

Dear Dr. Hargraves,

Thank you again for editing this manuscript. I have amended the manuscript, this time highlighting the edits of this round in red, which are almost exclusively in the Model Evaluation section. The blue highlights from the last round of edits are still highlighted. Below I reply to your comment in dark green, and my reply in black.

Yours sincerely,

A handwritten signature in black ink that reads "Mark Baird". The signature is written in a cursive, slightly slanted style.

Mark Baird

Good progress is being made, but this paper doesn't yet meet the standard for a GMD paper.

Thank you.

Model description papers need to contain sufficient evaluation to show that the model behaves as expected, and the evidence must be comprehensible to those outside of the group of people developing the model.

I have significantly improved the Model Evaluation section.

The part of the model equations that will be least familiar to marine BGC modellers will be the equations for microalgae growth and chlorophyll synthesis. For many in the community these will also be the most important component, since while the benthic component of BGC models vary between groups due to different habitats, all marine BGC models include the plankton.

As a result, I have included a new section "11.1 Analysis of microalgae growth and pigment synthesis dynamics". The analysis considers the common question challenge of marine BGC modellers of capturing the changing physiological response of microalgae with depth and cell size. The analysis adds a new figure and 35 lines of text, showing the model conforms to the classic understanding of the phenomena and assists the reader to understand the unique aspects of the model.

In this case the evaluation is performed with reference to previous evaluations of previous model versions or parts of the same model. This is an acceptable approach. However, the evaluation needs to be presented in a form that is useful to readers outside of the EMS model development community. This means that much more description and explanation of the results is required in the main manuscript (as suggested by the reviewer), with essential plots being brought from the supplement into the main manuscript.

In addition to highlighting the chlorophyll dynamics as found in the earlier submission, I have now included both nutrient (phosphorus, nitrate and ammonium) and carbon chemistry dynamics. I have also expanded the explanation of the model evaluation to give better understanding of the skill metrics and explanation of the differing performance of elements of the model.

Thank you.

# CSIRO Environmental Modelling Suite (EMS): Scientific description of the optical and biogeochemical models (vB3p0).

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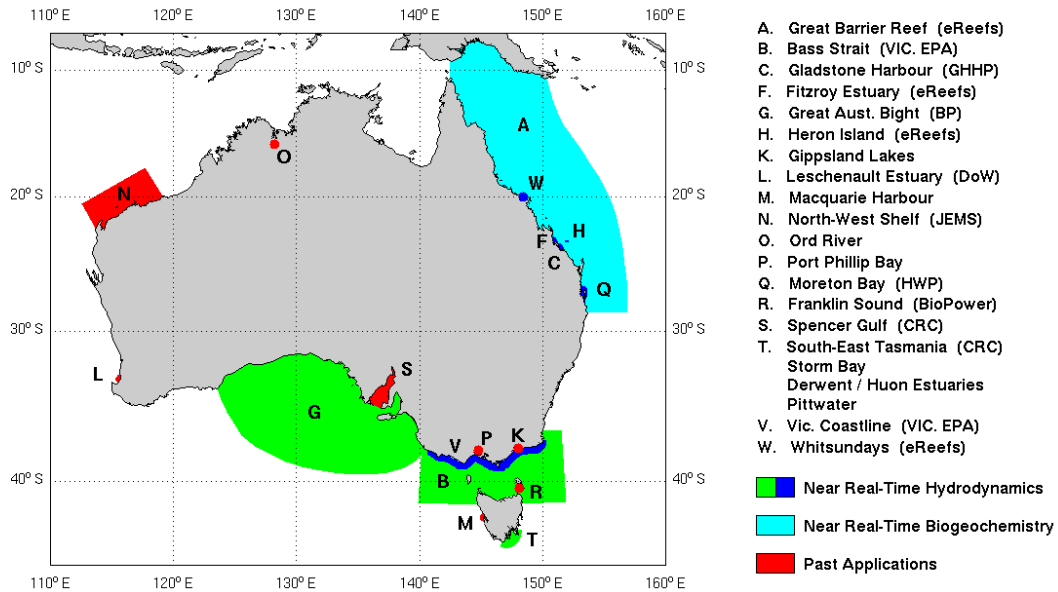
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## Abstract.

Since the mid 1990s, Australia's Commonwealth Science Industry and Research Organisation (CSIRO) has developed a biogeochemical (BGC) model for coupling with a hydrodynamic and sediment model for application in estuaries, coastal waters and shelf seas. The suite of coupled models is referred to as the CSIRO Environmental Modelling Suite (EMS) and has been applied at tens of locations around the Australian continent. At a mature point in the BGC model's development, this paper presents a full mathematical description, as well as links to the freely available code and User Guide. The mathematical description is structured into processes so that the details of new parameterisations can be easily identified, along with their derivation. In the EMS the underwater light field is simulated by a spectrally-resolved optical model that calculates vertical light attenuation from the scattering and absorption of 20+ optically-active constituents. The BGC model itself cycles carbon, nitrogen, phosphorous and oxygen through multiple phytoplankton, zooplankton, detritus and dissolved organic and inorganic forms in multiple water column and sediment layers. The water column is dynamically coupled to the sediment to resolve deposition, resuspension and benthic-pelagic biogeochemical fluxes. With a focus on shallow waters, the model also includes particularly-detailed representations of benthic plants such as seagrass, macroalgae and coral polyps. A second focus has been on, where possible, the use of geometric derivations of physical limits to constrain ecological rates, which generally requires population-based rates to be derived from initially considering the size and shape of individuals. For example, zooplankton grazing considers encounter rates of one predator on a prey field based on summing relative motion of the predator with the prey individuals and the search area; chlorophyll synthesis includes a geometrically-derived self-shading term; and the bottom coverage of benthic plants is calculated from their biomass using an exponential form derived from geometric arguments. This geometric approach has led to a more algebraically-complicated set of equations when compared to more empirical biogeo-

## COASTAL ENVIRONMENTAL MODELLING TEAM



**Figure 1.** Model domains of the CSIRO EMS hydrodynamic and biogeochemical applications from 1996 onwards. Additionally, EMS was used for the nation-wide Simple Estuarine Response Model (SERM) that was applied generically around Australia's 1000+ estuaries (Baird et al., 2003). Brackets refer to specific funding bodies. EMS has also been applied in the Los Lagos region of Chile. A full list of past and current applications and funding bodies is available at: <https://research.csiro.au/cem/projects/>.

chemical model formulations. But while being algebraically-complicated, the model has fewer unconstrained parameters and is therefore simpler to move between applications than it would otherwise be. The version of EMS described here is implemented in the eReefs project that is delivering a near real time coupled hydrodynamic, sediment and biogeochemical simulation of the Great Barrier Reef, northeast Australia, and its formulation provides an example of the application of geometric reasoning in the formulation of aquatic ecological processes.

**Keywords.** Great Barrier Reef, mechanistic model, geometric derivation

## 1 Introduction

The first model of marine biogeochemistry was developed more than 70 years ago to explain phytoplankton blooms (Riley, 1947). Today the modelling of estuarine, coastal and global biogeochemical systems has been used for a wide variety of

applications including coastal eutrophication (Madden and Kemp, 1996; Baird et al., 2003), shelf carbon and nutrient dynamics (Yool and Fasham, 2001; Dietze et al., 2009), plankton ecosystem diversity (Follows et al., 2007), ocean acidification (Orr et al., 2005), impact of local developments such as fish farms and sewerage treatment plants (Wild-Allen et al., 2010), fishery production (Stock et al., 2008) and operational forecasting (Fennel et al., 2019), to name a few. As a result of these varied applications, a diverse range of biogeochemical models have emerged, with some models developed over decades and being capable of investigating a suite of biogeochemical phenomena (Butenschön et al., 2016). With model capabilities typically dependent on the history of applications for which a particular model has been funded, and perhaps even the backgrounds and interests of the developers themselves, significant differences exist between models. Thus it is vital that biogeochemical models are accurately described in full (e.g. Butenschön et al. (2016); Aumont et al. (2015) and Dutkiewicz et al. (2015)), so that model differences can be understood, and, where useful, innovations shared between modelling teams.

Estuarine, coastal and shelf modelling projects undertaken over the past 20+ years by Australia's national science agency, the Commonwealth Science Industry and Research Organisation (CSIRO), have led to the development of the CSIRO Environmental Modelling Suite (EMS). EMS contains a suite of hydrodynamic, transport, sediment, optical and biogeochemical models that can be run coupled or sequentially. The EMS biogeochemical model, the subject of this paper, has been applied around the Australian coastline (Fig. 1) leading to characteristics of the model which have been tailored to the Australian environment and its challenges.

Australian shelf waters range from tropical to temperate, micro- to macro-tidal, with shallow waters containing coral, seagrass or algae-dominated benthic communities. With generally narrow continental shelves, and being surrounded by two poleward-flowing boundary currents (Thompson et al., 2009), primary production in Australian coastal environments is generally limited by dissolved nitrogen in marine environments, phosphorus in freshwaters, and unlimited by silica and iron. The episodic nature of rainfall on the Australian continent, especially in the tropics, and a lack of snow cover, delivers intermittent but occasionally extreme river flows to coastal waters. With a low population density, continent-wide levels of human impacts are small relative to other continents, but can be significant locally, often due to large isolated developments such as dams, irrigation schemes, mines and ports. Global changes such as ocean warming and acidification affect all regions. The EMS BGC model has many structural features similar to other models (e.g. multiple plankton functional types, nutrient and detrital pools, an increasing emphasis on optical and carbon chemistry components). Nonetheless, the geographical characteristics of, and anthropogenic influences on, the Australian continent have shaped the development of EMS, and led to a BGC model with many unique features.

As the national science body, CSIRO needed to develop a numerical modelling system that could be deployed across the broad range of Australian coastal environments and capable of resolving multiple anthropogenic impacts. With a long coastline (60,000+ km by one measure), containing over 1000 estuaries, an Australian-wide configuration has insufficient resolution to be used for many applied environmental challenges. Thus, in 1999, the EMS biogeochemical model development was targeted to increase its applicability across a range of ecosystems. In particular, given limited resources to model a large number of environments / ecosystems, developments aimed to minimise the need for re-parameterisation of biogeochemical processes for each application. Two innovations arose from this imperative: 1. the software development of a process-based modelling

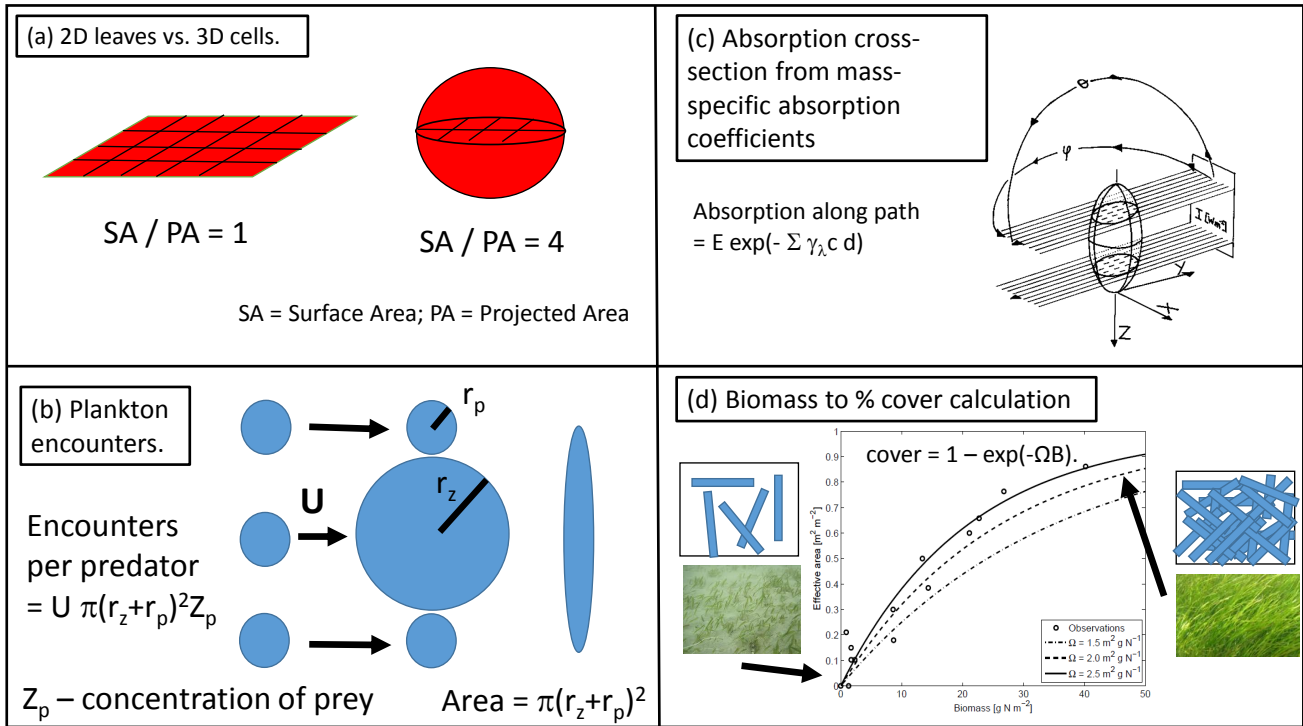
architecture, such that processes could be included, or excluded, while using the same executable file; and 2. the use, where possible, of geometric descriptions of physical limits to ecological processes as a means of reducing parameter uncertainty (Baird et al., 2003). It is the use of these geometric descriptions that has led to the greatest differences between EMS and other aquatic biogeochemical models.

5 In the aquatic sciences there has been a long history of experimental and process studies that use geometric arguments to quantify ecological processes, but these derivations have rarely been applied in biogeochemical models, with notable exceptions (microalgal light absorption and plankton sinking rates generally, surface area to volume considerations (Reynolds, 1984), size-focused trait-based modelling (Litchman and Klausmeier, 2008)). By prioritising geometric arguments, EMS has included a number of previously-published geometric forms including diffusion limitation of microalgae nutrient uptake (Hill  
10 and Whittingham, 1955), absorption cross-sections of microalgae (Fig. 2C, Duysens (1956); Kirk (1975); Morel and Bricaud (1981)), diffusion limits to macroalgae and coral nutrient uptake (Munk and Riley, 1952; Atkinson and Bilger, 1992; Zhang et al., 2011), and encounter-rate limitation of grazing rates (Fig. 2B, Jackson (1995)).

Perhaps the most important consequence of using geometric constraints in the BGC model is the representation of benthic flora as two dimensional surfaces, while plankton are represented as three dimensional suspended objects (Baird et al., 2003).  
15 Thus leafy benthic plants such as macroalgae take up nutrients and absorb light on a 2D surface. In contrast, nutrient uptake to microalgae occurs through a 3D field while light uptake of the 3D cell is limited by the 2D projected area (Fig. 2A). These contrasting geometric properties, from which the model equations are derived, generates greater potential light absorption relative to nutrient uptake of benthic communities relative to the same potential light absorption relative to nutrient uptake in unicellular algae (Baird et al., 2004). In the most simple terms, this can be related to the surface area to projected area of a  
20 leaf being 1/4 times that of a microalgae cell (Fig. 2A). Thus the competition for nutrients, ultimately being driven by light absorption and its rate compared to nutrient uptake, is explicitly determined by the contrasting geometries of cells and leaves.

In addition to geometric constraints derived by others, a number of novel geometric descriptions have been introduced into the EMS BGC model, including:

1. Geometric derivation of the relationship between biomass,  $B$ , and fraction of the bottom covered,  $A_{eff} = 1 - \exp(-\Omega B)$ ,  
25 where  $\Omega$  is the nitrogen-specific leaf area (Sec. 6).
2. Impact of self-shading on chlorophyll synthesis quantified by the incremental increase in absorption with the increase in pigment content (Sec. 5.1.3).
3. Mass-specific absorption coefficients of photosynthetic pigments have been better utilised to determine phytoplankton absorption cross-sections (Duysens, 1956; Kirk, 1975; Morel and Bricaud, 1981) through the availability of a library of  
30 mass-specific absorption coefficients (Clementson and Wojtasiewicz, 2019), and their wavelength correction using the refractive index of the solvent used in the laboratory determinations (Fig. 5).
4. The space-limitation of zooxanthellae within coral polyps using zooxanthellae projected areas in a two layer gastrodermal cell anatomy (Sec. 6.3.1).



**Figure 2.** Examples of geometric descriptions of ecological processes. (a) The relative difference in the 2D experience to nutrient and light fields of leaves compared to the 3D experience of cells, as typified by the ratio of surface area (coloured) to projected area (hashed area); (b) The encounter rate of prey per individual predator as a function of the radius of encounter (the sum the predator and prey radii) and the relative motion and prey concentration following Jackson (1995); (c) The use of ray tracing and the mass-specific absorption coefficient to calculate an absorption cross section for a randomly oriented spheroid following (Kirk, 1975); (d) Fraction of the bottom covered as seen from above as a result of increasing the number of randomly placed leaves (Baird et al., 2016a). Based on the assumption that leaves are randomly placed, the cover reaches  $1 - \exp(-1) = 0.63$  when the sum of the shaded areas induced by all individual leaves equals the ground area (i.e. a Leaf Area Index of 1).

5. Preferential ammonium uptake, which is often calculated using different half-saturation coefficients of nitrate and ammonium uptake (Lee et al., 2002), is determined by allowing ammonium uptake to proceed up to the diffusion limit. Should this diffusion limit not meet the required demand, nitrate uptake supplements the ammonium uptake. This representation has the benefit that no additional parameters are required to assign preference, with the same approach applied for both microalgae and benthic plants (Sec. 9.1).

To be clear, these geometric definitions have their own set of assumptions (e.g. a single cell size for a population), and simplifications (e.g. spherical shape). Nonetheless, the effort to apply geometric descriptions of physical limits across the BGC

model appears to have been beneficial, as measured by the minimal amount of re-parameterisation that has been required to apply the model to contrasting environments. Of the above mentioned new formulations, the most useful and easily applied is the bottom cover calculation (Fig. 2D). In fact it is so simple, and such a clear improvement on empirical forms as demonstrated in Baird et al. (2016a), that it is likely to have been applied in other ecological / biogeochemical models, although we are  
5 unaware of any other implementation.

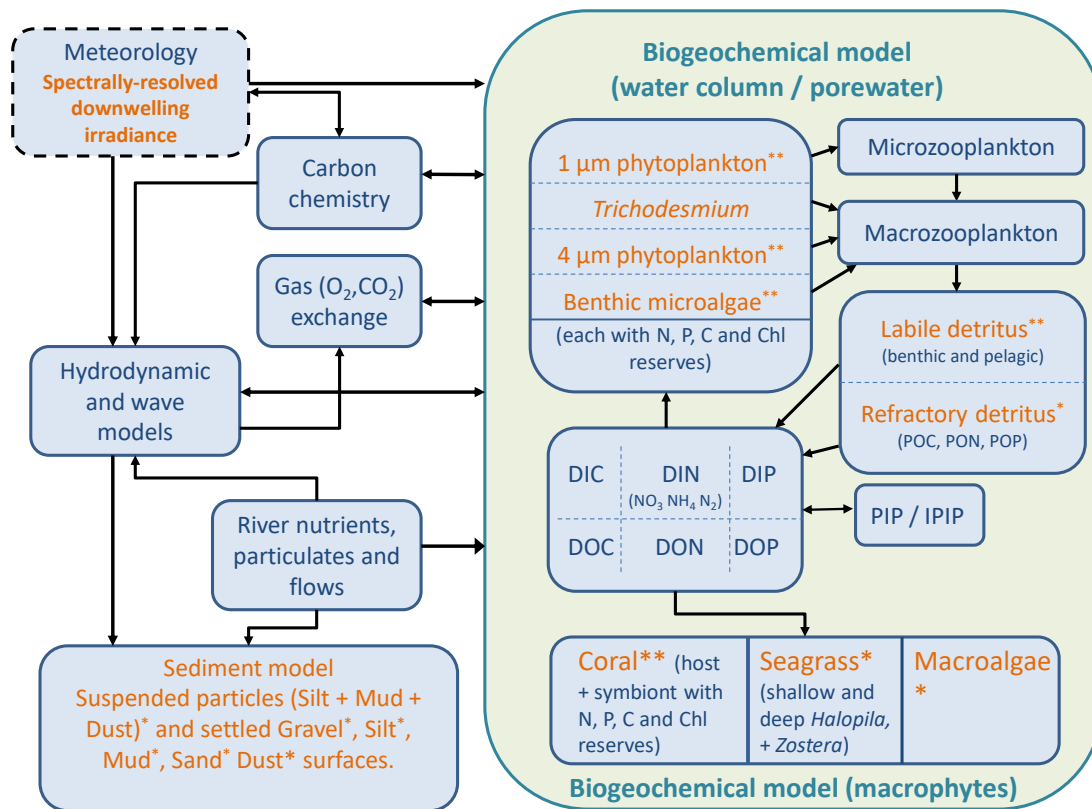
The geometrically-constrained relationship between bottom cover and seagrass biomass,  $B$ , is  $\text{cover} = 1 - \exp(-\Omega B)$  and can be used to illustrate how geometric arguments can produce model equations with tightly-constrained parameters. This geometric relationship contains only one parameter,  $\Omega$ , that is the initial slope between cover and biomass. At low biomass there is no overlapping of leaves, so the  $\Omega$  is the area of leaves per unit of biomass (or nitrogen-specific leaf area), and has been  
10 determined by many authors on hundreds of types of seagrass. Comparison with data is shown in Appendix A of Baird et al. (2016a) and Fig. 2D. Thus by using geometric arguments in developing the equation, the form contains only one parameter which has a physical meaning that is tightly constrained.

In addition to using geometric descriptions, there are a few other features unique to the EMS BGC model including:

1. Calculation of scalar irradiance from downwelling irradiance, vertical attenuation and a photon balance within a layer  
15 (Sec. 4.1.2).
2. An oxygen balance achieved through use of biological and chemical oxygen demand tracers (Sec. 10.3.2).
3. The stoichiometric link of excess photons to reactive oxygen production in zooxanthallae.

## 1.1 Manuscript outline

20 This document provides a summary of the biogeochemical processes included in the model (Sec. 2), a summary of the transport model that integrates the advection-diffusion and sinking terms (Sec. 3), and full descriptions of the optical (Sec. 4) and ecological (Sec. 5 - Sec. 10) model equations. The description of both the optical and biogeochemical models is divided into the primary environmental zones: pelagic, epibenthic and sediment, as well as processes that are common to all zones. Sec. 9 details parameterisations that are common across numerous ecological processes, such as temperature dependence, and  
25 Sec. 10 provides details of the numerical integration techniques. Further sections detail the model evaluation (Sec. 11), code availability (Sec. 12) and test case generation (Sec. 13). The Discussion (Sec. 14) details how past and present applications have influenced the development of the EMS BGC model, and anticipates some future developments. Finally, the Supplementary Material provides a tables of processes, state variables and parameters, with both mathematical and numerical code details, and additional model evaluation from the Great Barrier Reef configuration.



**Figure 3.** Schematic of CSIRO Environmental Modelling Suite, illustrating the biogeochemical processes in the water column, epipelagic and sediment zones, as well as the carbon chemistry and gas exchange used in vB3p0 for the Great Barrier Reef application. Orange labels represent components that scatter or absorb light.

## 2 Overview of the EMS optical and biogeochemical models

The optical model undertakes calculations at distinct wavelengths of light (say 395, 405, 415, ... 705 nm) representative of individual wavebands (say 400-410, 410-420 nm etc.) of the vertically-resolved downwelling and scalar irradiance that are used by the biogeochemical model to drive photosynthesis. The optical model includes the effect of Earth-Sun distance, sun angle, surface albedo and refraction on the downwelling surface irradiance. In the water column, the model attenuates light based on the spectrally-resolved total absorption and scattering of microalgae, detritus, dissolved organic matter, inorganic particles and the water itself (Fig. 3). The light reaching the bottom is further attenuated by macroalgae, seagrass, corals and benthic microalgae.

The biogeochemical model is organised into 3 zones: pelagic, epibenthic and sediment. Depending on the grid formulation the pelagic zone may have one or several layers of similar or varying thickness. The epibenthic zone overlaps with the lowest



pelagic layer and the top sediment layer and shares the same dissolved and suspended particulate material fields. The sediment is modelled in multiple layers with a thin layer of easily resuspendable material overlying thicker layers of more consolidated sediment.

5 Dissolved and particulate biogeochemical tracers are advected and diffused throughout the model domain in an identical fashion to temperature and salinity. Additionally, biogeochemical particulate substances sink and are resuspended in the same way as sediment particles. Biogeochemical processes are organized into pelagic processes of phytoplankton and zooplankton growth and mortality, detritus remineralisation and fluxes of dissolved oxygen, nitrogen and phosphorus; epibenthic processes of growth and mortality of macroalgae, seagrass and corals, and sediment based processes of plankton mortality, microphyto-

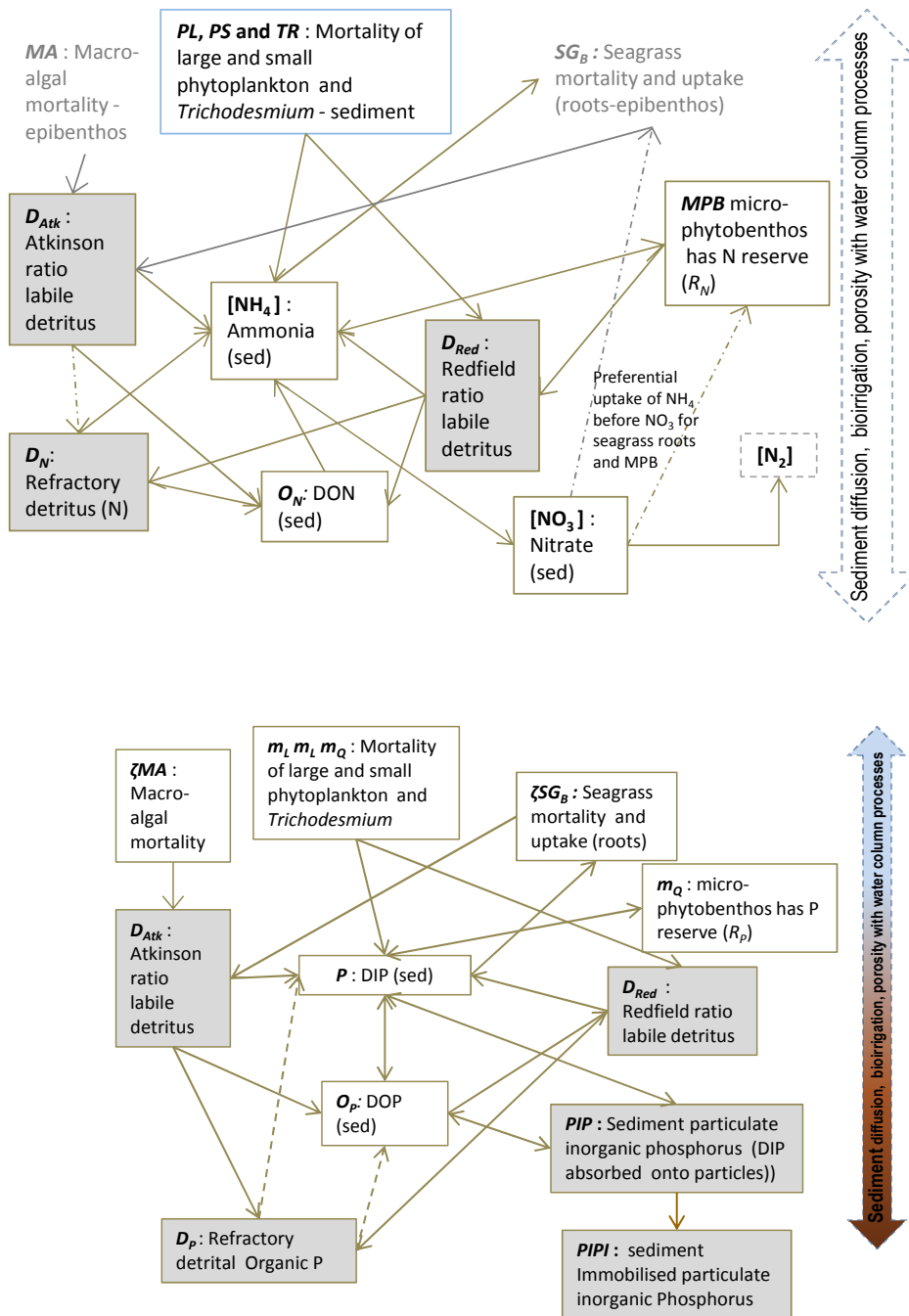
10 The biogeochemical model considers four groups of microalgae (small and large phytoplankton representing the functionality of photosynthetic cyanobacteria and diatoms respectively, microphytobenthos and *Trichodesmium*), four macrophytes types (seagrass types corresponding to *Zostera*, *Halophila*, deep *Halophila* and macroalgae) and coral communities. For temperate system applications of the EMS, dinoflagellates, *Nodularia* and multiple macroalgal species have also been characterised (Wild-Allen et al., 2013; Hadley et al., 2015a)

15 Photosynthetic growth is determined by concentrations of dissolved nutrients (nitrogen and phosphate) and photosynthetically active radiation. Autotrophs take up dissolved ammonium, nitrate, phosphate and inorganic carbon. Microalgae incorporate carbon (C), nitrogen (N) and phosphorus (P) at the Redfield ratio (106C:16N:1P) while macrophytes do so at the Atkinson ratio (550C:30N:1P). Microalgae contain two pigments (chlorophyll *a* and an accessory pigment), and have variable carbon:pigment ratios determined using a photoadaptation model.

20 Micro- and meso-zooplankton graze on small and large phytoplankton respectively, at rates determined by particle encounter rates and maximum ingestion rates. Additionally large zooplankton consume small zooplankton. Of the grazed material that is not incorporated into zooplankton biomass, half is released as dissolved and particulate carbon, nitrogen and phosphate, with the remainder forming detritus. Additional detritus accumulates by mortality. Detritus and dissolved organic substances are remineralised into inorganic carbon, nitrogen and phosphate with labile detritus transformed most rapidly (days), refractory  
25 detritus slower (months) and dissolved organic material transformed over the longest timescales (years). The production (by photosynthesis) and consumption (by respiration and remineralisation) of dissolved oxygen is also included in the model and depending on prevailing concentrations, facilitates or inhibits the oxidation of ammonium to nitrate and its subsequent denitrification to di-nitrogen gas which is then lost from the system.

30 Additional water column chemistry calculations are undertaken to solve for the equilibrium carbon chemistry ion concentrations necessary to undertake ocean acidification (OA) studies, and to consider sea-air fluxes of oxygen and carbon dioxide. The adsorption and desorption of phosphorus onto inorganic particles as a function of the oxic state of the water is also considered.

In the sediment porewaters, similar remineralisation processes occur as in the water column (Fig. 4). Additionally, nitrogen is denitrified and lost as N<sub>2</sub> gas while phosphorus can become adsorbed onto inorganic particles, and become permanently immobilised in sediments.



**Figure 4.** Schematic of sediment nitrogen and phosphorus pools and fluxes. Processes represented include phytoplankton mortality, detrital decomposition, denitrification (nitrogen only), phosphorus adsorption (phosphorus only) and microphytobenthic growth.

## 2.1 Structure of the model description

The biogeochemical model presented in this paper is process-based. That is, the rate of change of each ecological state variable is determined by a mathematical representation of each process that moves mass between one variable and another, conserving total mass. For dissolved inorganic phosphorus, the equation in the bottom water column layer (excluding advection, diffusion and particle sinking) could be written as:

$$\begin{aligned} \frac{dP}{dt} = & - \sum^4 \text{microalgae uptake} - \sum^3 \text{seagrass uptake} - \text{macroalgae uptake} - \text{zooxanthallae uptake} \\ & - \text{water column / sediment porewater exchange} - \text{phosphorus adsorption/desorption} \\ & + \sum^4 \text{microalgae respiration} + \sum^3 \text{seagrass respiration} + \text{macroalgae respiration} + \text{zooxanthallae respiration} \\ & + \sum^2 \text{zooplankton sloppy feeding} + \sum^2 \text{zooplankton respiration} + \text{remineralisation of labile detritus} \\ & + \text{remineralisation of refractory detritus} + \text{remineralisation of dissolved organic matter} \end{aligned}$$

As the number of processes in the model has grown, the representation of all the terms affecting one variables has become unworkable. Thus, instead of presenting the full equation for each state variable, we present the full set of equations for each process.

### 2.1.1 Presentation of process equations

In Sec. 5 - Sec. 10 descriptions are sorted by processes, such as microalgae growth, coral growth, food web interactions. This organisation allows the model to be explained, with individual notation, in self-contained chunks. For each process the complete set of model equations, parameter values and state variables are given in tables. Within each process the equations are required to conserve mass of oxygen, carbon, nitrogen and phosphorus. Furthermore each process description is independent of any other processes in the model. As the code itself allows the inclusion / exclusion of processes at runtime, the process-based structuring of the scientific description aligns with the architecture of the numerical code.

### 2.1.2 Model stoichiometry

The model contains state variables that quantify the mass of carbon, nitrogen, phosphorus and oxygen, as well as state variables that contain stoichiometrically-constant combinations of carbon, nitrogen, phosphorus (O:C:N:P of 110:106:16:1 for plankton and animals; 554:550:30:1 for benthic plants). While a number of state variables and parameters are specified in units of nitrogen, the model could equally be specified by carbon or phosphorus. Furthermore, while the structural material of microalgae (including benthic microalgae and zooxanthallae) is at the Redfield ratio, changing reserves in microalgae of fixed carbon, nitrogen and phosphorus mean that the microalgae have a variable stoichiometry. Furthermore, the model has separate state variables for refractory detrital carbon, nitrogen and phosphorus, meaning detritus also has a variable stoichiometry. As ex-

plained later, we also represent stoichiometric coefficients in the model equations as integers, a simple approximation to make the mathematical equations easier to read.

### 3 Transport model

The local rate of change of concentration of each dissolved and particulate constituent,  $C$ , contains sink/source terms,  $S_C$ , which are described in length in this document, and the advection, diffusion and sinking terms:

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla^2 C = \nabla \cdot (K \nabla C) + w_{sink} \frac{\partial C}{\partial z} + S_C \quad (1)$$

where the symbol  $\nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$ ,  $\mathbf{v}$  is the velocity field,  $K$  is the eddy diffusion coefficient which varies in space and time, and  $w_C$  is the local sinking rate (positive downwards) and the  $z$  co-ordinate is positive upwards. The calculation of  $\mathbf{v}$  and  $K$  is described in the hydrodynamic model (Herzfeld, 2006; Gillibrand and Herzfeld, 2016). The advection-diffusion terms of Eq. 1, based on the continuum hypothesis for a fluid (Vichi et al., 2007), are solved by either an in-line advection scheme with the baroclinic timestep of the hydrodynamic model, or an offline transport scheme using a potentially much longer timestep (Gillibrand and Herzfeld, 2016). Options for advection and transport schemes in EMS include mass conservative Lagrangian and flux-form approaches described in Herzfeld (2006) and Gillibrand and Herzfeld (2016).

The microalgae are particulates that contain internal concentrations of dissolved nutrients (C, N, P) and pigments that are specified on a per cell basis. To conserve mass, the local rate of change of the concentration of microalgae,  $B$ , multiplied by the content of the cell,  $R$ , is given by:

$$\frac{\partial(BR)}{\partial t} + \mathbf{v} \cdot \nabla^2 (BR) = \nabla \cdot (K \nabla (BR)) + w_C \frac{\partial(BR)}{\partial z} + S_{BR} \quad (2)$$

For more information see Sec. 5.1.6 and Sec. 3.1 of Baird et al. (2004) which describes the coupling of the plankton component of the biogeochemical model to the Princeton Ocean Model.

### 4 Optical model

The optical model calculates the spectrally-resolved light field in each vertical column and uses it to drive the photosynthesis of phytoplankton and benthic plants in the biogeochemical model. Following the terminology of aquatic optics (Mobley, 1994), we divide the description of the model into calculations of inherent optical properties (IOPs) followed by apparent optical properties (AOPs). IOPs are properties of the medium (e.g. scattering and absorption) and do not depend on the ambient light field. The optical model uses the value of the optically-active state variables, and their mass-specific absorption and scattering properties, to calculate the total absorption and scattering. AOPs are those properties that depend both on the medium (the IOPs) and on the surface light field (e.g. downwelling and scalar irradiance). Thus the optical model uses the vertical distribution of IOPs, and the surface light field, to determine the vertical distribution of the AOPs.

## 4.1 Water column optical model

### 4.1.1 Inherent optical properties (IOPs)

*Phytoplankton absorption.* The model contains 4 phytoplankton types (small and large phytoplankton, benthic mircoalgae and *Trichodesmium*), each with a unique ratio of internal concentration of accessory photosynthetic pigments to chlorophyll-*a*. To calculate the absorption due to each pigment, we use a database of spectrally-resolved mass-specific absorption coefficients (Clementson and Wojtasiewicz, 2019). As it can be assumed that accessory pigments stay in a constant ratio to chlorophyll-*a*, the model needs only a state variable for chlorophyll-*a* for each phytoplankton type. The model then calculates the chlorophyll-*a* specific absorption coefficient due to all pigments by using the Chl-*a* state variable, the ratio of concentration of the accessory pigment to chlorophyll-*a*, and the mass-specific absorption coefficient of each of the accessory pigments. Thus the chlorophyll-*a* specific absorption coefficient due to all photosynthetic pigments for small phytoplankton at wavelength  $\lambda$ ,  $\gamma_{small,\lambda}$ , is given by:

$$\gamma_{small,\lambda} = 1.0\gamma_{Chla,\lambda} + 0.35\gamma_{Zea,\lambda} + 0.05\gamma_{Echi,\lambda} + 0.1\gamma_{\beta-car,\lambda} + 2\gamma_{PE,\lambda} + 1.72\gamma_{PC,\lambda} \quad (3)$$

where Chla is the pigment chlorophyll-*a*, Zea is zeaxanthin, Echi is echinenone,  $\beta$ -car is beta-carotene, PE is phycoerithin, and PC is phycocyanin, and the ratios of chlorophyll-*a* to accessory pigment concentration are determined from Wojtasiewicz and Stoń-Egiert (2016). Note that the coefficient in Eq. 3 for Chla is 1.0 because the ratio of chlorophyll-*a* to chlorophyll-*a* is 1. The resulting chlorophyll-*a* specific absorption coefficient is shown in Fig. 5.

Similarly for large phytoplankton and microphytobenthos (Wright et al., 1996):

$$\gamma_{large,\lambda} = 1.0\gamma_{Chla,\lambda} + 0.6\gamma_{Fuco,\lambda} \quad (4)$$

where Fuco is fucoxanthin. And for *Trichodesmium* (Carpenter et al., 1993) :

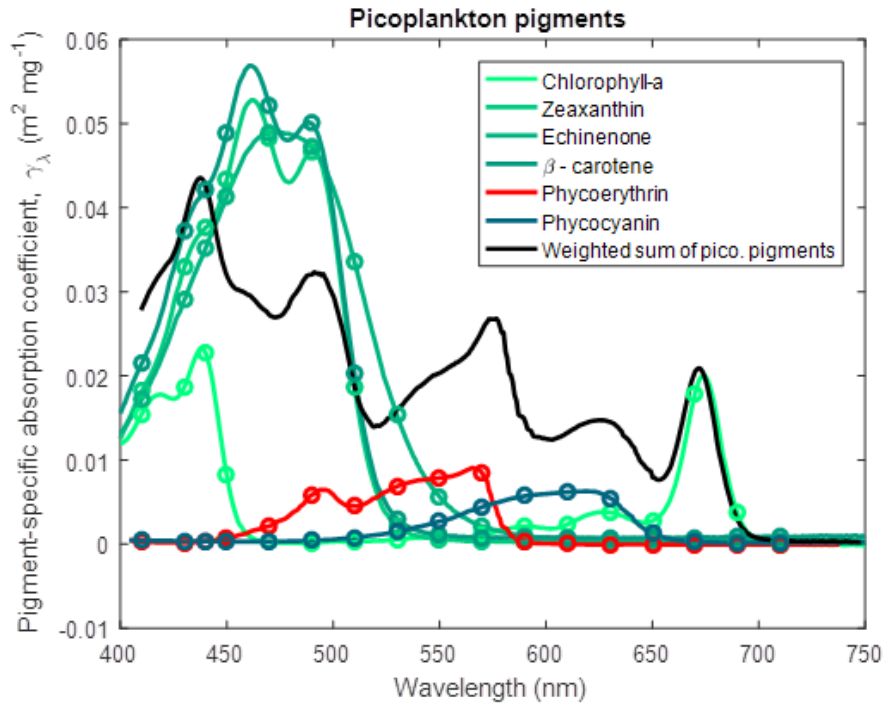
$$\gamma_{Tricho,\lambda} = 1.0\gamma_{Chla,\lambda} + 0.1\gamma_{Zea,\lambda} + 0.02\gamma_{Myxo,\lambda} + 0.09\gamma_{\beta-car,\lambda} + 2.5\gamma_{PE,\lambda} \quad (5)$$

where Myxo is myxoxanthophyll.

The absorption cross-section at wavelength  $\lambda$  ( $\alpha_\lambda$ ) of a spherical cell of radius ( $r$ ), chlorophyll-*a* specific absorption coefficient ( $\gamma_\lambda$ ), and homogeneous intracellular chlorophyll-*a* concentration ( $c_i$ ) can be calculated using geometric optics (i.e., ray tracing without considering internal scattering) and is given by (Duysens, 1956; Kirk, 1975):

$$\alpha_\lambda = \pi r^2 \left( 1 - \frac{2(1 - (1 + 2\gamma_\lambda c_i r)e^{-2\gamma_\lambda c_i r})}{(2\gamma_\lambda c_i r)^2} \right) \quad (6)$$

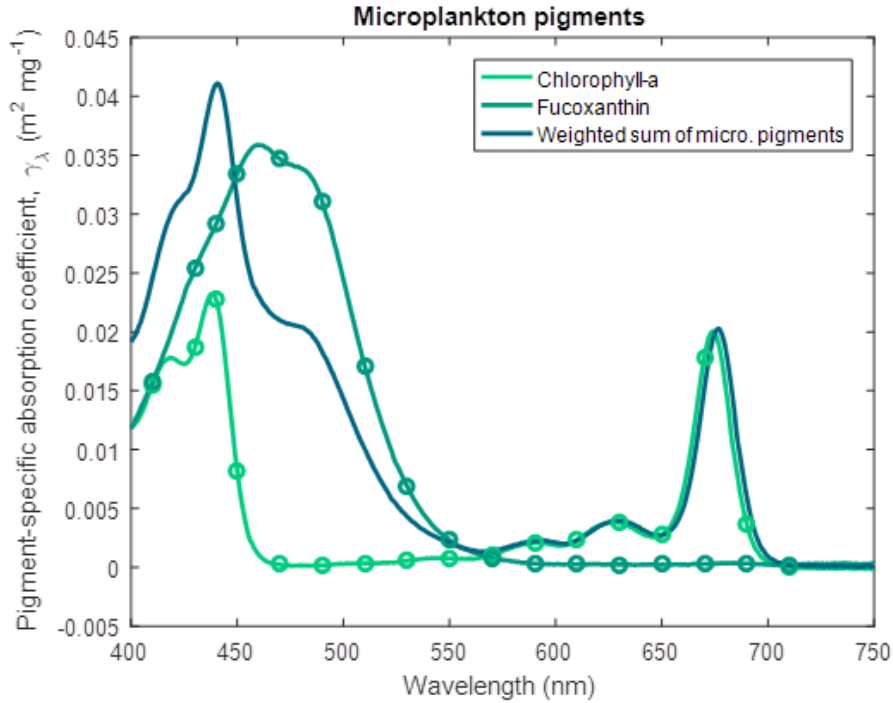
where  $\pi r^2$  is the projected area of a sphere, and the bracketed term is 0 for no absorption ( $\gamma c_i r = 0$ ) and approaches 1 as the cell becomes fully opaque ( $\gamma c_i r \rightarrow \infty$ ). Note that the bracketed term in Eq. 6 is mathematically equivalent to the dimensionless efficiency factor for absorption,  $Q_a$  (used in Morel and Bricaud (1981), Finkel (2001) and Bohren and Huffman (1983)), of homogeneous spherical cells with an index of refraction close to that of the surrounding water. Note that the intracellular chlorophyll concentration,  $c_i$ , changes as a result of chlorophyll synthesis (described later in Eq. 36).



**Figure 5.** Pigment-specific absorption coefficients for the dominant pigments found in small phytoplankton determined using laboratory standards in solvent in a 1 cm vial. Green and red lines are photosynthetic pigments constructed from 563 measured wavelengths. Circles represent the wavelengths at which the optical properties are calculated in the simulations. The black line represents the weighted sum of the photosynthetic pigments (Eq. 3), with the weighting calculated from the ratio of each pigment concentration to chlorophyll *a*. The spectra are wavelength-shifted from their raw measurement by the ratio of the refractive index of the solvent to the refractive index of water (1.352 for acetone used with chlorophyll *a* and  $\beta$ -carotene; 1.361 for ethanol used with zeaxanthin, echinenone; 1.330 for water used with phycoerythrin, phycocyanin).

The use of an absorption cross-section of an individual cell has two significant advantages. Firstly, the same model parameters used here to calculate absorption in the water column are used to determine photosynthesis by individual cells, including the effect of packaging of pigments within cells. Secondly, the dynamic chlorophyll concentration determined later can be explicitly included in the calculation of phytoplankton absorption. Thus the absorption of a population of  $n$  cell  $m^{-3}$  is given by  $n\alpha m^{-1}$ , while an individual cell absorbs  $\alpha E_o$  light, where  $E_o$  is the scalar irradiance.

*Coloured Dissolved Organic Matter (CDOM) absorption.* Two equations for CDOM absorption are presently being trialled. The two schemes are:



**Figure 6.** Pigment-specific absorption coefficients for the dominant pigments found in large phytoplankton and microphytobenthos determined using laboratory standards in solvent in a 1 cm vial. The aqua line represents the weighted sum of the photosynthetic pigments (Eq. 4), with the weighting calculated from the ratio of each pigment concentration to chlorophyll *a*. See Fig. 5 for more details. Fucoxanthin was dissolved in ethanol.

