014). Recent innovative work in marine modelling has demonstrated the use of a range of emergent properties in evaluation of marine models, from the relationship between phytoplankton density and grazing rates (Anderson et al., 2010) to relationships between chlorophyll concentrations and phytoplankton community composition and nutrient stoichiometry (de Mora et al., 2016).

Here, we evaluate the eReefs biogeochemical and optical model products against three emergent properties: (a) the relationship between chlorophyll *a* and phytoplankton community size structure reported by Hirata et al. (2011); b) the relationship between annual river discharge and photic depth on the mid- and outer-shelf of the Great Barrier Reef reported by Fabricius et al. (2014) and Fabricius et al. (2016); and c) the observed water quality conditions in fronts of river flood plumes as identified from optical properties observable from satellites (Devlin et al., 2015).

2. METHODS

We accessed eReefs model outputs available via www.ereefs.info from the most recent biogeochemical model run (GBR4_H2p0_B2p0_Chyd_Dcrt). This provides a Jan 1, 2011 to Oct 20, 2016 simulation on a 4 km grid-scale, using version 2.0 of both the eReefs hydrodynamic and biogeochemical models forced with best available catchment loads (primarily derived from Source catchment models – for more detail, refer to www.ereefs.info).

For the phytoplankton community structure evaluation, 30,000 points in space and time were randomly sampled from a sub-surface layer of model output for the 15th day of each January, April, July, and October during the five-year simulation period for which model outputs are so far available (i.e. 2011 to 2016). At each of these points, the percent large phytoplankton (i.e. microphytoplankton, 4 x 10^{-6} µm radius) and the percent small phytoplankton (corresponding to pico- and nano-phytoplankton; 1 x 10^{-6} µm radius) were calculated, and plotted against modelled chlorophyll *a*.

For the photic depth versus river discharge evaluation, we adopted the region boundaries described by Fabricius et al. (2016) and calculated the mean estimated Secchi depth in each region over the course of each "water year" (defined by Fabricius et al. (2016) as 1 October to 30 September) from the simulated profiles of light attenuation at 490 nm using the relationship given by Lee et al. (2015) (i.e. Secchi depth = $1/Kd_{490}$). Annual discharge from the North Wet Tropics region was calculated as the sum of gauged flow from the Daintree, Barron, Mulgrave, Russell, North Johnstone, and South Johnstone Rivers plus 30% of the discharge from the Burdekin River, while annual discharge from the South Wet Tropics was taken as the sum of the discharge from the Mulgrave, Russell, North Johnstone, South Johnstone, Tully and Herbert Rivers, plus 50% of discharge from the Burdekin River, following Fabricius et al. (2016). At this time, we have not adjusted for ungauged catchment areas, so our estimated annual discharges are somewhat different from those reported by Fabricius et al. (2016).

For the flood-plume water quality characterisation, we used the optical model to classify flood plume classes from 2011-2014 wet-season model results, as described by Baird et al. (submitted), then randomly sampled 20,000 surface points with salinity<34 from each plume class.

3. RESULTS AND DISCUSSION

Simulated percent large and percent small phytoplankton shows a clear relationship with simulated total chlorophyll *a* from large and small phytoplankton combined, as shown in Figure 1. The relationship corresponds closely to the relationship observed by Hirata et al. (2011) from a global marine database.