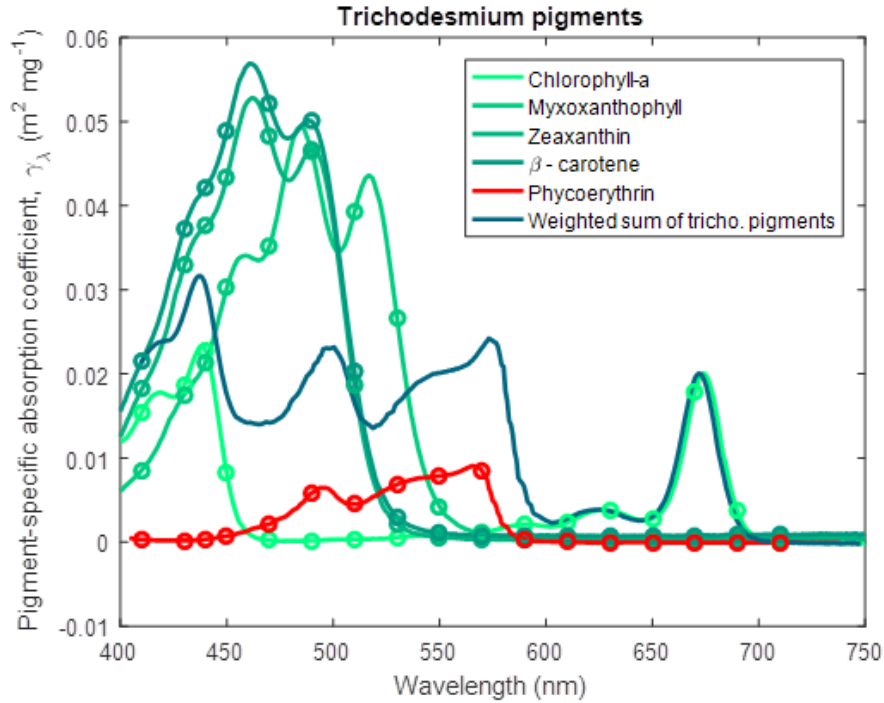
*Scheme 1.* The absorption of CDOM,  $a_{CDOM,\lambda}$ , is determined from a relationship with salinity in the region (Schroeder et al., 2012):

$$a_{CDOM,443} = -0.0332S + 1.2336 \quad (7)$$

where  $S$  is the salinity. In order to avoid unrealistic extrapolation, the salinity used in this relationship is the minimum of the model salinity and 36. In some cases coastal salinities exceed 36 due to evaporation. The absorption due to CDOM at other wavelengths is calculated using a CDOM spectral slope for the region (Blondeau-Patissier et al., 2009):

$$a_{CDOM,\lambda} = a_{CDOM,443} \exp(-S_{CDOM}(\lambda - 443.0)) \quad (8)$$

where  $S_{CDOM}$  is an approximate spectral slope for CDOM, with observations ranging from 0.01 to 0.02  $nm^{-1}$  for significant concentrations of CDOM. Lower magnitudes of the spectral slope generally occur at lower concentrations of CDOM (Blondeau-Patissier et al., 2009).



**Figure 7.** Pigment-specific absorption coefficients for the dominant pigments found in *Trichodesmium* determined using laboratory standards in solvent in a 1 cm vial. The aqua line represents the weighted sum of the photosynthetic pigments (Eq. 5), with the weighting calculated from the ratio of each pigment concentration to chlorophyll *a*. See Fig. 5 for more details. Myxoxanthophyll was dissolved in acetone.

*Scheme 2.* The absorption of CDOM,  $a_{CDOM,\lambda}$ , is directly related to the concentration of dissolved organic carbon,  $D_C$ .

$$a_{CDOM,\lambda} = k_{CDOM,443}^* D_C \exp(-S_{CDOM}(\lambda - 443.0)) \quad (9)$$

where  $k_{CDOM,443}^*$  is the dissolved organic carbon-specific CDOM absorption coefficient at 443 nm.

Both schemes have drawbacks. Scheme 2, using the concentration of dissolved organic carbon, is closer to reality, but is likely to be sensitive to poorly-known parameters such as remineralisation rates and initial detrital concentrations. Scheme 1, a function of salinity, will be more stable, but perhaps less accurate, especially in estuaries where hypersaline waters may have large estuarine loads of coloured dissolved organic matter.

*Absorption due to non-algal particulate material.* The waters of the Great Barrier Reef contain suspended sediments originating from various marine sources, such as the white calcium carbonate fragments generated by coral erosion, and sediments derived from terrestrial sources such as granite (Soja-Woźniak et al., 2019). The model uses spectrally-resolved mass-specific absorption coefficients (and also total scattering measurements) from a database of laboratory measurements conducted on



	Symbol	Value
<i>Constants</i>		
Speed of light	$c$	$2.998 \times 10^8 \text{ m s}^{-1}$
Planck constant	$h$	$6.626 \times 10^{-34} \text{ J s}^{-1}$
Avogadro constant	$A_V$	$6.02 \times 10^{23} \text{ mol}^{-1}$
<sup>a</sup> Total scattering coefficient of phytoplankton	$b_{phy}$	$0.2 \text{ (mg Chl } a \text{ m}^{-2})^{-1}$
<sup>b</sup> Azimuth-independent scattering coefficient	$g_i$	0.402
<sup>b</sup> Azimuth-dependent scattering coefficient	$g_{ii}$	0.180
<sup>c</sup> CDOM-specific absorption coefficient at 443 nm	$k_{CDOM,443}^*$	$0.02 \text{ m}^2 \text{ mg C}^{-1}$
<sup>c</sup> Spectral slope of CDOM absorption	$S_{CDOM}$	$0.012 \text{ nm}^{-1}$
<sup>d</sup> Linear remote-sensing reflectance coefficient	$g_0$	$0.0895 \text{ sr}^{-1}$
<sup>d</sup> Quadratic remote-sensing reflectance coefficient	$g_1$	$0.1247 \text{ sr}^{-1}$

**Table 1.** Constants and parameter values used in the optical model. <sup>a</sup> Kirk (1994). <sup>b</sup> Kirk (1991) using an average cosine of scattering of 0.924 (Mobley, 1994). <sup>c</sup> Blondeau-Patissier et al. (2009) see also Cherukuru et al. (2019). <sup>d</sup> Brando et al. (2012). <sup>e</sup> Vaillancourt et al. (2004).

	Symbol	Units
Downwelling irradiance at depth $z$ , wavelength $\lambda$	$E_{d,z,\lambda}$	$\text{W m}^{-2}$
Scalar irradiance at depth $z$ , wavelength $\lambda$	$E_{o,z,\lambda}$	$\text{W m}^{-2}$
In water azimuth angle	$\theta$	rad
Fractional backscattering	$u_\lambda$	-
Below-surface remote-sensing reflectance	$r_{rs,\lambda}$	$\text{sr}^{-1}$
Above-surface remote-sensing reflectance	$R_{rs,\lambda}$	$\text{sr}^{-1}$
Thickness of model layer	$h$	m
Optical depth weighting function	$w_{z,\lambda}$	
Vertical attenuation coefficient	$K_\lambda$	$\text{m}^{-1}$
Total absorption coefficient	$a_{T,\lambda}$	$\text{m}^{-1}$
Total scattering coefficient	$b_{T,\lambda}$	$\text{m}^{-1}$
Absorption cross-section	$\alpha_\lambda$	$\text{m}^2 \text{ cell}^{-1}$
Concentration of cells	$n$	$\text{cell m}^{-3}$

**Table 2.** State and derived variables in the water column optical model.

either pure mineral suspensions, or mineral mixtures, at two ranges of size distributions (Fig. 8, Stramski et al. (2007)). In this model version we use the calcium carbonate sample CAL1 for  $\text{CaCO}_3$ -based particles

For the terrestrially-sourced particles we used observations from Gladstone Harbour in the central GBR (Fig. 9). These IOPs gave a realistic surface colour for the Queensland river sediment plumes (Baird et al., 2016b). In the model, optically-active non-algal particulates (NAPs) includes the inorganic particulates (such as sand and mud, see Sec. 7.1) and detritus. We assumed the optical properties of the detritus was the same as the optical properties in Gladstone Harbour, although open ocean studies have used a detrital absorption that is more like CDOM (Dutkiewicz et al., 2015).

The absorption due to calcite-based NAP is given by:

$$a_{NAP_{CaCO_3},\lambda} = c_1 NAP_{CaCO_3} \quad (10)$$

where  $c_1$  is the mass-specific, spectrally-resolved absorption coefficient determine from laboratory experiments (Fig. 8). The absorption due to non-calcite NAPs,  $NAP_{non-CaCO_3}$ , combined with detritus, is given by:

$$a_{NAP_{non-CaCO_3},\lambda} = c_2 NAP_{non-CaCO_3} + \left( \frac{550}{30} \frac{12}{14} D_{Atk} + \frac{106}{16} \frac{12}{14} D_{Red} + D_C \right) / 10^6 \quad (11)$$

where  $c_2$  is the mass-specific, spectrally-resolved absorption coefficient determine from field measurements (Fig. 9),  $NAP_{non-CaCO_3}$  is quantified in  $kg\ m^{-3}$ ,  $D_{Atk}$  and  $D_{Red}$  are quantified in  $mg\ N\ m^{-3}$  and  $D_C$  is quantified in  $mg\ C\ m^{-3}$ .

*Total absorption.* The total absorption,  $a_{T,\lambda}$ , is given by:

$$a_{T,\lambda} = a_{w,\lambda} + a_{NAP_{non-CaCO_3},\lambda} + a_{NAP_{CaCO_3},\lambda} + a_{CDOM,\lambda} + \sum_{x=1}^N n_x \alpha_{x,\lambda} \quad (12)$$

where  $a_{w,\lambda}$  is clear water absorption (Fig. 10) and  $N$  is the number of phytoplankton classes (see Table 4).

*Scattering.* The total scattering coefficient is given by

$$b_{T,\lambda} = b_{w,\lambda} + c_1 NAP_{non-CaCO_3} + c_2 NAP_{CaCO_3} + b_{phy,\lambda} \sum_{x=1}^N n_x c_{i,x} V_x \quad (13)$$

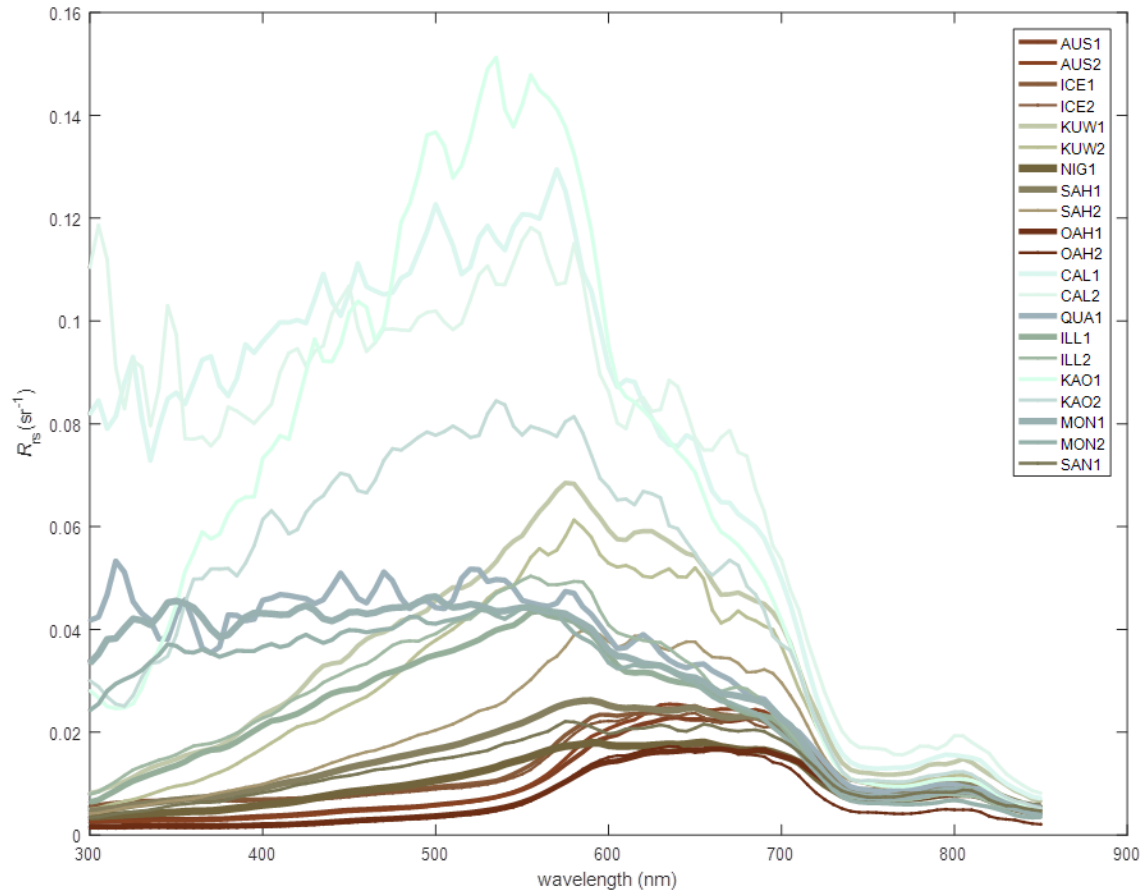
where  $NAP$  is the concentration of non-algal particulates,  $b_{w,\lambda}$  is the scattering coefficient due to clear water (Fig. 10),  $c_1$  and  $c_2$  are the spectrally-resolved, mass-specific coefficients (Figs. 8 & 9) and phytoplankton scattering is the product of the chlorophyll-specific phytoplankton scattering coefficient,  $b_{phy,\lambda}$ , and the water column chlorophyll concentration of all classes,  $\sum n_x c_{i,x} V_x$  (where  $c_i$  is the chlorophyll concentration in the cell, and  $V$  is the cell volume). The value for  $b_{phy,\lambda}$  is set to  $0.2\ (mg\ Chl\ a\ m^{-2})^{-1}$  for all wavelengths, a typical value for marine phytoplankton (Kirk, 1994). For more details see Baird et al. (2007b).

*Backscattering* In addition to the IOPs calculated above, the calculation of remote-sensing reflectance uses a backscattering coefficient,  $b_b$ , which has a component due to pure seawater, and a component due to algal and non-algal particulates. The backscattering ratio is a coarse resolution representation of the volume scattering function, and is the ratio of the forward and backward scattering.

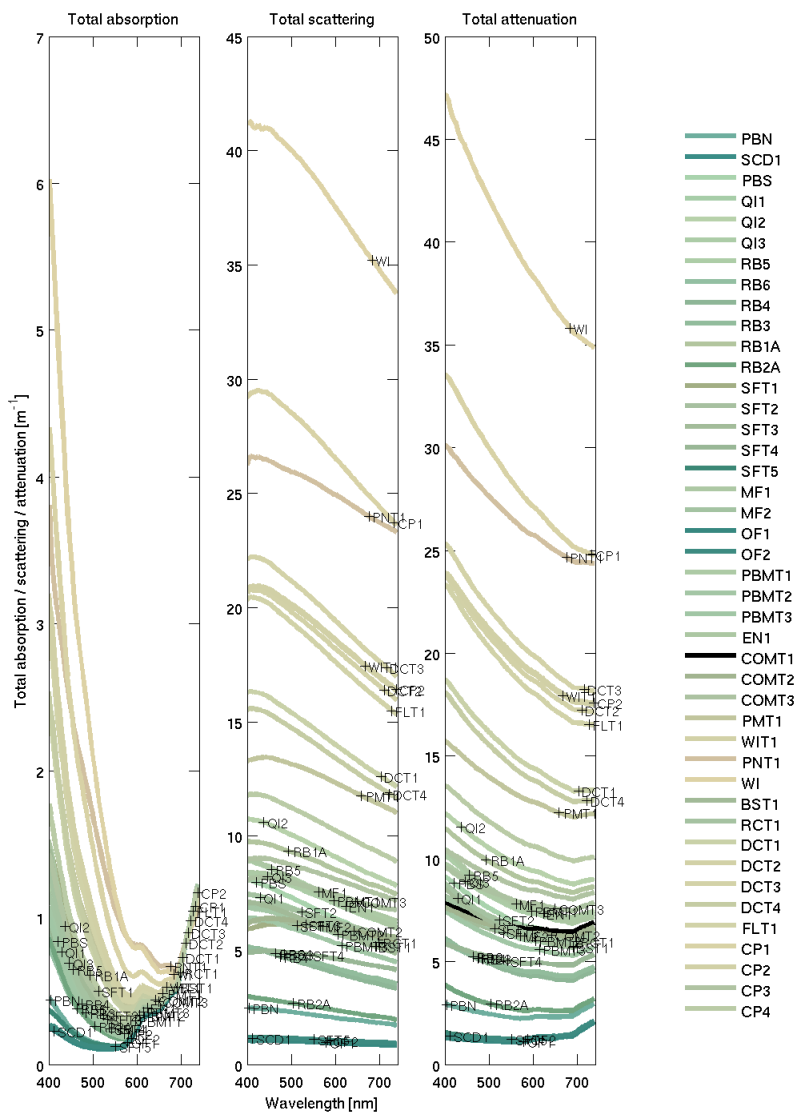
The backscattering coefficient for clear water is 0.5, a result of isotropic scattering of the water molecule.

The particulate component of backscattering for phytoplankton is strongly related to cell carbon (and therefore cell size) and the number of cells (Vaillancourt et al., 2004):

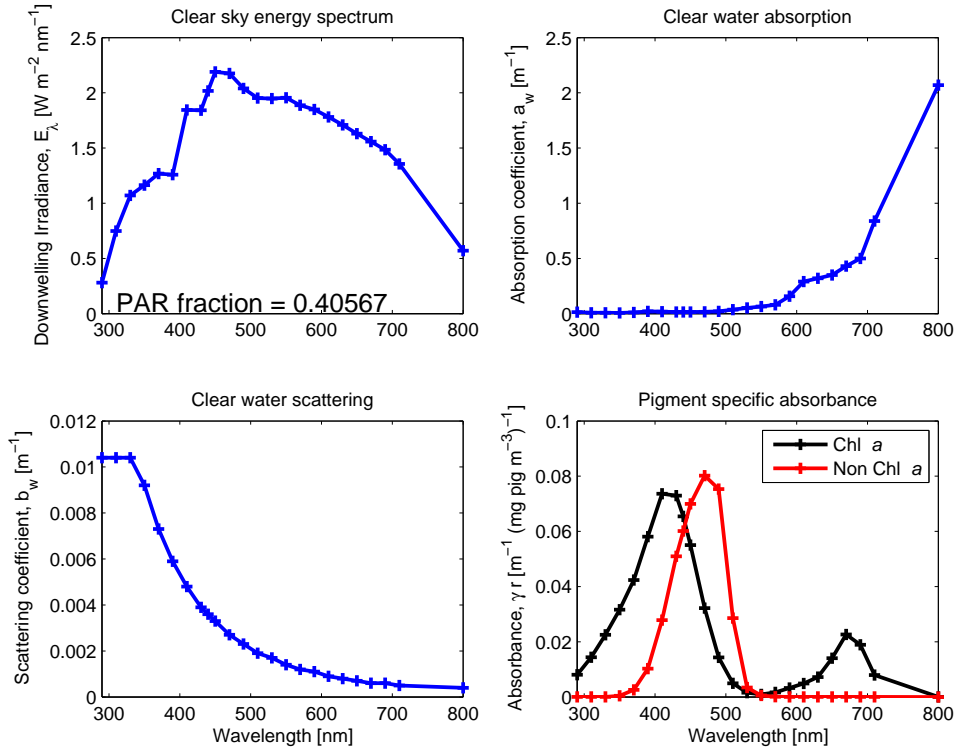
$$b_{bphy,\lambda}^* = 5 \times 10^{-15} m_C^{1.002} \quad (R^2 = 0.97) \quad (14)$$



**Figure 8.** The remote-sensing reflectance of the 21 mineral mixtures suspended in water as measured by Stramski et al. (2007). Laboratory measurements of absorption and scattering properties are used to calculate remote-sensing reflectance (Baird et al., 2016b). Line colouring corresponds to that produced by the mineral suspended in clear water as calculated using the MODIS true color algorithm (Gumley et al., 2010). CAL1, with a median particle diameter of  $2 \mu\text{m}$ , is used for  $\text{Mud}_{\text{CaCO}_3}$ .



**Figure 9.** Inherent optical properties (total absorption and total scattering) at sample sites in Gladstone Harbour on 13-19 September 2013 (Babcock et al., 2015). The line colour is rendered like Fig. 8. The site labelling is ordered in time, from the first sample collected during neap tides at the top, to the last sample collected at spring tides on the bottom. The IOPs used for the  $\text{Mud}_{\text{non-CaCO}_3}$  end-member is from the WIT site at the centre of the harbour, was dominated by inorganic particles. The measured concentration of NAP at the site was  $33.042 \text{ mg L}^{-1}$ , and is used to calculate mass-specific IOPs.



**Figure 10.** Spectrally-resolved energy distribution of sunlight, clear water absorption, and clear water scattering (Smith and Baker, 1981). The fraction of solar radiation between 400 and 700 nm for clear sky irradiance at the particular spectral resolution is given in the top left panel. The centre of each waveband used in the model simulations is identified by a cross on each curve. The bottom right panel shows the pigment-specific absorption of Chl *a* and generic photosynthetic carotenoids (Ficek et al., 2004) that were used in earlier versions of this model (Baird et al., 2016b) before the mass-specific absorption coefficients of multiple accessory pigments was implemented (Figs. 5, 6 & 7).

where  $m_C$  is the carbon content of the cells, here in  $\text{pg cell}^{-1}$ .

For inorganic particles, backscattering can vary between particle mineralogies, size, shape, and at different wavelengths, resulting, with spectrally-varying absorption, in the variety of colours that we see from suspended sediments. Splitting sediment types by mineralogy only, the backscattering ratio for carbonate and non-carbonate particles is given in Table 3.

- 5 The backscatter due to phytoplankton is approximately 0.02. To account for a greater backscattering ratio, and therefore backscatter, at low wavelengths (Fig. 4 of Vaillancourt et al. (2004)), we linearly increased the backscatter ratio from 0.02 at 555 nm to 0.04 at 470 nm. Above and below 555 nm and 470 nm respectively the backscatter ratio remained constant.

The total backscatter then becomes:

$$b_{b,\lambda} = \tilde{b}_w b_{w,\lambda} + b_{bphy,\lambda}^* n + \tilde{b}_{b,NAP_{non-CaCO_3},\lambda} c_1 NAP_{non-CaCO_3} + \tilde{b}_{b,NAP_{CaCO_3},\lambda} c_2 NAP_{non-CaCO_3} NAP_{CaCO_3} \quad (15)$$

- 10 where the backscatter ratio of pure seawater,  $\tilde{b}_w$ , is 0.5,  $n$  is the concentration of cells, and for particulate matter (NAP and detritus),  $\tilde{b}_{b,NAP,\lambda}$ , is variable (Table 3) and the coefficients  $c_1$  and  $c_2$  come from the total scattering equations above.

	Wavelength [nm]								
	412.0	440.0	488.0	510.0	532.0	595.0	650.0	676.0	715.0
Carbonate	0.0209	0.0214	0.0224	0.0244	0.0216	0.0201	0.0181	0.0170	0.0164
Terrestrial	0.0028	0.0119	0.0175	0.0138	0.0128	0.0134	0.0048	0.0076	0.0113

**Table 3.** Particulate backscattering ratio for carbonate and non-carbonate minerals based on samples at Lucinda Jetty Coastal Observatory, a site at the interface on carbonate and terrestrial bottom sediment (Soja-Woźniak et al., 2019).

#### 4.1.2 Apparent optical properties (AOPs)

The optical model is forced with the downwelling short wave radiation just above the sea surface, based on remotely-sensed cloud fraction observations and calculations of top-of-the-atmosphere clear sky irradiance and solar angle. The calculation of downwelling radiation and surface albedo (a function of solar elevation and cloud cover) is detailed in the hydrodynamic scientific description (<https://research.csiro.au/cem/software/ems/ems-documentation/>, Sec 9.1.1).

The downwelling irradiance just above the water interface is split into wavebands using the weighting for clear sky irradiance (Fig. 10). Snell's law is used to calculate the azimuth angle of the mean light path through the water,  $\theta_{sw}$ , as calculated from the atmospheric azimuth angle,  $\theta_{air}$ , and the refraction of light at the air/water interface (Kirk, 1994):

$$\frac{\sin \theta_{air}}{\sin \theta_{sw}} = 1.33 \quad (16)$$

10 *Calculation of in-water light field.* Given the IOPs determined above, the exact solution for AOPs would require a radiative transfer model (Mobley, 1994), which is too computationally-expensive for a complex ecosystem model such as developed here. Instead, the in-water light field is solved for using empirical approximations of the relationship between IOPs and AOPs (Kirk, 1991; Mobley, 1994).

The vertical attenuation coefficient at wavelength  $\lambda$  when considering absorption and scattering,  $K_\lambda$ , is given by:

$$15 \quad K_\lambda = \frac{a_{T,\lambda}}{\cos \theta_{sw}} \sqrt{1 + (g_i \cos \theta_{sw} - g_{ii}) \frac{b_{T,\lambda}}{a_{T,\lambda}}} \quad (17)$$

The term outside the square root quantifies the effect of absorption, where  $a_{T,\lambda}$  is the total absorption. The term within the square root of Eq. 17 represents scattering as an extended pathlength through the water column, where  $g_i$  and  $g_{ii}$  are empirical constants and take values of 0.402 and 0.180 respectively. The values of  $g_i$  and  $g_{ii}$  depend on the average cosine of scattering. For filtered water with scattering only due to water molecules, the values of  $g_i$  and  $g_{ii}$  are quite different to natural waters. But 20 for waters ranging from coastal to open ocean, the average cosine of scattering varies by only a small amount (0.86 - 0.95, Kirk (1991)), and thus uncertainties in  $g_i$  and  $g_{ii}$  do not strongly affect  $K_\lambda$ .

The downwelling irradiance at wavelength  $\lambda$  at the bottom of a layer  $h$  thick,  $E_{d,\lambda,bot}$ , is given by:

$$E_{d,bot,\lambda} = E_{d,top,\lambda} e^{-K_\lambda h} \quad (18)$$

where  $E_{d,top,\lambda}$  is the downwelling irradiance at wavelength  $\lambda$  at the top of the layer and  $K_\lambda$  is the vertical attenuation coefficient at wavelength  $\lambda$ , a result of both absorption and scattering processes.

Assuming a constant attenuation rate within the layer, the average downwelling irradiance at wavelength  $\lambda$ ,  $E_{d,\lambda}$ , is given by:

$$5 \quad E_{d,\lambda} = \frac{1}{h} \int_{bot}^{top} E_{d,z,\lambda} e^{-K_\lambda z} dz = \frac{E_{d,top,\lambda} - E_{d,bot,\lambda}}{K_\lambda h} \quad (19)$$

We can now calculate the scalar irradiance,  $E_o$ , for the calculation of absorbing components, from downwelling irradiance,  $E_d$ . The light absorbed within a layer must balance the difference in downwelling irradiance from the top and bottom of the layer (since scattering in this model only increases the pathlength of light), thus:

$$E_{o,\lambda} a_{T,\lambda} h = E_{d,top,\lambda} - E_{d,bot,\lambda} = E_{d,\lambda} K_\lambda h \quad (20)$$

10 Cancelling  $h$ , the scalar irradiance as a function of downwelling irradiance is given by:

$$E_{o,\lambda} = \frac{E_{d,\lambda} K_\lambda}{a_{T,\lambda}} \quad (21)$$

This correction conserves photons within the layer, although it is only as good as the original approximation of the impact of scattering and azimuth angle on vertical attenuation (Eq. 17).

*Vertical attenuation of heat.* The vertical attenuation of heat is given by:

$$15 \quad K_{heat} = - \int \frac{1}{E_{d,z,\lambda}} \frac{\partial E_{d,z,\lambda}}{\partial z} d\lambda \quad (22)$$

and the local heating by:

$$\frac{\partial T}{\partial t} = - \frac{1}{\rho c_p} \int \frac{\partial E_{d,\lambda}}{\partial z} d\lambda \quad (23)$$

where  $T$  is temperature,  $\rho$  is the density of water, and  $c_p = 4.1876 \text{ J m}^{-3} \text{ K}^{-1}$  is the specific heat of water. This calculation does not feed back to the hydrodynamic model.

## 20 4.2 Epibenthic optical model

The spectrally-resolved light field at the base of the water column is attenuated, [from top to bottom](#), by macroalgae, seagrass (*Zostera* then shallow and then deep forms of *Halophila*), followed by the zooxanthellae in corals. The downwelling irradiance at wavelength  $\lambda$  after passing through each macroalgae and seagrass species is given by,  $E_{below,\lambda}$ :

$$E_{below,\lambda} = E_{d,above,\lambda} e^{-A_\lambda \Omega_X X} \quad (24)$$

25 where  $E_{above,\lambda}$  for macroalgae is  $E_{d,bot,\lambda}$ , the downwelling irradiance of the bottom water column layer,  $A_\lambda$  is the leaf-specific absorbance,  $\Omega$  is the nitrogen specific leaf area, and  $X$  is the leaf nitrogen biomass.

The light absorbed by corals is assumed to be entirely due to zooxanthellae, and is given by:

$$E_{below,\lambda} = E_{above,\lambda} e^{-n\alpha_\lambda} \quad (25)$$

where  $n = CS/m_{N,CS}$  is the areal density of zooxanthellae cells and  $\alpha_\lambda$  is the absorption cross-section of a cell a result of the absorption of multiple pigment types.

- 5 The optical model for microphytobenthic algae, and the bottom reflectance due to sediment and bottom types, is described in Sec. 7.1.

### 4.3 Sediment optical model

The optical model in the sediment only concerns the benthic microalgae growing in the porewaters of the top sediment layer. The calculation of light absorption by benthic microalgae assumes they are the only attenuating component in a layer that  
 10 lies on top layer of sediment, with a perfectly absorbing layer below and no scattering by any other components in the layer. Thus no light penetrates through to the second sediment layer where benthic microalgae also reside. Thus the downwelling irradiance at wavelength  $\lambda$  at the bottom of a layer,  $E_{d,\lambda,bot}$ , is given by:

$$E_{d,bot,\lambda} = E_{d,top,\lambda} e^{-n\alpha_\lambda h} \quad (26)$$

where  $E_{d,top,\lambda}$  is the downwelling irradiance at wavelength  $\lambda$  at the top of the layer and  $\alpha_\lambda$  is the absorption cross-section of  
 15 the cell at wavelength  $\lambda$ , and  $n$  is the concentration of cells in the layer. The layer thickness used here,  $h$ , is the thickness of the top sediment layer, so as to convert the concentration of cells in that layer,  $n$ , into the areal concentration of cells in the biofilm,  $nh$ .

Given no scattering in the cell, and that the vertical attenuation coefficient is independent of azimuth angle, the scalar irradiance that the benthic microalgae are exposed to in the surface biofilm is given by:

$$20 \quad E_{o,\lambda} = (E_{d,top,\lambda} - E_{d,bot,\lambda}) / (n\alpha_\lambda h) \quad (27)$$

The photons captured by each cell, and the microalgae process, follow the same equations as for the water column (Sec. 5.1.3).

## 5 Pelagic processes

### 5.1 Microalgae

The model contains four [functional groups](#) of suspended microalgae: small and large phytoplankton, microphytobenthos and  
 25 *Trichodesmium*. The growth from internal reserves for each of the functional groups is identical and explained below. The differences in the ecological interactions of the four functional groups are summarised in Table 4. *Trichodesmium*, a nitrogen fixers, also contains additional processes described below.



	small phyto.	large phyto.	benthic phyto.	<i>Trichodesmium</i>
Radius ( $\mu\text{m}$ )	1	4	10	5
<sup>a</sup> Maximum growth rate ( $\text{d}^{-1}$ )	1.6	1.4	0.839	0.2
Sink rate ( $\text{m d}^{-1}$ )				variable
Surface sediment growth	×	×	✓	×
Nitrogen fixation	×	×	×	✓
Water column mort.	✓	✓	×	✓
Sediment mort.	✓	✓	✓	✓

**Table 4.** Traits of suspended microalgae.<sup>a</sup> At  $T_{ref} = 20^\circ\text{C}$ .

### 5.1.1 Microalgal growth

The growth of microalgae has been modelled in many ways, from simple exponential growth and logistic growth curves, to single and multiple-nutrient based curves, through to equations that contain a state variable for the physiological state of the cell (variously described as stores, quotas, reserves etc.) and to consider the complex processing of photons in the microalgal photosystem.

It is now common for complex biogeochemical models to contain state variables for the physiological state variables of each of potentially limiting nutrients (Baretta-Bekker et al., 1997; Vichi et al., 2007) and include adaptation to photosystems (Geider et al., 1998). In the context of many different microalgae models, the model that is described here has taken another path again. As articulated above, we chose to base nutrient uptake and light absorption on using geometric constraints. This meant that any growth model needed to be formulated around the maximum rate of supply of each of the limiting nutrients (and light) (see Fig. 2 of Baird et al. (2006)).

In the microalgae model (most fully described in Baird et al. (2001)), the uptake of nutrients and light absorption increases the reserves of nutrients and light, as quantified by a reserve,  $R$ , which has units of mass per cell. In the equations we often use a normalised reserve,  $R^*$ , which is a quantity between zero and one (Tab. 5). The reserves are in turn consumed to generate structural material. Thus the total content of nitrogen in the microalgae is equal to the sum of the structural material and the reserves.

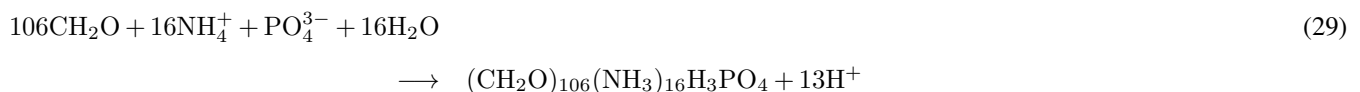
The model considers the diffusion-limited supply of dissolved inorganic nutrients (N and P) and the absorption of light, delivering N, P and fixed C to the internal reserves of the cell (Fig. 11). Nitrogen and phosphorus are taken directly into the reserves, but carbon is first fixed through photosynthesis (Kirk, 1994):



Variable	Symbol	Units
Scalar irradiance	$E_o$	$\text{W m}^{-2}$
Dissolved inorganic nitrogen (DIN)	$N$	$\text{mg N m}^{-3}$
Dissolved inorganic phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Dissolved inorganic carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$
Dissolved oxygen	$[\text{O}_2]$	$\text{mg O m}^{-3}$
Reserves of nitrogen	$R_N$	$\text{mg N cell}^{-1}$
Reserves of phosphorus	$R_P$	$\text{mg P cell}^{-1}$
Reserves of carbon	$R_C$	$\text{mg C cell}^{-1}$
Maximum reserves of nitrogen	$R_N^{\max}$	$\text{mg N cell}^{-1}$
Maximum reserves of phosphorus	$R_P^{\max}$	$\text{mg P cell}^{-1}$
Maximum reserves of carbon	$R_C^{\max}$	$\text{mg C cell}^{-1}$
Normalised reserves of nitrogen	$R_N^* \equiv R_N / R_N^{\max}$	-
Normalised reserves of phosphorus	$R_P^* \equiv R_P / R_P^{\max}$	-
Normalised reserves of carbon	$R_C^* \equiv R_C / R_C^{\max}$	-
Intracellular Chl $a$ concentration	$c_i$	$\text{mg m}^{-3}$
Structural phytoplankton biomass	$B$	$\text{mg N m}^{-3}$
Absorption cross-section	$\alpha$	$\text{m}^2 \text{cell}^{-1}$
Diffusion shape factor	$\psi$	$\text{m cell}^{-1}$
Wavelength	$\lambda$	$\text{nm}$
Maximum Chl $a$ synthesis rate	$k_{\text{Chl}}^{\max}$	$\text{mg Chl m}^{-3} \text{d}^{-1}$
Photon absorption-weighted opaqueness	$\bar{\Theta}$	-
Non-dimensional absorption	$\rho_\lambda = \gamma_\lambda c_i r$	-

**Table 5.** State and derived variables for the microalgae growth model. DIN is given by the sum of nitrate and ammonium concentrations,  $[\text{NO}_3] + [\text{NH}_4]$ .

The internal reserves of C, N, and P are consumed to form structural material at the Redfield ratio (Redfield et al., 1963):



- 5 where we have represented nitrogen as ammonium ( $\text{NH}_4$ ) in Eq. 29. When the nitrogen source to the cell is nitrate,  $\text{NO}_3$ , it is assumed to lose its oxygen at the cell wall (Sec. 9.1). The growth rate of microalgae is given by the maximum growth rate,  $\mu^{\max}$ , multiplied by the normalised reserves,  $R^*$ , of each of N, P and C:

$$\mu = \mu^{\max} R_N^* R_P^* R_C^* \quad (30)$$

The mass of the reserves (and therefore the total C:N:P:Chl *a* ratio) of the cell depends on the interaction of the supply and consumption rates (Fig. 11). When consumption exceeds supply, and the supply rates are non-Redfield, the normalised internal reserves of the non-limiting nutrients approach 1 while the limiting nutrient becomes depleted. Thus the model behaves like a 'Law of the Minimum' growth model, except during fast changes in nutrient supply rates.

5 The molar ratio of a cell, the addition of structural material and reserves, is given by:

$$C : N : P = 106(1 + R_C^*) : 16(1 + R_N^*) : 1 + R_P^* \quad (31)$$

### 5.1.2 Nutrient uptake

The diffusion-limited nutrient uptake to a single phytoplankton cell,  $J$ , is given by:

$$J = \psi D (C_b - C_w) \quad (32)$$

10 where  $\psi$  is the diffusion shape factor ( $= 4\pi r$  for a sphere),  $D$  is the molecular diffusivity of the nutrient,  $C_b$  is the average extracellular nutrient concentration, and  $C_w$  is the concentration at the wall of the cell. The diffusion shape factor is determined by equating the divergence of the gradient of the concentration field to zero ( $\nabla^2 C = 0$ ).

A semi-empirical correction to Eq. 32, to account for fluid motion around the cell, and the calculation of non-spherical diffusion shape factors, has been applied in earlier work (Baird and Emsley, 1999). For the purposes of biogeochemical modelling  
15 these uncertain corrections for small scale turbulence and non-spherical shape are not quantitatively important, and have not been pursued here.

Numerous studies have considered diffusion-limited transport to the cell surface at low nutrient concentrations saturating to a physiologically-limited nutrient uptake from the cell wall (Hill and Whittingham, 1955; Pasciak and Gavis, 1975; Mann and Lazier, 2006) at higher concentrations. The physiological limitation is typically considered using a Michaelis-Menten type  
20 equation. Here we simply consider the diffusion-limited uptake to be saturated by the filling-up of reserves,  $(1 - R^*)$ . Thus, nutrient uptake is given by:

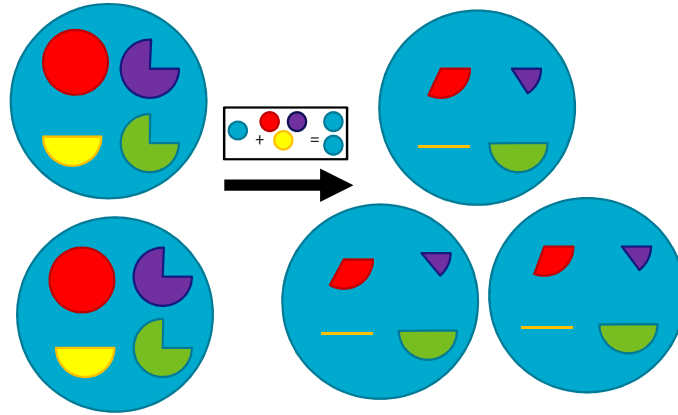
$$J = \psi D C_b (1 - R^*) \quad (33)$$

where  $R^*$  is the normalised reserve of the nutrient being considered. As shown later when considering preferential ammonium uptake, under extreme limitation relative to other nutrients,  $R^*$  approaches 0, and uptake approaches the diffusion limitation.

### 25 5.1.3 Light capture and chlorophyll synthesis

Light absorption by microalgae cells has already been considered above Eq. 6. The same absorption cross-section,  $\alpha$ , is used to calculate the capture of photons:

$$\frac{\partial R_C^*}{\partial t} = (1 - R_C^*) \frac{(10^9 hc)^{-1}}{A_V} \int \alpha_\lambda E_{o,\lambda} d\lambda \quad (34)$$



**Figure 11.** Schematic of the process of microalgae growth from internal reserves. Blue circle - structural material; Red pie - nitrogen reserves; Purple pie - phosphorus reserves; Yellow pie - carbon reserves; Green pie - pigment content. Here a circular pie has a value of 1, representing the normalised reserve (a value between 0 and 1). The box shows that to generate structural material for an additional cell requires the equivalent of 100 % internal reserves of carbon, nitrogen and phosphorus of one cell. This figure shows the discrete growth of 2 cells to 3, requiring both the generation of new structural material from reserves and the reserves being diluted as a result of the number of cells in which they are divided increasing from 2 to 3. Thus the internal reserves for nitrogen after the population increases from 2 to 3 is given by: two from the initial 2 cells, minus one for building structural material of the new cell, shared across the 3 offspring, to give 1/3. The same logic applies to carbon and phosphorus reserves, with phosphorus reserves being reduced to 1/6, and carbon reserves being exhausted. In contrast, pigment is not required for structural material so the only reduction is through dilution; the 3/4 content of 2 cells is shared among 3 cells to equal 1/2 in the 3 cells. This schematic shows one limitation of a population-style model whereby reserves are 'shared' across the population (as opposed to individual based modelling, Beckmann and Hense (2004)). A proof of the conservation of mass for this scheme, including under mixing of populations of suspended microalgae, is given in Baird et al. (2004). The model equations also include terms affecting internal reserves through nutrient uptake, light absorption, respiration and mortality that are not shown in this simple schematic.

where  $(1 - R_C^*)$  accounts for the reduced capture of photons as the reserves becomes saturated, and  $\frac{(10^9 hc)^{-1}}{A_V}$  converts from energy to photons. The absorption cross-section is a function of intracellular pigment concentration, which is a dynamic variable determined below. While a drop-off of photosynthesis occurs as the carbon reserves become replete, this formulation does not consider photoinhibition due to photooxidation, although it has been considered elsewhere for zooxanthallae (Baird et al., 2018).

The dynamic C:Chl component determines the rate of synthesis of pigment based on the incremental benefit of adding pigment to the rate of photosynthesis. This calculation includes both the reduced benefit when carbon reserves are replete,  $(1 - R_C^*)$ , and the reduced benefit due to self-shading,  $\chi$ . The factor  $\chi$  is calculated for the derivative of the absorption cross-section per unit projected area (see Eq. 6),  $\alpha/PA$ , with non-dimensional group  $\rho = \gamma c_i r$ . For a sphere of radius  $r$  (Baird et al.,

2013):

$$\frac{1}{PA} \frac{\partial \alpha}{\partial \rho} = \frac{1 - e^{-2\rho}(2\rho^2 + 2\rho + 1)}{\rho^3} = \chi \quad (35)$$

where  $\chi$  represents the area-specific incremental rate of change of absorption with  $\rho$ . The rate of chlorophyll synthesis is given by:

$$\frac{\partial c_i}{\partial t} = k_{\text{Chl}}^{\text{max}}(1 - R_C^*)\bar{\chi} \quad \text{if } C : \text{Chl} > \theta_{\text{min}} \quad (36)$$

where  $k_{\text{Chl}}^{\text{max}}$  is the maximum rate of synthesis and  $\theta_{\text{min}}$  is the minimum C:Chl ratio. Below  $\theta_{\text{min}}$ , pigment synthesis is zero. Both self-shading, and the rate of photosynthesis itself, are based on photon absorption rather than energy absorption (Table 6), as experimentally shown in Nielsen and Sakshaug (1993).

For each phytoplankton type the model considers multiple pigments with distinct absorption spectra. The model needs to represent all photo-absorbing pigments as the C:Chl model calculates the pigment concentration based on that required to maximise photosynthesis. If only Chl *a* was represented, the model would predict a Chl *a* concentration that was accounting for the absorption of Chl *a* and the auxiliary pigments, thus over-predicting the Chl *a* concentration when compared to observations. Thus the Chl-*a* predicted by the model is like a HPLC-determined Chl-*a* concentration, and not the sum of the photosynthetic pigments.

#### 5.1.4 Carbon fixation / respiration

When photons are captured (photosynthesis) there is an increase in reserves of carbon,  $k_I(1 - R_C^*)$  (Eq. 48), and an accompanying uptake of dissolved inorganic carbon,  $\frac{106}{1060} 12k_I(1 - R_C^*)$  (Eq. 44), and release of oxygen,  $\frac{106}{1060} 32k_I(1 - R_C^*)$  (Eq. 45), per cell to the water column (Table 6).

Additionally, there is a basal respiration, representing a constant cost of cell maintenance. The loss of internal reserves,  $\mu_B^{\text{max}} m_{B,C} \phi R_C^*$ , results in a gain of water column dissolved inorganic carbon per cell,  $\frac{106}{1060} \frac{12}{14} \mu_B^{\text{max}} \phi R_C^*$ , as well as a loss in water column dissolved oxygen per cell,  $\frac{106}{1060} \frac{32}{14} \mu_B^{\text{max}} \phi R_C^*$  (Table 6). The loss in water column dissolved oxygen per cell represents an instantaneous respiration of the fixed carbon of the reserves. Basal respiration decreases internal reserves, and therefore growth rate, but does not directly lead to cell mortality at zero carbon reserves. Implicit in this scheme is that the basal cost is higher when the cell has more carbon reserves,  $R_C^*$ .

A linear mortality term, resulting in the loss of structural material and carbon reserves, is considered later.

#### 5.1.5 Application of single cell rates to a population

As mentioned above, the nutrient uptake and light absorption rates are calculated on a per cell basis. This has allowed geometric considerations to be explicitly used, and contrasts with most biogeochemical models that formulate planktonic rates based on

population interactions. However, the state variables for microalgae (and zooplankton) are for the population. Therefore, rates per cell need to be multiplied by the number of cells to obtain population rates. In the case of microalgae, the number of cells  $n$  is given by  $B/m_{B,N}$ . It should be noted that firstly this assumes all cells in the population are identical, and that the state variable for the population,  $B$ , is quantifying only the nitrogen (or oxygen, carbon and phosphorus) associated with the structural material. It should also be noted that all cells in a population have the same quantity in their reserves.

### 5.1.6 Conservation of mass of microalgae model

The conservation of mass during transport, growth and mortality is proven in Baird et al. (2004). Briefly, for microalgal growth, total concentration of nitrogen in microalgae cells is given by  $B + BR_N^*$ . For conservation of mass, the time derivatives must equate to zero:

$$10 \quad \frac{\partial B}{\partial t} + \frac{\partial (R_N B / R_N^{max})}{\partial t} = 0. \quad (37)$$

using the product rule to differentiate the second term on the LHS:

$$\frac{\partial B}{\partial t} + \frac{\partial B}{\partial t} \frac{R_N}{R_N^{max}} + \frac{B}{R_N^{max}} \frac{\partial R_N}{\partial t} = 0 \quad (38)$$

Where:

$$\frac{\partial B}{\partial t} = +\mu_B^{max} R_C^* R_N^* R_P^* B \quad (39)$$

$$15 \quad \frac{\partial B}{\partial t} \frac{R_N}{R_N^{max}} = +\mu_B^{max} R_C^* R_N^* R_P^* B \frac{R_N}{R_N^{max}} \quad (40)$$

$$\frac{B}{R_N^{max}} \frac{\partial R_N}{\partial t} = -B(1 + R_N^*) \mu_B^{max} R_C^* R_N^* R_P^* \frac{R_N}{R_N^{max}} \quad (41)$$

Thus demonstrating conservation of mass when  $m_{B,N} = R_N^{max}$ , as used here.

20 The state variables, equations and parameter values are listed in Tables 5, 6 and 7 respectively. The equations in Table 6 described nitrogen uptake from the DIN pool, where the partitioning between nitrate and ammonium due to preferential ammonium uptake is described in Sec. 9.1. Earlier published versions of the microalgae model are described with multiple nutrient limitation (Baird et al., 2001), with variable C:N ratios (Wild-Allen et al., 2010) and variable C:Chl ratios (Baird et al., 2013). Further, demonstration of the conservation of mass during transport is given in Baird et al. (2004). Here the microalgae model  
 25 is presented with variable C:Chl ratios (with an additional auxiliary pigment), and both nitrogen and phosphorus limitation, and a preference for ammonium uptake when compared to nitrate.

## 5.2 Nitrogen-fixing *Trichodesmium*

The growth of *Trichodesmium* follows the microalgae growth and C:Chl model above, with the following additional processes of nitrogen fixation and physiological-dependent buoyancy adjustment, as described in Robson et al. (2013). Additional parameter values for *Trichodesmium* are given in Table 8.

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$$\frac{\partial N}{\partial t} = -\psi D_N N(1 - R_N^*)(B/m_{B,N}) \quad (42)$$

$$\frac{\partial P}{\partial t} = -\psi D_P P(1 - R_P^*)(B/m_{B,N}) \quad (43)$$

$$\frac{\partial DIC}{\partial t} = -\left(\frac{106}{1060} 12k_I(1 - R_C^*) - \frac{106}{16} \frac{12}{14} \mu_B^{\max} \phi R_C^*\right)(B/m_{B,N}) \quad (44)$$

$$\frac{\partial [O_2]}{\partial t} = \left(\frac{106}{1060} 32k_I(1 - R_C^*) - \frac{106}{16} \frac{32}{14} \mu_B^{\max} \phi R_C^*\right)(B/m_{B,N}) \quad (45)$$

$$\frac{\partial R_N}{\partial t} = \psi D_N N(1 - R_N^*) - \mu_B^{\max} (m_{B,N} + R_N) R_P^* R_N^* R_C^* \quad (46)$$

$$\frac{\partial R_P}{\partial t} = \psi D_P P(1 - R_P^*) - \mu_B^{\max} (m_{B,P} + R_P) R_P^* R_N^* R_C^* \quad (47)$$

$$\frac{\partial R_C}{\partial t} = k_I(1 - R_C^*) - \mu_B^{\max} (m_{B,C} + R_C) R_P^* R_N^* R_C^* - \mu_B^{\max} \phi m_{B,C} R_C^* \quad (48)$$

$$\frac{\partial B}{\partial t} = \mu_B^{\max} R_P^* R_N^* R_C^* B \quad (49)$$

$$\frac{\partial c_i}{\partial t} = k_{\text{Chl}}^{\max} (1 - R_C^*) \bar{\chi} - \mu_P^{\max} R_P^* R_N^* R_C^* c_i \quad (50)$$

$$\psi = 4\pi r \quad (51)$$

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int \alpha_\lambda E_{o,\lambda} d\lambda \quad (52)$$

$$\alpha_\lambda = \pi r^2 \left(1 - \frac{2(1 - (1 + 2\rho_\lambda)e^{-2\rho_\lambda})}{4\rho_\lambda^2}\right) \quad (53)$$

$$\bar{\chi} = \int \chi_\lambda E_{o,\lambda} d\lambda \Big/ \int E_{o,\lambda} d\lambda \quad (54)$$

$$\chi_\lambda = \frac{1}{\pi r^2} \frac{\partial \alpha_\lambda}{\partial \rho_\lambda} = \frac{1 - e^{-2\rho_\lambda} (2\rho_\lambda^2 + 2\rho_\lambda + 1)}{\rho_\lambda^3} \quad (55)$$

$$\rho_\lambda = \gamma c_i r \quad (56)$$


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**Table 6.** Microalgae growth model equations. The term  $B/m_{B,N}$  is the concentration of cells. The equation for organic matter formation gives the stoichiometric constants; 12 g C mol C<sup>-1</sup>; 32 g O mol O<sub>2</sub><sup>-1</sup>. The equations are for scalar irradiance specified as an energy flux.

	Symbol	Value
<i>Constants</i>		
<sup>d</sup> Molecular diffusivity of NO <sub>3</sub>	$D_N$	$f(T, S) \text{ m}^2 \text{ s}^{-1}$
<sup>d</sup> Molecular diffusivity of PO <sub>4</sub>	$D_P$	$f(T, S) \text{ m}^2 \text{ s}^{-1}$
Speed of light	$c$	$2.998 \times 10^8 \text{ m s}^{-1}$
Planck constant	$h$	$6.626 \times 10^{-34} \text{ J s}^{-1}$
Avogadro constant	$A_V$	$6.02 \times 10^{23} \text{ mol}^{-1}$
<sup>a</sup> Pigment-specific absorption coefficient	$\gamma_{\text{pig}, \lambda}$	$f(\text{pig}, \lambda) \text{ m}^{-1} (\text{mg m}^{-3})^{-1}$
<sup>d</sup> Minimum C:Chl ratio	$\theta_{\text{min}}$	20.0 wt/wt
<i>Allometric relationships</i>		
<sup>b</sup> Carbon content	$m_{B,C}$	$12010 \times 9.14 \times 10^3 V \text{ mg C cell}^{-1}$
<sup>c</sup> Maximum intracellular Chl <i>a</i> concentration	$c_i^{\text{max}}$	$2.09 \times 10^7 V^{-0.310} \text{ mg Chl m}^{-3}$
Nitrogen content of phytoplankton	$m_{B,N}$	$\frac{14}{12} \frac{16}{106} m_{B,C} \text{ mg N cell}^{-1}$

**Table 7.** Constants and parameter values used in the microalgae model.  $V$  is cell volume in  $\mu\text{m}^3$ . <sup>a</sup> Figs. 5 & 6 & 7, <sup>b</sup>Straila (1997), <sup>c</sup> Finkel (2001), Sathyendranath et al. (2009) using HPLC-determination which isolate Chl-*a*; <sup>d</sup> Li and Gregory (1974).

### 5.2.1 Nitrogen fixation

Nitrogen fixation occurs when the DIN concentration falls below a critical concentration,  $DIN_{\text{crit}}$ , typically 0.3 to 1.6  $\mu\text{mol L}^{-1}$  (i.e. 4 to 20  $\text{mg N m}^{-3}$ , Robson et al. (2013)), at which point *Trichodesmium* produce nitrogenase to allow fixation of N<sub>2</sub>. It is assumed that nitrogenase becomes available whenever ambient DIN falls below the value of  $DIN_{\text{crit}}$  and carbon and phosphorus are available to support nitrogen uptake. The rate of change of internal reserves of nitrogen,  $R_N$ , due to nitrogen fixation if  $DIN < DIN_{\text{crit}}$  is given by:

$$N_{\text{fix}} = \frac{\partial R_N}{\partial t} \Big|_{N_{\text{fix}}} = \max(4\pi r D_{\text{NO}_3} DIN_{\text{crit}} R_P^* R_C^* (1 - R_N^*) - 4\pi r D_{\text{NO}_3} [\text{NO}_3 + \text{NH}_4] (1 - R_N^*), 0) \quad (57)$$

where  $N_{\text{fix}}$  is the rate of nitrogen fixation per cell and  $r$  is the radius of the individual cell. Using this formulation, *Trichodesmium* is able to maintain its nitrogen uptake rate at that achieved through diffusion limited uptake at  $DIN_{\text{crit}}$  even when  $DIN$  drops below  $DIN_{\text{crit}}$ , provided phosphorus and carbon reserves,  $R_P^*$  and  $R_C^*$  respectively, are available.

The energetic cost of nitrogen fixation is represented as a fixed proportion of carbon fixation,  $f_{N_{\text{fix}}}$ , equivalent to a reduction in quantum efficiency, and as a proportion,  $f_{\text{nitrogenase}}$ , of the nitrogen fixed:

$$\frac{\partial R_C}{\partial t} = -(1 - f_{N_{\text{fix}}})(1 - f_{\text{nitrogenase}})k_I \quad (58)$$

where  $k_I$  is the rate of photon absorption per cell obtain from the microalgal growth model (Table 6).



	Symbol	Value
Maximum growth rate	$\mu^{max}$	0.2 d <sup>-1</sup>
<sup>b</sup> Ratio of xanthophyll to Chl <i>a</i>	$f_{xan}$	0.5
Linear mortality	$m_L$	0.10 d <sup>-1</sup>
Quadratic mortality	$m_Q$	0.10 d <sup>-1</sup> (mg N m <sup>-3</sup> ) <sup>-1</sup>
Cell radius	$r$	5 $\mu$ m
Colony radius	$r_{col}$	5 $\mu$ m
Max. cell density	$\rho_{max}$	1050 kg m <sup>-3</sup>
Min. cell density	$\rho_{min}$	900 kg m <sup>-3</sup>
Critical threshold for N fixation	$DIN_{crit}$	10 mg N m <sup>-3</sup>
Fraction of energy used for nitrogenase	$f_{nitrogenase}$	0.07
Fraction of energy used for N fixation	$f_{Nfix}$	0.33
Nitrogen gas in equilibrium with atm.	[N <sub>2</sub> ]	2 × 10 <sup>4</sup> mg N m <sup>-3</sup>

**Table 8.** Parameter values used in the *Trichodesmium* model (Robson et al., 2013). <sup>b</sup> The major accessory pigments in *Trichodesmium* are the red-ish phycourobilin and phycoerythrobilin (Subramaniam et al., 1999). For simplicity in this model their absorption cross-section is approximated by photosynthetic xanthophyll, which has an absorption peak approximately 10 nm less than the phycourobilin.

### 5.2.2 Buoyancy adjustment

The rate of change of *Trichodesmium* biomass,  $B$ , as a result of density difference between the cell and the water, is approximated by Stokes' Law:

$$\frac{\partial B}{\partial t} = -\frac{2}{9} \frac{gr_{col}^2}{\mu} (\rho - \rho_w) \frac{\partial B}{\partial z} \quad (59)$$

- 5 where  $z$  is the distance in the vertical (+ve up),  $\mu$  is the dynamic viscosity of water,  $g$  is acceleration due to gravity,  $r_{col}$  is the equivalent spherical radius of the sinking mass representing a colony radius,  $\rho_w$  is the density of water, and  $\rho$  is the cell density is given by:

$$\rho = \rho_{min} + R_C^* (\rho_{max} - \rho_{min}) \quad (60)$$

- 10 where  $R_C^*$  is the normalised carbon reserves of the cell (see above), and  $\rho_{min}$  and  $\rho_{max}$  are the densities of the cell when there is no carbon reserves and full carbon reserves respectively. Thus, when light reserves are depleted, the cell is more buoyant, facilitating the retention of *Trichodesmium* in the surface waters.

Variable	Symbol	Units
Ammonium concentration	$[\text{NH}_4]$	$\text{mg N m}^{-3}$
Water column Dissolved Inorganic Carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$
Water column Dissolved Inorganic Phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Water column Particulate Inorganic Phosphorus (PIP)	$PIP$	$\text{mg P m}^{-3}$
Water column Non-Algal Particulates (NAP)	$NAP$	$\text{kg m}^{-3}$
Water column dissolved oxygen concentration	$[\text{O}_2]$	$\text{mg O m}^{-3}$

**Table 9.** State and derived variables for the water column inorganic chemistry model.

### 5.3 Water column inorganic chemistry

#### 5.3.1 Carbon chemistry

The major pools of dissolved inorganic carbon species in the ocean are  $\text{HCO}_3^-$ ,  $\text{CO}_3^-$ , and dissolved  $\text{CO}_2$ , which influence the speciation of  $\text{H}^+$ , and  $\text{OH}^-$  ions, and therefore pH. The interaction of these ions reaches an equilibrium in seawater within a few tens of seconds (Zeebe and Wolf-Gladrow, 2001). In the biogeochemical model here, where calculation timesteps are of order tens of minutes, it is reasonable to assume that the carbon chemistry system is at equilibrium.

The Ocean-Carbon Cycle Model Intercomparison Project (OCMIP) has developed numerical methods to quantify air-sea carbon fluxes and carbon dioxide system equilibria (Najjar and Orr, 1999). Here we use a modified version of the OCMIP-2 Fortran code developed for MOM4 (GFDL Modular Ocean Model version 4, (Griffies et al., 2004)). The OCMIP procedures quantify the state of the carbon dioxide ( $\text{CO}_2$ ) system using two prognostic variables, the concentration of dissolved inorganic carbon,  $DIC$ , and total alkalinity,  $A_T$ . The value of these prognostic variables, along with salinity and temperature, are used to calculate the pH and partial pressure of carbon dioxide,  $p\text{CO}_2$ , in the surface waters using a set of governing chemical equations which are solved using a Newton-Raphson method (Najjar and Orr, 1999).

One alteration from the global implementation of the OCMIP scheme is to increase the search space for the iterative scheme from  $\pm 0.5$  pH units (appropriate for global models) to  $\pm 2.5$ . With this change, the OCMIP scheme converges over a broad range of  $DIC$  and  $A_T$  values (Munhoven, 2013).

For more details see Mongin and Baird (2014); Mongin et al. (2016b).

#### 5.3.2 Nitrification

Nitrification is the oxidation of ammonium with oxygen, to form nitrite followed by the rapid oxidation of these nitrites into nitrates. This is represented in a one step processes, with the rate of nitrification given by:

$$\frac{\partial[\text{NH}_4]}{\partial t} = -\tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]}{K_{nit,O} + [\text{O}_2]} \quad (67)$$

where the equations and parameter values are defined in Tables 10 and 11.



$$\frac{\partial[\text{NH}_4]}{\partial t} = -\tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]}{K_{nit,O} + [\text{O}_2]} \quad (62)$$

$$\frac{\partial[\text{O}_2]}{\partial t} = -2\tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]}{K_{nit,O} + [\text{O}_2]} \quad (63)$$

$$\frac{\partial[\text{NO}_3]}{\partial t} = \tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]}{K_{nit,O} + [\text{O}_2]} \quad (64)$$

$$\frac{\partial P}{\partial t} = \tau_{Pabs} \left( \frac{PIP}{k_{Pads,wc} NAP} - \frac{[\text{O}_2]P}{K_{\text{O}_2,abs} + [\text{O}_2]} \right) \quad (65)$$

$$\frac{\partial PIP}{\partial t} = -\tau_{Pabs} \left( \frac{PIP}{k_{Pads,wc} NAP} - \frac{[\text{O}_2]P}{K_{\text{O}_2,abs} + [\text{O}_2]} \right) \quad (66)$$

**Table 10.** Equations for the water column inorganic chemistry.

Description	Symbol	Units
Maximum rate of nitrification in the water column	$\tau_{nit,wc}$	$0.1 \text{ d}^{-1}$
Oxygen half-saturation constant for nitrification	$K_{nit,O}$	$500 \text{ mg O m}^{-3}$
Rate of P adsorbed/desorbed equilibrium	$\tau_{Pabs}$	$0.04 \text{ d}^{-1}$
Isothermic const. P adsorption for NAP	$k_{Pads,wc}$	$30 \text{ kg NAP}^{-1}$
Oxygen half-saturation for P adsorption	$K_{\text{O}_2,abs}$	$2000 \text{ mg O m}^{-3}$

**Table 11.** Constants and parameter values used in the water column inorganic chemistry.

### 5.3.3 Phosphorus absorption - desorption

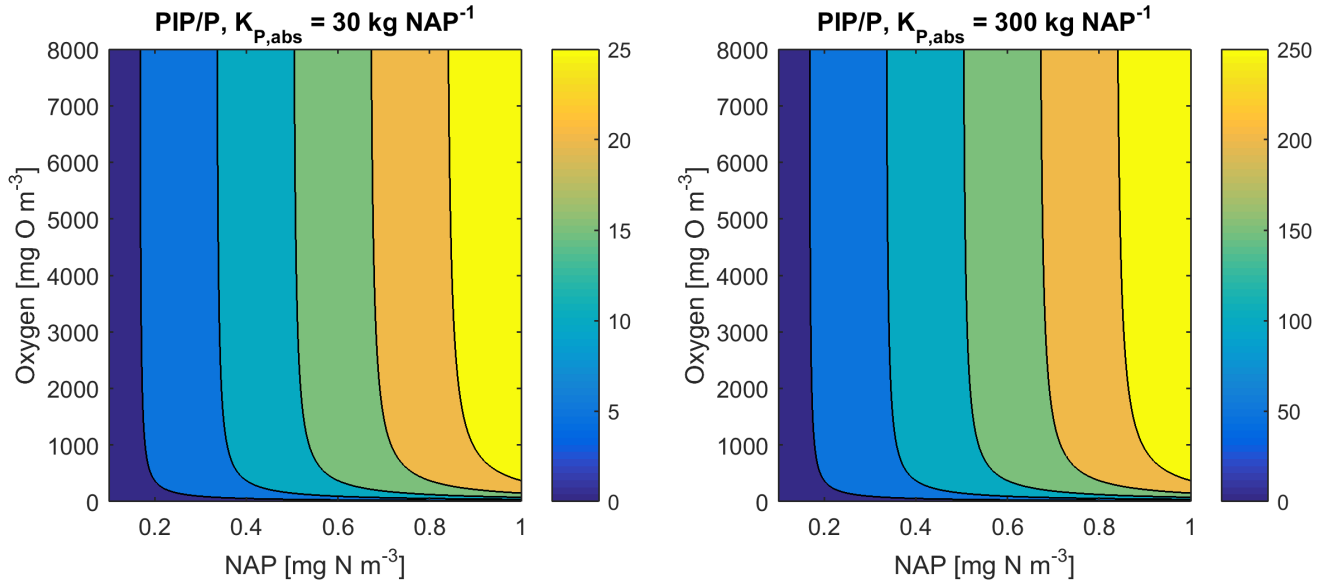
The rate of phosphorus desorption from particulates is given by:

$$\frac{\partial P}{\partial t} = \tau_{Pabs} \left( \frac{PIP}{k_{Pads,wc} NAP} - \frac{[\text{O}_2]P}{K_{\text{O}_2,abs} + [\text{O}_2]} \right) = -\frac{\partial PIP}{\partial t} \quad (68)$$

where  $[\text{O}_2]$  is the concentration of oxygen,  $P$  is the concentration of dissolved inorganic phosphorus,  $PIP$  is the concentration of particulate inorganic phosphorus,  $NAP$  is the sum of the non-algal inorganic particulate concentrations, and  $\tau_{Pabs}$ ,  $k_{Pads,wc}$  and  $K_{\text{O}_2,abs}$  are model parameters described in Table 11.

At steady-state, the  $PIP$  concentration is given by:

$$PIP = k_{Pads,wc} P \frac{[\text{O}_2]}{K_{\text{O}_2,abs} + [\text{O}_2]} NAP \quad (69)$$



**Figure 12.** Phosphorus adsorption - desorption equilibria,  $K_{O_2,abs} = 74 \text{ mg O m}^{-3}$ .

As an example for rivers flowing into the eReefs configuration,  $[O_2] = 7411 \text{ mg m}^{-3}$  (90% saturation at  $T = 25$ ,  $S = 0$ ),  $NAP = 0.231 \text{ kg m}^{-3}$ ,  $k_{Pads,wc} = 30 \text{ kg NAP}^{-1}$ ,  $K_{O_2,abs} = 74 \text{ mg O m}^{-3}$ ,  $P = 4.2 \text{ mg m}^{-3}$ , thus the ratio  $PIP/DIP = 6.86$  (see Fig. 12).

Limited available observations of absorption-desorption include from the Johnstone River (Pailles and Moody, 1992) and the GBR (Monbet et al., 2007).

#### 5.4 Zooplankton herbivory

In the simple food web of the model, herbivory involves small zooplankton consuming small phytoplankton, and large zooplankton consuming large phytoplankton, microphytobenthos and *Trichodesmium*. For simplicity the state variables and equations are only given for small plankton grazing (Tables 12, 14), but the parameters are given for all grazing terms (Table 13).

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The rate of zooplankton grazing is determined by the encounter rate of the predator and all its prey up until the point at which it saturates the growth of the zooplankton (Eq. 77), and then it is constant. This is effectively a Hollings Type I grazing response (Gentleman, 2002). Under the condition of multiple prey types, there is no preferential grazing other than that determined by the chance of encounter. The encounter rate is the result of the relative motion of individuals brought about by diffusive (Eq. 79), swimming (Eq. 80), and shear (Eq. 81) determined relative velocities (Eq. 82) (Jackson, 1995; Baird, 2003). One particular advantage of formulating the encounter rate on individuals is that should the number of populations considered in the model

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change (i.e. an additional phytoplankton class is added), there is no need for empirical coefficients in the model to change. More recent uses of encounter based grazing functions are described in Flynn and Mitra (2016).

5 Unlike the microalgae, zooplankton does not contain reserves of nutrients and fixed carbon, and therefore has a fixed stoichiometry of the Redfield ratio. As the zooplankton are grazing on the phytoplankton that contain internal reserves of nutrients an addition flux of dissolved inorganic nutrients ( $gR_N^*$  for nitrogen) is returned to the water column (for more details see Sec. 5.4.1).

#### 5.4.1 Conservation of mass in zooplankton grazing

It is important to note that the microalgae model presented above represents internal reserves of nutrients, carbon and chlorophyll as a per cell quantity. Using this representation there are no losses of internal quantities with either grazing or mortality. However the implication of their presence is represented in the ( $gR_N^*$ ) terms (Table 14) that return the reserves to the water column. These terms represent the fast return of a fraction of phytoplankton nitrogen due to processes like "sloppy eating".

15 An alternative and equivalent formulation would be to consider total concentration of microalgal reserves in the water column, then the change in water column concentration of reserves due to mortality (either grazing or natural mortality) must be considered. This alternate representation will not be undertaken here as the above considered equations are fully consistent, but it is worth noting that the numerical solution of the model within the EMS package represents total water column concentrations of internal reserves, and therefore must include the appropriate loss terms due to mortality.

#### 5.5 Zooplankton carnivory

Large zooplankton consume small zooplankton. This process uses similar encounter rate and consumption rate limitations calculated for zooplankton herbivory (Table 14). As zooplankton contain no internal reserves, the equations are simplified from the herbivory case to those listed in Table 15). Assuming that the efficiency of herbivory,  $\gamma$ , is equal to that of carnivory, and therefore assigned the same parameter, the additional process of carnivory adds no new parameters to the biogeochemical model.

#### 5.6 Zooplankton respiration

25 In the model there is no change in water column oxygen concentration if organic material is exchanged between pools with the same elemental ratio. Thus, when zooplankton consume phytoplankton no oxygen is consumed due to the consumption of phytoplankton structural material ( $B_P$ ). However, the excess carbon reserves represent a pool of fixed carbon, which when released from the phytoplankton must consume oxygen. Further, zooplankton mortality and growth inefficiency results in detrital production, which when remineralised consumes oxygen. Additionally, carbon released to the dissolved inorganic pool during inefficiency grazing on phytoplankton structural material also consumes oxygen. Thus zooplankton respiration is implicitly captured in these associated processes.

Variable	Symbol	Units
Ammonium concentration	$[\text{NH}_4]$	$\text{mg N m}^{-3}$
Water column dissolved Inorganic Carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$
Water column dissolved Inorganic Phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Water column dissolved oxygen concentration	$[\text{O}_2]$	$\text{mg O m}^{-3}$
Reserves of phytoplankton nitrogen	$R_N$	$\text{mg N cell}^{-1}$
Reserves of phytoplankton phosphorus	$R_P$	$\text{mg P cell}^{-1}$
Reserves of phytoplankton carbon	$R_C$	$\text{mmol photon cell}^{-1}$
Maximum reserves of nitrogen	$R_N^{\text{max}}$	$\text{mg N cell}^{-1}$
Maximum reserves of phosphorus	$R_P^{\text{max}}$	$\text{mg P cell}^{-1}$
Maximum reserves of carbon	$R_C^{\text{max}}$	$\text{mmol photon cell}^{-1}$
Normalised reserves of nitrogen	$R_N^* \equiv R_N / R_N^{\text{max}}$	-
Normalised reserves of phosphorus	$R_P^* \equiv R_P / R_P^{\text{max}}$	-
Normalised reserves of carbon	$R_C^* \equiv R_C / R_C^{\text{max}}$	-
Phytoplankton structural biomass	$B$	$\text{mg N m}^{-3}$
Zooplankton biomass	$Z$	$\text{mg N m}^{-3}$
Detritus at the Redfield ratio	$D_{Red}$	$\text{mg N m}^{-3}$
Zooplankton grazing rate	$g$	$\text{mg N m}^{-3} \text{ s}^{-1}$
Encounter rate coefficient due to molecular diffusion	$\phi_{diff}$	$\text{m}^3 \text{ s}^{-1} \text{ cell Z}^{-1}$
Encounter rate coefficient due to relative motion	$\phi_{rel}$	$\text{m}^3 \text{ s}^{-1} \text{ cell Z}^{-1}$
Encounter rate coefficient due to turbulent shear	$\phi_{shear}$	$\text{m}^3 \text{ s}^{-1} \text{ cell Z}^{-1}$
Phytoplankton cell mass	$m_{B,N}$	$\text{mg N cell}^{-1}$
Zooplankton cell mass	$m_{Z,N}$	$\text{mg N cell}^{-1}$

**Table 12.** State and derived variables for the zooplankton grazing. Zooplankton cell mass,  $m_Z = 16000 \times 14.01 \times 10.5 V_Z \text{ mg N cell}^{-1}$ , where  $V_Z$  is the volume of zooplankton (Hansen et al., 1997).

Description	Symbol	Small	Large
Maximum growth rate of zooplankton at $T_{ref}$ ( $d^{-1}$ )	$\mu_Z$	4.0	1.33
Nominal cell radius of zooplankton ( $\mu m$ )	$r_Z$	5	320
Growth efficiency of zooplankton	$E_Z$	0.462	0.426
Fraction of growth inefficiency lost to detritus	$\gamma_Z$	0.5	0.5
Swimming velocity ( $\mu m s^{-1}$ )	$U_Z$	200	3000
Constants			
Boltzmann's constant	$\kappa$	$1.38066 \times 10^{-23}$	$J K^{-1}$
Viscosity	$\nu$	$10^{-6}$	$m^2 s^{-1}$
Dissipation rate of TKE	$\epsilon$	$10^{-6}$	$m^3 s^{-1}$
Oxygen half-saturation for aerobic respiration	$K_{OA}$	256	$mg O m^{-3}$

**Table 13.** Constants and parameter values used for zooplankton grazing. Dissipation rate of turbulent kinetic energy (TKE) is considered constant.

### 5.7 Non-grazing plankton mortality

The rate of change of plankton biomass,  $B$ , as a result of natural mortality is given by:

$$\frac{\partial B}{\partial t} = -m_L B - m_Q B^2 \quad (91)$$

where  $m_L$  is the linear mortality coefficient and  $m_Q$  is the quadratic mortality coefficient.

- 5 A combination of linear and quadratic mortality rates are used in the model. When the mortality term is the sole loss term, such as zooplankton in the water column or benthic microalgae in the sediments, a quadratic term is employed to represent increasing predation / viral disease losses in dense populations. For suspended microalgae we have used only a linear term (i.e.  $m_Q = 0$ ). Linear terms have been used to represent a basal respiration rate.

As described in Sec 5.1.6, the mortality terms need to account for the internal properties of lost microalgae.

- 10 For definitions of the state variables see Tables 16 & 17.

### 5.8 Air-sea gas exchange

Air-sea gas exchange is calculated using wind speed (we choose a cubic relationship, Wanninkhof and McGillis (1999)), saturation state of the gas (described below) and the Schmidt number of the gas (Wanninkhof, 1992). The transfer coefficient,  $k$ , is given by:

$$15 \quad k = \frac{0.0283}{360000} u_{10}^3 (Sc/660)^{-1/2} \quad (102)$$

where  $0.0283 \text{ cm hr}^{-1}$  is an empirically-determined constant (Wanninkhof and McGillis, 1999),  $u_{10}$  is the short-term steady wind at 10 m above the sea surface [ $m s^{-1}$ ], the Schmidt number,  $Sc$ , is the ratio of the diffusivity of momentum and that of the

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$$\frac{\partial[\text{NH}_4]}{\partial t} = g(1-E)(1-\gamma) + gR_N^* \quad (70)$$

$$\frac{\partial P}{\partial t} = g \frac{1}{16} \frac{31}{14} (1-E)(1-\gamma) + \frac{1}{16} \frac{31}{14} gR_P^* \quad (71)$$

$$\frac{\partial DIC}{\partial t} = g \frac{106}{16} \frac{12}{14} (1-E)(1-\gamma) + \frac{106}{16} \frac{12}{14} gR_C^* \quad (72)$$

$$\frac{\partial B}{\partial t} = -g \quad (73)$$

$$\frac{\partial Z}{\partial t} = Eg \quad (74)$$

$$\frac{\partial D_{Red}}{\partial t} = g(1-E)\gamma \quad (75)$$

$$\frac{\partial [\text{O}_2]}{\partial t} = -\frac{\partial DIC}{\partial t} \frac{32}{12} \frac{[\text{O}_2]}{K_{OA} + [\text{O}_2]} \quad (76)$$

$$g = \min \left[ \mu_Z^{max} Z/E, \frac{Z}{m_{ZL}} (\phi_{diff} + \phi_{rel} + \phi_{shear}) B \right] \quad (77)$$

$$\phi = \phi_{diff} + \phi_{rel} + \phi_{shear} \quad (78)$$

$$\phi_{diff} = (2\kappa T / (3\rho\nu))(1/r_Z + 1/r_B)(r_B + r_Z) \quad (79)$$

$$\phi_{rel} = \pi(r_Z + r_B)^2 U_{eff} \quad (80)$$

$$\phi_{shear} = 1.3\sqrt{\epsilon/\nu}(r_Z + r_B)^3 \quad (81)$$

$$U_{eff} = (U_B^2 + 3U_Z^2)/3U_Z \quad (82)$$


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**Table 14.** Equations for zooplankton grazing. The terms represent a predator  $Z$  consuming a phytoplankton  $B$ . Notes (1) If the zooplankton diet contains multiple phytoplankton classes, and grazing is prey saturated, then phytoplankton loss must be reduced to account for the saturation by other types of microalgae; (2)  $\frac{Z}{m_Z}$  is the number of individual zooplankton; (3) Phytoplankton pigment is lost to water column without being conserved. Chl  $a$  has chemical formulae  $\text{C}_{55}\text{H}_{72}\text{O}_5\text{N}_4\text{Mg}$ , and a molecular weight of  $893.49 \text{ g mol}^{-1}$ . The uptake (and subsequent remineralisation) of molecules for chlorophyll synthesis could make up a maximum (at  $\text{C:Chl} = 20$ ) of  $(660/893)/20$  and  $(56/893)/20 \times (16/106) \times (14/12)$ , or  $\sim 4$  and  $\sim 2$  per cent of the exchange of C and N between the cell and water column, and will cancel out over the lifetime of a cell. Thus the error in ignoring chlorophyll loss to the water column is small.



$$\frac{\partial[\text{NH}_4]}{\partial t} = g(1-E)(1-\gamma) \quad (83)$$

$$\frac{\partial P}{\partial t} = g \frac{1}{16} \frac{31}{14} (1-E)(1-\gamma) \quad (84)$$

$$\frac{\partial DIC}{\partial t} = g \frac{106}{16} \frac{12}{14} (1-E)(1-\gamma) \quad (85)$$

$$\frac{\partial Z_S}{\partial t} = -g \quad (86)$$

$$\frac{\partial Z_L}{\partial t} = Eg \quad (87)$$

$$\frac{\partial D_{Red}}{\partial t} = g(1-E)\gamma \quad (88)$$

$$\frac{\partial [\text{O}_2]}{\partial t} = -\frac{\partial DIC}{\partial t} \frac{32}{12} \frac{[\text{O}_2]}{K_{OA} + [\text{O}_2]} \quad (89)$$

$$g = \min \left[ \mu_{Z_L}^{max} Z_L / E, \frac{Z_L}{m_{Z,N}} (\phi_{diff} + \phi_{rel} \phi_{shear}) Z_S \right] \quad (90)$$

**Table 15.** Equations for zooplankton carnivory, represent large zooplankton  $Z_L$  consuming small zooplankton  $Z_S$ . The parameters values and symbols are given in Table 13 and Table 12

Description	water column		sediment	
	linear	quadratic	linear	quadratic
	$\text{d}^{-1}$	$\text{d}^{-1} (\text{mg N m}^{-3})^{-1}$	$\text{d}^{-1}$	$\text{d}^{-1} (\text{mg N m}^{-3})^{-1}$
Small phytoplankton	0.1	-	1	-
Large phytoplankton	0.1	-	10	-
Microphytobenthos	-	-	-	0.0001
<i>Trichodesmium</i>	0.1	0.1	-	-

**Table 16.** Constants and parameter values used for plankton mortality.

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$$\frac{\partial[\text{NH}_4]}{\partial t} = m_{L,B}BR_N^* \quad (92)$$

$$\frac{\partial DIP}{\partial t} = \frac{1}{16} \frac{31}{14} m_{L,B}BR_P^* \quad (93)$$

$$\frac{\partial DIC}{\partial t} = \frac{106}{16} \frac{12}{14} m_{L,B}BR_C^* \quad (94)$$

$$\frac{\partial[\text{O}_2]}{\partial t} = -\frac{\partial DIC}{\partial t} \frac{32}{12} \frac{[\text{O}_2]}{K_{OA} + [\text{O}_2]} \quad (95)$$

$$\frac{\partial B}{\partial t} = -m_{L,B}B \quad (96)$$

$$\frac{\partial D_{Red}}{\partial t} = m_{L,B}B \quad (97)$$


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**Table 17.** Equations for linear phytoplankton mortality.

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$$\frac{\partial Z_S}{\partial t} = -m_{Q,ZS}Z_S^2 \quad (98)$$

$$\frac{\partial Z_L}{\partial t} = -m_{Q,ZL}Z_L^2 \quad (99)$$

$$\frac{\partial D_{Red}}{\partial t} = f_{Z2det} (m_{Q,ZS}Z_S^2 + m_{Q,ZL}Z_L^2) \quad (100)$$

$$\frac{\partial[\text{NH}_4]}{\partial t} = (1 - f_{Z2det}) (m_{Q,ZS}Z_S^2 + m_{Q,ZL}Z_L^2) \quad (101)$$


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**Table 18.** Equations for the zooplankton mortality.  $f_{Z2det}$  is the fraction of zooplankton mortality that is remineralised, and is equal to 0.5 for both small and large zooplankton.

exchanging gas, and is given by a cubic temperature relationship (Wanninkhof, 1992). Finally, a conversion factor of  $360000 \text{ m s}^{-1} (\text{cm hr}^{-1})^{-1}$  is used.

In practice the hydrodynamic model can contain thin surface layers as the surface elevation moves between z-levels. Further, physical processes of advection and diffusion and gas fluxes are done sequentially, allowing concentrations to build up through a single timestep. To avoid unrealistic changes in the concentration of gases in thin surface layers, the shallowest layer thicker than 20 cm receives all the surface fluxes.

### 5.8.1 Oxygen

The saturation state of oxygen  $[\text{O}_2]_{sat}$  is determined as a function of temperature and salinity following Weiss (1970). The change in concentration of oxygen in the surface layer due to a sea-air oxygen flux (positive from sea to air) is given by:

$$10 \quad \frac{\partial[\text{O}_2]}{\partial t} = k_{\text{O}_2} ([\text{O}_2]_{sat} - [\text{O}_2]) / h \quad (103)$$

where  $k_{\text{O}_2}$  is the transfer coefficient for oxygen (Eq. 102),  $[\text{O}_2]$  is the dissolved oxygen concentration in the surface waters, and  $h$  is the thickness of the surface layer of the model into which sea-air flux flows.

### 5.8.2 Carbon dioxide

The change in surface dissolved inorganic carbon concentration,  $DIC$ , resulting from the sea-air flux (+ve from sea to air) of carbon dioxide is given by:

$$15 \quad \frac{\partial DIC}{\partial t} = k_{\text{CO}_2} ([\text{CO}_2]_{atm} - [\text{CO}_2]) / h \quad (104)$$

where  $k_{\text{CO}_2}$  the transfer coefficient for carbon dioxide (Eq. 102),  $[\text{CO}_2]$  is the dissolved carbon dioxide concentration in the surface waters determined from  $DIC$  and  $A_T$  using the carbon chemistry equilibria calculations described in Sec 5.3.1,  $[\text{CO}_2]_{atm}$  is the partial pressure of carbon dioxide in the atmosphere, and  $h$  is the thickness of the surface layer of the model into which sea-air flux flows.

Note the carbon dioxide flux is not determined by the gradient in  $DIC$ , but the gradient in  $[\text{CO}_2]$ . At pH values around 8,  $[\text{CO}_2]$  makes up only approximately 1/200th of  $DIC$  in seawater, significantly reducing the air-sea exchange. Counteracting this reduced gradient, note that changing  $DIC$  results in an approximately 10 fold change in  $[\text{CO}_2]$  (quantified by the Revelle factor (Zeebe and Wolf-Gladrow, 2001)). Thus, the gas exchange of  $\text{CO}_2$  is approximately  $1/200 \times 10 = 1/20$  of the oxygen flux for the same proportional perturbation in  $DIC$  and oxygen. At a  $Sc$  number of 524 ( $25^\circ\text{C}$  seawater) and a wind speed of  $12 \text{ m s}^{-1}$ , 1 m of water equilibrates with  $\text{CO}_2$  in the atmosphere with an e-folding timescale of approximately 1 day.

## 6 Epibenthic processes

In the model, benthic communities are quantified as a biomass per unit area, or areal biomass. At low biomass, the community is composed of a few specimens spread over a small fraction of the bottom, with no interaction between the nutrient and energy acquisition of individuals. Thus, at low biomass the areal fluxes are a linear function of the biomass.

- 5 As biomass increases, the individuals begin to cover a significant fraction of the bottom. For nutrient and light fluxes that are constant per unit area, such as downwelling irradiance and sediment releases, the flux per unit biomass decreases with increasing biomass. Some processes, such as photosynthesis in a thick seagrass meadow or nutrient uptake by a coral reef, become independent of biomass (Atkinson, 1992) as the bottom becomes completely covered. To capture the non-linear effect of biomass on benthic processes, we use an effective projected area fraction,  $A_{eff}$ .
- 10 To restate, at low biomass, the area on the bottom covered by the benthic community is a linear function of biomass. As the total leaf area approaches and exceeds the projected area, the projected area for the calculation of water-community exchange approaches 1, and becomes independent of biomass. This is represented using:

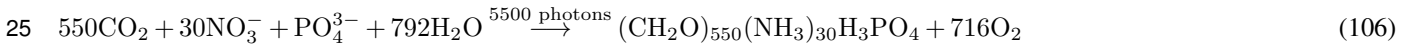
$$A_{eff} = 1 - \exp(-\Omega_B B) \quad (105)$$

- where  $A_{eff}$  is the effective projected area fraction of the benthic community ( $\text{m}^2 \text{m}^{-2}$ ),  $B$  is the biomass of the benthic community ( $\text{g N m}^{-2}$ ), and  $\Omega_B$  is the nitrogen-specific leaf area coefficient ( $\text{m}^2 \text{g N}^{-1}$ ). For further explanation of  $\Omega_B$  see Baird et al. (2016a).

- The parameter  $\Omega_B$  is critical: it provides a means of converting between biomass and fractions of the bottom covered, and is used in calculating the absorption cross-section of the leaf and the nutrient uptake of corals and macroalgae. That  $\Omega_B$  has a simple physical explanation, and can be determined from commonly undertaken morphological measurement (see below), gives us confidence in its use throughout the model.

### 6.1 Macroalgae

The macroalgae model considers the diffusion-limited supply of dissolved inorganic nutrients (N and P) and the absorption of light, delivering N, P and fixed C respectively. Unlike the microalgae model, no internal reserves are considered, implying that the macroalgae has a fixed stoichiometry that can be specified as:



where the stoichiometry is based on Atkinson and Smith (1983) (see also Baird and Middleton (2004); Hadley et al. (2015a, b)). Note that when ammonium is taken up instead of nitrate there is a slightly different  $\text{O}_2$  balance (Sec. 9.1). In the next section will consider the maximum nutrient uptake and light absorption, and then bring them together to determine the realised growth rate.

Variable	Symbol	Units
Downwelling irradiance	$E_d$	$\text{W m}^{-2}$
Macroalgae biomass	$MA$	$\text{g N m}^{-2}$
Water column detritus, C:N:P = 550:30:1	$D_{Atk}$	$\text{g N m}^{-3}$
Effective projected area of macroalgae	$A_{eff}$	$\text{m}^2 \text{m}^{-2}$
Leaf-specific absorptance	$A_{L,\lambda}$	-
Bottom stress	$\tau$	$\text{N m}^{-2}$
Wavelength	$\lambda$	nm
Bottom water layer thickness	$h_{wc}$	m

**Table 19.** State and derived variables for the macroalgae model. For simplicity in the equations all dissolved constituents are given in grams, although elsewhere they are shown in milligrams.

### 6.1.1 Nutrient uptake

Nutrient uptake by macroalgae is a function of nutrient concentration, water motion (Hurd, 2000) and internal physiology. The maximum flux of nutrients is specified as a mass transfer limit per projected area of macroalgae and is given by (Falter et al., 2004; Zhang et al., 2011):

$$5 \quad S_x = 2850 \left( \frac{2\tau}{\rho} \right)^{0.38} \text{Sc}_x^{-0.6}, \text{Sc}_x = \frac{\nu}{D_x} \quad (107)$$

where  $S_x$  is the mass transfer rate coefficient of element  $x = \text{N, P}$ ,  $\tau$  is the shear stress on the bottom,  $\rho$  is the density of water and  $\text{Sc}_x$  is the Schmidt number. The Schmidt number is the ratio of the diffusivity of momentum,  $\nu$ , and mass,  $D_x$  (Tab. 7), and varies with temperature, salinity and nutrient species. The rate constant  $S$  can be thought of as the height of water cleared of mass per unit of time by the water-macroalgae exchange.

### 10 6.1.2 Light capture

The calculation of light capture by macroalgae involves estimating the fraction of light that is incident upon the leaves, and the fraction that is absorbed. The rate of photon capture is given by:

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int E_{d,\lambda} (1 - \exp(-A_{L,\lambda} \Omega_{MA} MA)) \lambda d\lambda \quad (108)$$

where  $h$ ,  $c$  and  $A_V$  are fundamental constants,  $10^9 \text{ nm m}^{-1}$  accounts for the typical representation of wavelength,  $\lambda$  in nm, and  $A_{L,\lambda}$  is the spectrally-resolved leaf-specific absorptance. As shown in Eq. 105, the term  $1 - \exp(-\Omega_{MA} MA)$  gives the effective projected area fraction of the community. In the case of light absorption of macroalgae, the exponent is multiplied by the leaf-specific absorptance,  $A_{L,\lambda}$ , to account for the transparency of the leaves. At low macroalgae biomass, absorption

at wavelength  $\lambda$  is equal to  $E_{d,\lambda}A_{L,\lambda}\Omega_{MA}MA$ , increasing linearly with biomass as all leaves at low biomass are exposed to full light (i.e. there is no self-shading). At high biomass, the absorption by the community asymptotes to  $E_{d,\lambda}$ , at which point increasing biomass does not increase the absorption as all light is already absorbed.

For more details on the calculation of  $\Omega_{MA}$  see Baird et al. (2016a).