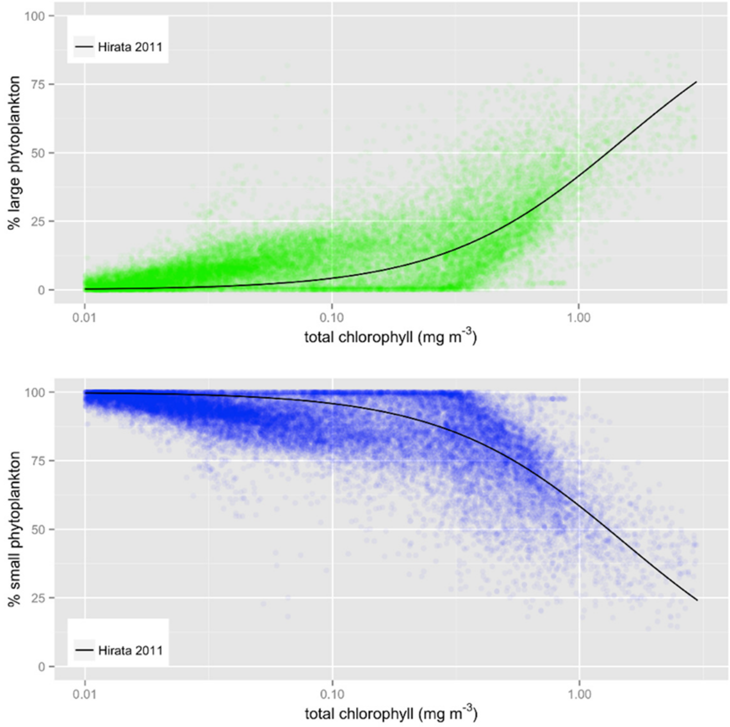

Figure 1. Relationship between phytoplankton size class and chlorophyll *a* concentration. Dots show 3000 randomly sampled points from the eReefs marine models. Lines indicated fits to observed data from a global database, taken from Hirata (2011). The "large" size class here refers to microphytoplankton (1 x10^{-6} µm radius in the model), while "small" encompasses pico- and nano-phytoplankton (4 x10^{-6} µm radius).

Annual mean modelled Secchi depth on the North and South Wet Tropics Mid Shelf and Outer Shelf is inversely correlated with annual river discharge (Figure 2), as reported by Fabricius et al. (2016). Where individual years deviated from the expected line, examination of modelled and satellite-observed flood plume paths provides an explanation: in 2012, for example, the Burdekin River plume dispersed to the East rather than to the North-East, as is more common, and hence had less influence on Wet Tropics Great Barrier Reef waters than would otherwise be expected (i.e. an influence equivalent to a smaller annual discharge with a more typical northward path from the mouth of the Burdekin). Model results show higher estimated Secchi depth in low discharge years than the remotely sensed photic depth estimates reported by Fabricius et al. (2016), particularly in the South Wet Tropics. This may be due to the difference in algorithm used to estimate photic depth, or to model or observational errors. Also potentially important is the difference in time of day – model output is provided at midday, when solar zenith is near its maximum, while the Fabricius et al. (2016) results are calculated from MODIS observations, typically made at around 10 a.m., when solar zenith is lower, which will produce lower photic depths. The model indicates that the increased light attenuation in the outer shelf regions following high-flow wet seasons is primarily due to chlorophyll rather than sediments.