### 5 6.1.3 Growth

The growth rate combines nutrient, light and maximum organic matter synthesis rates following:

$$\mu_{MA} = \min \left[ \mu_{MA}^{max}, \frac{30}{5500} 14 \frac{k_I}{MA}, \frac{S_N A_{eff} N}{MA}, \frac{30}{1} \frac{14}{31} \frac{S_P A_{eff} P}{MA} \right] \quad (109)$$

and the production of macroalgae is given by  $\mu_{MA}MA$ . We have used the commonly applied multiple minimum function (von Liebig, 1840), although it is noted that others use the multiple of limitation terms (Fasham, 1993). The microalgae model described above uses dynamical reserves to determine the growth rate. The growth approximated using dynamical reserves closer approximates a multiple minimum function than a multiple of minimum terms, so it was deemed more appropriate to use a multiple minimum function for macroalgae and seagrass for which internal reserves were not resolved.

As per seagrass, that the maximum growth rates sits within the minimum operator. This allows the growth of macroalgae to be independent of temperature at low light, but still have an exponential dependence at maximum growth rates (Baird et al., 2003).

### 6.1.4 Mortality

Mortality is defined as a simple linear function of biomass:

$$\frac{\partial MA}{\partial t} = -\zeta_{MA}MA \quad (121)$$

A quadratic formulation is not necessary as both the nutrient and light capture rates become independent of biomass as  $MA \gg 1/\Omega_{MA}$ . Thus the steady-state biomass of macroalgae under nutrient limitation is given by:

$$(MA)_{SS} = \frac{S_N A_{eff} N}{\zeta} \quad (122)$$

and for light-limited growth by:

$$(MA)_{SS} = \frac{k_I}{\zeta} \quad (123)$$

The full macroalgae equations, parameters and symbols are listed in Tables 19, 20 and 21.

$$\frac{\partial N}{\partial t} = -\mu_{MA}MA/h_{wc} \quad (110)$$

$$\frac{\partial P}{\partial t} = -\frac{1}{30} \frac{31}{14} \mu_{MA}MA/h_{wc} \quad (111)$$

$$\frac{\partial DIC}{\partial t} = -\frac{550}{30} \frac{12}{14} \mu_{MA}MA/h_{wc} \quad (112)$$

$$\frac{\partial [O_2]}{\partial t} = \frac{716}{30} \frac{32}{14} (\mu_{MA}MA)/h_{wc} \quad (113)$$

$$\frac{\partial MA}{\partial t} = \mu_{MA}MA - \zeta_{MA}MA \quad (114)$$

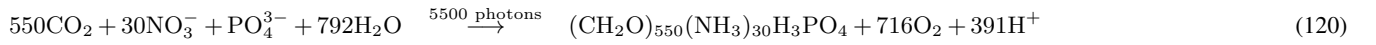
$$\frac{\partial D_{Atk}}{\partial t} = \zeta_{MA}MA/h_{wc} \quad (115)$$

$$\mu_{MA} = \min \left[ \mu_{MA}^{max}, \frac{30}{5500} 14 \frac{k_I}{MA}, \frac{S_N A_{eff} N}{MA}, \frac{30}{1} \frac{14}{31} \frac{S_P A_{eff} P}{MA} \right] \quad (116)$$

$$S_x = 2850 \left( \frac{2\tau}{\rho} \right)^{0.38} Sc^{-0.6}, S_c = \frac{\nu}{D_x} \quad (117)$$

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int E_{d,\lambda} (1 - \exp(-A_{L,\lambda} \Omega_{MA} MA)) \lambda d\lambda \quad (118)$$

$$A_{eff} = 1 - \exp(-\Omega_{MA} MA) \quad (119)$$



**Table 20.** Equations for the macroalgae model. Other constants and parameters are defined in Table 21. 14 g N mol N<sup>-1</sup>; 12 g C mol C<sup>-1</sup>; 31 g P mol P<sup>-1</sup>; 32 g O mol O<sub>2</sub><sup>-1</sup>. Uptake shown here is for nitrate, see Sec. 9.1 for ammonium uptake.

	Symbol	Value	Units
<i>Parameters</i>			
Maximum growth rate of macroalgae	$\mu_{MA}^{max}$	1.0	d <sup>-1</sup>
Nitrogen-specific area of macroalgae	$\Omega_{MA}$	1.0	(g N m <sup>-2</sup> ) <sup>-1</sup>
<sup>a</sup> Leaf-specific absorptance	$A_{L,\lambda}$	~ 0.7	-
Mortality rate	$\zeta_{MA}$	0.01	d <sup>-1</sup>

**Table 21.** Constants and parameter values used to model macroalgae. <sup>a</sup>Spectrally-resolved values

Variable	Symbol	Units
Downwelling irradiance	$E_d$	$\text{W m}^{-2}$
Porewater DIN concentration	$N_s$	$\text{g N m}^{-3}$
Porewater DIP concentration	$P_s$	$\text{g P m}^{-3}$
Water column DIC concentration	$DIC$	$\text{g C m}^{-3}$
Water column oxygen concentration	$[O_2]$	$\text{g O m}^{-3}$
Above-ground seagrass biomass	$SG_A$	$\text{g N m}^{-2}$
Below-ground seagrass biomass	$SG_B$	$\text{g N m}^{-2}$
Detritus at 550:30:1 in sediment	$D_{Atk, sed}$	$\text{g N m}^{-3}$
Effective projected area of seagrass	$A_{eff}$	$\text{m}^2 \text{ m}^{-2}$
Bottom stress	$\tau$	$\text{N m}^{-2}$
Thickness of sediment layer $l$	$h_{s,l}$	m
Bottom water layer thickness	$h_{wc}$	m
Wavelength	$\lambda$	nm
Translocation rate	$\Upsilon$	$\text{g N m}^{-2} \text{ s}^{-1}$
Porosity	$\phi$	-

**Table 22.** State and derived variables for the seagrass model. For simplicity in the equations all dissolved constituents are given in grams, although elsewhere they are shown in milligrams. The bottom water column thickness varies is spatially-variable, depending on bathymetry.

## 6.2 Seagrass

Seagrasses are quantified per  $\text{m}^2$  with a constant stoichiometry (C:N:P = 550:30:1) for both above-ground,  $SG_A$ , and below-ground,  $SG_B$ , biomass, and can translocate organic matter at this constant stoichiometry between the two stores of biomass. Growth occurs only in the above-ground biomass, but losses (grazing, decay etc.) occur in both. Multiple seagrass varieties are represented. The varieties are modelled using the same equations for growth, respiration and mortality, but with different parameter values.



$$\frac{\partial N_w}{\partial t} = - \left( \mu_{SG} - \frac{\mu_{SG}^{max} \bar{N}_s}{K_{SG,N} + \bar{N}_s} \right) / h_{wc} \quad (124)$$

$$\frac{\partial P_w}{\partial t} = - \left( \frac{1}{30} \frac{31}{14} \mu_{SG} - \frac{\mu_{SG}^{max} \bar{P}_s}{K_{SG,P} + \bar{P}_s} \right) / h_{wc} \quad (125)$$

$$\frac{\partial N_{s,l}}{\partial t} = -f_{N,l} / (h_{s,l} \phi_l) \quad (126)$$

$$\frac{\partial P_{s,l}}{\partial t} = -\frac{1}{30} \frac{31}{14} f_{P,l} / (h_{s,l} \phi_l) \quad (127)$$

$$\frac{\partial DIC}{\partial t} = -\frac{550}{30} \frac{12}{14} (\mu_{SG_A} SG_A) / h_{wc} \quad (128)$$

$$\frac{\partial [O_2]}{\partial t} = \frac{716}{30} \frac{32}{14} (\mu_{SG_A} SG_A) / h_{wc} \quad (129)$$

$$\frac{\partial SG_A}{\partial t} = \mu_{SG_A} SG_A - (\zeta_{SG_A} + \zeta_{SG,\tau}) \left( SG_A - \frac{f_{seed}}{\Omega_{SG}} (1 - f_{below}) \right) - \Upsilon \quad (130)$$

$$\frac{\partial SG_B}{\partial t} = -(\zeta_{SG_B} + \zeta_{SG,\tau}) \left( SG_B - \frac{f_{seed}}{\Omega_{SG}} f_{below} \right) + \Upsilon \quad (131)$$

$$\begin{aligned} \frac{\partial D_{Atk,seed}}{\partial t} &= \left( (\zeta_{SG_A} + \zeta_{SG,\tau}) \left( SG_A - \frac{f_{seed}}{\Omega_{SG}} (1 - f_{below}) \right) \right) / (h_{sed} \phi) \\ &+ \left( (\zeta_{SG_B} + \zeta_{SG,\tau}) \left( SG_B - \frac{f_{seed}}{\Omega_{SG}} f_{below} \right) \right) / (h_{sed} \phi) \end{aligned} \quad (132)$$

$$\mu_{SG_A} = \min \left[ \frac{\mu_{SG}^{max} \bar{N}_s}{K_{SG,N} + \bar{N}_s} + S_{NA_{eff}} N, \frac{\mu_{SG}^{max} \bar{P}_s}{K_{SG,P} + \bar{P}_s} + S_{PA_{eff}} P, \frac{30}{5500} 14 \frac{\max(0, k_I - k_{resp})}{SG_A} \right] \quad (133)$$

$$\bar{N}_s = \frac{\sum_{l=1}^L N_{s,l} h_{s,l} \phi_l}{\sum_{l=1}^L h_{s,l} \phi_l} \quad (134)$$

$$\bar{P}_s = \frac{\sum_{l=1}^L P_{s,l} h_{s,l} \phi_l}{\sum_{l=1}^L h_{s,l} \phi_l} \quad (135)$$

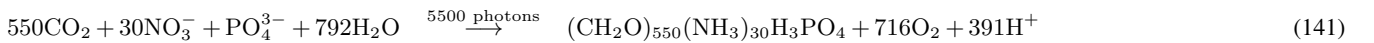
$$f_{N,l} = \frac{N_{s,l} h_{s,l} \phi_l}{\sum_{l=1}^L N_{s,l} h_{s,l} \phi_l} \mu_{SG} SG_A \quad (136)$$

$$f_{P,l} = \frac{P_{s,l} h_{s,l} \phi_l}{\sum_{l=1}^L P_{s,l} h_{s,l} \phi_l} \mu_{SG} SG_A \quad (137)$$

$$k_I = \frac{(10^9 h_C)^{-1}}{A_V} \int E_{d,\lambda} (1 - \exp(-A_{L,\lambda} \Omega_{SG} SG_A \sin \beta_{blade})) \lambda d\lambda \quad (138)$$

$$k_{resp} = 2 \left( E_{comp} A_L \Omega_{SG} \sin \beta_{blade} - \frac{5500}{30} \frac{1}{14} \zeta_{SG_A} \right) SG_A \quad (139)$$

$$\Upsilon = \left( f_{below} - \frac{SG_B}{SG_B + SG_A} \right) (SG_A + SG_B) \tau_{tran} \quad (140)$$



**Table 23.** Equations for the seagrass model. Other constants and parameters are defined in Table 24. The equation for organic matter formation gives the stoichiometric constants; 14 g N mol N<sup>-1</sup>; 12 g C mol C<sup>-1</sup>; 31 g P mol P<sup>-1</sup>; 32 g O mol O<sub>2</sub><sup>-1</sup>.

	Symbol	<i>Zostera capricorni</i>		<i>Halophila ovalis</i>		<i>Halophila decipens</i>		Units
<i>Parameters</i>								
<sup>a</sup> Maximum growth rate of seagrass	$\mu_{SG}^{max}$	0.4	0.4	0.4	0.4	0.4	0.4	d <sup>-1</sup>
<sup>b</sup> Nitrogen-specific area of seagrass	$\Omega_{SG}$	1.5	1.9	1.9	1.9	1.9	1.9	(g N m <sup>-2</sup> ) <sup>-1</sup>
<sup>c</sup> Leaf-specific absorbance	$A_{L,\lambda}$	~ 0.7	~ 0.7	~ 0.7	~ 0.7	~ 0.7	~ 0.7	-
<sup>d</sup> Fraction biomass below ground	$f_{below}$	0.75	0.25	0.25	0.5	0.5	0.5	-
<sup>e</sup> Translocation rate	$\tau_{tran}$	0.033	0.033	0.033	0.033	0.033	0.033	d <sup>-1</sup>
<sup>f</sup> Half-saturation P uptake	$K_{SG,P}$	96	96	96	96	96	96	mg P m <sup>-3</sup>
<sup>g</sup> Half-saturation N uptake	$K_{SG,N}$	420	420	420	420	420	420	mg N m <sup>-3</sup>
<sup>h</sup> Compensation scalar PAR irradiance	$E_{comp}$	4.5	2.0	2.0	1.5	1.5	1.5	mol photon m <sup>-2</sup> d <sup>-1</sup>
<sup>h</sup> Leaf loss rate	$\zeta_{SG,A}$	0.04	0.08	0.08	0.06	0.06	0.06	d <sup>-1</sup>
<sup>h</sup> Root loss rate	$\zeta_{SG,B}$	0.004	0.004	0.004	0.004	0.004	0.004	d <sup>-1</sup>
Seed biomass as a fraction of 63 % cover	$f_{seed}$	0.01	0.01	0.01	0.01	0.01	0.01	-
<sup>i</sup> Seagrass root depth	$z_{root}$	0.15	0.08	0.08	0.05	0.05	0.05	m
Sine of nadir canopy bending angle	$\sin \beta_{blade}$	0.5	1.0	1.0	1.0	1.0	1.0	-
Mortality critical shear stress	$\tau_{SG,shear}$	1.0	1.0	1.0	1.0	1.0	1.0	N m <sup>-2</sup>
Mortality shear stress time-scale	$\tau_{SG,time}$	0.5	0.5	0.5	0.5	0.5	0.5	d
Max. shear stress loss rate	$\zeta_{SG,\tau}^{max}$	2	2	2	2	2	2	d <sup>-1</sup>

**Table 24.** Constants and parameter values used to model seagrass. <sup>a</sup>  $\times 2$  for nighttime  $\times 2$  for roots; <sup>b</sup> *Zostera* - calculated from leaf characteristics in (Kemp et al., 1987; Hansen et al., 2000), *Halophila ovalis* - calculated from leaf dimensions in Vermaat et al. (1995) -  $\Omega_{SG}$  can also be determined from specific leaf area such as determined in Cambridge and Lamberts (1998) for 9 Australian seagrass species; <sup>c</sup> Spectrally-resolved values in Baird et al. (2016a); <sup>d</sup> Duarte and Chiscano (1999); <sup>e</sup> loosely based on Kaldy et al. (2013); <sup>f</sup> *Thalassia testudinum* Gras et al. (2003); <sup>g</sup> *Thalassia testudinum* (Lee and Dunton, 1999); <sup>h</sup> Chartrand et al. (2012); Longstaff (2003); Chartrand et al. (2017); <sup>i</sup> Roberts (1993).

Here we present just the equations for the seagrass submodel. A description of the seagrass processes of growth, translocation between roots and leaves, and mortality has been published in Baird et al. (2016a), along with a comparison to observations from Gladstone Harbour on the northeast Australian coast.

### 6.3 Coral polyps

5 The coral polyp parameterisation consists of a microalgae growth model to represent zooxanthellae growth based on Baird et al. (2013), and the parameterisation of coral - zooxanthellae interaction based on the host - symbiont model of Gustafsson et al. (2013), a new photoadaptation, photoinhibition and reaction centre dynamics models. The extra detail on the zooxanthellae photosystem is required due to its important role in thermal-stress driven coral bleaching (Yonge, 1930; Suggett et al., 2008).

#### 6.3.1 Coral host, symbiont and the environment

10 The state variables for the coral polyp model (Table 25) include the biomass of coral tissue,  $CH$  ( $\text{g N m}^{-2}$ ), and the structure material of the zooxanthellae cells,  $CS$  ( $\text{mg N m}^{-2}$ ). The structure material of the zooxanthellae,  $CS$ , in addition to nitrogen, contains carbon and phosphorus at the Redfield ratio. The zooxanthellae cells also contain reserves of nitrogen,  $R_N$  ( $\text{mg N m}^{-2}$ ), phosphorus,  $R_P$  ( $\text{mg P m}^{-2}$ ), and carbon,  $R_C$  ( $\text{mg C m}^{-2}$ ).

15 The zooxanthellae light absorption capability is resolved by considering the time-varying concentrations of pigments chlorophyll  $a$ ,  $Chl$ , diadinoxanthin,  $X_p$ , and diatoxanthin  $X_h$ , for which the state variable represents the areal concentration. A further three pigments, chlorophyll  $c_2$ , peridinin, and  $\beta$ -carotene are considered in the absorption calculations, but their concentrations are in fixed ratios to chlorophyll  $a$ . Exchanges between the coral community and the overlying water can alter the water column concentrations of dissolved inorganic carbon,  $DIC$ , nitrogen,  $N$ , and phosphorus,  $P$ , as well as particulate phytoplankton,  $B$ , zooplankton,  $Z$ , and detritus,  $D$ , where multiple nitrogen, plankton and detritus types are resolved (Table 25).

20 The coral host is able to assimilate particulate organic nitrogen either through translocation from the zooxanthellae cells or through the capture of water column organic detritus and/or plankton. The zooxanthellae varies its intracellular pigment content depending on potential light limitation of growth, and the incremental benefit of adding pigment, allowing for the package effect (Baird et al., 2013). The coral tissue is assumed to have a Redfield C:N:P stoichiometry (Redfield et al., 1963), as shown by Muller-Parker et al. (1994). The zooxanthellae are modelled with variable C:N:P ratios (Muller-Parker et al., 25 1994), based on a structure material at the Redfield ratio, but with variable internal reserves. The fluxes of C, N and P with the overlying water column (nutrient uptake and detrital / mucus release) can therefore vary from the Redfield ratio.

An explanation of the individual processes follows, with tables in the Appendix listing all the model state variables (Table 25), derived variables (Table 26), equations (Tables 27, 28, 29 and 30), and parameters values (Tables 31 and 32).

30 Here we present just the equations for the coral submodel. The description of the coral processes has been published in Baird et al. (2018), along with a comparison to observations from the Great Barrier Reef on the northeast Australian coast. The effect of coral calcification on water column properties is described below.

Variable	Symbol	Units
Dissolved inorganic nitrogen (DIN)	$N$	$\text{mg N m}^{-3}$
Dissolved inorganic phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Zooxanthellae biomass	$CS$	$\text{mg N m}^{-2}$
Reserves of nitrogen	$R_N$	$\text{mg N cell}^{-1}$
Reserves of phosphorus	$R_P$	$\text{mg P cell}^{-1}$
Reserves of carbon	$R_C$	$\text{mg C cell}^{-1}$
Coral biomass	$CH$	$\text{g N m}^{-2}$
Suspended phytoplankton biomass	$B$	$\text{mg N m}^{-3}$
Suspended zooplankton biomass	$Z$	$\text{mg N m}^{-3}$
Suspended detritus at 106:16:1	$D_{Red}$	$\text{mg N m}^{-3}$
Macroalgae biomass	$MA$	$\text{mg N m}^{-3}$
Temperature	$T$	$^{\circ}\text{C}$
Absolute salinity	$S_A$	$\text{kg m}^{-3}$
zooxanthellae chlorophyll $a$ concentration	$Chl$	$\text{mg m}^{-2}$
zooxanthellae diadinoxanthin concentration	$X_p$	$\text{mg m}^{-2}$
zooxanthellae diatoxanthin concentration	$X_h$	$\text{mg m}^{-2}$
Oxidised reaction centre concentration	$Q_{ox}$	$\text{mg m}^{-2}$
Reduced reaction centre concentration	$Q_{red}$	$\text{mg m}^{-2}$
Inhibited reaction centre concentration	$Q_{in}$	$\text{mg m}^{-2}$
Reactive oxygen species concentration	$[\text{ROS}]$	$\text{mg m}^{-2}$
Chemical oxygen demand	$COD$	$\text{mg O}_2 \text{ m}^{-3}$

**Table 25.** Model state variables for the coral polyp model. Note that water column variables are 3 dimensional, benthic variables are 2 dimensional, and unnormalised reserves are per cell.

### 6.3.2 Coral calcification

The rate of coral calcification is a function of the water column aragonite saturation,  $\Omega_a$ , and the normalised reserves of fixed carbon in the symbiont,  $R_C^*$ . The rates of change of DIC and total alkalinity,  $A_T$ , in the bottom water column layer of thickness  $h_{wc}$  due to calcification becomes:

$$5 \quad \frac{\partial DIC}{\partial t} = -12gA_{eff}/h_{wc} \quad (186)$$

$$\frac{\partial A_T}{\partial t} = -2gA_{eff}/h_{wc} \quad (187)$$

Variable	Symbol	Units
Downwelling irradiance	$E_d$	$\text{W m}^{-2}$
Maximum reserves of nitrogen	$R_N^{\max}$	$\text{mg N cell}^{-1}$
Maximum reserves of phosphorus	$R_P^{\max}$	$\text{mg P cell}^{-1}$
Maximum reserves of carbon	$R_C^{\max}$	$\text{mg C cell}^{-1}$
Normalised reserves of nitrogen	$R_N^* \equiv R_N/R_N^{\max}$	-
Normalised reserves of phosphorus	$R_P^* \equiv R_P/R_P^{\max}$	-
Normalised reserves of carbon	$R_C^* \equiv R_C/R_C^{\max}$	-
Intracellular chlorophyll <i>a</i> concentration	$c_i$	$\text{mg m}^{-3}$
Intracellular diadinoxanthin concentration	$x_p$	$\text{mg m}^{-3}$
Intracellular diatoxanthin concentration	$x_h$	$\text{mg m}^{-3}$
Total reaction centre concentration	$Q_T$	$\text{mg m}^{-2}$
Total active reaction centre concentration	$Q_a$	$\text{mg m}^{-2}$
Concentration of zooxanthellae cells	$n$	$\text{cell m}^{-2}$
Thickness of the bottom water column layer	$h_{wc}$	m
Effective projected area fraction	$A_{eff}$	$\text{m}^2 \text{m}^{-2}$
Area density of zooxanthellae cells	$n_{CS}$	$\text{cell m}^{-2}$
Absorption cross-section	$\alpha$	$\text{m}^2 \text{cell}^{-1}$
Rate of photon absorption	$k_I$	$\text{mol photon cell}^{-1} \text{s}^{-1}$
Photon-weighted average opaqueness	$\bar{\chi}$	-
Maximum Chl. synthesis rate	$k_{\text{Chl}}^{\max}$	$\text{mg Chl m}^{-3} \text{d}^{-1}$
Density of water	$\rho$	$\text{kg m}^{-3}$
Bottom stress	$\tau$	$\text{N m}^{-2}$
Schmidt number	$Sc$	-
Mass transfer rate coefficient for particles	$S_{part}$	$\text{m d}^{-1}$
Heterotrophic feeding rate	$G$	$\text{g N m}^{-2} \text{d}^{-1}$
Wavelength	$\lambda$	nm
Translocation fraction	$f_{tran}$	-
Active fraction of oxidised reaction centres	$a_{Q_{ox}}^*$	-

**Table 26.** Derived variables for the coral polyp model.

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$$\frac{\partial N}{\partial t} = -S_N N(1 - R_N^*) A_{eff} \quad (142)$$

$$\frac{\partial P}{\partial t} = -S_P P(1 - R_P^*) A_{eff} \quad (143)$$

$$\frac{\partial DIC}{\partial t} = - \left( \frac{106}{1060} 12 k_I \frac{Q_{ox}}{Q_T} a_{Q_{ox}}^* (1 - R_C^*) - \frac{106}{16} \frac{12}{14} \mu_{CS}^{\max} \phi R_C^* \right) (CS/m_{B,N}) \quad (144)$$

$$\frac{\partial [O_2]}{\partial t} = \left( \frac{106}{1060} 32 k_I \frac{Q_{ox}}{Q_T} a_{Q_{ox}}^* (1 - R_C^*) - \frac{106}{16} \frac{32}{14} \mu_{CS}^{\max} \phi R_C^* \right) (CS/m_{B,N}) \quad (145)$$

$$\frac{\partial R_N}{\partial t} = S_N N(1 - R_N^*) / (CS/m_{B,N}) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_{B,N} + R_N) \quad (146)$$

$$\frac{\partial R_P}{\partial t} = S_P P(1 - R_P^*) / (CS/m_{B,N}) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_{B,P} + R_P) \quad (147)$$

$$\frac{\partial R_C}{\partial t} = k_I \left( \frac{Q_{ox}}{Q_T} \right) a_{Q_{ox}}^* (1 - R_C^*) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_{B,C} + R_C) - \mu_{CS}^{\max} \phi m_{B,C} R_C^* \quad (148)$$

$$\frac{\partial CS}{\partial t} = \mu_{CS}^{\max} R_P^* R_N^* R_C^* CS - \zeta_{CS} CS \quad (149)$$

$$\frac{\partial c_i}{\partial t} = (k_{Chl}^{\max} (1 - R_C^*) (1 - Q_{in}/Q_T) \bar{\chi} - \mu_P^{\max} R_P^* R_N^* R_C^* c_i) (CS/m_{B,N}) \quad (150)$$

$$\frac{\partial X_p}{\partial t} = \Theta_{xan2chl} (k_{Chl}^{\max} (1 - R_C^*) (1 - Q_{in}/Q_T) \bar{\chi}) - 8(Q_{in}/Q_T - 0.5)^3 \tau_{xan} \Phi(X_p + X_h) \quad (151)$$

$$\frac{\partial X_h}{\partial t} = 8(Q_{in}/Q_T - 0.5)^3 \tau_{xan} \Phi(X_p + X_h) \quad (152)$$

$$\frac{\partial CS}{\partial t} = (1 - f_{tran}) \mu_{CS} CS - \zeta_{CS} CS + f_{remin} \frac{\zeta_{CH}}{A_{eff}} CH^2 \quad (154)$$

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int \alpha_\lambda E_{d,\lambda} d\lambda \quad (155)$$

$$S_x = 2850 \left( \frac{2\tau}{\rho} \right)^{0.38} S_{c_x}^{-0.6}, S_{c_x} = \frac{\nu}{D_x} \quad (156)$$

$$\Phi = 1 - 4 \left( \frac{X_p}{X_p + X_h} - 0.5 \right)^2 \text{ or } \Phi = 1 \quad (157)$$


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**Table 27.** Equations for the interactions of coral host, symbiont and environment excluding bleaching loss terms that appear in Table 30. The term  $CS/m_{B,N}$  is the concentration of zoothaxellae cells. The equation for organic matter formation gives the stoichiometric constants; 12 g C mol C<sup>-1</sup>; 32 g O mol O<sub>2</sub><sup>-1</sup>.

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$$\frac{\partial CH}{\partial t} = G' - \frac{\zeta_{CH}}{A_{eff}} CH^2 \quad (158)$$

$$\frac{\partial B}{\partial t} = -S_{part} A_{eff} B \frac{G'}{G} / h_{wc} \quad (159)$$

$$\frac{\partial Z}{\partial t} = -S_{part} A_{eff} Z \frac{G'}{G} / h_{wc} \quad (160)$$

$$\frac{\partial D_{Red}}{\partial t} = \left( -S_{part} A_{eff} D_{Red} \frac{G'}{G} + (1 - f_{remin}) \frac{\zeta_{CH}}{A_{eff}} CH^2 \right) / h_{wc} \quad (161)$$

$$f_{tran} = \frac{\pi r_{CS}^2 n_{CS}}{2CH\Omega_{CH}} \quad (162)$$

$$G = S_{part} A_{eff} (B + Z + D_{Red}) \quad (163)$$

$$G' = \min[\min[\mu_{CH}^{max} CH - f_{tran} \mu_{CS} CS - \zeta_{CS} CS, 0], G] \quad (164)$$

$$A_{eff} = 1 - \exp(-\Omega_{CH} CH) \quad (165)$$


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**Table 28.** Equations for the coral polyp model. The term  $CS/m_{B,N}$  is the concentration of zoothaxellae cells. The equation for organic matter formation gives the stoichiometric constants; 12 g C mol  $C^{-1}$ ; 32 g O mol  $O_2^{-1}$ . Other constants and parameters are defined in Table 32.

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$$\frac{\partial Q_{ox}}{\partial t} = -k_{In} m_{RCH} \left( \frac{Q_{ox}}{Q_T} \right) (1 - a_{Q_{ox}}^* (1 - R_C^*)) + f_2(T) R_N^* R_P^* R_C^* Q_{in} \quad (166)$$

$$\frac{\partial Q_{red}}{\partial t} = k_{In} m_{RCH} \left( \frac{Q_{ox}}{Q_T} \right) (1 - a_{Q_{ox}}^* (1 - R_C^*)) - k_{In} m_{RCH} \frac{Q_{red}}{Q_T} \quad (167)$$

$$\frac{\partial Q_{in}}{\partial t} = -268 m_{RCH} Q_{in} + k_{In} m_{RCH} \frac{Q_{red}}{Q_T} \quad (168)$$

$$\frac{\partial [ROS]}{\partial t} = -f(T) R_N^* R_P^* R_C^* [ROS] + 32 \frac{1}{10} k_{In} m_{RCH} \left( \frac{Q_{in}}{Q_T} \right) \quad (169)$$


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**Table 29.** Equations for symbiont reaction centre dynamics. Bleaching loss terms appear in Table 30.

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$\frac{\partial[\text{NH}_4]}{\partial t}$	$= \min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] CSR_N^*/h_{wc}$	(170)
$\frac{\partial P}{\partial t}$	$= \frac{1}{16} \frac{31}{14} \min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] CSR_P^*/h_{wc}$	(171)
$\frac{\partial DIC}{\partial t}$	$= \frac{106}{16} \frac{12}{14} \min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] CSR_C^*/h_{wc}$	(172)
$\frac{\partial[\text{O}_2]}{\partial t}$	$= \frac{\partial DIC}{\partial t} \frac{32}{12} \frac{[\text{O}_2]^2}{K_{\text{O}_A}^2 + [\text{O}_2]^2}$	(173)
$\frac{\partial[\text{COD}]}{\partial t}$	$= \frac{\partial DIC}{\partial t} \frac{32}{12} \left( 1 - \frac{[\text{O}_2]^2}{K_{\text{O}_A}^2 + [\text{O}_2]^2} \right)$	(174)
$\frac{\partial CS}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] CS$	(175)
$\frac{\partial R_N}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] R_N$	(176)
$\frac{\partial R_P}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] R_P$	(177)
$\frac{\partial R_C}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] R_C$	(178)
$\frac{\partial Chl}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] Chl$	(179)
$\frac{\partial X_p}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] X_p$	(180)
$\frac{\partial X_h}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] X_h$	(181)
$\frac{\partial Q_{\text{ox}}}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] Q_{\text{ox}}$	(182)
$\frac{\partial Q_{\text{red}}}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] Q_{\text{red}}$	(183)
$\frac{\partial Q_{\text{in}}}{\partial t}$	$= -\min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] Q_{\text{in}}$	(184)
$\frac{\partial D_{\text{Red}}}{\partial t}$	$= \min \left[ \gamma, \max \left[ 0, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_{\text{O}}} \right] \right] CS/h_{wc}$	(185)

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**Table 30.** Equations describing the expulsion of zooxanthellae, and the resulting release of inorganic and organic molecules into the bottom water column layer.



	Symbol	Value
<i>Constants</i>		
Molecular diffusivity of NO <sub>3</sub>	$D$	$f(T, S_A) \sim 17.5 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
Speed of light	$c$	$2.998 \times 10^8 \text{ m s}^{-1}$
Planck constant	$h$	$6.626 \times 10^{-34} \text{ J s}^{-1}$
Avogadro constant	$A_V$	$6.02 \times 10^{23} \text{ mol}^{-1}$
<sup>a</sup> Pigment-specific absorption coefficients	$\gamma_\lambda$	$f(\text{pig}, \lambda) \text{ m}^{-1} (\text{mg m}^{-3})^{-1}$
Kinematic viscosity of water	$\nu$	$f(T, S_A) \sim 1.05 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$
<i>Parameters</i>		
<sup>b</sup> Nitrogen content of zooxanthellae cells	$m_N$	$5.77 \times 10^{-12} \text{ mol N cell}^{-1}$
<sup>c</sup> Carbon content of zooxanthellae cells	$m_C$	$(106/16) m_N \text{ mol C cell}^{-1}$
<sup>d</sup> Maximum intracellular Chl concentration	$c_i^{\text{max}}$	$3.15 \times 10^6 \text{ mg Chl m}^{-3}$
Radius of zooxanthellae cells	$r_{CS}$	$5 \mu\text{m}$
Maximum growth rate of coral	$\mu_{CH}^{\text{max}}$	$0.05 \text{ d}^{-1}$
<sup>e</sup> Rate coefficient of particle capture	$S_{part}$	$3.0 \text{ m d}^{-1}$
Maximum growth rate of zooxanthellae	$\mu_{CS}^{\text{max}}$	$0.4 \text{ d}^{-1}$
Quadratic mortality coefficient of polyps	$\zeta_{CH}$	$0.01 \text{ d}^{-1} (\text{g N m}^{-2})^{-1}$
Linear mortality of zooxanthellae	$\zeta_{CS}$	$0.04 \text{ d}^{-1}$
<sup>g</sup> Remineralised fraction of coral mortality	$f_{remin}$	$0.5$
Nitrogen-specific host area coefficient of polyps	$\Omega_{CH}$	$2.0 \text{ m}^2 \text{ g N}^{-1}$
Fractional (of $\mu_{CS}^{\text{max}}$ ) respiration rate	$\phi$	$0.1$

**Table 31.** Constants and parameter values used to model coral polyps.  $V$  is zooxanthellae cell volume in  $\mu\text{m}^3$ . <sup>a</sup>Baird et al. (2016a), <sup>c</sup>Redfield et al. (1963) and Kirk (1994), <sup>d</sup>Finkel (2001), <sup>e</sup>Ribes and Atkinson (2007); Wyatt et al. (2010), <sup>f,g</sup>Gustafsson et al. (2013, 2014).

	Symbol	Value
<i>Parameters</i>		
Maximum growth rate of zooxanthellae	$\mu_{CS}^{max}$	1 d <sup>-1</sup>
Rate coefficient of xanthophyll switching	$\tau_{xan}$	1/600 s <sup>-1</sup>
<sup>a</sup> Atomic ratio of Chl a to RCII in <i>Symbiodinium</i>	$A_{RCII}$	500 mol Chl mol RCII <sup>-1</sup>
<sup>a</sup> Stoichiometric ratio of RCII units to photons	$m_{RCII}$	0.1 mol RCII mol photon <sup>-1</sup>
Maximum rate of zooxanthellae expulsion	$\gamma$	1 d <sup>-1</sup>
Oxygen half-saturation for aerobic respiration	$K_{OA}$	500 mg O m <sup>-3</sup>
Molar mass of Chl a	$M_{Chla}$	893.49 g mol <sup>-1</sup>
<sup>b</sup> Ratio of Chl a to xanthophyll	$\Theta_{chla2xan}$	0.2448 mg Chl mg X <sup>-1</sup>
<sup>b</sup> Ratio of Chl a to Chl c	$\Theta_{chla2chlc}$	0.1273 mg Chl-a mg Chl-c <sup>-1</sup>
<sup>b</sup> Ratio of Chl a to peridinin	$\Theta_{chla2per}$	0.4733 mg Chl mg <sup>-1</sup>
<sup>b</sup> Ratio of Chl a to $\beta$ -carotene	$\Theta_{chla2caro}$	0.0446 mg Chl mg <sup>-1</sup>
<sup>c</sup> Lower limit of ROS bleaching	[ROS <sub>threshold</sub> ]	$5 \times 10^{-4}$ mg O cell <sup>-1</sup>

**Table 32.** Constants and parameter values used in the coral bleaching model. <sup>a</sup>In Suggett et al. (2009). <sup>b</sup> ratio of constant terms in multivariate analysis in Hochberg et al. (2006). <sup>c</sup>Fitted parameter based on the existence of non-bleaching threshold (Suggett et al., 2009), and a comparison of observed bleaching and model output in the  $\sim 1$  km model.

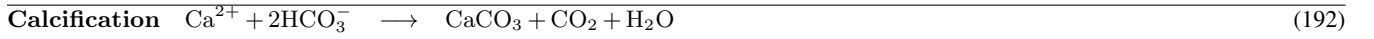
$$g = k_{day}(\Omega_a - 1)(R_C^*)^2 + k_{night}(\Omega_a - 1) \quad (188)$$

where  $g$  is the rate of net calcification,  $k_{day}$  and  $k_{night}$  are defined in Table 31 with habitat-specific values (Anthony et al., 2011; Mongin and Baird, 2014). The fluxes are scaled by the effective projected area of the community,  $A_{eff}$ . The power of 2 for  $R_C^*$  ensures that generally light replete symbionts provide the host with sufficient energy for calcification.

### 6.3.3 Dissolution of shelf carbonate sands

In addition to the dissolution of carbonate sands on a growing coral reef, which is captured in the net dissolution quantified above, the marine carbonates on the continental shelf dissolve (Eyre et al., 2018). Like above, the dissolution of marine carbonates is approximated as a source of DIC and alkalinity but does not affect the properties (mass, porosity etc.) of the underlying sediments.

We assume carbonate dissolution from the sediment bed is proportional to the fraction of the total surface sediment is composed of either sand or mud carbonates. Other components, whose fraction do not release DIC and alkalinity, including carbonate gravel and non-carbonate mineralogies. Thus the change in  $DIC$  and  $A_T$  in the bottom water column layer is given



$$\frac{\partial A_T}{\partial t} = -2gA_{eff}/h_{wc} \quad (193)$$

$$\frac{\partial DIC}{\partial t} = -12gA_{eff}/h_{wc} \quad (194)$$

$$g = k_{day}(\Omega_a - 1)(R_C^*)^2 + k_{night}(\Omega_a - 1) \quad (195)$$

$$\Omega_a = \frac{[\text{CO}_3^{2-}][\text{Ca}^{2+}]}{K_{sp}} \quad (196)$$



$$\frac{\partial A_T}{\partial t} = 2d_{\text{CaCO}_3} \left( \frac{Mud_{\text{CaCO}_3} + Sand_{\text{CaCO}_3}}{M} \right) / h_{wc} \quad (198)$$

$$\frac{\partial DIC}{\partial t} = 12d_{\text{CaCO}_3} \left( \frac{Mud_{\text{CaCO}_3} + Sand_{\text{CaCO}_3}}{M} \right) / h_{wc} \quad (199)$$

$$d_{\text{CaCO}_3} = -11.51\Omega_a + 33.683 \quad (200)$$


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**Table 33.** Equations for coral polyp calcification and dissolution. The concentration of carbonate ions,  $[\text{CO}_3^{2-}]$ , is determined from equilibrium carbon chemistry as a function of  $A_T$ ,  $DIC$ , temperature and salinity, and the concentration of calcium ions,  $[\text{Ca}^{2+}]$ , is a mean oceanic value.  $12 \text{ g C mol C}^{-1}$ . Other constants and parameters are defined in Table 31.

by:

$$\frac{\partial DIC}{\partial t} = -12d_{\text{CaCO}_3} \left( \frac{Mud_{\text{CaCO}_3} + Sand_{\text{CaCO}_3}}{M} \right) / h_{wc} \quad (189)$$

$$\frac{\partial A_T}{\partial t} = -2d_{\text{CaCO}_3} \left( \frac{Mud_{\text{CaCO}_3} + Sand_{\text{CaCO}_3}}{M} \right) / h_{wc} \quad (190)$$

- 5 where  $M$  is the total mass of surface layer inorganic sediments (see Sec. 7),  $d_{\text{CaCO}_3}$  is the dissolution rate of  $\text{CaCO}_3$ , and is the reverse reaction to calcification and  $h_{wc}$  is the thickness of the water column layer. The dissolution rate,  $d_{\text{CaCO}_3}$  [ $\text{mmol m}^{-2} \text{ d}^{-1}$ ] is assumed to be a function of  $\Omega_a$  (Eyre et al., 2018):

$$d_{\text{CaCO}_3} = -11.51\Omega_a + 33.683 \quad (191)$$

Name	Nom. size $\mu\text{m}$	Sinking vel. $\text{m d}^{-1}$	Organic	Origin	Phosphorus adsorption	Colour
Gravel $\text{CaCO}_3$	$10^4$	60,480	N	I	N	W
Gravel non- $\text{CaCO}_3$	$10^4$	60,480	N	I	N	B
Sand $\text{CaCO}_3$	$10^2$	172.8	N	I	N	W
Sand non- $\text{CaCO}_3$	$10^2$	172.8	N	I	N	B
Mud $\text{CaCO}_3$	30	17.2	N	I	Y	W
Mud non- $\text{CaCO}_3$	30	17.2	N	I	Y	B
FineSed	30	17.2	N	C	Y	B
Dust	1	1	N	C	Y	B
$D_{Atk}$	-	10	Y	OM	N	B
$D_{Red}$	-	10	Y	OM	N	B
$D_C, D_N, D_P$	-	100	Y	OM	N	B

**Table 34.** Characteristics of the particulate classes. Y - Yes, N - No, I - initial condition, C - catchment, OM - remineralisation from organic matter, B - brown, W - white (Condie et al., 2009; Margvelashvili, 2009).

## 7 Sediment processes

### 7.1 Brief summary of processes in the sediments

The EMS model contains a multi-layered sediment compartment with time and space-varying vertical layers, and the same horizontal grid as the water column and epibenthic models. All state variables that exist in the water column layers have an equivalent in the sediment layers. The dissolved tracers are given as a concentration in the porewater, while the particulate tracers are given as a concentration per unit volume (see Sec. 10.3.2).

The sediment model contains inorganic particles of different sizes (Dust, Mud, Sand and Gravel) and different mineralogies (carbonate and non-carbonate) (Tab. 34). The sediment model includes the processes of particulate advection and mixing in the water column, resuspension sinking and settling, as well as sediment overturning and bioturbation (Margvelashvili, 2009).

10 These processes, along with initial conditions, determine the mass of each inorganic particulate type in the sediments.

The critical shear stress for resuspension, and the sinking rates, are generally larger for large particles, while and mineralogy only affects the optical properties. The size-class Dust comes only in a non-carbonate mineralogy, and the Mud-carbonate class contains a category of FineSed-mineral that has the same physical and optical properties as Mud-mineral, except that it is initialised with a zero value and only enters the domain from rivers.

15 The organic matter classes are discussed in the Sec. 8.1. The inorganic and organic particulate classes are summarised in Table 34, and undergo resuspension, sinking, settling, sediment overturning and bioturbation in a manner similar to the inorganic particulates.

Variable	Symbol	Units
Ammonium concentration	$[\text{NH}_4]$	$\text{mg N m}^{-3}$
Sediment Dissolved Inorganic Carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$
Sediment Dissolved Inorganic Phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Sediment Particulate Inorganic Phosphorus (PIP)	$PIP$	$\text{mg P m}^{-3}$
Sediment Immobilised Particulate Inorganic Phosphorus (PIPI)	$PIPI$	$\text{mg P m}^{-3}$
Sediment Non-Algal Particulates (NAP)	$NAP$	$\text{kg m}^{-3}$
Sediment dissolved oxygen concentration	$[\text{O}_2]$	$\text{mg O m}^{-3}$

**Table 35.** State and derived variables for the sediment inorganic chemistry model.

Description	Symbol	Units
Maximum rate of nitrification in the water column	$\tau_{nit,wc}$	$0.1 \text{ d}^{-1}$
Maximum rate of nitrification in the sediment	$\tau_{nit,sed}$	$20 \text{ d}^{-1}$
Oxygen half-saturation constant for nitrification	$K_{\text{O}_2,nit}$	$500 \text{ mg O m}^{-3}$
Maximum rate of denitrification	$\tau_{denit}$	$0.8 \text{ d}^{-1}$
Oxygen half-saturation constant for de-nitrification	$K_{\text{O}_2,denit}$	$10000 \text{ mg O m}^{-3}$
Rate of P adsorbed/desorbed equilibrium	$\tau_{Pabs}$	$0.04 \text{ d}^{-1}$
Isothermic const. P adsorption for NAP	$k_{Pads,wc}$	$300 \text{ kg NAP}^{-1}$
Oxygen half-saturation for P adsorption	$K_{\text{O}_2,abs}$	$2000 \text{ mg O m}^{-3}$
Rate of P immobilisation	$\tau_{Pimm}$	$0.0012 \text{ d}^{-1}$

**Table 36.** Constants and parameter values used in the sediment inorganic chemistry.

## 7.2 Sediment chemistry

### 7.2.1 Sediment nitrification - denitrification

Nitrification in the sediment is similar to the water-column, but with a sigmoid rather than hyperbolic relationship at low oxygen, for numerical reasons (Eq. 206). Denitrification occurs only in the sediment.

### 5 7.2.2 Sediment phosphorus absorption - desorption

Sediment phosphorus absorption - desorption is similar to water column (Eq. 208).

There is an additional pool of immobilised particulate inorganic phosphorus,  $PIPI$ , which accumulates in the model over time as  $PIP$  becomes immobilised, and represents permanent sequestration (Eq. 209).



(203)

$$\frac{\partial[\text{NH}_4]}{\partial t} = -\tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]^2}{K_{\text{O}_2,nit}^2 + [\text{O}_2]^2} \quad (204)$$

$$\frac{\partial[\text{O}_2]}{\partial t} = -2\frac{32}{14}\tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]^2}{K_{\text{O}_2,nit}^2 + [\text{O}_2]^2} + 2\frac{32}{14}\tau_{denit}[\text{NO}_3] \frac{K_{\text{O}_2,denit}}{K_{\text{O}_2,denit} + [\text{O}_2]} \quad (205)$$

$$\frac{\partial[\text{NO}_3]}{\partial t} = \tau_{nit,wc}[\text{NH}_4] \frac{[\text{O}_2]^2}{K_{\text{O}_2,nit}^2 + [\text{O}_2]^2} - \tau_{denit}[\text{NO}_3] \frac{K_{\text{O}_2,denit}}{K_{\text{O}_2,denit} + [\text{O}_2]} \quad (206)$$

$$\frac{\partial P}{\partial t} = \left( \tau_{Pabs} \left( \frac{PIP}{k_{Pads, sed} NAP} - \frac{[\text{O}_2]P}{K_{\text{O}_2,abs} + [\text{O}_2]} \right) \right) / \phi \quad (207)$$

$$\frac{\partial PIP}{\partial t} = -\tau_{Pabs} \left( \frac{PIP}{k_{Pads,wc} NAP} - \frac{[\text{O}_2]P}{K_{\text{O}_2,abs} + [\text{O}_2]} \right) - \tau_{Pimm} PIP \quad (208)$$

$$\frac{\partial PIP_I}{\partial t} = \tau_{Pimm} PIP \quad (209)$$


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**Table 37.** Equations for the sediment inorganic chemistry.