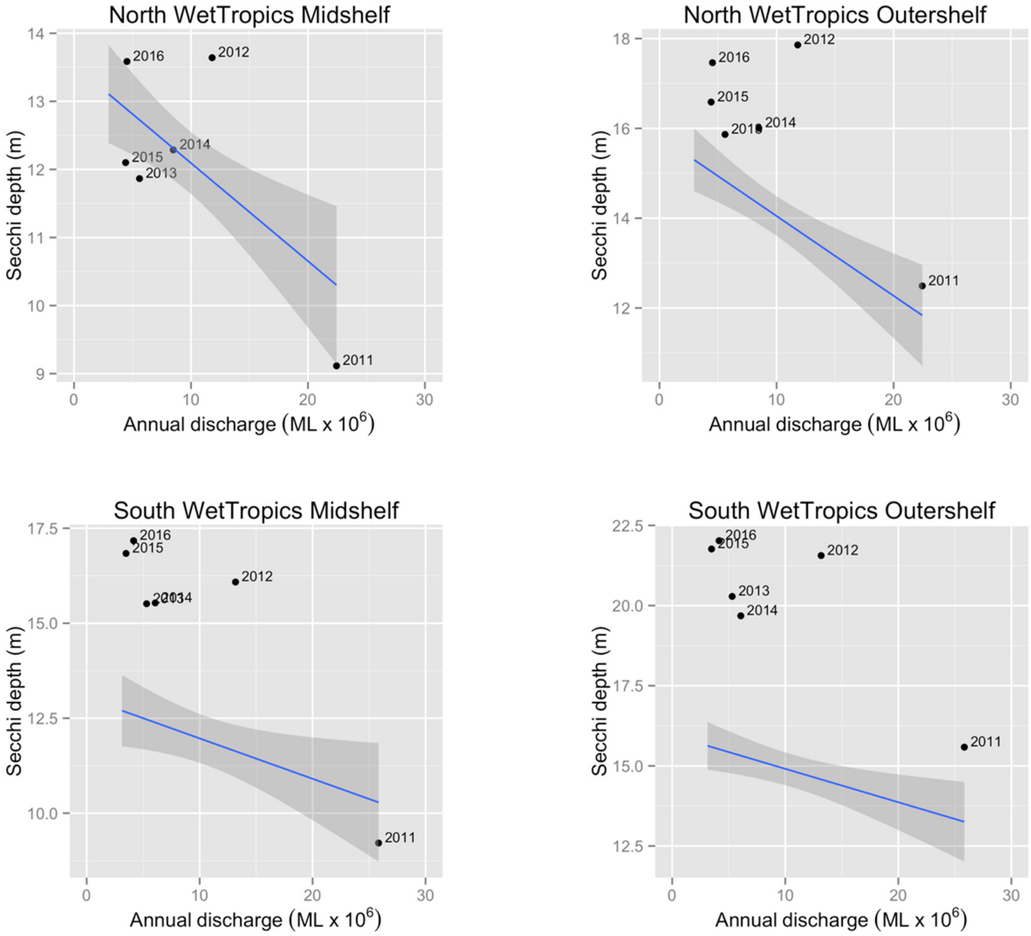

Figure 2. Relationship between North and South Wet Tropics gauged river discharge and modelled mean annual photic depth in the North and South Wet Tropics Mid-shelf and Outer-shelf regions (region boundaries as defined by Fabricius et al. (2016)). Blue lines and shaded regions show a linear best fit (with confidence interval) to the photic depth estimates for 2002 to 2013 reported by Fabricius et al. (2016) (digitised from original figures and replotted against our discharge estimates).

Figure 3 and Figure 4 allow comparison of *in situ* observed water quality in Great Barrier Reef flood plumes (Devlin et al., 2015) with modelled wet-season flood-plume water quality. The model shows that water quality conditions within flood plumes are highly variable, and the full range of variability may not be entirely captured by the (relatively sparse) marine monitoring data. In general, the observed range and distribution of dissolved inorganic nitrogen and phosphorus, suspended sediment concentrations, chlorophyll *a* and light attenuation in modelled flood plumes correspond well to those observed in the marine monitoring program, bearing in mind that flood plume extents and conditions vary from year to year. Dissolved inorganic nitrogen and phosphorus concentrations in the modelled flood plumes appear to be a little lower than typically observed, with a faster decline from concentrations in plume class 1 (near the mouths of rivers) towards marine conditions. Alongside limitations of the marine models such as dilution by the 4 km model grid, this may be due to the limitations of the river load data used as boundary conditions, or may be an artefact of sampling and filtration methods in the marine monitoring program.

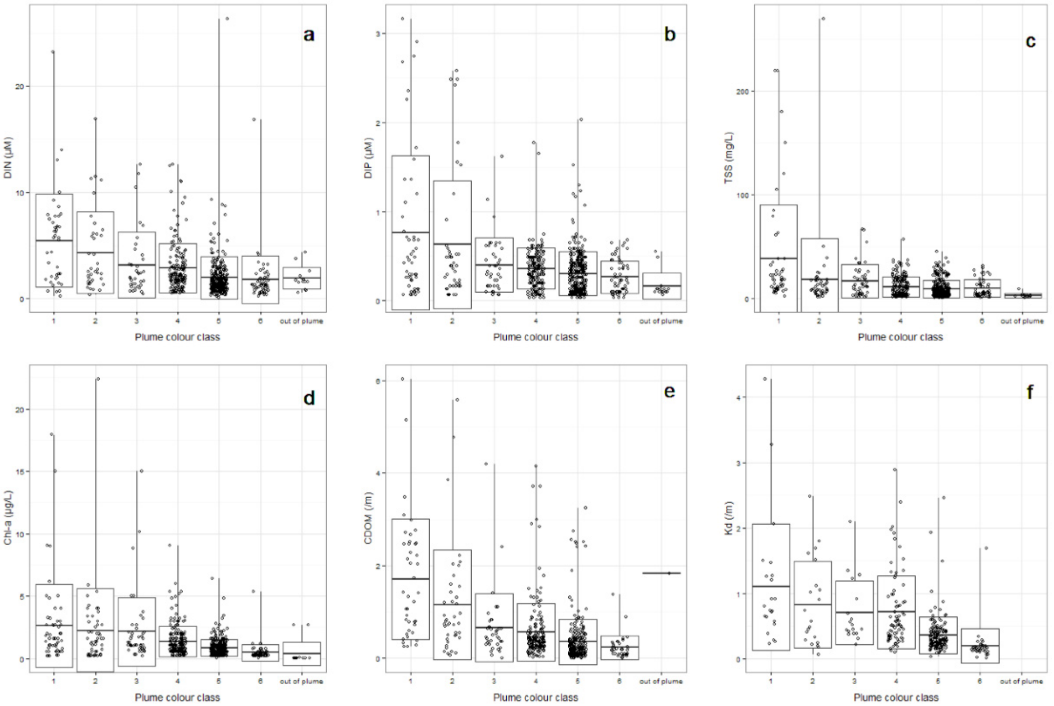

Figure 3. Properties of Great Barrier Reef flood plumes sampled *in situ* between 2007 and 2015, grouped by optical plume class detected from MODIS satellite images. (a) Dissolved Inorganic Nitrogen, DIN (µM) and (b) Dissolved Inorganic Phosphorus, DIP (µM), the three main optical attenuating components of (c) TSS (mg/L), (d) chlorophyll-a (mg/m^3), (e) CDOM (m^{-1}), and (f) light attenuation (Kd, m^{-1}). From Devlin et al. (2015), reproduced under the Creative Commons Attribution 4.0 International License. Box plots show the 25th, 50th and 75th percentiles of observations (shown as points, with jitter applied so that individual points can be distinguished). Lines show the complete range of observations.