## 8 Common water / epibenthic / sediment processes

### 8.1 Detritus remineralisation

The non-living components of C, N, and P cycles include the particulate labile and refractory pools, and a dissolved pool (Fig. 4). The labile detritus has a pool at the Redfield ratio,  $D_{Red}$ , and at the Atkinson ratio,  $D_{Atk}$ , resulting from dead organic matter at these ratios. The labile detritus from both pools then breaks down into refractory detritus and dissolved organic matter. The refractory detritus and dissolved organic matter pools are quantified by individual elements (C, N, P), in order to account for the mixed source of labile detritus. Finally, a component of the breakdown of each of these pools is returned to dissolved inorganic components. The variables, parameters and equations can be found in Tables 38, 40 & 39 respectively.

As the refractory and dissolved components are separated into C, N and P components, this introduces the possibility to have P components break down quicker than C and N. This is specified as the breakdown rate of P relative to N,  $\Phi_{RD_P}$  and  $\Phi_{DOM_P}$  respectively for refractory and dissolved detritus respectively.

Variable	Symbol	Units
Ammonium concentration	$[\text{NH}_4]$	$\text{mg N m}^{-3}$
Dissolved Inorganic Carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$
Dissolved Inorganic Phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$
Dissolved oxygen concentration	$[\text{O}_2]$	$\text{mg O m}^{-3}$
Labile detritus at Redfield ratio	$D_{Red}$	$\text{mg N m}^{-3}$
Labile detritus at Atkinson ratio	$D_{Atk}$	$\text{mg N m}^{-3}$
Refractory Detritus C	$D_C$	$\text{mg C m}^{-3}$
Refractory Detritus N	$D_N$	$\text{mg N m}^{-3}$
Refractory Detritus P	$D_P$	$\text{mg P m}^{-3}$
Dissolved Organic C	$O_C$	$\text{mg C m}^{-3}$
Dissolved Organic N	$O_N$	$\text{mg N m}^{-3}$
Dissolved Organic P	$O_P$	$\text{mg P m}^{-3}$
Chemical Oxygen Demand (COD)	$COD$	$\text{mg O m}^{-3}$

**Table 38.** State and derived variables for the detritus remineralisation model in both the sediment and water column.

### 8.1.1 Anaerobic and anoxic respiration

The processes of remineralisation, phytoplankton mortality and zooplankton grazing return carbon dioxide to the water column. In oxic conditions, these processes consume oxygen in a ratio of  $DIC : \frac{32}{12}[\text{O}_2]$ . At low oxygen concentrations, the oxygen consumed is reduced:

$$5 \quad \frac{\partial[\text{O}_2]}{\partial t} = -\frac{\partial DIC}{\partial t} \frac{32}{12} \frac{[\text{O}_2]^2}{K_{OA}^2 + [\text{O}_2]^2} \quad (223)$$

where  $K_{OA} = 256 \text{ mg O m}^{-3}$  is the half-saturation constant for anoxic respiration (Boudreau, 1996). A sigmoid saturation term is used because it is more numerically stable as the oxygen concentration approaches 0. The anoxic component of remineralisation results in an increased chemical oxygen demand (COD):

$$\frac{\partial COD}{\partial t} = \frac{\partial DIC}{\partial t} \frac{32}{12} \left( 1 - \frac{[\text{O}_2]^2}{K_{OA}^2 + [\text{O}_2]^2} \right) \quad (224)$$

10 COD is a dissolved tracer, with the same units as oxygen.

When oxygen and COD co-exist they react to reduce both, following:

$$\frac{\partial[\text{O}_2]}{\partial t} = -\tau_{COD} \min[COD, 8000] \frac{[\text{O}_2]}{8000} \quad (225)$$

$$\frac{\partial COD}{\partial t} = -\tau_{COD} \min[COD, 8000] \frac{[\text{O}_2]}{8000} \quad (226)$$

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$\frac{\partial D_{Red}}{\partial t}$	$= -r_{Red}D_{Red}$	(210)
$\frac{\partial D_{Atk}}{\partial t}$	$= -r_{Atk}D_{Atk}$	(211)
$\frac{\partial D_C}{\partial t}$	$= \frac{106}{16} \frac{12}{14} \zeta_{Red} r_{Red} D_{Red} + \frac{550}{30} \frac{12}{14} \zeta_{Atk} r_{Atk} D_{Atk} - r_R D_C$	(212)
$\frac{\partial D_N}{\partial t}$	$= \zeta_{Red} r_{Red} D_{Red} + \zeta_{Atk} r_{Atk} D_{Atk} - r_R D_N$	(213)
$\frac{\partial D_P}{\partial t}$	$= \frac{1}{16} \frac{31}{14} \zeta_{Red} r_{Red} D_{Red} + \frac{1}{30} \frac{31}{14} \zeta_{Atk} r_{Atk} D_{Atk} - \Phi_{RD_P} r_R D_P$	(214)
$\frac{\partial O_C}{\partial t}$	$= \frac{106}{16} \frac{12}{14} \vartheta_{Red} r_{Red} D_{Red} + \frac{550}{30} \frac{12}{14} \vartheta_{Atk} r_{Atk} D_{Atk} + \vartheta_{Ref} r_R D_C - r_O O_C$	(215)
$\frac{\partial O_N}{\partial t}$	$= \vartheta_{Red} r_{Red} D_{Red} + \vartheta_{Atk} r_{Atk} D_{Atk} + \vartheta_{Ref} r_R D_N - r_O O_N$	(216)
$\frac{\partial O_P}{\partial t}$	$= \frac{1}{16} \frac{31}{14} \vartheta_{Red} r_{Red} D_{Red} + \frac{1}{30} \frac{31}{14} \vartheta_{Atk} r_{Atk} D_{Atk} + \vartheta_{Ref} \Phi_{RD_P} r_R D_P - \Phi_{DOM_P} r_O O_P$	(217)
$\frac{\partial [NH_4]}{\partial t}$	$= r_{Red} D_{Red} (1 - \zeta_{Red} - \vartheta_{Red})$	(218)
	$+ r_{Atk} D_{Atk} (1 - \zeta_{Atk} - \vartheta_{Atk}) + r_R D_N (1 - \vartheta_{Ref}) + r_O O_N$	
$\frac{\partial DIC}{\partial t}$	$= \frac{106}{16} \frac{12}{14} r_{Red} D_{Red} (1 - \zeta_{Red} - \vartheta_{Red})$	(219)
	$+ \frac{550}{30} \frac{12}{14} r_{Atk} D_{Atk} (1 - \zeta_{Atk} - \vartheta_{Atk}) + r_R D_C (1 - \vartheta_{Ref}) + r_O O_C$	
$\frac{\partial P}{\partial t}$	$= \frac{1}{16} \frac{31}{14} r_{Red} D_{Red} (1 - \zeta_{Red} - \vartheta_{Red})$	(220)
	$+ \frac{1}{30} \frac{31}{14} r_{Atk} D_{Atk} (1 - \zeta_{Atk} - \vartheta_{Atk}) + \Phi_{RD_P} r_R D_P (1 - \vartheta_{Ref}) + \Phi_{DOM_P} r_O O_P$	
$\frac{\partial [O_2]}{\partial t}$	$= -\frac{32}{12} \frac{\partial DIC}{\partial t} \frac{[O_2]^2}{K_{O_A}^2 + [O_2]^2}$	(221)
$\frac{\partial [COD]}{\partial t}$	$= \frac{32}{12} \frac{\partial DIC}{\partial t} \left( 1 - \frac{[O_2]^2}{K_{O_A}^2 + [O_2]^2} \right)$	(222)

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**Table 39.** Equations for detritus remineralisation in the water column and sediment.



Description	Symbol	Red	Atk	Refractory	Dissolved
Detritus breakdown rate ( $\text{d}^{-1}$ )	$r_{Red,Atk,R,O}$	0.04	0.01	0.001	0.0001
Fraction of detritus to refractory	$\zeta_{Red,Atk}$	0.19	0.19	-	-
Fraction of detritus to DOM	$\vartheta_{Red,Atk,R}$	0.1	0.1	0.05	
Breakdown rate of P relative to N	$\Phi_{R,O}$	N/A	N/A	2	2

**Table 40.** Constants and parameter values used in the water column detritus remineralisation model. Red = Redfield ratio (C:N:P = 106:16:1); Atk = Atkinson ratio (C:N:P = 550:30:1); Ref = Refractory. See Lønberg et al. (2017).

	Labile Det., $D_{Red}$	Refractory Det., $D$	Dissolved Organic, $O$
Redfield	25	-	-
Carbon	-	27	767
Nitrogen	-	4.75	135
Phosphorus	-	0.66	18.7

**Table 41.** Steady-state detrital and dissolved organic C, N and P concentrations for primary production equal to  $2 \text{ mg N m}^{-1}$

where  $8000 \text{ mg O m}^{-3}$  is approximately the saturation concentration of oxygen in seawater, and  $\tau_{COD}$  is the timescale of this reduction. The term  $\min[COD, 8000]$  is required because  $COD$  represents the end stage of anoxic reduction and can become large for long simulations. Even with this limitation, if  $\tau_{COD} = 1 \text{ hr}^{-1}$ , the processes in Eqs. 225 and 226 proceed faster than most of the other porewater processes.

## 5 9 Common ecological parameterisations

Most of the ecological processes contain a temperature-dependence and, for those uptaking dissolved inorganic nitrogen, preferential ammonium uptake. To simplify the description of the above processes, these common parameterisations are described separately in this section. An additional processes common to all variables, and across multiples zones, is the diffusive sediment / water exchange.

### 10 9.1 Preferential uptake of ammonium

The model contains two forms of dissolved inorganic nitrogen (DIN), dissolved ammonium ( $\text{NH}_4$ ) and dissolved nitrate ( $\text{NO}_3$ ):

$$N = [\text{NH}_4] + [\text{NO}_3] \quad (227)$$

where  $N$  is the concentration of DIN,  $[\text{NH}_4]$  is the concentration of dissolved ammonium and  $[\text{NO}_3]$  is the concentration of nitrate. In the model, the ammonium component of the DIN pool is assumed to be taken up first by all primary producers, followed by the nitrate, with the caveat that the uptake of ammonium cannot exceed the diffusion limit for ammonium. The underlying principle of this assumption is that photosynthetic organisms can entirely preference ammonium, but that the uptake of ammonium is still limited by diffusion to the organism's surface.

As the nitrogen uptake formulation varies for the different autotrophs, the formulation of the preference of ammonium also varies. The diffusion coefficient of ammonium and nitrate are only 3 % different, so for simplicity we have used the nitrate diffusion coefficient for both.

Thus, for microalgae (Eq. 42) and *Trichodesmium* (Eq. 57), that both contain internal reserves of nitrogen, the partitioning of nitrogen uptake is given by:

$$\frac{\partial N}{\partial t} = -\psi D_N N (1 - R_N^*) (B/m_{B,N}) \quad (228)$$

$$\frac{\partial [\text{NH}_4]}{\partial t} = -\min[\psi D_N N (1 - R_N^*), \psi D_N [\text{NH}_4]] (B/m_{B,N}) \quad (229)$$

$$\frac{\partial [\text{NO}_3]}{\partial t} = -(\psi D_N N (1 - R_N^*) - \min[\psi D_N N (1 - R_N^*), \psi D_N [\text{NH}_4]]) (B/m_{B,N}) \quad (230)$$

For macroalgae (Eq. 110) and seagrass leaves (Eq. 124), which also have diffusion limits to uptake, but are not represented with internal reserves of nitrogen, the terms are:

$$\frac{\partial N}{\partial t} = -\mu_{MA} M A \quad (231)$$

$$\frac{\partial [\text{NH}_4]}{\partial t} = -\min[S A_{eff} [\text{NH}_4], \mu_{MA} M A] \quad (232)$$

$$\frac{\partial [\text{NO}_3]}{\partial t} = -(\mu_{MA} M A - \min[S A_{eff} [\text{NH}_4], \mu_{MA} M A]) \quad (233)$$

Zooxanthellae is a combination of the two cases above, because in the model they contain reserves like microalgae, but the uptake rate is across a 2D surface like macroalage.

In the case of nutrient uptake by seagrass roots (Eq. 126), which has a saturating nitrogen uptake functional form, the terms are:

$$\frac{\partial N_s}{\partial t} = -\mu_{SG} S G \quad (234)$$

$$\frac{\partial [\text{NH}_4]_s}{\partial t} = -\min\left[\mu_{SG} S G, \frac{\mu_{SG}^{max} [\text{NH}_4]_s S G}{K_N + [\text{NH}_4]_s}\right] \quad (235)$$

$$\frac{\partial [\text{NO}_3]_s}{\partial t} = -\left(\mu_{SG} S G - \min\left[\mu_{SG} S G, \frac{\mu_{SG}^{max} [\text{NH}_4]_s S G}{K_N + [\text{NH}_4]_s}\right]\right) \quad (236)$$

where  $K_N$  is a function of the ratio of above ground to below ground biomass described in Baird et al. (2016a).

One feature worth noting is that the above formulation for preferential ammonium uptake requires no additional parameters, which is different to other classically applied formulations (Fasham et al., 1990) that require a new parameter, potentially for each autotroph. This simple use of the geometric constraint has an important role in reducing model complexity.

## 9.2 Oxygen release during nitrate uptake

For all autotrophs, the uptake of a nitrate ion results in the retention of the one nitrogen atom in their reserves or structural material, and the release of the three oxygen atoms into the water column or porewaters.

$$\frac{\partial[\text{O}]}{\partial t} = -\frac{48}{14} \frac{\partial[\text{NO}_3]}{\partial t} \quad (237)$$

- 5 The oxygen that is part of the structural material is assumed to have been taken up through photosynthesis.

For simplicity, in the equations for autotroph driven changes in dissolved oxygen above, we have assumed that DIN uptake is ammonium. Thus after partitioning on nitrogen uptake, the term Eq. 237 needs to be added to change in oxygen in microalgae (Eq. 42), *Trichodesmium* (Eq. 57) and other autotrophs.

## 9.3 Temperature dependence of ecological rates

- 10 Physiological rate parameters (maximum growth rates, mortality rates, remineralisation rates) have a temperature dependence that is determined from:

$$r_T = r_{T_{ref}} Q_{10}^{(T-T_{ref})/10} \quad (238)$$

where  $r_T$  is the physiological rate parameter (e.g.  $\mu$ ,  $\zeta$  etc.) at temperature  $T$ ,  $T_{ref}$  is the reference temperature (nominally 20°C for GBR),  $r_{T_{ref}}$  the physiological rate parameter at temperature  $T_{ref}$ ,  $Q_{10}$  is the Q10 temperature coefficient and represents

- 15 the rate of change of a biological rate as a result of increasing temperature by 10°C.

Note that while physiological rates may be temperature-dependent, the ecological processes they are included in may not. For example, for extremely light-limited growth, all autotrophs capture light at a rate independent of temperature. With the reserves of nutrients replete, the steady-state realised growth rate,  $\mu$ , becomes the rate of photon capture,  $k$ . This can be shown algebraically:  $\mu = \mu^{max} R_C^* = k(1 - R^*)$ , where  $R^*$  is the reserves of carbon. Rearranging,  $R^* = k/(\mu^{max} + k)$ . At

20  $k \ll \mu^{max}$ ,  $R^* = k/\mu^{max}$ , thus  $\mu = \mu^{max} k/\mu^{max} = k$ . This corresponds with observations of no temperature dependence of photosynthesis at low light levels (Kirk, 1994).

Similar arguments show that extremely nutrient limited autotrophs will have the same temperature dependence to that of the diffusion coefficient. Thus, the autotroph growth model has a temperature-dependence that adjust appropriately to the physiological condition of the autotroph, and is a combination of constant, exponential, and polynomial expressions.

- 25 Physiological rates in the model that are not temperature dependent are: mass transfer rate constant for particulate grazing by corals,  $S_{part}$ ; net coral calcification  $g$ ; maximum chlorophyll synthesis,  $k_{chl}^{max}$ ; and rate of translocation between leaves and roots in seagrass,  $\tau_{tran}$ .

## 9.4 Diffusive exchange of dissolved tracers across sediment-water interface

- Due to the thin surface sediment layer, and the potentially large epibenthic drawdown of porewater dissolved tracers, the
- 30 exchange of dissolved tracers between the bottom water column layer and the top sediment layer is solved in the same numerical

operation as the ecological tracers (other transport processes occurring between ecological timesteps). The flux,  $J$ , is given by:

$$J = k(C_s - C) \quad (239)$$

where  $C$  and  $C_s$  are the concentration in water column and sediment respectively,  $k = 4.6 \times 10^{-7} \text{ m s}^{-1}$  is the transfer coefficient. In the model parameterisation,  $k = D/h$  where  $D = 3 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$  is the diffusion coefficient and  $h = 0.0065 \text{ mm}$  is the thickness of the diffusive layer.

While in reality  $k$  would vary with water column and sediment hydrodynamics as influenced by community type etc, these complexities has not been considered. In addition to the diffusive flux between the sediment and water column, particulate deposition entrains water column water into the sediments, and particulate resuspension releases porewaters into the water column. Sediment model details can be found at: <https://research.csiro.au/cem/software/ems/ems-documentation/>.

## 10 Numerical integration

### 10.1 Splitting of physical and ecological integrations

The numerical solution of the time-dependent advection-diffusion-reaction equations for each of the ecological tracers is implemented through sequential solving of the partial differential equations (PDEs) for advection and diffusion, and the ordinary differential equations (ODEs) for reactions. This technique, called operator splitting, is common in geophysical science (Hundsdoerfer and Verwer, 2003; Butenschön et al., 2012).

Under the sequential operator splitting technique used, first the advection-diffusion processes are solved for the period of the time-step (15 min - 1 hour, Table 42). The value of the tracers at the end of this PDE integration, and the initial time, are then used as initial conditions for the ODE integration. After the ODE integration has run for the same time period, the values of the tracers are updated, and time is considered to have moved forward just one time-step. The integration continues to operate sequentially for the whole model simulation. The errors due to operator splitting can be significant (Butenschön et al., 2012), although tests in relatively coarse (4 km) models show that reducing the time-step from 60 min to 30 min does not substantially change the model solution. For higher resolution models shorter time scales are required to resolve finer scale motion, and its interaction with ecological processes.

The PDE solvers are described in the physical model description available at:

[www.emg.cmar.csiro.au/www/en/emg/software/EMS/hydrodynamics.html](http://www.emg.cmar.csiro.au/www/en/emg/software/EMS/hydrodynamics.html).

The code allows 4-5th and 7-8th order adaptive ODE solvers following Dormand and Prince (1980), as well as the Euler method and adaptive first and second order solvers. The preferred scheme is the adaptive 4th-5th order (similar to ode45 in MATLAB), and implement in numerous biogeochemical models (Yool, 1997). This requires 7 function evaluations for the first step and 6 for each step after. A tolerance of  $1 \times 10^{-5}$  is required for the integration step to be accepted.

The solution of the ecological equations are independent for each vertical column, and depend only on the layers above through which the light has propagated. For an  $n_{wc}$ -layer water column and  $n_{sed}$ -layer sediment, the integrator sequentially

solves the top  $n_{wc} - 1$  water column layers; the  $n$ th water column layer, epibenthic and top sediment layer together; and then the  $n_{sed} - 1$  to bottom sediment layers.

Description	Values
Timestep of hydrodynamic model	90 s
<sup>a</sup> Timestep of ODE ecological model	3600 s
Timestep of optical and carbon chemistry models	3600 s
Optical model resolution in PAR	~ 20 nm
ODE integrator	Adaptive 4th-5th order (Dormand and Prince, 1980)
ODE tolerance	$10^{-5}$
Maximum number of ODE steps in ecology	2000
Maximum number of iterations in carbon chemistry	100
Accuracy of carbon chemistry calculations	$[H^+] = 10^{-12}$ mol

**Table 42.** Integration details. Optical wavelengths (nm): 290 310 330 350 370 390 410 430 440 450 470 490 510 530 550 570 590 610 630 650 670 690 710 800.<sup>a</sup>Since the integrator is 4-5th order, the ecological derivatives are evaluated at least every approximately  $3600/5 = 900$  s, and more regularly for stiff equations. The ODE tolerance is a fraction of the value of the state variable.

## 10.2 Optical integration

The inherent and apparent optical properties are calculated between the physical and ecological integrations. The light climate used for each ecological timestep is that calculated at the start time of the ecological integration. The spectral resolution of 25 wavebands has been chosen to resolve the absorption peaks associated with Chl *a*, and to span the optical wavelengths. As IOPs can be calculated at any wavelength given the model state, IOPs and AOPs at observed wavelengths are recalculated after the integration.

Additionally, the wavelengths integrated have been chosen such that the lower end of one waveband and the top end of another fall on 400 and 700 nm respectively, allowing precise calculation of photosynthetically available radiation (PAR).

## 10.3 Additional integration details

### 10.3.1 Approximation of stoichiometric coefficients

In this model description we have chosen to explicitly include atomic mass as integer values, so that the conversion are more readable in the equations than if they had all been rendered as mathematical symbols. Nonetheless these values are more precisely given in the numerical code (Table 43).

It is worth remembering that the atomic masses are approximations assuming the ratio of isotopes found in the Periodic Table (Atkins, 1994), based on the natural isotopic abundance of the Earth. So, for example,  $^{14}\text{N}$  and  $^{15}\text{N}$  have atomic masses

of 14.00307 and 15.00011 respectively, with  $^{14}\text{N}$  making up 99.64 % of the abundance on Earth. Thus the value 14.01 comes from  $14.00307 \times 99.64 + 15.00011 \times 0.36 = 14.0067$ . The isotopic discrimination in the food web of 3 ppt per trophic level would increase the mean atomic mass by  $(15.00011 - 14.00307) \times 0.003 = 0.003$  per trophic level. Perhaps more importantly, if the model had state variables for  $^{14}\text{N}$  and  $^{15}\text{N}$ , then the equations would change to contain coefficients of 14 for the  $^{14}\text{N}$  isotope equations, and 15 for the  $^{15}\text{N}$  isotope equations, that would be applied in the numerical code using 14.00 and 15.00 respectively.

Element	Value in symbolic equations	Value in code
Nitrogen, N	14	14.01
Carbon, C	12	12.01
Oxygen, O <sub>2</sub>	32	32.00
Phosphorus, P	31	30.97

**Table 43.** Atomic mass of the C, N, P and O<sub>2</sub>, both in the model description where two significant figures are used for brevity, and in the numerical code, where precision is more important.

### 10.3.2 Mass conservation in water column and sediment porewaters

The model checks the conservation of Total C,  $TC$ , Total N,  $TN$ , Total P,  $TP$ , and oxygen,  $[\text{O}_2]$ , within each grid cell at each time step using the following conservation laws. To establish mass conservation, the sum of the change in mass (of N, P, C and O) with time and the mass of sinks / sources (such as sea-air fluxes, denitrification) must equate to zero.

The total mass and conservation equations are same for the water column and porewaters, with the caveats that (1) air-sea fluxes only affect surface layers of the water, (2) denitrification only occurs in the sediment, and (3) the porosity,  $\phi$ , of the water column is 1. In the sediment, the concentration of particulates is given in per unit volume of space, while the concentration of dissolved tracers is given in per unit volume of porewater. The concentration of dissolved tracer,  $X$ , per unit space is given by  $\phi X$ .

Thus the total carbon in a unit volume of space, and its conservation, are given by:

$$TC = \phi(DIC + O_C) + \left( \frac{550}{30} \frac{12}{14} D_{Atk} + D_C + \frac{106}{16} \frac{12}{14} (D_{red} + \sum B(1 + R_C^*) + \sum Z) \right) \quad (240)$$

$$\frac{\partial TC}{\partial t} + \underbrace{k_{\text{CO}_2} ([\text{CO}_2] - [\text{CO}_2]_{\text{atm}})}_{\text{sea-air flux}} / h = 0 \quad (241)$$

The total nitrogen in a unit volume of space, and its conservation, are given by:

$$TN = \phi([\text{NO}_3] + [\text{NH}_4] + O_N) + \left( D_{Atk} + D_{red} + D_N + \sum B(1 + R_N^*) + \sum Z \right) \quad (242)$$

$$\frac{\partial TN}{\partial t} + (\text{denitrification} - \text{nitrogen fixation}) / \phi - \text{dust input} / h = 0 \quad (243)$$

The total phosphorus in a unit volume of space, and its conservation, are given by:

$$TP = \phi(DIP + O_P) + PIP + PIP_I + \frac{1}{30} \frac{31}{14} D_{Atk} + D_P + \frac{1}{16} \frac{31}{14} \left( D_{red} + \sum B(1 + R_P^*) + \sum Z \right) \quad (244)$$

5

$$\frac{\partial TP}{\partial t} - \text{dust input} / h = 0 \quad (245)$$

The concept of oxygen conservation in the model is more subtle than that of C, N and P due to the mass of oxygen in the water molecules themselves not being considered. When photosynthesis occurs, C is transferred from the dissolved phase to reserves within the cell. With both dissolved and particulate pools considered, mass conservation of C is straightforward. In contrast to C, during photosynthesis oxygen is drawn from the water molecules (i.e. H<sub>2</sub>O), whose mass is not being considered, and released into the water column. Conversely, when organic matter is broken down oxygen is consumed from the water column and released as H<sub>2</sub>O.

In order to obtain a mass conservation for oxygen, the concept of Biological Oxygen Demand (BOD) is used. Often BOD represents the biological demand for oxygen in say a 5 day incubation, BOD<sub>5</sub>. Here, for the purposes of mass conservation checks, we use BOD<sub>∞</sub>, the oxygen demand over an infinite time for breakdown. This represents the total oxygen removed from the water molecules for organic matter creation.

Anaerobic respiration reduces BOD<sub>∞</sub> without reducing O<sub>2</sub>, but instead creating reduced-oxygen species. This is accounted for in the oxygen balance by the prognostic tracer Chemical Oxygen Demand (COD). In other biogeochemical modelling studies this is represented by a negative oxygen concentration.

Thus at any time point the biogeochemical model will conserve the oxygen concentration minus BOD<sub>∞</sub> minus COD, plus or minus any sources and sinks such as sea-air fluxes. The total oxygen minus BOD<sub>∞</sub> minus COD in a unit volume of water, and its conservation, is given by:

$$[O_2] + \frac{48}{14} [NO_3] - BOD_{\infty} - COD =$$

$$\phi \left( [O_2] + \frac{48}{14} [NO_3] - COD + \frac{32}{12} O_C \right) - \left( \frac{550}{30} \frac{32}{14} D_{Atk} + \frac{32}{12} D_C + \frac{106}{16} \frac{32}{14} \left( D_{red} + \sum B_N(1 + R_C^*) \right) \right) \quad (246)$$

$$\frac{\partial ([O_2] + \frac{48}{14} [NO_3] - BOD_{\infty} - COD)}{\partial t} + \mathcal{R} - \underbrace{\frac{k_{O_2} ([O_2]_{sat} - [O_2])}{h}}_{\text{sea-air flux}} - \underbrace{2 \frac{106}{16} \frac{32}{14} \tau_{nit,wc} [NH_4] \frac{[O_2]}{K_{nit,O} + [O_2]}}_{\text{nitrification}} = 0 \quad (247)$$

where  $\mathcal{R}$  is respiration of organic matter.

In addition to dissolved oxygen, BOD and COD, nitrate ( $\text{NO}_3$ ) appears in the oxygen mass balance. This is necessary because the N associated with nitrate uptake is not taken into the autotrophs, but rather released into the water column or porewater. Other entities that contain oxygen in the ocean include the water molecule ( $\text{H}_2\text{O}$ ) and the phosphorus ion ( $\text{PO}_4$ ).

- 5 In the case of water, this oxygen reservoir is considered very large, with the small flux associated with its change balanced by BOD. In the case of  $\text{PO}_4$ , this is a small reservoir. As oxygen remains bound to P through the entire processes of uptake into reserves and incorporated into structural material and then release, it is not necessary to include it in the oxygen balance for the purposes of ensuring consistency. Nonetheless, strictly the water column and porewater oxygen reservoirs could include a term  $+\frac{64}{31}[\text{PO}_4]$ , and the BOD would have similar quantities for reserves and structural material.

### 10 10.3.3 Mass conservation in the epibenthic

Mass conservation in the epibenthos requires consideration of fluxes between the water column, porewaters and the epibenthic organisms (macroalgae, seagrass and coral hosts and symbionts).

The total carbon in the epibenthos, and its conservation, is given by:

$$TC = \frac{550}{30} \frac{12}{14} (MA + SG_A + SG_B) + \frac{106}{16} \frac{12}{14} (CS(1 + R_C^*) + CH) \quad (248)$$

15

$$\frac{\partial TC}{\partial t} \Big|_{epi} + h_{wc} \frac{\partial TC}{\partial t} \Big|_{wc} + h_{sed} \frac{\partial TC}{\partial t} \Big|_{sed} + \underbrace{12(gA_{eff} - d_{CaCO_3})}_{\text{coral calcification - dissolution}} = 0 \quad (249)$$

where  $h_{wc}$  and  $h_{sed}$  are the thickness of the bottom water column and top sediment layers,  $R_C^*$  is the normalised internal reserves of carbon in zooxanthallae,  $12g$  is the rate coral calcification per unit area of coral,  $A_{eff}$  is the area of the bottom covered by coral per  $\text{m}^{-2}$ , and the diffusion terms between porewaters and the water column cancel, so do not appear in

- 20 the equations. Note the units of mass of  $CS$  needs to be in g N, and some configurations may have multiple seagrass and macroalgae species.

Similarly for nitrogen, phosphorus and oxygen in the epibenthos:

$$TN = MA + SG_A + SG_B + CS(1 + R_N^*) + CH \quad (250)$$

$$25 \frac{\partial TN}{\partial t} \Big|_{epi} + h_{wc} \frac{\partial TN}{\partial t} \Big|_{wc} + h_{sed} \frac{\partial TN}{\partial t} \Big|_{sed} = 0 \quad (251)$$

$$TP = \frac{1}{30} \frac{31}{14} (MA + SG_A + SG_B) + \frac{1}{16} \frac{31}{14} (CS(1 + R_P^*) + CH) \quad (252)$$

$$\frac{\partial TP}{\partial t} \Big|_{epi} + h_{wc} \frac{\partial TP}{\partial t} \Big|_{wc} + h_{sed} \frac{\partial TP}{\partial t} \Big|_{sed} = 0 \quad (253)$$



$$BOD_{\infty} = \frac{550}{30} \frac{32}{14} (MA + SG_A + SG_B) + \frac{106}{16} \frac{32}{14} (CS(1 + R_C^*) + CH) \quad (254)$$

$$-\frac{\partial BOD_{\infty}}{\partial t} \Big|_{epi} + h_{wc} \frac{\partial ([O_2] - BOD_{\infty})}{\partial t} \Big|_{wc} + h_{sed} \frac{\partial ([O_2] - BOD_{\infty})}{\partial t} \Big|_{sed} = 0 \quad (255)$$

5 where there is no dissolved oxygen in the epibenthos.

### 10.3.4 Wetting and drying

When a water column becomes dry (the sea level drops below the seabed depth) ecological processes are turned off.

### 10.3.5 Unconditional stability

In addition to the above standard numerical techniques, a number of innovations are used to ensure model solutions are reached.

10 Should an integration step fail in a grid cell, no increment of the state variables occurs, and the model continues with a warning flag registered (as `Ecology Error`). Generally the problem does not reoccur due to the transport of tracers alleviating the stiff point in phase space of the model.

## 11 Model evaluation

The EMS BGC model has been deployed in a range of environments around Australia, and with each deployment skill assess-  
 15 ment has been undertaken (for a history of these applications see Sec. 14). Recently, the EMS BGC model has been thoroughly assessed against remotely-sensed and in situ observations on the Great Barrier Reef (GBR), as part of the eReefs project (Schiller et al., 2014; Steven et al., 2019). The assessment of version B1p0 of the eReefs marine model configuration of the EMS included a range of model configurations (4 km, 1 km and relocatable fine resolution versions) (Herzfeld et al., 2016). The optical and carbon chemistry outputs were assessed in Baird et al. (2016b) and Mongin et al. (2016b) respectively.

20 A more recent assessment of the BGC model (vB2p0) in the GBR compared simulations against a range of in situ observations that included 24 water quality moorings, 2 nutrient sampling programs (with a total of 18 stations) and time-series of taxon-specific plankton abundance. In addition to providing a range of skill metrics, the assessment included analysis of seasonal plankton dynamics (Skerratt et al., 2019).

In this section we assess version B3p0 in the 4 km GBR configuration. First we consider the behaviour of the microalgae  
 25 physiology as a means to understanding the dynamics of the microalgal growth model. Secondly, the techniques and observations used in Skerratt et al. (2019) have been applied to the model version described in this paper (vB3p0) with highlights discussed here, and the full analysis appearing in the Supplementary Material.

## 11.1 Analysis of microalgae growth and pigment synthesis dynamics

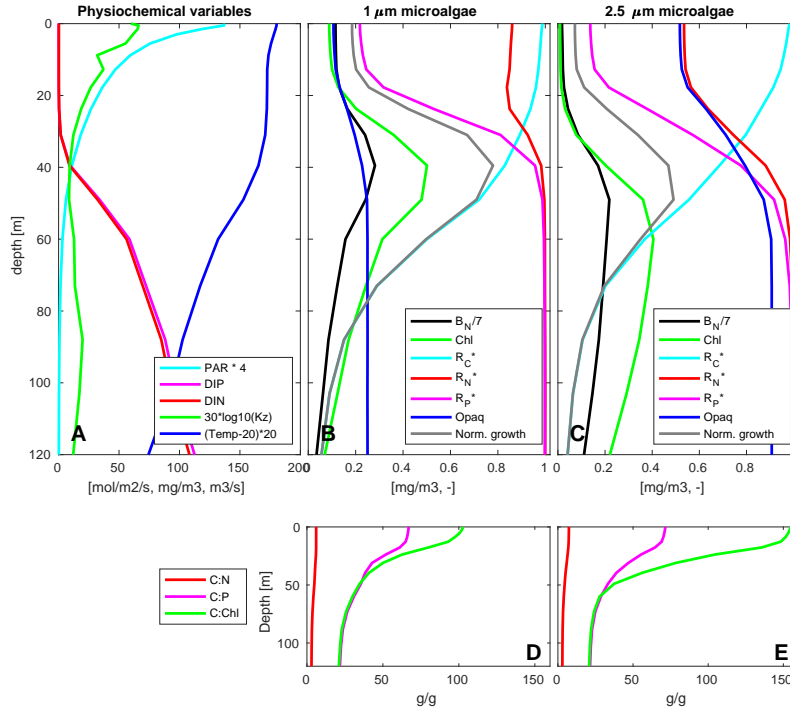
The microalgae growth model (Sec. 5.1.1) was derived from first quantifying the fluxes into a cell of energy or fixed carbon, N, P and O. Each flux adds to the reserves of that element in the cell. A second process, the consumption of reserves to create microalgae structural material with a constant stoichiometry (C:N:P = 106:16:1), increases the number of cells, but reduces the reserves of each element both per cell, and of the population. Thus, the microalgae in the growth model are generating organic matter at the Redfield ratio while being exposed to external nutrient fields at non-Redfield ratios. At the same time as the microalgae grow, the model represents the synthesis of chlorophyll based on the cell's need for more carbon fixation and the benefit of adding pigment on the rate of photon absorption.

To illustrate these dynamics, we look at a vertical profile of a deep site in the Coral Sea with a 1  $\mu\text{m}$  and 2.5  $\mu\text{m}$  radius microalgae (Fig. 13). The expectation is that, for the same environmental conditions, the 1  $\mu\text{m}$  cell will be less nutrient-limited and more light-limited than the 2.5  $\mu\text{m}$  cell – a result of the 1  $\mu\text{m}$  cell having a greater diffusion rate per unit volume than the larger cell. Further, that near-surface cells will be more nutrient-limited, deeper cells more light-limited, with light-limited cells having more pigment per cell.

In addition to being a measure of the quantity of nutrient reserves, normalised reserves ( $R^*$ ) of each nutrient is a metric of how limiting that nutrient is, with one being unlimited, and zero being completely limited. At the surface at midday, the 1  $\mu\text{m}$  cells have a biomass of  $0.2 \text{ mg m}^{-3}$  (Fig. 13B). The cells are strongly phosphorus limited ( $R_P^* = 0.22$ ), slightly nitrogen limited ( $R_N^* = 0.86$ ), and almost light unlimited ( $R_C^* = 0.99$ ). The realised growth rate, as a fraction of the maximum growth rate, is  $R_C^* R_N^* R_P^* = 0.19$ . The larger cells are more nutrient limited ( $R_P^* = 0.14$ ,  $R_N^* = 0.54$ ), and again light unlimited ( $R_C^* = 0.98$ ), realising a normalised growth rate of 0.07 (Fig. 13C).

The elemental ratios of the microalgae can be calculated from the reserves [in wt/wt: C:N =  $(12/14)(106/16)(1 + R_C^*)/(1 + R_N^*)$ ; C:P =  $(12/31)(106/1)(1 + R_C^*)/(1 + R_P^*)$ ]. The C:N and C:P ratios are both higher in the nutrient replete surface waters, with C:P varying more due to greater P limitation in the surface waters. A deep chlorophyll maximum has formed for the 1  $\mu\text{m}$  microalgae at 40 m, and for 2.5  $\mu\text{m}$  microalgae at 60 m. Here we will explain this distribution based on microalgae growth alone (ignoring grazing and sinking terms). The 1  $\mu\text{m}$  microalgae has a growth maximum at 40 m, as nutrients have become unlimiting and fixed carbon reserves are still relatively high ( $R_C^* = 0.8$ ). Growth below 50 m becomes primarily light-limited, so normalised growth is equal to normalised fixed carbon reserves. The 2.5  $\mu\text{m}$  microalgae are nutrient limited deeper into the water column, resulting in a deep growth maximum.

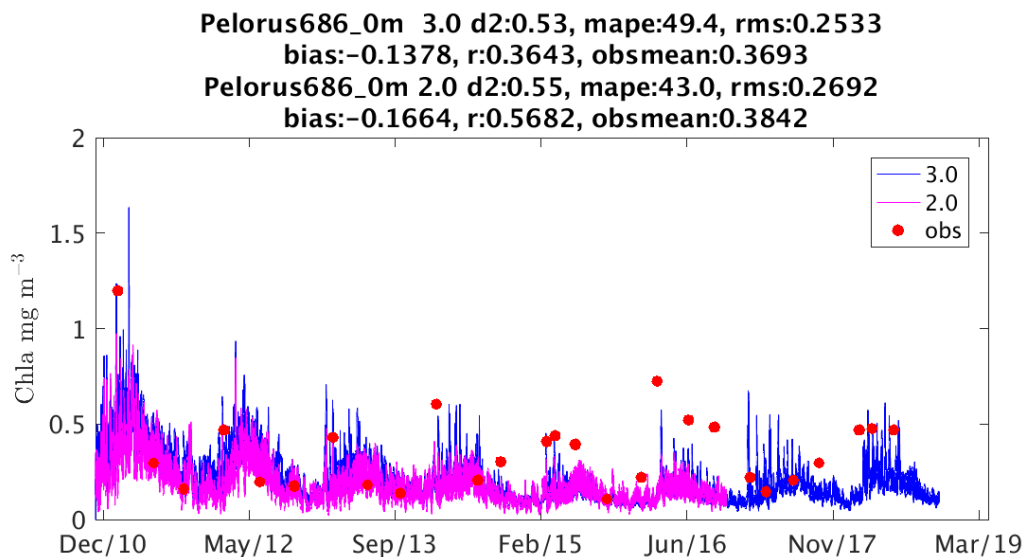
The 1 and 2.5  $\mu\text{m}$  cells have a slight biomass maximum at 40 and 50 m respectively, but the chlorophyll maximum is more pronounced (Fig. 13B, C). At the surface the 1  $\mu\text{m}$  microalgae have low pigment content and are therefore relatively transparent (opaqueness, or the absorption cross-section divided by the projected area,  $\alpha/(\pi r^2)$ , is 0.11), with a C:Chl ratio of 100 [g/g]. At the deep chlorophyll maxima for 1  $\mu\text{m}$  cells, the pigment content has increased, as shown by the C:Chl dropping to 20 [g/g], the maximum C:Chl ratio observed in the ocean (Sathyendranath et al., 2009), resulting in an opaqueness of 0.25. The 2.5  $\mu\text{m}$  cells are more light-limited than the smaller cells. At the surface, chlorophyll synthesis generates in 2.5  $\mu\text{m}$  cells an opaqueness of 0.52. Given the larger size of the cell, this is achieved at a C:Chl ratio of 150. At the 50 m deep chlorophyll



**Figure 13.** Vertical profiles of physiochemical variables (A) and physiological variables from 1  $\mu\text{m}$  (B, D) and 2.5  $\mu\text{m}$  (C, E) radii microalgae. Panel A: PAR – photosynthetically available radiation [ $\text{mol m}^{-2} \text{s}^{-1}$ ], Dissolved Inorganic Phosphorus (DIP,  $\text{mg P m}^{-3}$ ), Dissolved Inorganic Nitrogen (DIN,  $\text{mg N m}^{-3}$ ), Vertical diffusivity ( $K_z$   $\text{m}^3 \text{s}^{-1}$ ), temperature ( $^{\circ}\text{C}$ ); Panel B (1  $\mu\text{m}$ ) and C (2.5  $\mu\text{m}$ ): biomass of structural material in nitrogen ( $B_N$ ,  $\text{mg N m}^{-3}$ ), chlorophyll a concentration (Chl,  $\text{mg chl-a m}^{-3}$ ), normalised reserves of fixed carbon ( $R_C^*$ ), nitrogen ( $R_N^*$ ) and phosphorus ( $R_P^*$ ), cell opaqueness [absorption cross-section divided by projected area,  $\alpha/(\pi r^2)$ ] and normalised growth rate =  $R_C^* R_N^* R_P^*$ . Panel D (1  $\mu\text{m}$ ) and E (2.5  $\mu\text{m}$ ): stoichiometric ratios of carbon to nitrogen (C:N), phosphorus (C:P) and chlorophyll (C:Chl-a). PAR,  $K_z$ , temperature and  $B_N$  are all scaled for plotting.

maxima, the C:Chl dropped to 20, but in the larger cells this achieves an opaqueness of 0.91 (i.e. absorption cross-section is almost equal to the projected area).

In summary, the application of simple physical limits to uptake, a restraint of constant stoichiometric conversion to structural material, and cells synthesising chlorophyll to maximise photon absorption when light limited, generates the typical physiological properties of microalgae seen in vertical profiles in the ocean.



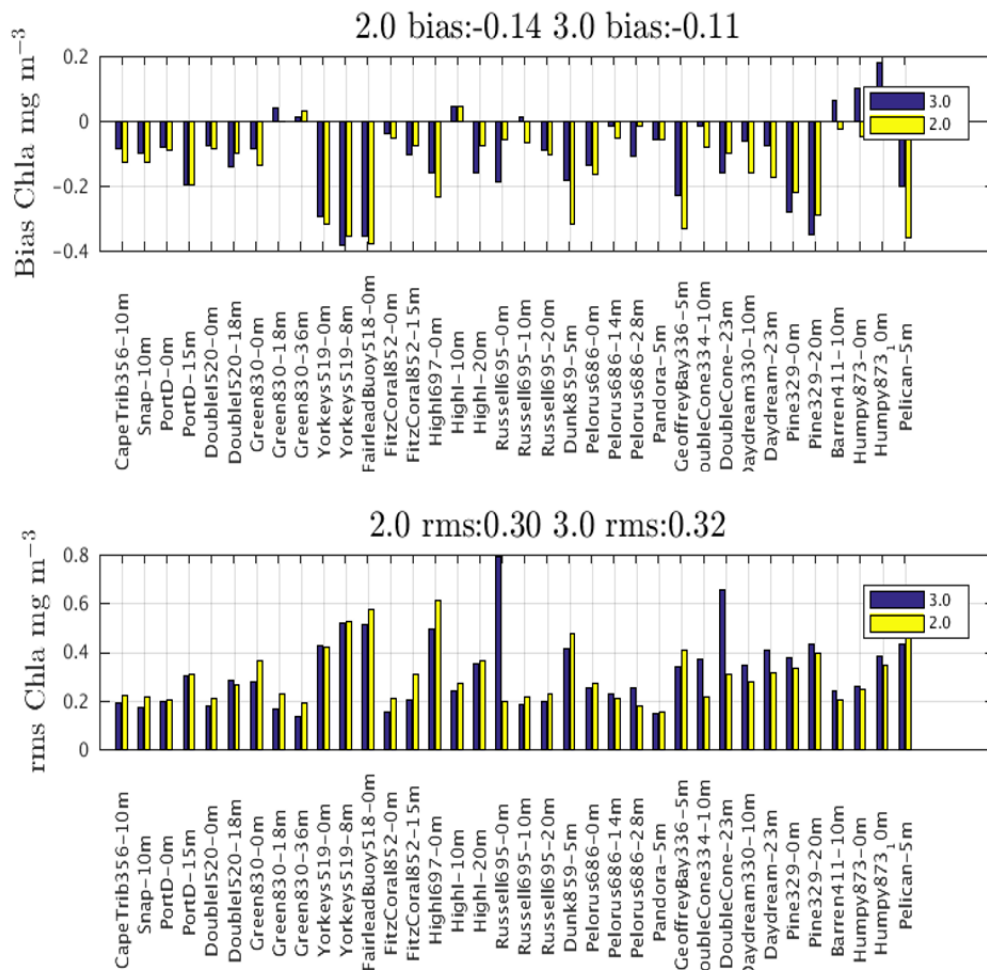
**Figure 14.** Observed surface chlorophyll concentration from chlorophyll extraction (red dots) at Pelorus Island Marine Monitoring Program site (146°29' E, 18°33' S) with a comparison to configurations vB2p0 (pink line) and vB3p0 (blue line). Statistics listed include the Willmott d2 metric (Willmott et al., 1985), mean absolute percent error (mape) and root mean square (rms) error.

## 11.2 Model assessment of the Great Barrier Reef (GBR) configuration

A detailed comparison of a GBR simulation against observations of Chl a concentration, dissolved inorganic carbon, nitrogen, phosphorus and ammonium, dissolved organic nitrogen and phosphorus, alkalinity, pH, aragonite saturation, mass of suspended sediments, turbidity and Secchi depth appears in the Supplementary Material (SM). Here we highlight the carbon chemistry, nutrient and plankton components that are driven by the BGC model.

### 11.2.1 Chlorophyll dynamics

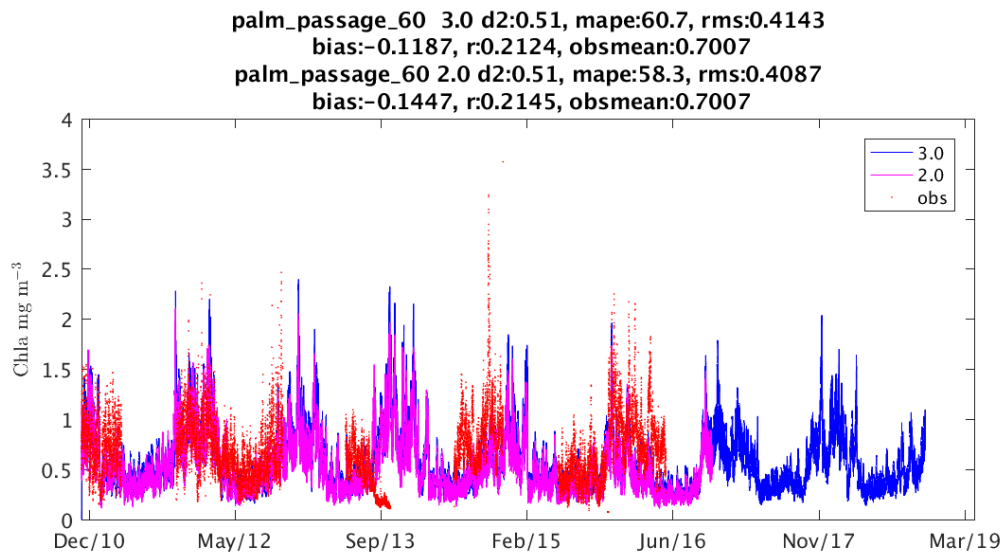
The most accurate measurements of water column chlorophyll concentrations in the GBR are obtained using high-performance liquid chromatography (HPLC) and chlorophyll extractions from water column samples. Chlorophyll extractions have been taken at 36 locations along the GBR (SM, Sec. E10; for site locations see SM, Sec. E1). As an example, a time-series at Pelorus Island in the central GBR (Fig. 14) shows large variability in both the observations and the simulations, driven by inter-annual climatic forcing, with 2011-2013 experiencing much greater river loads than 2014-2016, intra-annual trends driven by greater loads of nutrients during the wet season (Jan - Jun) than the remainder of the year, as well as monthly variability related to tidal movements and predator-prey oscillations. Even given this variability, comparison of the instantaneous state of the simulations



**Figure 15.** Skill metrics for the comparison of chlorophyll extracts at the Long Term Monitoring sites against observations for model version 2p0 and 3p0. For more information see Fig. 14 and SM, Sec. 10.

against extracted chlorophyll concentrations showed the model was able to achieve across all 36 sites a bias  $\pm$  root mean square (rms) error of  $-0.11 \pm 0.32$  mg m<sup>-3</sup> (Fig. 15).

- Moored fluorometers are generally less accurate than chlorophyll extractions, but provide a greater temporal resolution of chlorophyll dynamics. Here we show observations from a mooring at Palm Passage (Fig. 16), away from the influence of the river discharges and dependent primary on shelf break interactions. The observed time-series from 60 m depth show inter-annual variability in fluorescence related to primarily to a Oct - Mar maximum in intrusion events (for details of deployment



**Figure 16.** Observed chlorophyll fluorescence (red dots) at 60 m depth at the Palm Passage site with a comparison to configuration vB3p0 (blue) and vB2p0 (pink).

details and oceanographic processes see Benthuisen et al. (2016)), which are also seen in the vB3p0 simulations. Comparison to other moored fluorometers on the GBR (SM, Secs. 19 and 21) shows a range of predictive skill.

### 11.2.2 Nutrient dynamics

The model represents dissolved nitrate, ammonium and phosphorus nutrients. In the surface waters of the inshore GBR, nutrients are generally at very low concentrations, with modest increases seen each wet season. At High Island in the central GBR (Fig. 17), DIP has a mean concentration of  $2 \text{ mg m}^{-3}$ , with concentrations varying between 0 and  $5 \text{ mg m}^{-3}$ . The concentrations of nitrate and ammonium are both very low, with occasional peaks driven by river plume exposure. The simulated nutrients generally follow the expected time-varying patterns: peaks in the wet season, larger peaks in the wettest years (2011, 2012, 2013, 2018) and extremely low concentrations in the dry seasons. Across all sites (SM, Sec. E13), vB3p0 predicted DIP with a skill of (bias  $\pm$  rmse) of  $-0.88 \pm 2.17 \text{ mg P m}^{-3}$ , nitrate of  $-0.70 \pm 3.86 \text{ mg N m}^{-3}$  and ammonium of  $-0.77 \pm 1.63 \text{ mg N m}^{-3}$ .

### 11.2.3 Carbon chemistry

The model contains two state variables to represent the state of carbon chemistry, dissolved inorganic carbon and alkalinity, from which, at equilibrium and known temperature and salinity, other variables such as pH may be calculated. The biogeochemical model provides highly skilful predictions of pH and aragonite saturation (Fig. 18). This success is primarily due to the skill of the hydrodynamic model. The circulation produces a good representation of the alkalinity field, and the sea

surface temperature set an accurate difference in the partial pressure of CO<sub>2</sub> between the atmosphere and ocean. With these phenomenon accurately calculated, the model needs only to correctly predict the time-averaged wind-speed dependent air-sea flux. Further assessment of carbon chemistry properties along the entire length of the GBR (SM, Sec. E28) shows a bias ± rms error of DIC of  $-7.7 \pm 34.2 \text{ mmol m}^{-3}$ . Further skill assessment from inshore sites is available in Mongin et al. (2016b).

5

The outputs of all hindcasts in the eReefs project can be downloaded from:

<http://dapds00.nci.org.au/thredds/catalogs/fx3/catalog.html>

## 12 Code availability

10 The model web page is:

<https://research.csiro.au/cem/software/ems/>

The webpage links to an extensive User Guide for the entire EMS package, which contains any information that is generic across the hydrodynamic, sediment, transport and ecological models, such as input/output formats. A smaller Biogeochemical User Guide documents details relevant only to the biogeochemical and optical models (such as how to specify wavelengths for

15 the optical model), and a Biogeochemical Developer's Guide describes how to add additional processes to the code.

A permanent link to the Environmental Modelling Suite (EMS) C code used in this paper is (CSIRO, 2019):

<https://doi.org/10.25919/5e701c5c2d9c9>.

The code available is also available on GitHub at <https://github.com/csiro-coasts/EMS/> which continues to be developed. The version is labelled as vB3p0 is to distinguish it from earlier versions of the ecological library used in the

20 eReefs project and others. At the GitHub site, vB3p0 is referred to as ecology v1.1.1, is contained within EMS release v1.1 in the GitHub archive, and can be accessed at:

<https://github.com/csiro-coasts/EMS/releases/tag/v1.1.1>

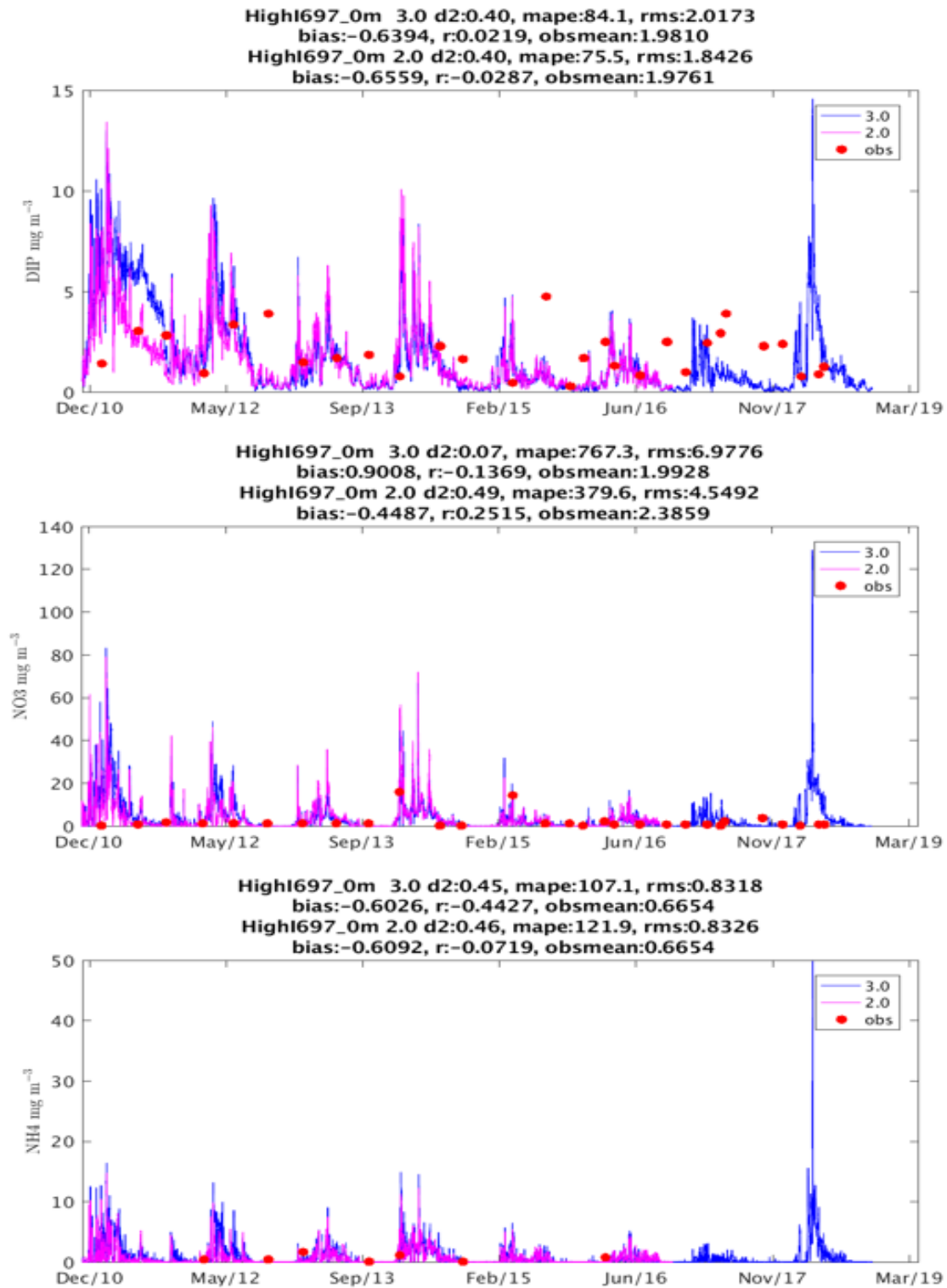
The list of processes that this paper describes are given in a configuration file in App. A. The library contains other processes that have been retained for backward comparability, or for other applications (i.e. mussel farms).

25 The method in which in differential equations described in this scientific description are incorporated into the model code are described in App. B.

## 13 Relocatable Coast and Ocean Model (RECOM)

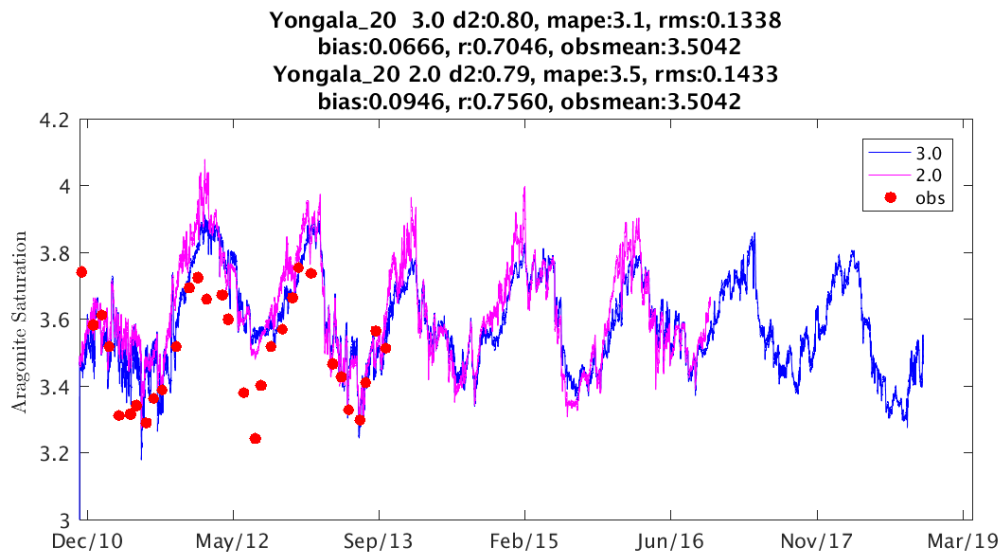
A web based interface, RECOM, has been developed to automate the process of downscaling the EMS model using an existing hindcast as boundary conditions (<https://research.csiro.au/ereefs/models/models-about/recom/>, including the RECOM User Manual). For the purposes of learning how to apply the EMS software available, RECOM provides

30



**Figure 17.** Dissolved inorganic phosphorus (top), nitrate (centre) and ammonium (bottom) concentrations at High Island, central GBR: observations (red dots), simulation vB2p0 (pink) and vB3p0 (blue). **79**





**Figure 18.** Aragonite saturation state calculated from temperature, DIC and alkalinity at 20 m depth at the IMOS Yongala mooring, central GBR: observations (red dots), simulation B2p0 (pink) and B3p0 (blue).

the user with the ability to generate a complete test case of a domain situated along the northeast Australian coastline. Once a RECOM simulation has been generated using the web interface, the entire simulation including source code, forcing and initial condition files, model configuration files and the model output can be downloaded. This allows the user to repeat the model simulation on their own computing system, and modify code, forcing, and output frequency as required. The technical details of RECOM are detailed in Baird et al. (2018), and in the RECOM User Manual.

## 14 Discussion

The EMS BGC model development has been a function of the historical applications of the model across a range of ecosystems, so it is worth giving a brief history of the model development.

### 14.1 History of the development of the EMS biogeochemical model

- 10 The EMS biogeochemical model was first developed as a nitrogen-based model for determining the assimilative capacity for sewerage discharged into Port Philip Bay, the embayment of the city of Melbourne (Harris et al., 1996). This study saw a focus on sediment processes such as denitrification, and demonstrated the ability of bay-wide denitrification to prevent change in the ecological state of the bay exposed to sewerage treatment plant loads (Murray and Parslow, 1997; Murray and Parslow, 1999). The basic structure of the model, and in particular the split of pelagic, epibenthic and sediment zones were in place for this

project. This zonation generated the ability to resolve processes in shallow water systems, and in particular to consider benthic flora in detail.

The next major study involved simulating a range of estuarine morphologies (salt wedge, tidal, lagoon, residence times) and forcings (river flow seasonality, nutrient inputs etc.) that were representative of Australia's 1000+ estuaries (Baird et al., 2003).

5 At this point carbon and phosphorus were included in the model, and the process of including physical limits to ecological processes begun (e.g. diffusion limitation of nutrient uptake and encounter rate limitation of grazing).

Following studies in the phosphorus-limited Gippsland Lakes and macro-tidal Ord River system led to the refinement of the phosphorus absorption / desorption processes. Further studies of the biogeochemical - sediment interactions in the sub-tropical Fitzroy River (Robson et al., 2006) and investigation of the impacts of a tropical cyclone (Condie et al., 2009), saw a stronger

10 link to remote observations. At this time the use of offline transport schemes were also implemented (such as the Moreton Bay model), allowing for an order of magnitude faster model integration (Gillibrand and Herzfeld, 2016).

The next major change in the BGC model involved implementing variable C:N:P ratios of microalgae through the introduction of reserves of energy, nitrogen and phosphorus (Wild-Allen et al., 2010), allowing for more accurate prediction of the elemental budgets and impacts of natural and anthropogenic forcing of the Derwent River estuary, southeast Tasmania. This study was followed up by a number of studies developing scenarios to inform management strategies of the region (Wild-Allen et al., 2011, 2013; Skerratt et al., 2013; Hadley et al., 2015a, b).

From 2010 onwards, EMS has been applied to consider the impacts of catchment loads on the Great Barrier Reef. The focus on water clarity led to the development of a spectrally-resolved optical model, and the introduction of simulated true colour (Baird et al., 2016b). The eReefs project was the first EMS application to consider corals, resulting in the introduction of the 20 host-symbiont coral system and equilibrium carbon chemistry (Mongin and Baird, 2014; Mongin et al., 2016b, a). Additionally, the calculation of model outputs that match remote-sensing observations allowed the model to be run in a data assimilating system, where the observation-model mis-match was based on remote-sensing reflectance (Jones et al., 2016).

The most recent application of the EMS BGC model has been for investigating the environmental impact of aquaculture in Los Lagos, Chile. For the Los Lagos application, new processes for fish farms, dinoflagellates and benthic filter feeders 25 were added, although these additions aren't described in this document. As a demonstration of the ability to add and remove processes, the Los Lagos application was run with the same EMS C executable file as the Great Barrier Reef application - just with the configuration files altered.

## 14.2 Comparison with other marine biogeochemical models

As introduced earlier, there are a number of complex marine biogeochemical model. The most similar model in scope and 30 approach to EMS is the ERSEM (European Regional Seas Ecosystem Model) model (Butenschön et al., 2016). Both ERSEM and EMS consider in detail pelagic, benthic and sediment processes, and could generally be described as functional group models. That is, the state variables, and the processes that link them, are chosen to represent groups of organisms that act in similar ways. This allows the complexity of real systems to be reduced to a tractable model. Many functional group style biogeochemical models exist, and were in fact the earliest models developed (Riley, 1947; Fasham, 1993; Sarmiento et al.,

1993). The most significant differences between EMS and ERSEM are (1) EMS concentrates more on benthic flora than ERSEM, while ERSEM considers lower trophic level ecosystem interactions such as fisheries that are not captured in EMS; and (2) while EMS and ERSEM have similar state variables and processes, EMS has a different set of governing equations that are based on geometric constraints of individuals while ERSEM, like most other functional biogeochemical models, has equations based on empirical relationships determined from population interactions.

The last two decades have seen additional modelling approaches emerge: trait-based models that consider changing processes rates as populations vary (Bruggeman and Kooijman, 2007); size-based models that determine rates based on organism size (Baird et al., 2007a); ecosystem-style models that consider a multiple "species" within a functional group, developing large food-webs (Fulton et al., 2014); and models that consider a large number of functional groups that is refined through competition between groups (Follows et al., 2007). These new approaches are applied primarily in pelagic ecosystems, where the generic nature of pelagic interactions encourages over-arching philosophies to model construction, and with considerable success (Dutkiewicz et al., 2015). The awkwardness of the variety of benthic communities (corals, seagrass, kelp etc.), and their prime role in shallow water, has meant that estuarine and coastal models have, like ERSEM and EMS, typically chosen the functional model approach (Madden and Kemp, 1996; Spillman et al., 2007).

### 14.3 Future developments in EMS

EMS has been developed to address specific scientific questions in Australia's coastal environment. As a result, the set of processes the EMS considers varies from those typically applied by other groups developing marine BGC models. Processes which have not been considered, but often are considered in marine BGC models, include iron and silicate limitation (which are not common on the Australian continental shelf or estuaries), photoinhibition of microalgae, explicit bacterial biomass. Each of these will be considered as the need arises.

A deliberate decision in the development of the EMS BGC model was made to avoid higher trophic level processes, such as fish dynamics and reproduction of long-lived species. This decision was made because: (1) including these longer time-scale, often highly non-linear, processes reduces the ability of development to concentrate on BGC processes; and (2) it was recognised that CSIRO has developed a widely-used ecosystem model (Atlantis, <https://research.csiro.au/atlantis/>, Fulton et al. (2014)), and that coupling the EMS with Atlantis takes advantage of complimentary strengths of the two modelling systems.

A recent capability introduced to EMS is the development of a relocatable capability (RECOM, Sec. 13), allowing model configurations (grid, river and meteorological forcing, ecological processes, boundary conditions) to be automatically generated. This capability will be a good test of the portability of the BGC model, and in particular the use of geometric description of physical limits to ecological processes.

Future enhancements in the EMS BGC model for tropical systems are likely to continue to pursue those components at risk from human impacts, such as dissolution of marine carbonates affecting sediment substrate and herbicide interactions with photosystems. We also expect to continue to refine the optical model, and in particular the relationship between particle size distribution and mass-specific scattering and absorption properties. In temperate systems, current and near-future deployments

of EMS in Australia will be focussed on coastal system characterisation for aquaculture, carbon sequestration and management decision support for the Blue Economy. Ongoing research includes improved methods for model validation against observations and translation of model outputs into knowledge that informs stakeholder decisions.

#### **14.4 Concluding thoughts**

- 5 The BGC model in the CSIRO EMS has developed unique parameterisation when compared to other marine biogeochemical models applied elsewhere due in part to a unique set of scientific challenges of the Australian coastline. It has proved to be useful in many applications, most notably the Great Barrier Reef where extensive observational datasets has allowed new process model development and detailed model skill assessment [(Baird et al., 2016b, a; Mongin et al., 2016b; Skerratt et al., 2019) and `eReefs.info`]. This document provides easy access to some of the novel process formulations that have been
- 10 important in this success, as well as a complete scientific description of version B3p0.

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*Author contributions.* All authors contributed to the CSIRO EMS BGC model through either proposing model formulations, writing significant components of the code, or through applying the model. The primary developers were Mark Baird, Karen Wild-Allen, John Parslow, Mathieu Mongin, Barbara Robson and Farhan Rizwi. Baird was the primary writer of the manuscript, and all co-authors contributed comments.

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Supplementary Material for:

## CSIRO Environmental Modelling Suite (EMS): Scientific description of the optical and biogeochemical models (vB3p0).

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## Contents

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- B. Code architecture
- C. State (prognostic) variables
- D. Parameter values
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## Appendix A: Process list of B3p0

The processes described in this paper are for version B3p0, which is invoked with a configuration file listing the processes in each of the domains water, sediment and epibenthic:

```
water
5 {
  tfactor
  viscosity
  moldiff
  values_common
10 remineralization
  microphytobenthos_spectral_grow_wc
  phytoplankton_spectral_grow_wc (small)
  phytoplankton_spectral_grow_wc (large)
  trichodesmium_mortality_wc
15 trichodesmium_spectral_grow_wc
  phytoplankton_spectral_mortality_wc (small)
  phytoplankton_spectral_mortality_wc (large)
  zooplankton_mortality_wc (small)
  zooplankton_mortality_wc (large)
20 zooplankton_large_carnivore_spectral_grow_wc
  zooplankton_small_spectral_grow_wc
  nitrification_wc
  p_adsorption_wc
  carbon_chemistry_wc
25 gas_exchange_wc (carbon, oxygen)
  light_spectral_wc (H, HPLC)
  massbalance_wc
  }
  epibenthos
30 {
  tfactor_epi ()
  values_common_epi ()
  macroalgae_spectral_grow_epi ()
  seagrass_spectral_grow_epi (Zostera)
35 seagrass_spectral_grow_epi (Halophila)
  seagrass_spectral_grow_epi (Deep)
  coral_spectral_grow_bleach_epi ()
```

```

coral_spectral_carb_epi(H)
macroalgae_mortality_epi()
seagrass_spectral_mortality_proto_epi(Zostera)
seagrass_spectral_mortality_proto_epi(Halophila)
5 seagrass_spectral_mortality_proto_epi(Deep)
massbalance_epi()
light_spectral_uq_epi(H)
diffusion_epi()
}
10 sediment
{
tfactor
viscosity
moldiff
15 values_common
remineralization
light_spectral_sed(HPLC)
microphytobenthos_spectral_grow_sed
carbon_chemistry_wc()
20 microphytobenthos_spectral_mortality_sed
phytoplankton_spectral_mortality_sed(small)
phytoplankton_spectral_mortality_sed(large)
zooplankton_mortality_sed(small)
zooplankton_mortality_sed(large)
25 trichodesmium_mortality_sed
nitrification_denitrification_sed
p_adsorption_sed
massbalance_sed()
}
30 or alternatively with a call in the configuration file: PROCESSFNAME B3p0.

```

Other processes in the `process_library` can be validly called, but their scientific description is not given in this paper. The header in the source code for each process file gives detail about its use within the code, such as any arguments that it requires (for example `seagrass_spectral_grow_epi` requires the seagrass type as an argument).



## Appendix B: Code architecture

This paper is a scientific description of the EMS ecological library (`/EMS/model/lib/ecology`). The ecological library consists primarily of a set of routines describing individual processes. The model chooses which processes it will include based on a configuration file (App. A provides the configuration file for B3p0). The model equations are primarily derivatives of the ecological state variables, and have been split in this paper into separate processes (such as a phytoplankton growth), thus aligning with the code (such as `phytoplankton_spectral_grow_wc.c`). This object-based approach allows individual processes to be included / excluded in a configuration file without re-writing the model code.

Within a process file, the routine containing the ecological derivatives is `<process_name>_calc`, and within that routine the ecological derivatives are stored within the array `y1`. Each element in the array `y1` stores the derivatives of a state variable. The index to the array for each state variable is determined within each process initialisation routine, `<process_name>_init`, and stored in the processes' workspace `ws`. In the case of nitrate, for example, the derivative held in `y1` will be the sum of the derivatives calculated in multiple processes (such as each autotrophic growth process, nitrification, denitrification, and each grazing and mortality process). The array of derivatives is then used by the model's adaptive integrator to update the model state, as held in the array `y`.

Some components of the ecological model are updated only once every time step without the derivatives being calculated. These include the optical and carbon chemistry model state variables. In these cases, the state variables, which are stored in the array `y`, are updated directly and this is done in either the routine `<process_name>_precalc` or `<process_name>_postcalc`.

### Appendix C: State (prognostic) variables

The below tables list the ecologically-relevant physical variables (Table C1), 10 dissolved (Table C2), 20 microalgal (Table C3), 2 zooplankton (Table C4), 7 non-living inorganic particulate (Table C5), 7 non-living organic particulate (Table C6) and 7 epibenthic plant (Table C7) and 5 coral polyp (Table C8) and 4 reaction centre (Table C9) state variables. All state variables that exist in the water column layers have an equivalent in the 5 sediment layers (and are specified by `<variable name>_sed`). The dissolved tracers are given as a concentration in the porewater, while the particulate tracers are given as a concentration per unit volume (see Sec. 10.3.2).

Name	Symbol	Units	Description
Temperature (temp)	$T$	°C	Water temperature
Salinity (salt)	$S$	PSU	Water salinity
Sea level elevation (eta)	$\eta$	m	Sea level elevation relative to mean sea level
Porosity (porosity)	$\phi$	-	Fraction of the volume made up of water
Bottom shear stress (us- trcw_skin)	$\tau$	N m <sup>-2</sup>	Shear stress due to currents and waves
Sand ripple height (PHYS- RIPH)	-	m	Physical dimension used for estimating bottom roughness due to ripples according to Grant and Madsen (1982)
Solar zenith (Zenith)	$\theta_{air}$	radians	Solar zenith angle is the angle between the zenith and the centre of the Sun's disc, taking a value of zero with the sun directly above, and $\pi/2$ when at, or below, the horizon.

**Table C1.** Long name (and variable name) in model output files, symbol and units used in this document, and a description of ecologically-relevant physical state and diagnostic variables.

Name	Symbol	Units	Description
Total alkalinity (alk)	$A_T$	$\text{mol kg}^{-1}$	Concentration of ions that can be converted to uncharged species by a strong acid. The model assumes $A_T = [\text{HCO}_3^-] + [\text{CO}_3^{2-}]$ , often referred to as carbonate alkalinity. Alkalinity and DIC together quantify the equilibrium state of the seawater carbon chemistry.
Nitrate (NO3)	$[\text{NO}_3^-]$	$\text{mg N m}^{-3}$	Concentration of nitrate. In the absence of nitrite $[\text{NO}_2^-]$ in the model, nitrate represents $[\text{NO}_3^-] + [\text{NO}_2^-]$ .
Ammonium (NH4)	$[\text{NH}_4^-]$	$\text{mg N m}^{-3}$	Concentration of dissolved ammonium.
Dissolved Inorganic Phosphorus (DIP)	$P$	$\text{mg P m}^{-3}$	Concentration of dissolved inorganic phosphorus, also referred to as orthophosphate or soluble reactive phosphorus, SRP, composed chiefly of $\text{HPO}_4^{2-}$ ions, with a small percentage present as $\text{PO}_4^{3-}$ .
Dissolved inorganic carbon (DIC)	$DIC$	$\text{mg C m}^{-3}$	Concentration of dissolved inorganic carbon, composed chiefly at seawater pH of $\text{HCO}_3^-$ , with a small percentage present as $\text{CO}_3^{2-}$ .
Dissolved oxygen (Oxygen)	$[\text{O}_2]$	$\text{mg O m}^{-3}$	Concentration of oxygen.
Chemical Oxygen Demand (COD)	$COD$	$\text{mg O m}^{-3}$	Concentration of products of anoxic respiration in oxygen units. This represents products such as hydrogen sulfide, $\text{H}_2\text{S}$ , that are produced during anoxic respiration and which, upon reoxidation of the water, will consume oxygen.
Dissolved Organic Carbon (DOR_C)	$O_C$	$\text{mg C m}^{-3}$	The concentration of carbon in dissolved organic compounds.
Dissolved Organic Nitrogen (DOR_N)	$O_N$	$\text{mg N m}^{-3}$	The concentration of nitrogen in dissolved organic compounds.
Dissolved Organic Phosphorus (DOR_P)	$O_P$	$\text{mg P m}^{-3}$	The concentration of phosphorus in dissolved organic compounds.

**Table C2.** Long name (and variable name) in model output files, symbol and units used in this document, and a description of all dissolved state variables. When the concentration of an ion is given, the chemical formulae appears in [ ] brackets.

Name	Symbol & Units	Description
Phytoplankton (*_N)	$N$ [mg N m <sup>-3</sup> ]	Total structural biomass of nitrogen of the phytoplankton population. All microalgae have a C:N:P ratio of the structural material of 106:16:1. Thus the mass of phosphorus in the structural material of a population with a biomass $B$ is given by: $\frac{1}{16} \frac{31}{14} B$ and the mass of carbon by: $\frac{106}{16} \frac{12}{14} B$ . The number of cells is given by $B/m_N$ .
Phytoplankton N reserves (*_NR)	$BR_N^*$ [mg N m <sup>-3</sup> ]	Total non-structural biomass of nitrogen of the phytoplankton population. Phytoplankton N reserves divided by Phytoplankton N is a number between 0 and 1 and represents the factor by which phytoplankton growth is inhibited due to the internal reserves of nitrogen.
Phytoplankton P reserves (*_PR)	$\frac{1}{16} \frac{31}{14} BR_P^*$ [mg P m <sup>-3</sup> ]	Total non-structural biomass of phosphorus of the phytoplankton population. Phytoplankton P reserves divided by (Phytoplankton N $\times \frac{1}{16} \frac{31}{14}$ ) is a number between 0 and 1 and represent the factor by which phytoplankton growth is inhibited due to the internal reserves of phosphorus.
Phytoplankton I reserves (*_I)	$\frac{1060}{16} \frac{1}{14} BR_I^*$ [mmol photon m <sup>-3</sup> ]	Total non-structural biomass of fixed carbon of the phytoplankton population, quantified in photons. Phytoplankton I reserves divided by (Phytoplankton N $\times \frac{1060}{16} \frac{1}{14}$ ) is a number between 0 and 1 and represent the factor by which phytoplankton growth is inhibited due to the internal reserves of energy (or fixed carbon).
Phytoplankton chlorophyll (*_Chl)	$nc_i V$ [mg m <sup>-3</sup> ]	Concentration of the chlorophyll $a$ pigment of the population. The four phytoplankton classes have two pigments, a chlorophyll $a$ -based pigment and an accessory pigment. As the pigment concentration adjusts to optimise photosynthesis, including the presence of the accessory pigment, the intracellular content, $c_i V$ , represents only the chlorophyll $a$ -based pigment. As the model does not distinguish between mono-vinyl and di-vinyl forms of chlorophyll, this $c_i$ represents either form, depending on the phytoplankton type.

**Table C3.** Long name (and variable name) in model output files, symbol and units used in this document, and description of all microalgae state variables in the model. The model contains four categories of phytoplankton (category shown as \* in left column, and given in brackets in following list): small (PhyS),  $r < 2 \mu\text{m}$  phytoplankton; large (PhyL);  $r > 2 \mu\text{m}$  phytoplankton; *Trichodesmium* (Tricho); nitrogen fixing phytoplankton; and benthic microalgae (MPB): fast-sinking diatoms that are suspended primarily in the top layer of sediment porewaters. The elemental ratio of phytoplankton including both structural material and reserves is given by: C:N:P =  $106(1 + R_C^*) : 16(1 + R_N^*) : (1 + R_P^*)$ . In the model description (this document) we have more correctly described fixed carbon as carbon reserves, while in the model outputs they are represented quantified as energy reserves. The relationship is 1 mg C of carbon reserves is equal to  $(1060/106)/12.01$  mmol photons of energy reserves.

Name	Symbol	Units	Description
Zooplankton	N (ZooS_N,	[mg N m <sup>-3</sup> ]	Total biomass of nitrogen in animals. With only small and large zooplankton categories
ZooL_N)	Z		resolved, small zooplankton represents the biomass of unicellular fast growing animals (protozoans) and large zooplankton represents the biomass of all other animals (metazoans). All zooplankton have a C:N:P ratio of 106:16:1. Thus the mass of phosphorus of a population with a biomass $Z$ is given by: $\frac{1}{16} \frac{31}{14} Z$ and the mass of carbon by: $\frac{106}{16} \frac{12}{14} Z$ .

**Table C4.** Long name (and variable name) in model output files, symbol, unit used in this document, and description of zooplankton state variables in the model.

Name	Symbol	Units	Description
Fine Sediment (FineSed)	<i>FineSed</i>	[kg m <sup>-3</sup> ]	Identical to Mud-mineral, except that it is initialised to zero in the model domain, and enters only from the catchments.
Dust (Dust)	<i>Dust</i>	[kg m <sup>-3</sup> ]	Very small sized, re-suspending particles with a sinking velocity of 1 m d <sup>-1</sup> and mass-specific optical properties based on observations in Gladstone Harbour.
Mud-mineral (Mud-mineral)	<i>Mud<sub>non-CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Small sized, re-suspending particles with a sinking velocity of 17 m d <sup>-1</sup> , and mass-specific optical properties based on observations in Gladstone Harbour.
Mud-carbonate (Mud-carbonate)	<i>Mud<sub>CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Small sized, re-suspending particles with a sinking velocity of 17 m d <sup>-1</sup> , and mass-specific optical properties based on observations of suspended carbonates at Lucinda Jetty.
Sand-mineral (Sand-mineral)	<i>Sand<sub>non-CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Medium sized, re-suspending particles with a sinking velocity of 173 m d <sup>-1</sup> and mass-specific optical properties based on observations in Gladstone Harbour.
Sand-carbonate (Sand-carbonate)	<i>Sand<sub>CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Medium sized, re-suspending particles with a sinking velocity of 173 m d <sup>-1</sup> and mass-specific optical properties based on observations of suspended carbonates at Lucinda Jetty.
Gravel-mineral (Gravel-mineral)	<i>Gravel<sub>non-CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Large, non-resuspending particles.
Gravel-carbonate (Gravel-carbonate)	<i>Gravel<sub>CaCO3</sub></i>	[kg m <sup>-3</sup> ]	Large, non-resuspending particles.

**Table C5.** Long name (and variable name) in model output files, symbol, unit used in this document, and description of all inorganic particulate state variables in the model.

Name	Symbol	Units	Description
Particulate Inorganic Phosphorus (PIP)	$P/IP$	[mg m <sup>-3</sup> ]	Phosphorus ions that are absorbed onto particles. It is considered a particulate with the same properties as Mud.
Immobilised Particulate Inorganic Phosphorus (PIPI)	$P/IPI$	[mg m <sup>-3</sup> ]	Phosphorus that is permanently removed from the system through burial of PIP.
Labile Detritus Nitrogen Plank (DetPL_N)	$D_{Red}$	[mg m <sup>-3</sup> ]	Concentration of N in labile (quickly broken down) organic matter with a C:N:P ratio of 106:16:1 derived from living microalgae, zooplankton, coral host tissue and zooxanthellae with the same C:N:P ratio. Thus the mass of phosphorus in $D_{Red}$ is given by: $\frac{1}{16} \frac{31}{14} D_{Red}$ and the mass of carbon by: $\frac{106}{16} \frac{12}{14} D_{Red}$ .
Labile Detritus Nitrogen Ben- thic (DetBL_N)	$D_{Atk}$	[mg m <sup>-3</sup> ]	Concentration of N in labile (quickly broken down) organic matter with a C:N:P ratio of 550:30:1 derived from living seagrass and macroalgae with the same C:N:P ratio. Thus the mass of phosphorus in $D_{Atk}$ is given by: $\frac{1}{30} \frac{31}{14} D_{Atk}$ and the mass of carbon by: $\frac{550}{30} \frac{12}{14} D_{Atk}$ .
Refractory Detritus Carbon (DetR_C)	$D_C$	[mg m <sup>-3</sup> ]	Concentration of carbon as particulate refractory (slowly breaking down) material. It is sourced only from the breakdown of labile detritus, and from rivers.
Refractory Detritus Nitrogen (DetR_N)	$D_N$	[mg m <sup>-3</sup> ]	Concentration of nitrogen as particulate refractory (slowly breaking down) material. It is sourced only from the breakdown of labile detritus, and from rivers.
Refractory Detritus Phosphorus (DetR_P)	$D_P$	[mg m <sup>-3</sup> ]	Concentration of phosphorus as particulate refractory (slowly breaking down) material. It is sourced only from the breakdown of labile detritus, and from rivers.

**Table C6.** Long name (and variable name) in model output files, symbol, unit used in this document, and description of all particulate detrital state variables in the model.

Name	Symbol	Description
Macroalgae (MA)	$MA$ [ $g\ N\ m^{-2}$ ]	Concentration of nitrogen biomass per $m^2$ of macroalgae. Macroalgae (or seaweed) grows above all other benthic plants (corals, seagrasses, benthic microalgae). It is parameterised as a non-calcifying leafy algae, with a C:N:P ratio of 550:30:1, and a formulation for calculating the percentage of the bottom covered as $1 - \exp(-\Omega_{MA} MA)$ . In the model, in the absence of both calcifying macroalgae (particularly <i>Halimeda</i> ) and unicellular epiphytes, macroalgae represents the biomass of all seaweeds and epiphytes.
Seagrass (SG)	$SG$ [ $g\ N\ m^{-2}$ ]	Concentration of nitrogen biomass per $m^2$ of a seagrass form parameterised to be similar to <i>Zostera</i> . This form captures light after it has passed through macroalgae and before it passes through <i>Halophila</i> . This form is better adapted to high light, low nutrient conditions than <i>Halophila</i> as a result of a deeper root structure and being able to shade it. See macroalgae for elemental ratio and bottom cover.
Halophila (SGH)	$SGH$ [ $g\ N\ m^{-2}$ ]	Concentration of nitrogen biomass per $m^2$ of a seagrass form parameterised to be similar to <i>Halophila ovalis</i> . This form captures light after it has passed through the <i>Zostera</i> seagrass form. The <i>Halophila ovalis</i> form is better adapted to low light conditions than <i>Zostera</i> , having a faster growth rate and lower minimum light requirement. See macroalgae for elemental ratio and bottom cover.
Deep seagrass (SGD)	$SGD$ [ $g\ N\ m^{-2}$ ]	Concentration of nitrogen biomass per $m^2$ of a seagrass form parameterised to be similar to <i>Halophila decipiens</i> . This form captures light after it has passed through the <i>Zostera</i> and <i>Halophila ovalis</i> seagrass form.
*root N	$*ROOT\_N$ [ $g\ N\ m^{-2}$ ]	Concentration of nitrogen biomass per $m^2$ in the roots of seagrass type * (SG, SGH or SGD). While this biomass in reality exists in multiple depths in the sediments, and in the model accesses multiple layers for nutrient uptake, it is quantified in the epibenthic compartment.

**Table C7.** Long name (and variable name) in model output files, units, symbol used in this document, and description of macroalgae and seagrass state variables in the model. The order in the above table corresponds to their vertical position, and therefore the order in which they access light. Benthic microalgae, being suspended in porewaters, is consider as a particulate in Table C5.



Name	Symbol	Description
Coral host N (CH_N)	$CH$ [g N m <sup>-2</sup> ]	Concentration of nitrogen biomass per m <sup>2</sup> of coral host tissue in the entire grid cell. Unlike other epibenthic variables, corals area is assumed to exist in communities that are potentially smaller than the grid size. The fraction of the grid cell covered by corals is given by $A_{CH}$ . Thus the biomass in the occupied region is given by $CH/A_{CH}$ . The percent coverage of the coral of the bottom for the whole cell is given by $A_{CH} (1 - \exp(-\Omega_{CH} CH/A_{CH}))$ . With only one type of coral resolved, $CH$ represents the biomass of all symbiotic corals. Since the model contains no other benthic filter-feeders, $CH$ best represent the sum of the biomass of all symbiotic filter-feeding organisms such as corals, sponges, clams etc. C:N:P is 106:16:1.
Coral symbiont N (CS_N)	$CS$ [mg N m <sup>-2</sup> ]	Concentration of nitrogen biomass per m <sup>2</sup> of coral symbiont cells, or zooxanthellae. To determine the density of cells, use $n = CS/m_N$ . The percentage of the bottom covered is given by $\frac{\pi}{2\sqrt{3}} n \pi r_{zo}^2$ , where $\pi r^2$ is the projected area of the cell, $n$ is the number of cells, and $\pi/(2\sqrt{3}) \sim 0.9069$ accounts for the maximum packaging of spheres. C:N:P is 106:16:1.
Coral symbiont chl (CS_Ch)	$nc_i V$ [mg chl m <sup>-2</sup> ]	Concentration of chlorophyll biomass per m <sup>2</sup> of coral symbiont cells.
Coral symbiont diadinoxanthin (CS_Xp)	$nx_p V$ [mg pig m <sup>-2</sup> ]	Concentration of the photosynthetic xanthophyll cycle pigment per m <sup>2</sup> of coral symbiont cells.
Coral symbiont diatoxanthin (CS_Xh)	$nx_h V$ [mg pig m <sup>-2</sup> ]	Concentration of heat dissipating xanthophyll cycle pigment biomass per m <sup>2</sup> of coral symbiont cells.

**Table C8.** Long name (and variable name) in model output files, units, symbol used in this document, and description of coral state variables in the model.

Name	Symbol	Description
Symbiont oxidised RC (CS_Qox)	$Q_{ox}$ [ $\text{mg N m}^{-2}$ ]	Concentration of symbiont reaction centres in an oxidised state per $\text{m}^2$ , residing in the symbiont, of in the entire grid cell.
Symbiont reduced RC (CS_Qred)	$Q_{red}$ [ $\text{mg N m}^{-2}$ ]	Concentration of symbiont reaction centres in a reduced state per $\text{m}^2$ , residing in the symbiont, of in the entire grid cell.
Symbiont inhibited RC (CS_Qin)	$Q_{in}$ [ $\text{mg N m}^{-2}$ ]	Concentration of symbiont reaction centres in an inhibited state per $\text{m}^2$ , residing in the symbiont, of in the entire grid cell.
Symbiont reactive oxygen gen (CS_RO)	[ $ROS$ ] [ $\text{mg N m}^{-2}$ ]	Concentration of reactive oxygen per $\text{m}^2$ , residing in the symbiont, of in the entire grid cell.

**Table C9.** Long name (and variable name) in model output files, units, symbol used in this document, and description of coral reaction state variables in the model.

### Appendix D: Parameter values used in eReefs biogeochemical model (B3p0).

The below five tables of parameters are specified for each run, and can be automatically generated by the EMS software after a simulation from the parameter file. At model initialisation the model produces a file `ecology_setup.txt` that contains a list of all the parameter values used, both those specified in the parameter file, and those using model defaults.