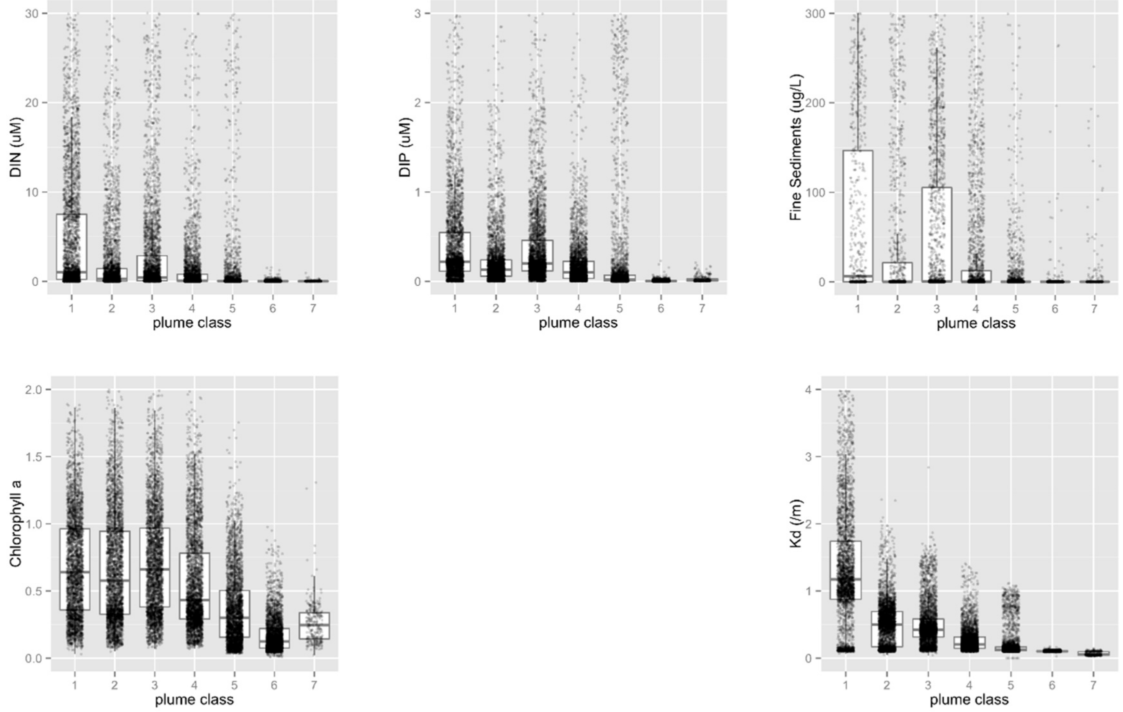

Figure 4. Properties of Great Barrier Reef flood plumes simulated by the eReefs marine models, 2011-2014. (CDOM is not directly simulated by the models). Box plots as described for Figure 3.

Similarly, chlorophyll *a* concentrations in modelled flood plumes appear a little lower than observed. This may be due to the use of phytoplankton groups in the model that are calibrated to the dominant marine conditions. In reality, flood-plume waters may include freshwater or euryhaline phytoplankton species.

4. CONCLUSIONS AND RECOMMENDATIONS

Evaluation of the eReefs models using a range of emergent properties provides an additional level of confidence in the performance of the models and their ability to simulate processes and conditions that are relevant to management and policy for the Great Barrier Reef. For the three emergent properties considered here, the eReefs models generally perform well, indicating that they are correctly representing the underlying processes that produce these larger, emergent patterns. Initial analyses of a 1 km grid-scale version of the biogeochemical model indicate that these properties persist with the finer grid-scale, with improved model performance.

We recommend that evaluation against emergent properties and large-scale system patterns be more widely adopted for process-based environmental models. Relevant emergent properties can be identified in collaboration with observational scientists working with the system of interest.

The approach used to assess the multi-dimensional properties of the model to data derived from observational or time-series monitoring programs may be of interest to other research groups.

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