5 For a more information see Robson et al. (2018).

Description	Name in code	Symbol	Value	Units
Reference temperature	Tref	$T_{ref}$	2.000000e+01	Deg C
Temperature coefficient for rate parameters	Q10	Q10	2.000000e+00	none
Nominal rate of TKE dissipation in water column	TKEeps	$\epsilon$	1.000000e-06	$\text{m}^2 \text{s}^{-3}$
Atmospheric CO2	xco2_in_air	$p\text{CO}_2$	3.964800e+02	ppmv
Concentration of dissolved N2	N2	$[\text{N}_2]_{gas}$	2.000000e+03	$\text{mg N m}^{-3}$
DOC-specific absorption of CDOM 443 nm	acdom443star	$k_C \text{DOM}_{443}$	1.300000e-04	$\text{m}^2 \text{mg C}^{-1}$

**Table D1.** Environmental parameters in eReefs biogeochemical model (B3p0).

Description	Name in code	Symbol	Value	Units
Chl-specific scattering coef. for microalgae	bphy	$b_{phy}$	2.000000e-01	$m^{-1}(mg\ Chla\ m^{-3})^{-1}$
Nominal N:Chl a ratio in phytoplankton by weight	NtoCHL	$R_{N:Chl}$	7.000000e+00	$g\ N(g\ Chla)^{-1}$
Maximum growth rate of PL at Tref	PLumax	$\mu_{PL}^{max}$	1.400000e+00	$d^{-1}$
Radius of the large phytoplankton cells	PLrad	$r_{PL}$	4.000000e-06	m
Natural (linear) mortality rate, large phytoplankton	PhyL_mL	$m_{L,PL}$	1.000000e-01	$d^{-1}$
Natural (linear) mortality rate in sed., large phyto.	PhyL_mL_sed	$m_{L,PL,sed}$	1.000000e+01	$d^{-1}$
Maximum growth rate of PS at Tref	PSumax	$\mu_{PS}^{max}$	1.600000e+00	$d^{-1}$
Radius of the small phytoplankton cells	PSrad	$r_{PS}$	1.000000e-06	m
Natural (linear) mortality rate, small phyto.	PhyS_mL	$m_{L,PS}$	1.000000e-01	$d^{-1}$
Natural (linear) mortality rate in sed., small phyto.	PhyS_mL_sed	$m_{L,PS,sed}$	1.000000e+00	$d^{-1}$
Maximum growth rate of MB at Tref	MBumax	$\mu_{MPB}^{max}$	8.390000e-01	$d^{-1}$
Radius of the MPB cells	MBrad	$r_{MPB}$	1.000000e-05	m
Natural (quadratic) mortality rate, MPB (in sed)	MPB_mQ	$m_{Q,MPB}$	1.000000e-04	$d^{-1}(mg\ N\ m^{-3})^{-1}$
Ratio of xanthophyll to chl a of PS	PSxan2chl	$\Theta_{xan2chl,PS}$	5.100000e-01	$mg\ mg^{-1}$
Ratio of xanthophyll to chl a of PL	PLxan2chl	$\Theta_{xan2chl,PL}$	8.100000e-01	$mg\ mg^{-1}$
Ratio of xanthophyll to chl a of MPB	MBxan2chl	$\Theta_{xan2chl,MPB}$	8.100000e-01	$mg\ mg^{-1}$
Maximum growth rate of Trichodesmium at Tref	Tricho_umax	$\mu_{MPB}^{max}$	2.000000e-01	$d^{-1}$
Radius of Trichodesmium colonies	Tricho_rad	$r_{MPB}$	5.000000e-06	m
Sherwood number for the Tricho dimensionless	Tricho_Sh	$Sh_{Tricho}$	1.000000e+00	none
Linear mortality for Tricho in sediment	Tricho_mL	$m_{L,Tricho}$	1.000000e-01	$d^{-1}$
Quadratic mortality for Tricho due to phages in wc	Tricho_mQ	$m_{Q,Tricho}$	1.000000e-01	$d^{-1}(mg\ N\ m^{-3})^{-1}$
Critical Tricho above which quadratic mortality applies	Tricho_crit		2.000000e-04	$mg\ N\ m^{-3}$
Minimum density of Trichodesmium	p_min	$\rho_{min,Tricho}$	9.000000e+02	$kg\ m^{-3}$
Maximum density of Trichodesmium	p_max	$\rho_{max,Tricho}$	1.050000e+03	$kg\ m^{-3}$
DIN conc below which Tricho N fixes	DINcrit	$DIN_{crit}$	1.000000e+01	$mg\ N\ m^{-3}$
Ratio of xanthophyll to chl a of Trichodesmium	Trichoxan2chl	$\Theta_{xan2chl,Tricho}$	5.000000e-01	$mg\ mg^{-1}$
Minimum carbon to chlorophyll a ratio	C2Chlmin	$\theta_{min}$	2.000000e+01	w/wt

**Table D2.** Phytoplankton parameters in eReefs biogeochemical model (B3p0).

Description	Name in code	Symbol	Value	Units
Maximum growth rate of ZS at Tref	ZSumax	$\mu_{max}^{ZS}$	4.000000e+00	d <sup>-1</sup>
Radius of the small zooplankton cells	ZStrad	$r_{ZS}$	5.000000e-06	m
Swimming velocity for small zooplankton	ZSswim	$U_{ZS}$	2.000000e-04	m s <sup>-1</sup>
Grazing technique of small zooplankton	ZSmeth		rect	none
Maximum growth rate of ZL at Tref	ZLumax	$\mu_{max}^{ZL}$	1.330000e+00	d <sup>-1</sup>
Radius of the large zooplankton cells	ZLrad	$r_{ZL}$	3.200000e-04	m
Swimming velocity for large zooplankton	ZLswim	$U_{ZL}$	3.000000e-03	m s <sup>-1</sup>
Grazing technique of large zooplankton	ZLmeth		rect	none
Growth efficiency, large zooplankton	ZL_E	$E_{ZL}$	4.260000e-01	none
Growth efficiency, small zooplankton	ZS_E	$E_{ZS}$	4.620000e-01	none
Natural (quadratic) mortality rate, large zooplankton	ZL_mQ	$m_{Q,ZL}$	1.200000e-02	d <sup>-1</sup> (mg N m <sup>-3</sup> ) <sup>-1</sup>
Natural (quadratic) mortality rate, small zooplankton	ZS_mQ	$m_{Q,ZS}$	2.000000e-02	d <sup>-1</sup> (mg N m <sup>-3</sup> ) <sup>-1</sup>
Fraction of growth inefficiency lost to detritus, large zoo.	ZL_FDG	$\gamma_{ZL}$	5.000000e-01	none
Fraction of mortality lost to detritus, large zoo.	ZL_FDM	N/A	1.000000e+00	none
Fraction of growth inefficiency lost to detritus, small zoo.	ZS_FDG	$\gamma_{ZS}$	5.000000e-01	none
Fraction of mortality lost to detritus, small zooplankton	ZS_FDM	N/A	1.000000e+00	none

**Table D3.** Zooplankton parameters in eReefs biogeochemical model (B3p0).

Description	Name in code	Symbol	Value	Units
Fraction of labile detritus converted to refractory detritus	F_LD_RD	$\zeta_{Red}$	1.900000e-01	none
Fraction of labile detritus converted to DOM	F_LD_DOM	$\vartheta_{Red}$	1.000000e-01	none
fraction of refractory detritus that breaks down to DOM	F_RD_DOM	$\vartheta_{Ref}$	5.000000e-02	none
Breakdown rate of labile detritus at 106:16:1	r_DetPL	$r_{Red}$	4.000000e-02	d <sup>-1</sup>
Breakdown rate of labile detritus at 550:30:1	r_DetBL	$r_{Atk}$	1.000000e-03	d <sup>-1</sup>
Breakdown rate of refractory detritus	r_RD	$r_R$	1.000000e-03	d <sup>-1</sup>
Breakdown rate of dissolved organic matter	r_DOM	$r_O$	1.000000e-04	d <sup>-1</sup>
Respiration as a fraction of umax	Plank_resp	$\phi$	2.500000e-02	none
Oxygen half-saturation for aerobic respiration	KO_aer	$K_{OA}$	2.560000e+02	mg O m <sup>-3</sup>
Maximum nitrification rate in water column	r_nit_wc	$\tau_{nit,wc}$	1.000000e-01	d <sup>-1</sup>
Maximum nitrification rate in water sediment	r_nit_sed	$\tau_{nit,sed}$	2.000000e+01	d <sup>-1</sup>
Oxygen half-saturation for nitrification	KO_nit	$K_{O_2,nit}$	5.000000e+02	mg O m <sup>-3</sup>
Rate at which P reaches adsorbed/desorbed equilibrium	Pads_r	$\tau_{Pabs}$	4.000000e-02	d <sup>-1</sup>
Freundlich Isothermic Const P adsorption to TSS in wc	Pads_Kwc	$k_{P,ads,wc}$	3.000000e+01	mg P kg TSS <sup>-1</sup>
Freundlich Isothermic Const P adsorption to TSS in sed	Pads_Ksed	$k_{P,ads,sed}$	7.400000e+01	mg P kg TSS <sup>-1</sup>
Oxygen half-saturation for P adsorption	Pads_KO	$K_{O_2,abs}$	2.000000e+03	mg O m <sup>-3</sup>
Exponent for Freundlich Isotherm	Pads_exp	$N/A$	1.000000e+00	none
Maximum denitrification rate	r_den	$\tau_{denit}$	8.000000e-01	d <sup>-1</sup>
Oxygen half-saturation constant for denitrification	KO_den	$K_{O_2,denit}$	1.000000e+04	mg O m <sup>-3</sup>
Rate of conversion of PIP to immobilised PIP	r_immob_PIP	$\tau_{Pimm}$	1.200000e-03	d <sup>-1</sup>

**Table D4.** Detritus parameters in eReefs biogeochemical model (B3p0).

Description	Name in code	Symbol	Value	Units
Sediment-water diffusion coefficient	EpiDiffCoeff	$D$	3.000000e-07	$\text{m}^2 \text{s}^{-1}$
Thickness of diffusive layer	EpiDiffDz	$h$	6.500000e-03	m
Maximum growth rate of MA at Tref	MAumax	$\mu_{MA}^{max}$	1.000000e+00	$\text{d}^{-1}$
Natural (linear) mortality rate, macroalgae	MA_mL	$\zeta_{MA}$	1.000000e-02	$\text{d}^{-1}$
Nitrogen-specific leaf area of macroalgae	MAleafden	$\Omega_{MA}$	1.000000e+00	$\text{m}^2 \text{g N}^{-1}$
Respiration as a fraction of umax	Benth_resp	$\phi$	2.500000e-02	none
net dissolution rate of sediment without coral	dissCaCO3_sed	$d_{sand}$	1.000000e-03	$\text{mmol C m}^{-2} \text{s}^{-1}$
Grid scale to reef scale ratio	CHarea	$A_{CH}$	1.000000e-01	$\text{m}^2 \text{m}^{-2}$
Nitrogen-specific host area of coral polyp	CHpolypden	$\Omega_{CH}$	2.000000e+00	$\text{m}^2 \text{g N}^{-1}$
Max. growth rate of Coral at Tref	CHumax	$\mu_{CH}^{max}$	5.000000e-02	$\text{d}^{-1}$
Max. growth rate of zooxanthellae at Tref	CSumax	$\mu_{CS}^{max}$	4.000000e-01	$\text{d}^{-1}$
Radius of the zooxanthellae	CSrad	$r_{CS}$	5.000000e-06	m
Quadratic mortality rate of coral polyp	CHmort	$\zeta_{CH}$	1.000000e-02	$(\text{g N m}^{-2})^{-1} \text{d}^{-1}$
Linear mortality rate of zooxanthellae	CSmort	$\zeta_{CS}$	4.000000e-02	$\text{d}^{-1}$
Fraction of coral host death translocated.	CHremin	$f_{remin}$	5.000000e-01	-
Rate coefficient for particle uptake by corals	Splank	$S_{part}$	3.000000e+00	$\text{m d}^{-1}$
Maximum daytime coral calcification	k_day_coral	$k_{day}$	1.320000e-02	$\text{mmol C m}^{-2} \text{s}^{-1}$
Maximum nighttime coral calcification	k_night_coral	$k_{night}$	6.900000e-03	$\text{mmol C m}^{-2} \text{s}^{-1}$
Carbonate sediment dissolution rate on shelf	dissCaCO3_shelf	$d_{shelf}$	1.000000e-04	$\text{mmol C m}^{-2} \text{s}^{-1}$
Age tracer growth rate per day	ageing_decay	$n/a$	1.000000e+00	$\text{d d}^{-1}$
Age tracer decay rate per day outside source	anti_ageing_decay	$\Phi$	1.000000e-01	$\text{d}^{-1}$
Bleaching ROS threshold	ROSthreshold	$\phi_{ROS}$	5.000000e-04	$\text{mg O cell}^{-1}$
Xanthophyll switching rate coefficient	Xanth_tau	$\tau_{xan}$	8.333333e-04	$\text{s}^{-1}$
Ratio of RCII to Chlorophyll a	chl2rcii	$A_{RCII}$	2.238413e-06	$\text{mol RCII g Chl}^{-1}$
Stoichiometric ratio of RCII units to photons	photon2rcii	$m_{RCII}$	1.000000e-07	$\text{mol RCII mol photon}^{-1}$
Maximum zooxanthellae expulsion rate	ROSmaxrate	$\gamma$	1.000000e+00	$\text{d}^{-1}$
Scaling of DetP to DOP, relative to N	r_RD_NtoP	$r_{RD_{NtoP}}$	2.000000e+00	-
Scaling of DOM to DIP, relative to N	r_DOM_NtoP	$r_{DOM_{NtoP}}$	1.500000e+00	-
Radius of Trichodesmium colonies	Tricho_colrad	$r_{Trichocolony}$	5.000000e-06	m

**Table D5.** Benthic parameters in eReefs biogeochemical model (B3p0), excluding seagrass

Description	Name in code	Symbol	Value	Units
Maximum growth rate of SG at Tref	SGumax	$\mu_{SG}^{max}$	4.000000e-01	d <sup>-1</sup>
Half-saturation of SG N uptake in SED	SG_KN	$K_{SG,N}$	4.200000e+02	mg N m <sup>-3</sup>
Half-saturation of SG P uptake in SED	SG_KP	$K_{SG,P}$	9.600000e+01	mg P m <sup>-3</sup>
Natural (linear) mortality rate aboveground seagrass	SG_mL	$\zeta_{SGA}$	3.000000e-02	d <sup>-1</sup>
Natural (linear) mortality rate belowground seagrass	SGROOT_mL	$\zeta_{SGB}$	4.000000e-03	d <sup>-1</sup>
Fraction (target) of SG biomass below-ground	SGfrac	$f_{below,SG}$	7.500000e-01	-
Time scale for seagrass translocation	SGtransrate	$\tau_{tran,SG}$	3.330000e-02	d <sup>-1</sup>
Nitrogen-specific leaf area of seagrass	SGleafden	$\Omega_{SG}$	1.500000e+00	m <sup>2</sup> g N <sup>-1</sup>
Seagrass seed biomass as fraction of 63 % cover	SGseedfrac	$f_{seed,SG}$	1.000000e-02	-
Sine of nadir Zostera canopy bending angle	SGorient	$\sin \beta_{blade,SG}$	5.000000e-01	-
Compensation irradiance for Zostera	SGmlr	$E_{comp,SG}$	4.500000e+00	mol m <sup>-2</sup>
Maximum depth for Zostera roots	SGrootdepth	$z_{root,SG}$	-1.500000e-01	m
Critical shear stress for SG loss	SG_tau_critical	$\tau_{SG,shear}$	1.000000e+00	N m <sup>-2</sup>
Time-scale for critical shear stress for SG loss	SG_tau_time	$\tau_{SG,time}$	4.320000e+04	s
Maximum growth rate of SGH at Tref	SGHumax	$\mu_{SGH}^{max}$	4.000000e-01	d <sup>-1</sup>
Half-saturation of SGH N uptake in SED	SGH_KN	$K_{SGH,N}$	4.200000e+02	mg N m <sup>-3</sup>
Half-saturation of SGH P uptake in SED	SGH_KP	$K_{SGH,P}$	9.600000e+01	mg P m <sup>-3</sup>
Nitrogen-specific leaf area of SGH	SGHleafden	$\Omega_{SGH}$	1.900000e+00	m <sup>2</sup> g N <sup>-1</sup>
Natural (linear) mortality rate, aboveground SGH	SGH_mL	$\zeta_{SGHA}$	6.000000e-02	d <sup>-1</sup>
Natural (linear) mortality rate, belowground SGH	SGHROOT_mL	$\zeta_{SGHB}$	4.000000e-03	d <sup>-1</sup>
Fraction (target) of SGH biomass below-ground	SGHfrac	$f_{below,SGH}$	5.000000e-01	-
Time scale for Halophila translocation	SGHtransrate	$\tau_{tran,SGH}$	3.330000e-02	d <sup>-1</sup>
Halophila seed biomass as fraction of 63 % cover	SGHseedfrac	$f_{seed,SGH}$	1.000000e-02	-
Sine of nadir Halophila canopy bending angle	SGHorient	$\sin \beta_{blade,SGH}$	1.000000e+00	-
Compensation irradiance for Halophila	SGHmlr	$E_{comp,SGH}$	2.000000e+00	mol m <sup>-2</sup>
Maximum depth for Halophila roots	SGHrootdepth	$z_{root,SGH}$	-8.000000e-02	m
Critical shear stress for SGH loss	SGH_tau_critical	$\tau_{SGH,shear}$	1.000000e+00	N m <sup>-2</sup>
Time-scale for critical shear stress for SGH loss	SGH_tau_time	$\tau_{SGH,time}$	4.320000e+04	s

**Table D6.** Seagrass parameters in eReefs biogeochemical model (B3p0).



Description	Name in code	Symbol	Value	Units
Maximum growth rate of SGD at Tref	SGDumax	$\mu_{SGD}^{max}$	4.000000e-01	d <sup>-1</sup>
Half-saturation of SGD N uptake in SED	SGD_KN	$K_{SGD,N}$	4.200000e+02	mg N m <sup>-3</sup>
Half-saturation of SGD P uptake in SED	SGD_KP	$K_{SGD,P}$	9.600000e+01	mg P m <sup>-3</sup>
Nitrogen-specific leaf area of SGD	SGDleafden	$\Omega_{SGD}$	1.900000e+00	m <sup>2</sup> g N <sup>-1</sup>
Natural (linear) mortality rate, aboveground SGD	SGD_mL	$\zeta_{SGDA}$	6.000000e-02	d <sup>-1</sup>
Natural (linear) mortality rate, belowground SGD	SGDROOT_mL	$\zeta_{SGDB}$	4.000000e-03	d <sup>-1</sup>
Fraction (target) of SGD biomass below-ground	SGDfrac	$f_{below,SGD}$	2.500000e-01	-
Time scale for deep SG translocation	SGDtransrate	$\tau_{tran,SGD}$	3.330000e-02	d <sup>-1</sup>
Deep SG seed biomass as fraction of 63 % cover	SGDseedfrac	$f_{seed,SGD}$	1.000000e-02	-
Sine of nadir deep SG canopy bending angle	SGDorient	$\sin \beta_{blade,SGD}$	1.000000e+00	-
Compensation irradiance for deep SG	SGDmlr	$E_{comp,SGD}$	1.500000e+00	mol m <sup>-2</sup>
Maximum depth for deep SG roots	SGDrootdepth	$z_{root,SGD}$	-5.000000e-02	m
Critical shear stress for deep SG loss	SGD_tau_critical	$\tau_{SGD,shear}$	1.000000e+00	N m <sup>-2</sup>
Time-scale for shear stress for deep SG loss	SGD_tau_time	$\tau_{SGD,time}$	4.320000e+04	s

**Table D7.** Deep seagrass parameters in eReefs biogeochemical model (B3p0).

# Appendix E. Assessment of eReefs biogeochemical simulation against observations

[Supplementary Material for Geoscientific Model Development: CSIRO

Environmental Modelling Suite (EMS): Scientific description of the optical and biogeochemical models (vB3p0)]

**Model version: gbr4\_H2p0\_**B3p0\_Chyd\_Dcrt

**Model run period: 1 Dec 2010 to 1 Nov 2018**

- Includes comparison with version **B2p0** where applicable

(Version Tuesday, 26 March 2019)

Wednesday, 3 June 2020

For more details of Methods see:

Skerratt J.H., M. Mongin, K. A. Wild-Allen, M. E. Baird, B. J. Robson, B. Schaffelke, M. Soja-Wozniak, N Margvelashvili, C. H. Davies, A. J. Richardson, A. D. L. Steven (2019) Simulated nutrient and plankton dynamics in the Great Barrier Reef (2011-2016). J. Mar. Sys. 192, 51-74.

## Document versions

*Thursday, 3 January 2019 version*

- Includes observation updates to MMP Turbidity and MMP chlorophyll mooring obs to November 2018: p111 to 125
- Includes the new MMP sites which have decreased the metrics for both Turbidity and Fluorescence. The metrics are better if we leave summer of 2011 in.
- Simulated turbidity has zeros (night-time) removed in the model run. p 118 to 125.
- Simulated Fluorescence is not as good as simulated Chl *a* against MMP mooring obs however obs are modified fluorescence based on Chl *a*
- Turbidity is presented at full extent of NTU and again with NTU under 20 (p119 and 125)
- The QC of the new set of MMP data remains excellent but doesn't appear as stringently QC'd as in the past with blanks and some unrealistic data.

*Friday, 4 January 2019 version*

- Scatter plots of fluorescence against Chl *a* for all MMP moorings and combined scatterplot at end

*Tuesday, 19 February 2019 version*

- Added parameter file for H3 version

*Wednesday, 20 February 2019 version*

- Added satellite photos depth of MMP and LTR sites and glossary

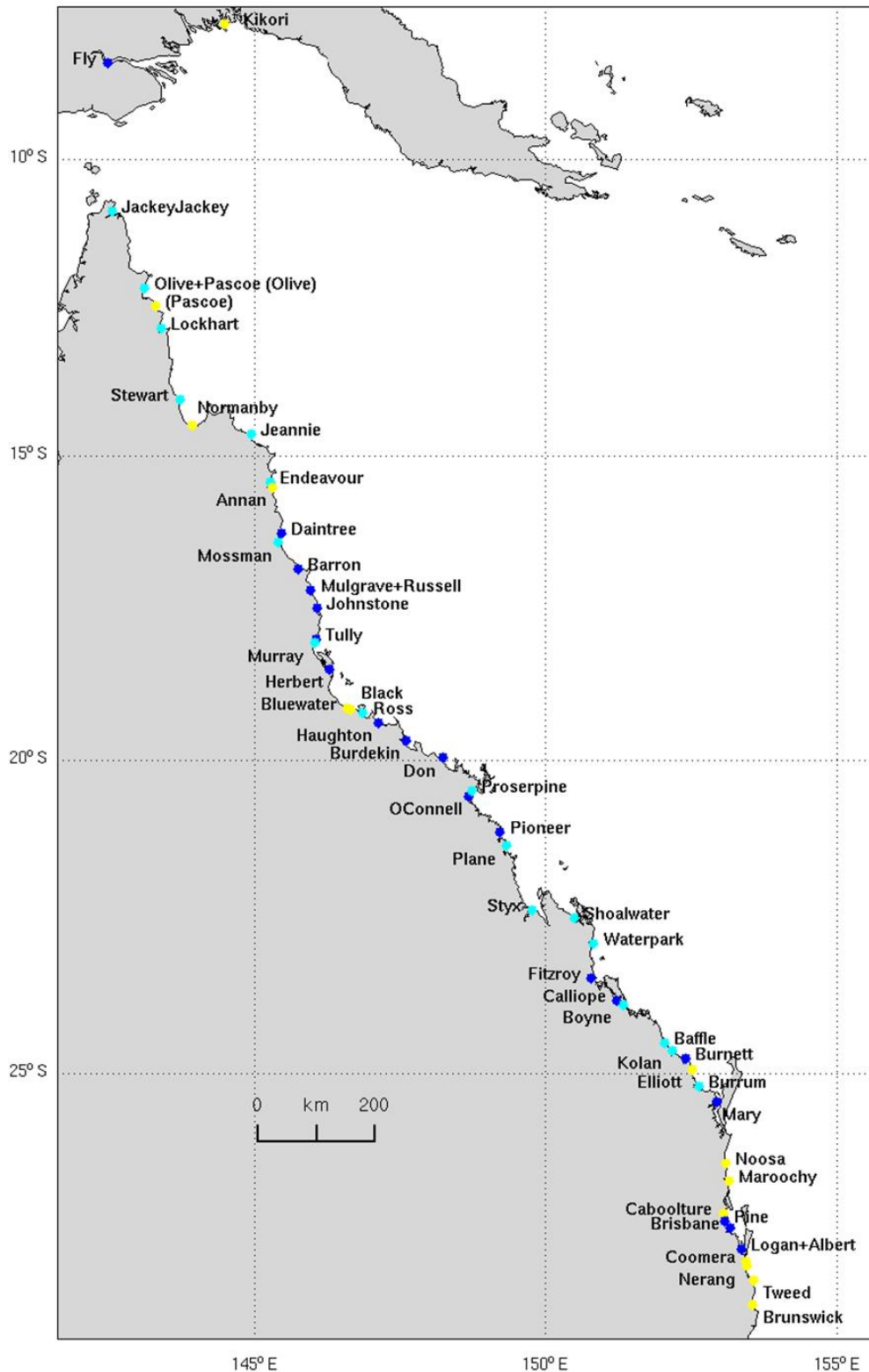
*Tuesday, 26 March 2019 version*

- Added correct NRS nutrient metrics and graphs with extended observational time series and NRS alkalinity extension of observed dates and inclusion of North Stradbroke island (GBRNSI)

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# 1. Map: River and catchments in eReef model



- Rivers and catchment model with hydro flow catchment loads B2p0 and B3p0
- Extra rivers in B3p0 where catchment in as point source loads
- Rivers in hydrodynamic model, some without flow, no catchment model data.

Figure 1 Map of Queensland rivers included in eReef model versions B2p0 and B3p0. Includes extra rivers for B3p0 in light blue

## 2. Map: AIMS and IMOS NRS sites used in eReef model

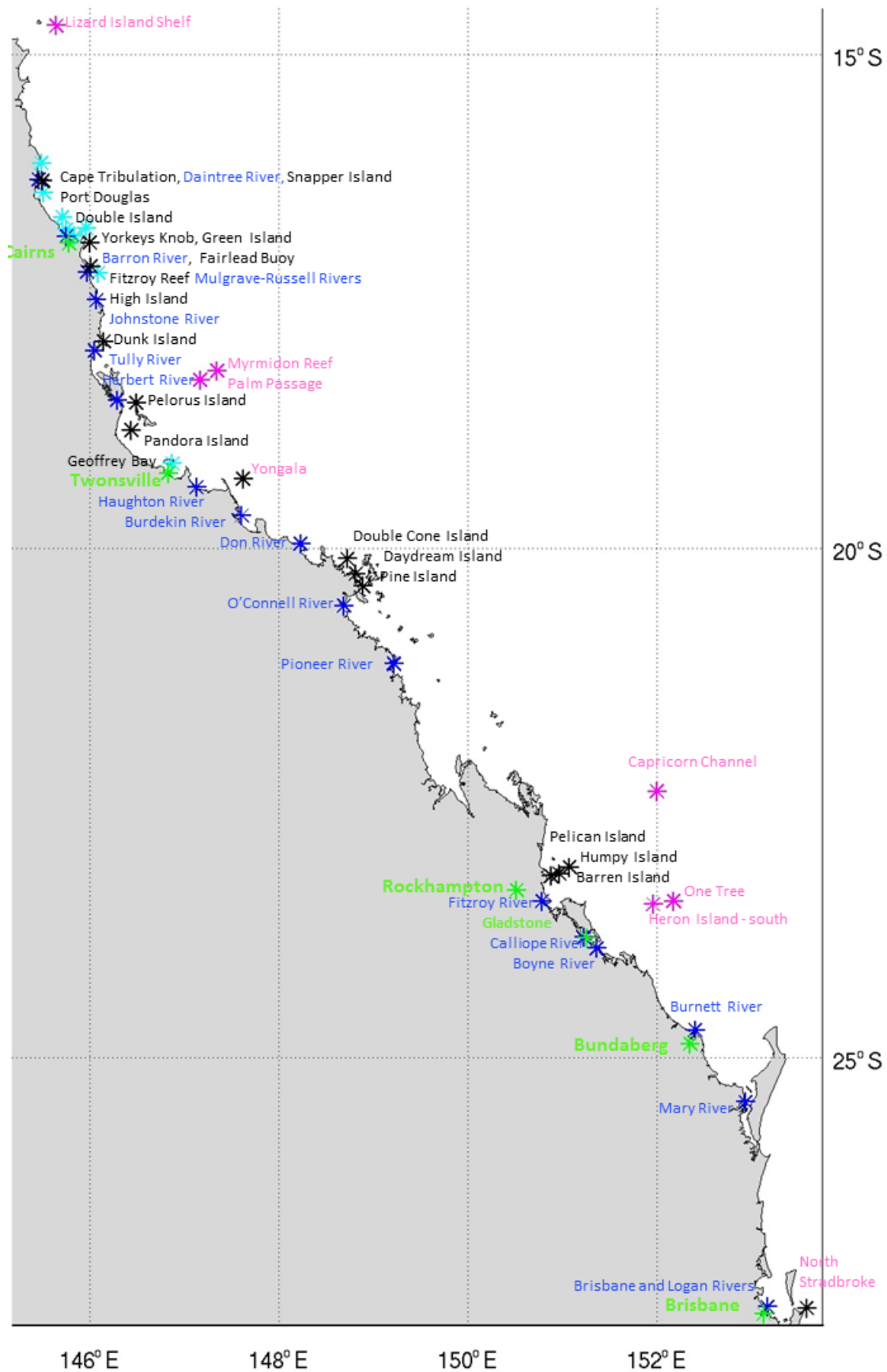
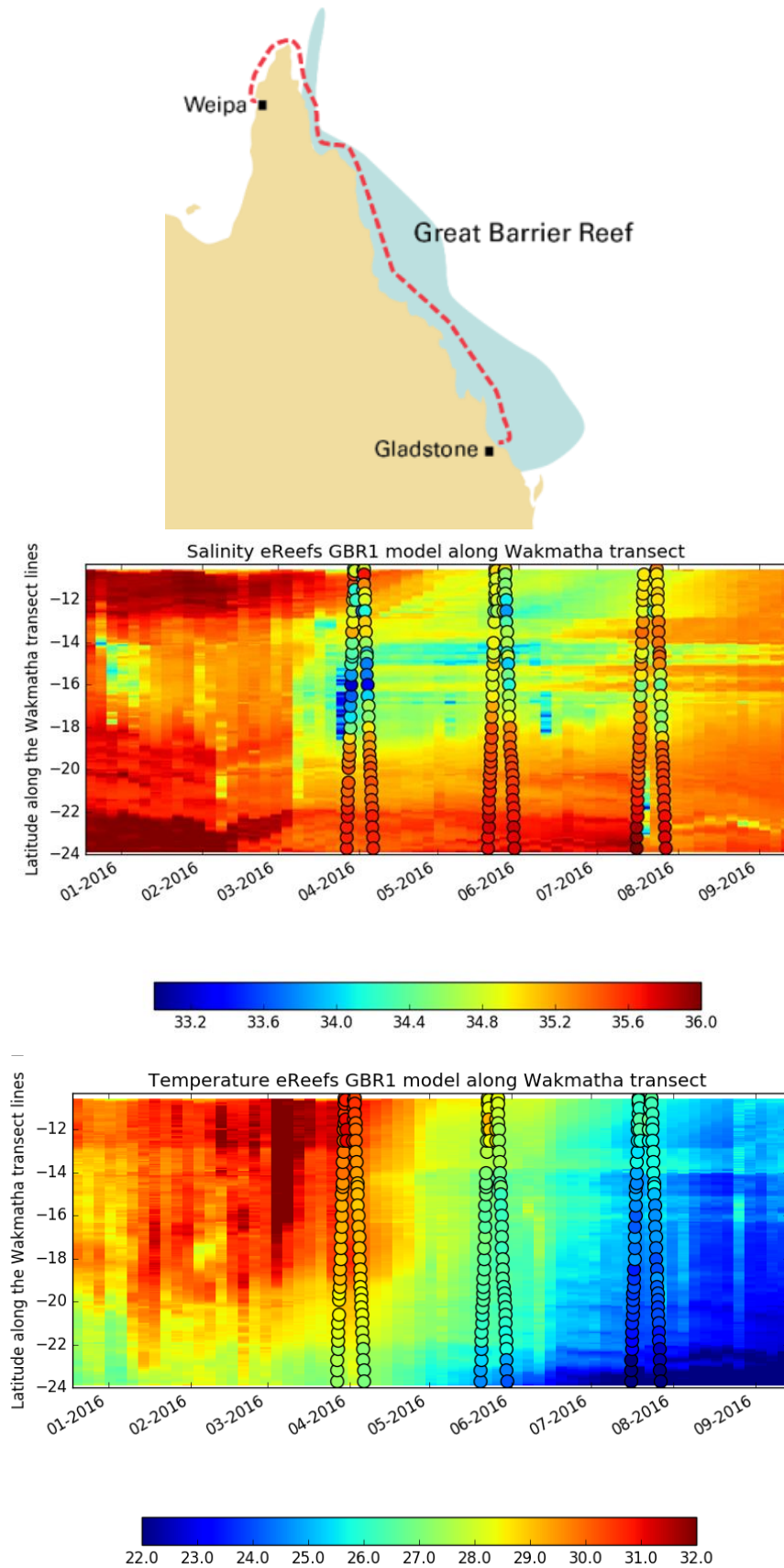


Figure 2 Map of observational sites in this report (black and pink), rivers (blue) and major towns (Green)

### 3. Map Wakmatha transect for Carbon Chemistry

Figure shows Wakmatha transect and temp and salinity comparison with GBR1 (see page 180 Wakmatha transect line for Carbon chemistry assessment of Wakmatha transect line)



## 4. eReefs Biogeochemical Model schematic

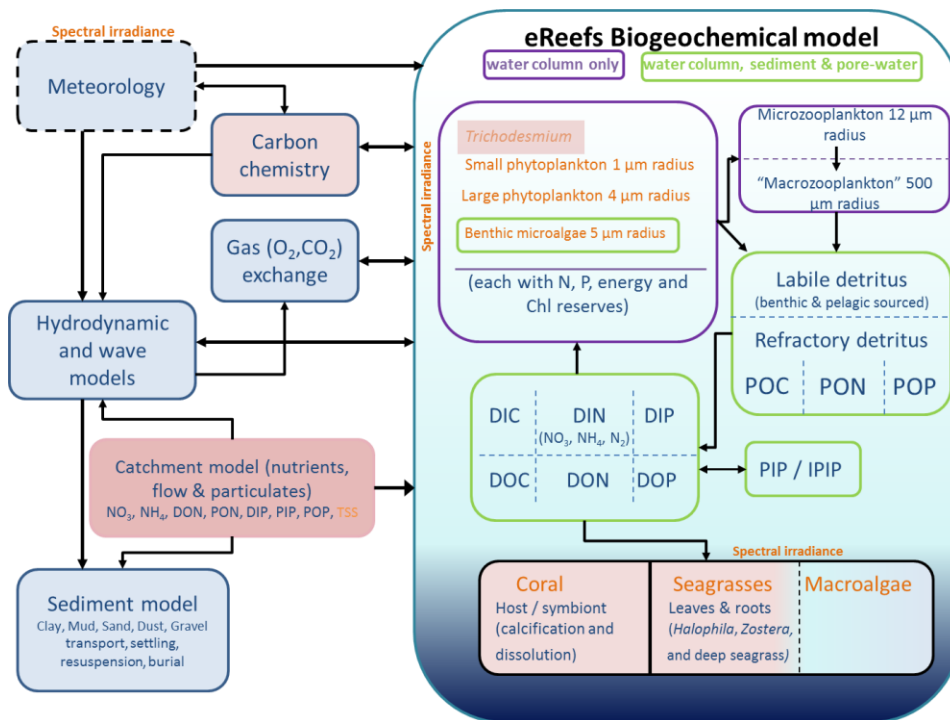


Figure 3. The eReefs modelling system, showing the linkages between hydrodynamic, wave, sediment and the optical and biogeochemical models, as well as the individual linkages within the biogeochemical model. The optically-active components are identified with orange font.

## 5. Model skill metrics description

To evaluate model skill, we consider; bias, the root mean square (RMS) error, the mean absolute error (MAE). and the modified Willmott index or 'd2' (Willmott et al., 1985). The Willmott index uses the sum of absolute values.

Model bias assesses whether the simulated variables are under- or over-predicting observed values. The RMS error is a measure of the absolute magnitude of the "error"/square deviation averaged over the time-series. An RMS or MAE of 0 indicates a perfect fit.

The Willmott index of agreement is designed to quantify errors that are unevenly distributed in time or space and reduce the influence of errors during periods of large observed mean or variance. The Willmott index is the ratio of the mean absolute error and the mean absolute deviation about the observed mean and varies between 0 and 1. A value of 1 indicates a perfect match ( $x = y$ ), and 0 indicates no agreement.

$$\text{Willmott} = 1 - \left[ \frac{\sum |x - y|}{\sum |x - \bar{y}| + (|y - \bar{y}|)} \right]$$

where  $x$  and  $y$  are vectors or arrays of time series data ( $x$  =observed,  $y$  = modelled).

A Willmott index above 0.7 is regularly obtained for high resolution models with high spatial and temporal observations for physical parameters such as salinity and temperature. In most cases for the eReefs model the salinity and temperature index was  $\geq 0.8$  when compared with observations (Appendix 1 of Herzfeld et al., 2016).



## 6. Abbreviations

AIMS	Australian Institute of Marine Science
AODN	Australian Ocean Data Network
B2p0	B2p0: biogeochemical model version 2.0
B3p0	B3p0: biogeochemical model version 3.0
CDOM	colour dissolved organic matter
Chl a	chlorophyll a
CTD	Conductivity Temperature Depth profiler
d2	Statistical metric, aka Willmott index ( see page 27)
DIN	dissolved inorganic nitrogen
DIN	Dissolved inorganic nitrogen (NH <sub>3</sub> plus NO <sub>x</sub> )
DIP	dissolved inorganic phosphorus
DOC	dissolved organic carbon
DON	dissolved organic nitrogen
DOP	dissolved organic phosphorus
ENSO	El Niño-Southern Oscillation
GBR	Great Barrier Reef
gbr4_H2p0_B3p0_Cb	gbr4 : model grid with approximate 4 km grid resolution, H2p0: hydrodynamic model version 2.0, B3p0: biogeochemical model version 3.0, Cb: catchment model baseline version using empirical SOURCE Catchments
GBRMP	Great Barrier Reef Marine Park
GBRMPA	Great Barrier Reef Marine Park Authority
GBRWHA	Great Barrier Reef World Heritage Area
IMOS	Integrated Marine and Observing System
Kd(PAR)	light attenuation coefficient
LTM	AIMS long term monitoring site
mae	mean absolute error
mape	mean absolute percentage error
MMP	AIMS Marine Monitoring Program
MODIS	Moderate Resolution Imaging Spectroradiometer
NH <sub>3</sub>	ammonia
NO <sub>x</sub>	nitrate plus nitrite
NRS	IMOS National reference station within the model grid these are Yongala (GBRYON) and North Stradbroke Island (GBRNSI)
NSI	North Stradbroke Island
NTU	Nephelometric Turbidity Unit
PON	particulate organic nitrogen
POP	particulate organic phosphorus
QA/QC	quality assurance/quality control
rms	root mean square
secchi	measurement of water transparency (depth in m)
TSS	total suspended solids
Willmott	statistical metric (see page 27)

## 7. Parameter tables for gbr4\_H2p0\_B3p0\_Cb

The following 4 pages give the parameters used in the model gbr4\_H2p0\_B3p0\_Cb.

Parameter description	Symbol	Units	Value	Reference
<b>Phytoplankton</b>				
Chl-specific scattering coefficient. for microalgae	bphy	m <sup>-1</sup> (mg Chl a m <sup>-3</sup> ) <sup>-1</sup>	0.2	Typical microalgae value, Kirk (1994)
Natural (linear) mortality rate, large phytoplankton	PhyL_mL	d <sup>-1</sup>	0.1	Not attributed
Natural (linear) mortality rate in sediment, large phytoplankton	PhyL_mL_sed	d <sup>-1</sup>	10	Not attributed
Natural (linear) mortality rate, small phytoplankton	PhyS_mL	d <sup>-1</sup>	0.1	Not attributed
Natural (linear) mortality rate in sediment, small phytoplankton	PhyS_mL_sed	d <sup>-1</sup>	1	Not attributed
Respiration as a fraction of umax	Plank_resp	none	0.025	Not attributed
Radius of the large phytoplankton cells	PLrad	m	0.000004	Not attributed
Maximum growth rate of PL at Tref	PLumax	d <sup>-1</sup>	1.4	CSIRO Parameter Library
Ratio of xanthophyll to chl a of PL	PLxan2chl	mg mg <sup>-1</sup>	0.81	CSIRO Parameter Library
Radius of the small phytoplankton cells	PSrad	m	0.000001	Not attributed
Maximum growth rate of PS at Tref	PSumax	d <sup>-1</sup>	1.6	CSIRO Parameter Library
Ratio of xanthophyll to chl a of PS	PSxan2chl	mg mg <sup>-1</sup>	0.51	CSIRO Parameter Library
<b>Trichodesmium</b>				
DIN conc below which <i>Trichodesmium</i> N fixes	DINcrit	mg N m <sup>-3</sup>	10	Lower end of Robson et al., (2013) 4-20 mg N m <sup>-3</sup>
Maximum density of <i>Trichodesmium</i>	p_max	kg m <sup>-3</sup>	1050	Not attributed
Minimum density of <i>Trichodesmium</i>	p_min	kg m <sup>-3</sup>	900	Not attributed
Radius of <i>Trichodesmium</i> colonies	Tricho_colrad	m	0.000005	Not attributed
Critical <i>Trichodesmium</i> above which quadratic mortality applies	Tricho_crit	mg N m <sup>-3</sup>	0.0002	Not used in code
Linear mortality for <i>Trichodesmium</i> in sediment	Tricho_mL	d <sup>-1</sup>	0.1	Not attributed
Quadratic mortality for <i>Trichodesmium</i> due to phages in water column	Tricho_mQ	d <sup>-1</sup> (mg N m <sup>-3</sup> ) <sup>-1</sup>	0.1	At steady-state, indep. of temp, Tricho_N ~ Tricho_umax / Tricho_mQ = 0.27 / 0.405 = 0.7 mg N m <sup>-3</sup> ~ 0.1 mg Chl m <sup>-3</sup>
<i>Trichodesmium</i> grazing preference	Tricho_pref	none	0	Not attributed
Radius of <i>Trichodesmium</i> colonies	Tricho_rad	m	0.000005	Not attributed
Sherwood number for the <i>Trichodesmium</i> dimensionless	Tricho_Sh	none	1	Not attributed
Maximum growth rate of <i>Trichodesmium</i> at Tref	Tricho_umax	d <sup>-1</sup>	0.2	Robson et al., 2013 + Parameter library
Ratio of xanthophyll to chl a of <i>Trichodesmium</i>	Trichoxan2chl	mg mg <sup>-1</sup>	0.5	Subramaniam et al. 1999. LO 44:618-627
<b>Microphytobenthos</b>				
Respiration as a fraction of umax	Benth_resp	none	0.025	Not attributed
Radius of the MPB cells	MBrad	m	0.00001	Not attributed
Maximum growth rate of MB at Tref	MBumax	d <sup>-1</sup>	0.839	CSIRO Parameter Library
Ratio of xanthophyll to chl a of MPB	MBxan2chl	mg mg <sup>-1</sup>	0.81	Not attributed
Natural (quadratic) mortality rate, microphytobenthos, applied in sediment	MPB_mQ	d <sup>-1</sup> (mg N m <sup>-3</sup> ) <sup>-1</sup>	0.0001	SS argument

## Parameter description

## Symbol

## Units

## Value

## Reference

## Zooplankton

Growth efficiency, large zooplankton	ZL_E	none	0.426	CSIRO Parameter Library, [0.341 (0.017900) Baird and Suthers, 2007 from Hansen et al (1997) LO 42: 687-704]
Fraction of growth inefficiency lost to detritus, large zooplankton	ZL_FDG	none	0.5	Not attributed
Fraction of mortality lost to detritus, large zooplankton	ZL_FDM	none	1	Not attributed
Natural (quadratic) mortality rate, large zooplankton	ZL_mQ	$d^{-1} (mg\ N\ m^{-3})^{-1}$	0.012	Not attributed
Diel vertical migration rate of ZL	ZLdvmrate	$m\ d^{-1}$	0	Not attributed
Grazing technique of large zooplankton	ZLmeth	none	rect	Not attributed
Light at which the	ZLpar	$mol\ photons\ m^{-2}\ s^{-1}$	1.00E-12	Not attributed
Radius of the large zooplankton cells	ZLrad	m	0.00032	Not attributed
Swimming velocity for large zooplankton	ZLswim	$m\ s^{-1}$	0.003	Not attributed
Maximum growth rate of ZL at Tref	ZLumax	$d^{-1}$	1.33	Not attributed
Growth efficiency, small zooplankton	ZS_E	none	0.462	CSIRO Parameter Library [0.3080000 (0.026600) Baird and Suthers, 2007 from Hansen et al (1997) LO 42: 687-704]
Fraction of growth inefficiency lost to detritus, small zooplankton	ZS_FDG	none	0.5	Not attributed
Fraction of mortality lost to detritus, small zooplankton	ZS_FDM	none	1	Not attributed
Natural (quadratic) mortality rate, small zooplankton	ZS_mQ	$d^{-1} (mg\ N\ m^{-3})^{-1}$	0.02	Not attributed
Grazing technique of small zooplankton	ZSmeth	none	rect	Not attributed
Radius of the small zooplankton cells	ZSrad	m	0.000005	Not attributed
Swimming velocity for small zooplankton	ZSswim	$m\ s^{-1}$	0.0002	Not attributed
Maximum growth rate of ZS at Tref	ZSumax	$d^{-1}$	4	Not attributed

## Coral

Quadratic mortality rate of coral polyp	CHmort	$(g\ N\ m^{-3})^{-1}\ d^{-1}$	0.01	Not attributed
Nitrogen-specific area of coral polyp density	CHpolypden	$m^2\ g\ N^{-1}$	2	Not attributed
Fraction of Host death translocated.	CHremin	-	0.5	Not attributed
Max. growth rate of Coral at Tref	CHumax	$d^{-1}$	0.05	Not attributed
Linear mortality rate of Zooxanthellae	CSmort	$d^{-1}$	0.04	Not attributed
Radius of the Zooxanthellae	CSrad	m	0.000005	Not attributed
Fraction of Zooxanthellae growth to Host.	CStoCHfrac	-	0.9	Gustafsson et al. (2013) Ecol. Mod. 250: 183-194
Max. growth rate of Zooxanthellae at Tref	CSumax	$d^{-1}$	0.4	Not attributed
Maximum daytime net coral calcification	k_day_coral	$mmol\ C\ m^{-2}\ s^{-1}$	0.0132	Anthony et al. (2013), Biogeosciences 10:4897-4909, Fig 5A: 50, 50, 35 55 $mmol\ m^{-2}\ h^{-1}$ for <i>Acropora aspera</i> n=4
Grid scale to reef scale ratio	CHarea	$m\ m^{-1}$	0.1	Not attributed
Maximum night time net coral calcification	k_night_coral	$mmol\ C\ m^{-2}\ s^{-1}$	0.0069	Anthony et al. (2013), Biogeosciences 10:4897-4909, Fig 5A: 20, 30, 20, 30 $mmol\ m^{-2}\ h^{-1}$ for <i>Acropora aspera</i> n=4
Rate coefficient for plankton uptake by corals	Splank	$m\ d^{-1}$	3	Ribes (2003), PARAMETER library analysis; Ribes and Atkinson (2007) Coral Reefs 26: 413-421

## Parameter description

## Symbol

## Units

## Value

## Reference

### Seagrass and Macroalgae

Half-saturation of SG N uptake in SED	SG_KN	$mg\ N\ m^{-3}$	420	Lee and Dunton (1999) 1204-1215. Table 3 <i>Zostera</i>
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Parameter description	Symbol	Units	Value	Reference
Half-saturation of SG P uptake in SED	SG_KP	mg P m <sup>-3</sup>	96	Gras et al. (2003) Aquatic Botany 76:299-315. Thalassia testudinum.
Natural (linear) mortality rate, seagrass	SG_mL	d <sup>-1</sup>	0.03	Fourquean et al. (2003) Chem. Ecol. 19: 373-390. Thalassia leaves with one component decay
Critical shear stress for SG loss	SG_tau_critical	N m <sup>-2</sup>	1	NESP project
Time-scale for critical shear stress for SG loss	SG_tau_efold	s	43200	NESP project
Half-saturation of SGD N uptake in SED	SGD_KN	mg N m <sup>-3</sup>	420	Not attributed
Half-saturation of SGD P uptake in SED	SGD_KP	mg P m <sup>-3</sup>	96	Not attributed
Natural (linear) mortality rate, aboveground SGD	SGD_mL	d <sup>-1</sup>	0.06	NESP project
Critical shear stress for SGD loss	SGD_tau_critical	N m <sup>-2</sup>	1	NESP project
Time-scale for critical shear stress for SGD loss	SGD_tau_efold	s	43200	NESP project
Fraction (target) of SGD biomass below-ground	SGDfrac	-	0.25	Duarte (1999) Aquatic Biol. 65: 159-174, Halophila ovalis.
Nitrogen-specific leaf area of SGD	SGDleafden	m <sup>2</sup> g N <sup>-1</sup>	1.9	Halophila ovalis: leaf dimensions from Vermaat et al. (1995)
Compensation irradiance for Halophila	SGDmlr	mol m <sup>-2</sup>	1.5	NESP project
Sine of nadir Deep Seagrass canopy bending angle	SGDorient	-	1	No source
Natural (linear) mortality rate, belowground SGD	SGDROOT_mL	d <sup>-1</sup>	0.004	NESP project
Maximum depth for Halophila roots	SGDrootdepth	m	-0.05	NESP project
Halophila seed biomass as fraction of 63 % cover	SGDseedfrac	-	0.01	Not attributed
Time scale for seagrass translocation	SGDtransrate	d <sup>-1</sup>	0.0333	Loosely based on Zostera marine Kaldy et al., 2013 MEPS 487:27-39
Maximum growth rate of SGD at Tref	SGDumax	d <sup>-1</sup>	0.4	x2 nighttime, x2 for roots.
Fraction (target) of SG biomass below-ground	SGfrac	-	0.75	Babcock (2015) Zostera capricornii
Half-saturation of SGH N uptake in SED	SGH_KN	mg N m <sup>-3</sup>	420	Not attributed
Half-saturation of SGH P uptake in SED	SGH_KP	mg P m <sup>-3</sup>	96	Not attributed
Natural (linear) mortality rate, seagrassH	SGH_mL	d <sup>-1</sup>	0.06	Fourquean et al. (2003) Chem. Ecol. 19: 373-390. Thalassia leaves with one component decay
Critical shear stress for SGH loss	SGH_tau_critical	N m <sup>-2</sup>	1	NESP project
Time-scale for critical shear stress for SGH loss	SGH_tau_efold	s	43200	NESP project
Fraction (target) of SGH biomass below-ground	SGHfrac	-	0.5	Babcock 2015, Halophila ovalis
Nitrogen-specific area of seagrass leaf	SGHleafden	m <sup>2</sup> g N <sup>-1</sup>	1.9	Halophila ovalis: leaf dimensions from Vermaat et al. (1995)
Compensation irradiance for SG	SGHmlr	mol m <sup>-2</sup>	2	Not attributed
Sine of nadir Halophila canopy bending angle	SGHorient	-	1	No source
Natural (linear) mortality rate, seagrassH	SGHROOT_mL	d <sup>-1</sup>	0.004	Fourquean et al. (2003) Chem. Ecol. 19: 373-390. Thalassia roots with one component decay
Maximum depth for Halophila roots	SGHrootdepth	m	-0.08	Roberts (1993) Aust. J. Mar. Fresh. Res. 44:85-100.
Halophila seed biomass as fraction of 63 % cover	SGHseedfrac	-	0.01	Not attributed
Time scale for seagrass translocation	SGHtransrate	d <sup>-1</sup>	0.0333	Loosely based on Zostera marine Kaldy et al., 2013 MEPS 487:27-39
Maximum growth rate of SGH at Tref	SGHumax	d <sup>-1</sup>	0.4	x2 night-time, x2 for roots.
Nitrogen-specific area of seagrass leaf	SGleafden	m <sup>2</sup> g N <sup>-1</sup>	1.5	Zostera capricornia: leaf dimensions Kemp et al (1987) Mar Ecol. Prog. Ser. 41:79-86.
Compensation irradiance for SG	SGmlr	mol m <sup>-2</sup>	4.5	Not attributed
SGorient	SGorient	-	0.5	Not attributed
Natural (linear) mortality rate, seagrass	SGROOT_mL	d <sup>-1</sup>	0.004	Fourquean et al. (2003) Chem. Ecol. 19: 373-390. Thalassia roots with one component decay
Maximum depth for Zostera roots	SGrootdepth	m	-0.15	Roberts (1993) Aust. J. Mar. Fresh. Res. 44:85-100.
Seagrass seed biomass as fraction of 63 % cover	SGseedfrac	-	0.01	No source
Time scale for seagrass translocation	SGtransrate	d <sup>-1</sup>	0.0333	Loosely based on Zostera marine Kaldy et al., 2013 MEPS 487:27-39
Maximum growth rate of SG at Tref	SGumax	d <sup>-1</sup>	0.4	x2 nighttime, x2 for roots.
Natural (linear) mortality rate, macroalgae	MA_mL	d <sup>-1</sup>	0.01	Not attributed
Nitrogen-specific area of macroalgae leaf	MAleafden	m <sup>2</sup> g N <sup>-1</sup>	1	Not attributed
Maximum growth rate of MA at Tref	MAumax	d <sup>-1</sup>	1	Not attributed

Parameter description	Symbol	Units	Value	Reference
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## Biogeochemistry

Reference temperature	Tref	Deg C	20	CSIRO Parameter Library
Temperature coefficient for rate parameters	Q10	none	2	CSIRO Parameter Library
Nominal rate of TKE dissipation in water column	TKEeps	$m^2 s^{-3}$	0.000001	Not attributed
Atmospheric CO2	xco2_in_air_dum	ppmv	396.48	Mean 2013 at Mauna Loa: <a href="http://co2now.org/current-co2/co2-now/">http://co2now.org/current-co2/co2-now/</a>
Wavelengths of light	Light_lambda	nm	Various*	Approx. 20 nm resolution with 10 nm about 440 nm. PAR (400-700) is integral of bands 2-22 (290 310 330 350 370 390 410 430 440 450 470 490 510 530 550 570 590 610 630 650 670 690 710 800)*
Nominal N:Chl a ratio in phytoplankton by weight	NtoChl	$g N (g Chl a)^{-1}$	7	Represents a C:Chl ratio of 39.25, Baird et al. (2013) Limnol. Oceanogr. 58: 1215-1226.
Concentration of dissolved N2	N2	$mg N m^{-3}$	2000	Robson et al. (2013)
Fraction of labile detritus converted to refractory detritus	F_LD_RD	none	0.19	Not attributed
Fraction of labile detritus converted to dissolved organic matter	F_LD_DOM	none	0.1	Not attributed
fraction of refractory detritus that breaks down to DOM	F_RD_DOM	none	0.05	Not attributed
Breakdown rate of labile detritus at 106:16:1	r_DetPL	$d^{-1}$	0.04	Not attributed
Breakdown rate of labile detritus at 550:30:1	r_DetBL	$d^{-1}$	0.001	Not attributed
Breakdown rate of refractory detritus	r_RD	$d^{-1}$	0.001	Not attributed
Breakdown rate of dissolved organic matter	r_DOM	$d^{-1}$	0.0001	Achieves approx. SS of global ocean at 20 C.
Oxygen half-saturation for aerobic respiration	KO_aer	$mg O m^{-3}$	256	Not attributed
Maximal nitrification rate in water column	r_nit_wc	$d^{-1}$	0.1	Not attributed
Maximal nitrification rate in water sediment	r_nit_sed	$d^{-1}$	20	Not attributed
Oxygen half-saturation for nitrification	KO_nit	$mg O m^{-3}$	500	Not attributed
Rate at which P reaches adsorbed/desorbed equilibrium	Pads_r	$d^{-1}$	0.04	Not attributed
Freundlich Isothermic Const P adsorption to TSS in water column	Pads_Kwc	$mg P kg TSS^{-1}$	30	Not attributed
Freundlich Isothermic Const P adsorption to TSS in sediment	Pads_Ksed	$mg P kg TSS^{-1}$	74	Not attributed
Oxygen half-saturation for P adsorption	Pads_KO	$mg O m^{-3}$	2000	Not attributed
Exponent for Freundlich Isotherm	Pads_exp	none	1	Not attributed
Maximum denitrification rate	r_den	$d^{-1}$	0.8	Not attributed
Oxygen half-inhibition of denitrification rate	KO_den	$mg O m^{-3}$	10000	Not attributed
Rate of conversion of PIP to immobilised PIP	r_immob_PIP	$d^{-1}$	0.0012	Not attributed
Sediment-water diffusion coefficient	EpiDiffCoeff	$m^2 s^{-1}$	3.00E-07	Not attributed
Thickness of diffusive layer	EpiDiffDz	m	0.0065	Not attributed
age tracer growth rate per day	ageing_decay	$d^{-1}$	1	Not attributed
age tracer decay rate per day outside source	anti_ageing_decay	$d^{-1}$	0.1	Not attributed
net dissolution rate of sediment without coral	dissCaCO3_sed	$mmol C m^{-2} s^{-1}$	0.001	Anthony et al. (2013), Biogeosciences 10:4897-4909, Fig 5E: -1 2 3 6 $mmol m^{-2} h^{-1}$
DOC-specific absorption of CDOM at 443 nm	acdom443star	$m^2 mg C^{-1}$	0.00013	Not attributed
Minimum carbon to chlorophyll ratio	C2Chlmin	wt/wt	20	Not attributed
swr scaling factor	SWRscale	none	1	Not attributed
Bleaching ROS threshold	ROSthreshold	-	5.00E-04	Not attributed
increased breakdown fraction DetrP to DOP	r_RD_NtoP	-	2	Not attributed
increased breakdown fraction DOMP to DIP	r_DOM_NtoP	-	1.5	Not attributed

## 8. Site and model grid depth of the MMP and NRS sites

MMP and NRS Sites	GBR4 grid depth (m)	Site depth (m)
Barren Island	24	15 - 19
Daydream Island	17	23 - 25
Double Cone Island	17	23 - 31
Dunk Island	9	9 - 10
Fitzroy Island	27	15 - 17
Geoffrey Bay	10	9 - 10
High Island	18	22 - 25
Humpy Island	13	12 - 19
North Stradbroke Island (NSI)	66	65 - 67
Pandora Island	17	13 - 14
Pelican Island	4	9 - 10
Pelorus Island	25	25 - 31
Pine Island	18	20 - 25
Russell Island	20	22 - 24
Snapper Island	22	8 - 11
Yongala	29	26 - 27

## 9. Site and depths for additional triannual sites or depths

AIMS additional Triannual Water Quality sites	Sampling Depths (m)		
Cape Tribulation	10		
Snapper Island	10		
Port Douglas	0	15	
Double Island	0	18	
Green Island	0	18	36
Yorkeys Knob	0	8	
Fairlead Buoy	0		
Fitzroy Reef	0	15	
High Island	0	10	20
Russell Island	0	10	20
Dunk Island	5		
Pelorus Island	0	14	28
Double Cone Island	10	23	
Daydream Island	10	23	
Pine Island	0	20	
Barren Island	10		
Humpy Island	0	10	

## 10. Simulated Chl *a* assessment against AIMS Long Term Monitoring

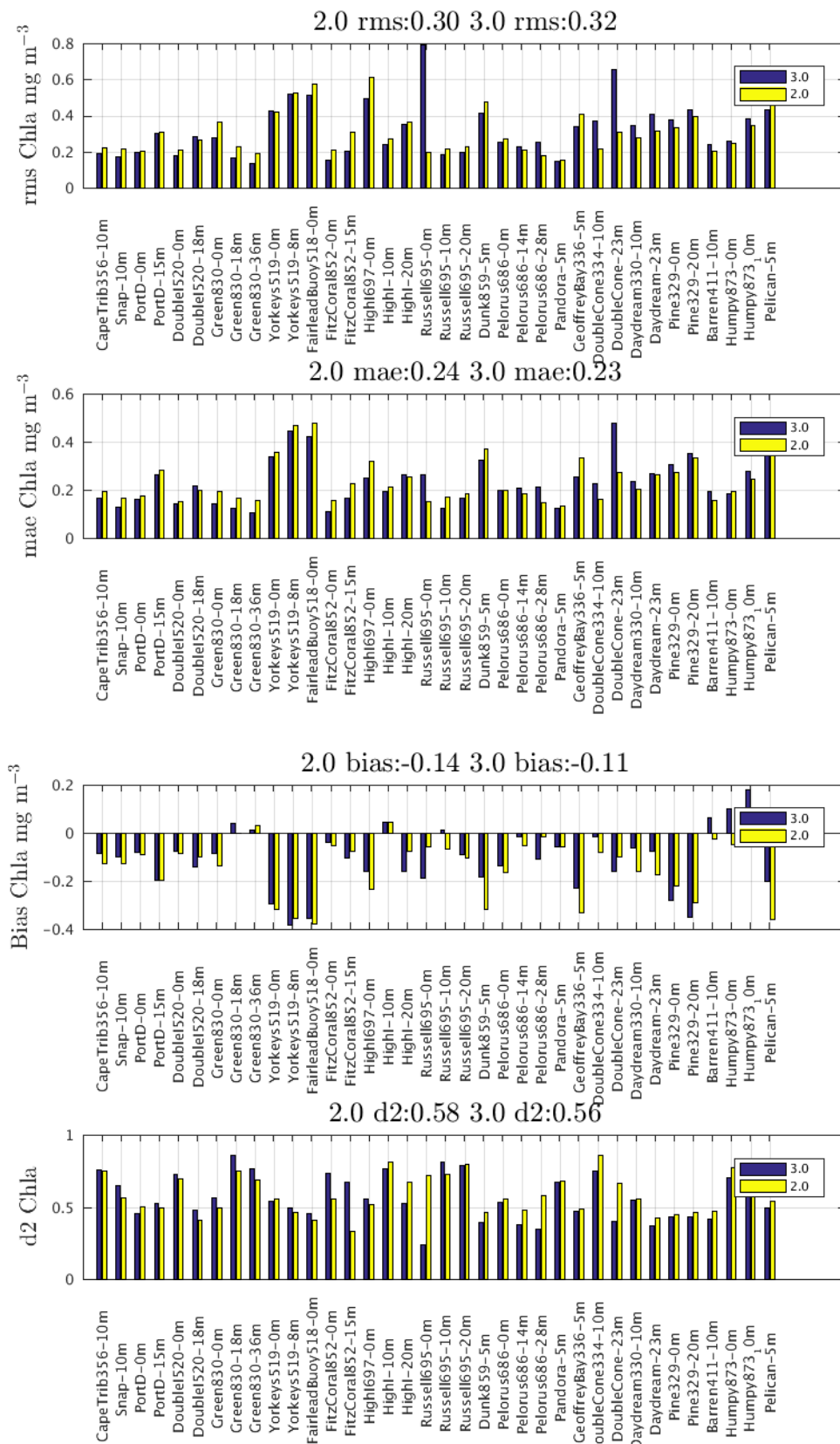
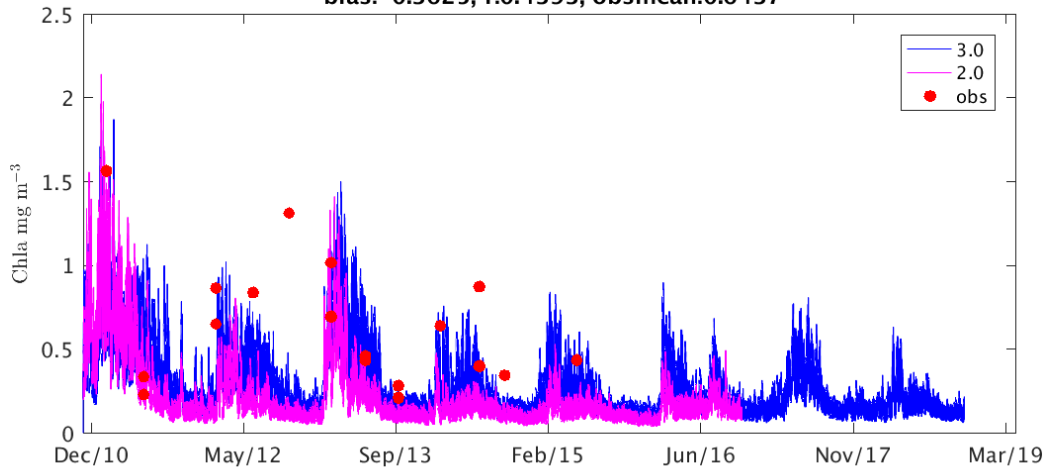
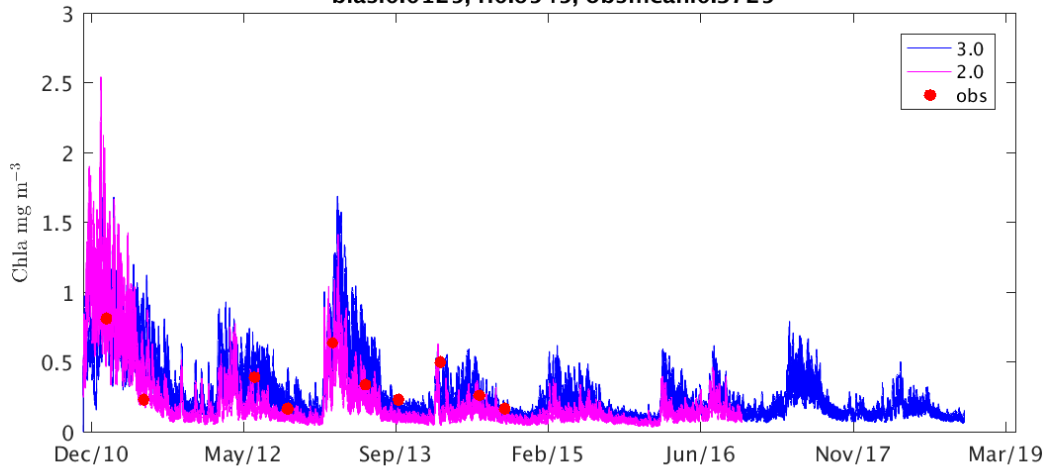


Figure 4 Metrics for Long Term Monitoring sites Chlorophyll assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27. mae: mean absolute error, rms root mean square

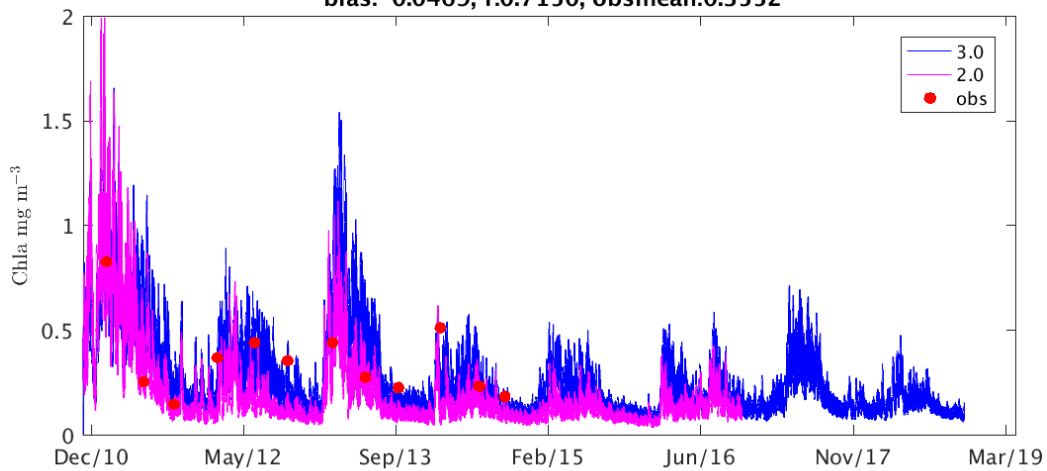
**Pelican\_5m 3.0 d2:0.49, mape:57.4, rms:0.4306**  
**bias:-0.2007, r:0.2329, obsmean:0.6437**  
**Pelican\_5m 2.0 d2:0.54, mape:56.6, rms:0.4907**  
**bias:-0.3625, r:0.4393, obsmean:0.6437**



**Humpy873\_10m 3.0 d2:0.63, mape:86.7, rms:0.3797**  
**bias:0.1801, r:0.5769, obsmean:0.3725**  
**Humpy873\_10m 2.0 d2:0.70, mape:55.6, rms:0.3449**  
**bias:0.0125, r:0.6545, obsmean:0.3725**

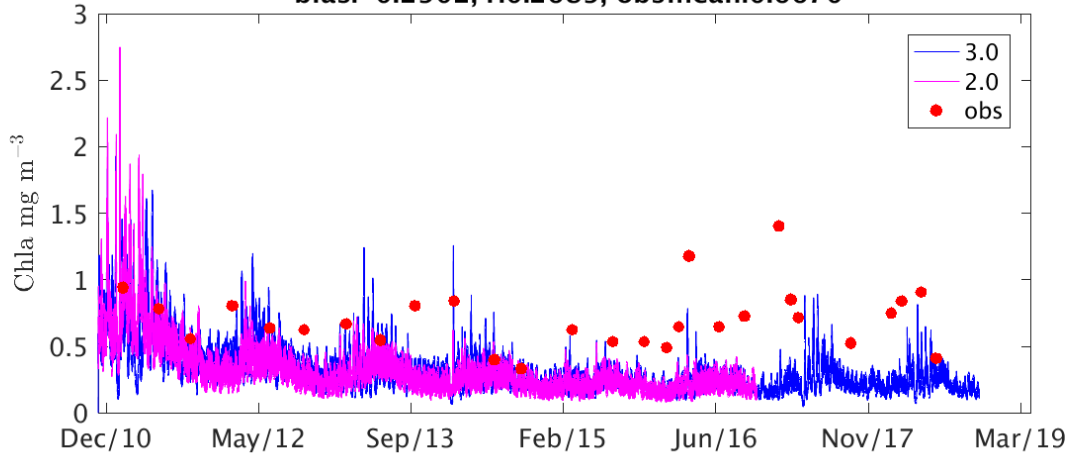


**Humpy873\_0m 3.0 d2:0.70, mape:58.6, rms:0.2604**  
**bias:0.1022, r:0.6019, obsmean:0.3552**  
**Humpy873\_0m 2.0 d2:0.77, mape:49.0, rms:0.2437**  
**bias:-0.0469, r:0.7150, obsmean:0.3552**

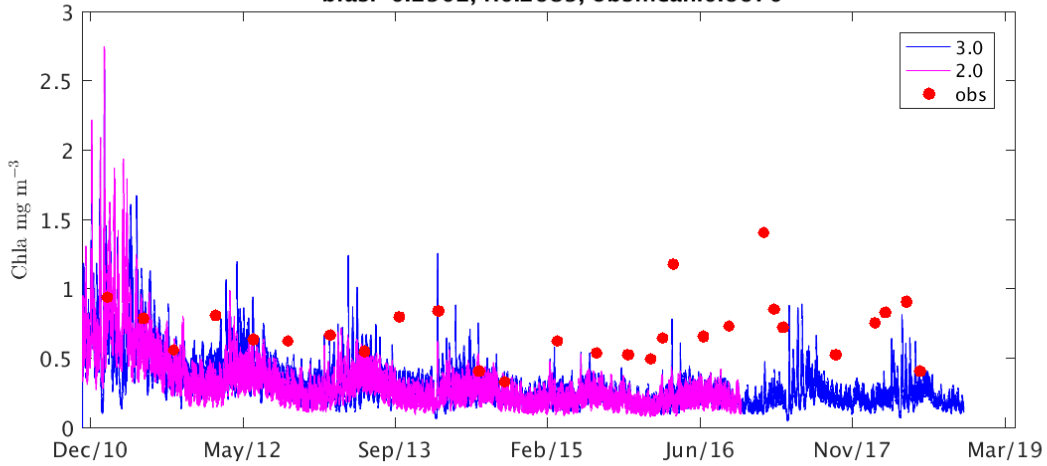




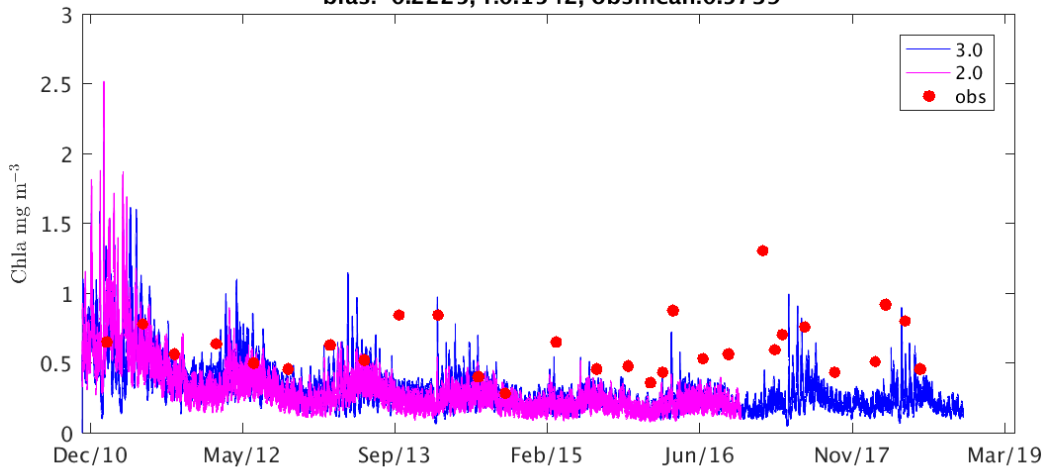
**Pine329\_20m 3.0 d2:0.43, mape:47.1, rms:0.4310**  
**bias:-0.3495, r:0.1346, obsmean:0.7053**  
**Pine329\_20m 2.0 d2:0.46, mape:46.7, rms:0.3931**  
**bias:-0.2902, r:0.2689, obsmean:0.6670**



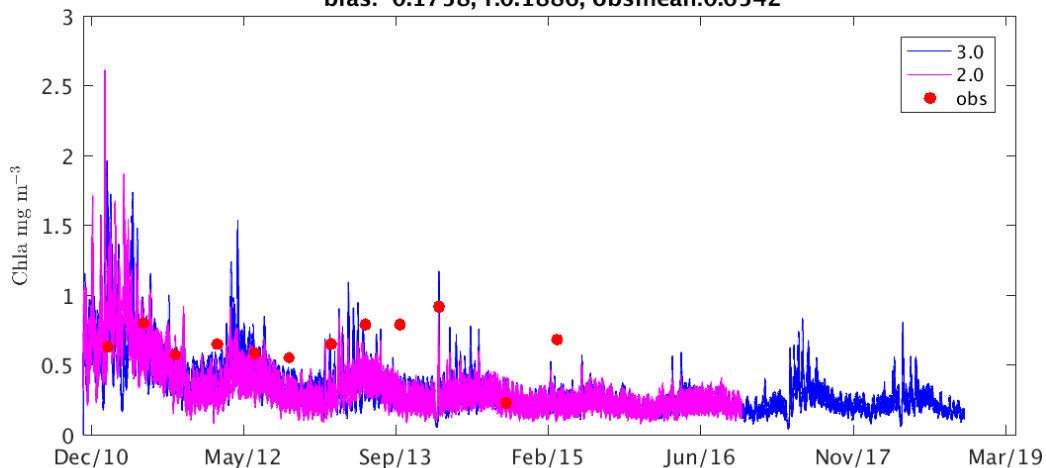
**Pine329\_20m 3.0 d2:0.43, mape:47.1, rms:0.4310**  
**bias:-0.3495, r:0.1346, obsmean:0.7053**  
**Pine329\_20m 2.0 d2:0.46, mape:46.7, rms:0.3931**  
**bias:-0.2902, r:0.2689, obsmean:0.6670**



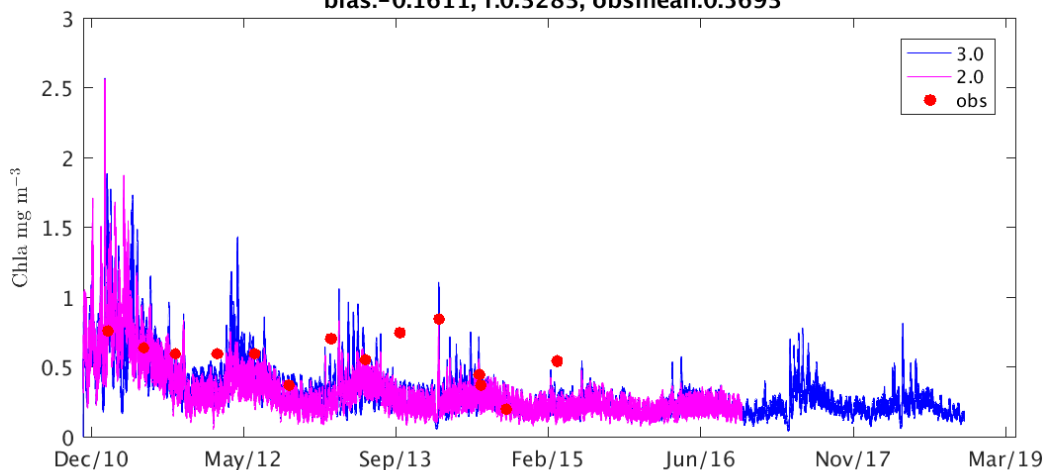
**Pine329\_0m 3.0 d2:0.43, mape:44.9, rms:0.3781**  
**bias:-0.2824, r:0.0450, obsmean:0.6195**  
**Pine329\_0m 2.0 d2:0.45, mape:43.6, rms:0.3312**  
**bias:-0.2225, r:0.1542, obsmean:0.5739**



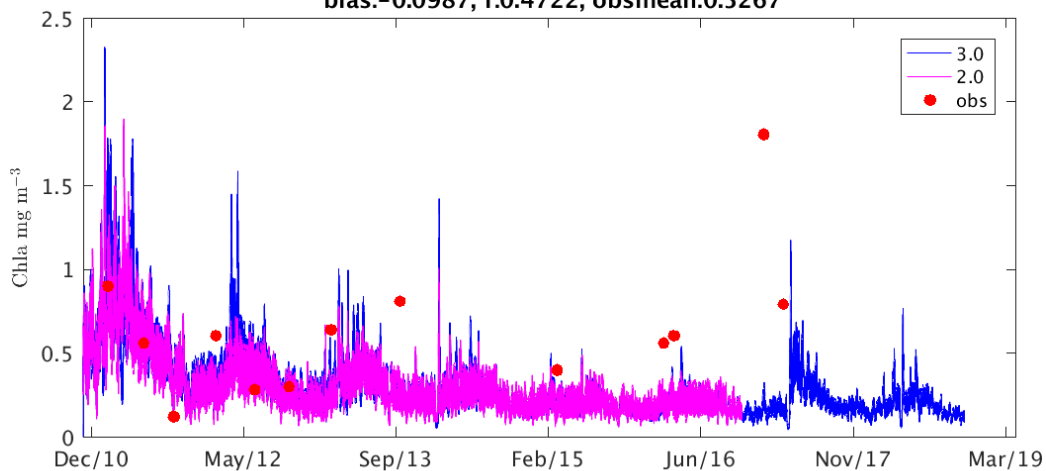
**Daydream\_23m 3.0 d2:0.37, mape:40.5, rms:0.4067**  
**bias:-0.0757, r:0.2319, obsmean:0.6542**  
**Daydream\_23m 2.0 d2:0.42, mape:39.6, rms:0.3114**  
**bias:-0.1758, r:0.1886, obsmean:0.6542**



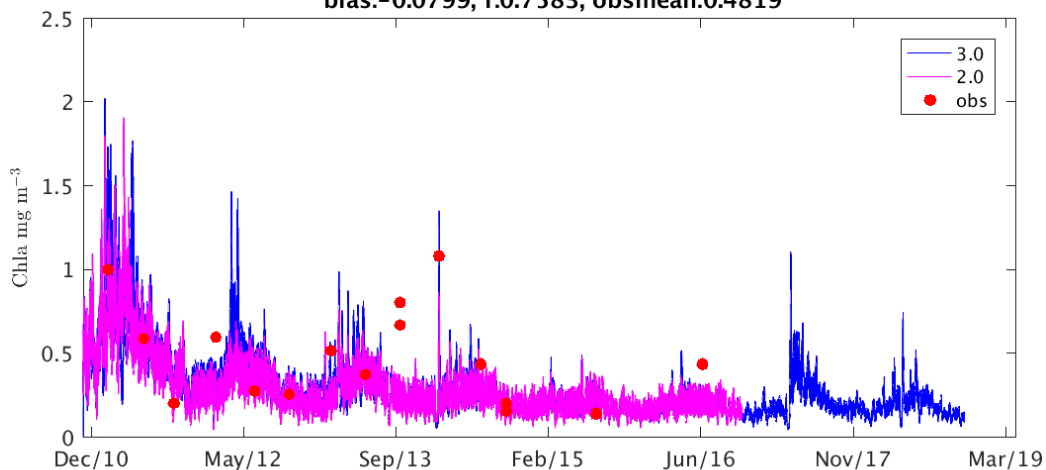
**Daydream330\_10m 3.0 d2:0.55, mape:35.5, rms:0.3463**  
**bias:-0.0645, r:0.4642, obsmean:0.5693**  
**Daydream330\_10m 2.0 d2:0.56, mape:31.6, rms:0.2735**  
**bias:-0.1611, r:0.3283, obsmean:0.5693**



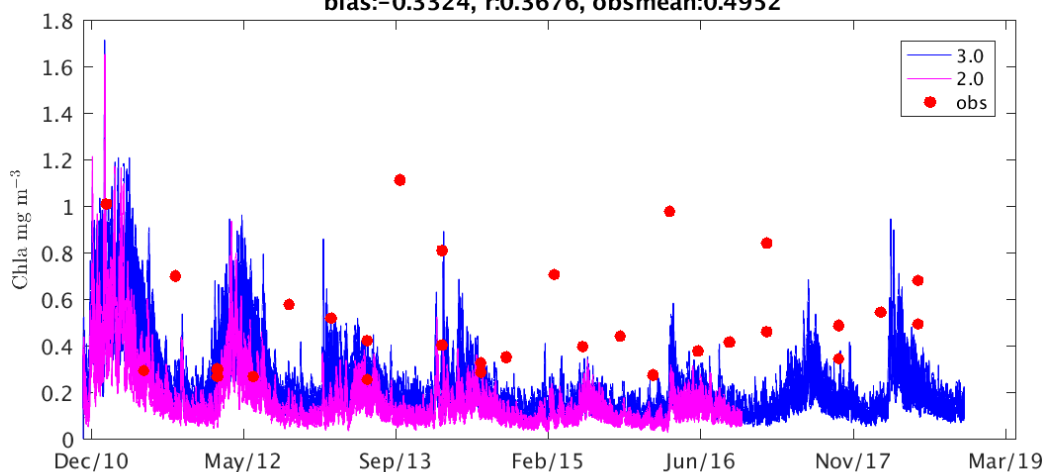
**DoubleCone\_23m 3.0 d2:0.40, mape:73.9, rms:0.6570**  
**bias:-0.1586, r:0.1348, obsmean:0.6454**  
**DoubleCone\_23m 2.0 d2:0.66, mape:58.4, rms:0.3045**  
**bias:-0.0987, r:0.4722, obsmean:0.5267**



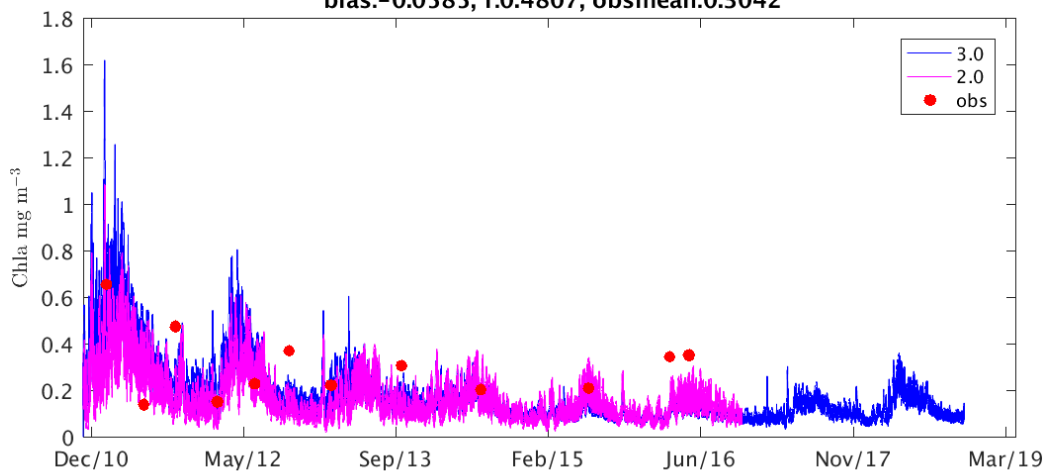
**DoubleCone334\_10m 3.0 d2:0.75, mape:38.2, rms:0.3694**  
**bias:-0.0143, r:0.6830, obsmean:0.4819**  
**DoubleCone334\_10m 2.0 d2:0.86, mape:30.5, rms:0.2147**  
**bias:-0.0799, r:0.7583, obsmean:0.4819**



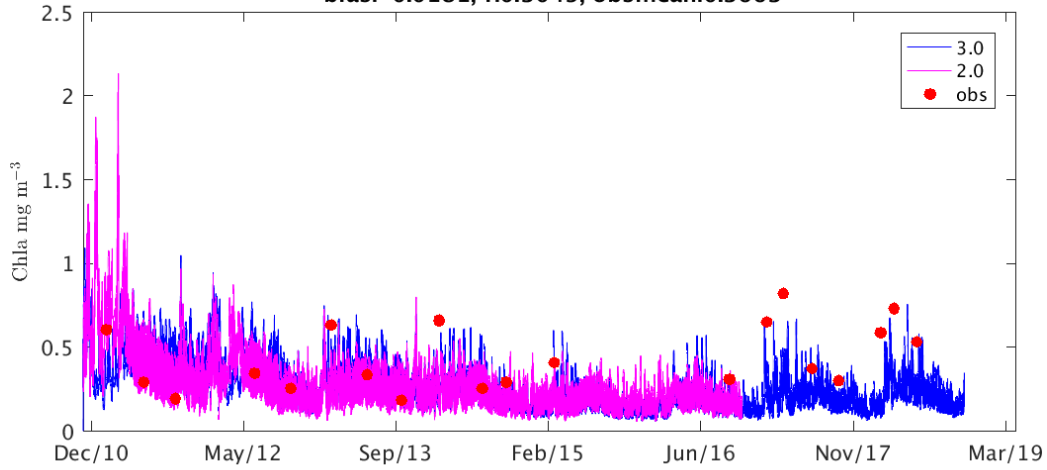
**GeoffreyBay336\_5m 3.0 d2:0.47, mape:45.2, rms:0.3352**  
**bias:-0.2301, r:0.2093, obsmean:0.5021**  
**GeoffreyBay336\_5m 2.0 d2:0.49, mape:63.0, rms:0.4065**  
**bias:-0.3324, r:0.3676, obsmean:0.4952**



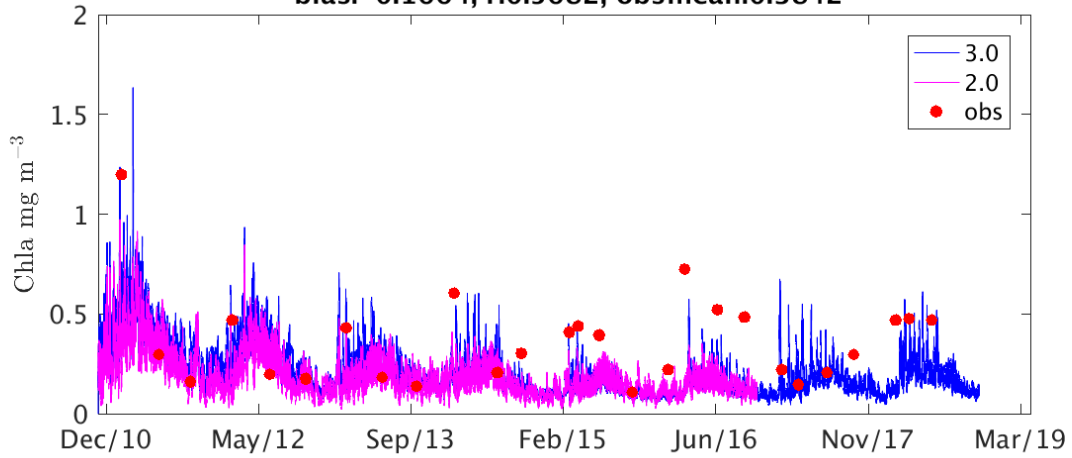
**Pandora\_5m 3.0 d2:0.67, mape:44.4, rms:0.1451**  
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**Pandora\_5m 2.0 d2:0.68, mape:51.8, rms:0.1546**  
**bias:-0.0585, r:0.4807, obsmean:0.3042**



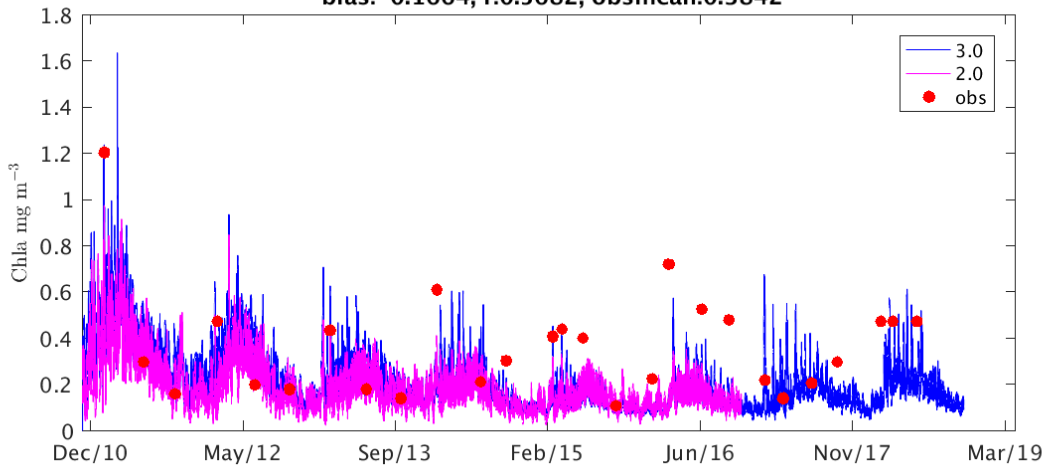
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 bias:-0.0181, r:0.3049, obsmean:0.3663



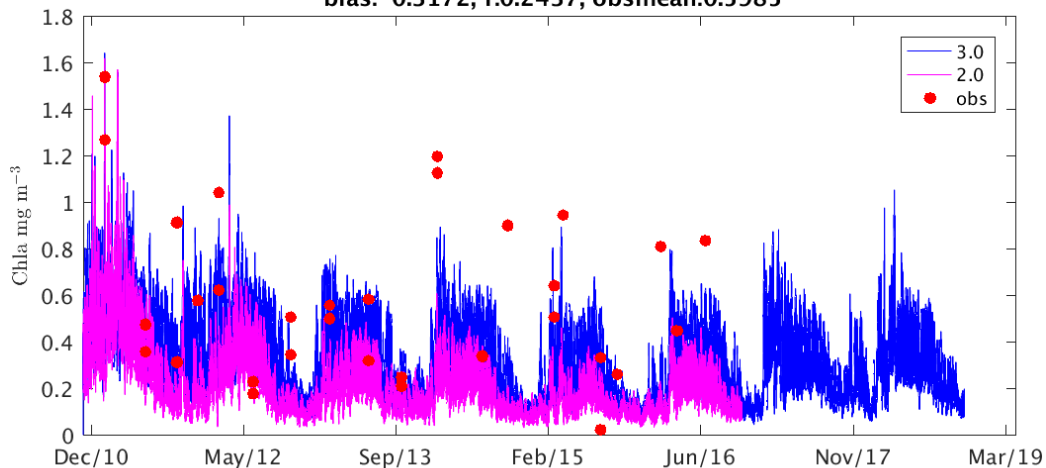
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 Pelorus686\_0m 2.0 d2:0.55, mape:43.0, rms:0.2692  
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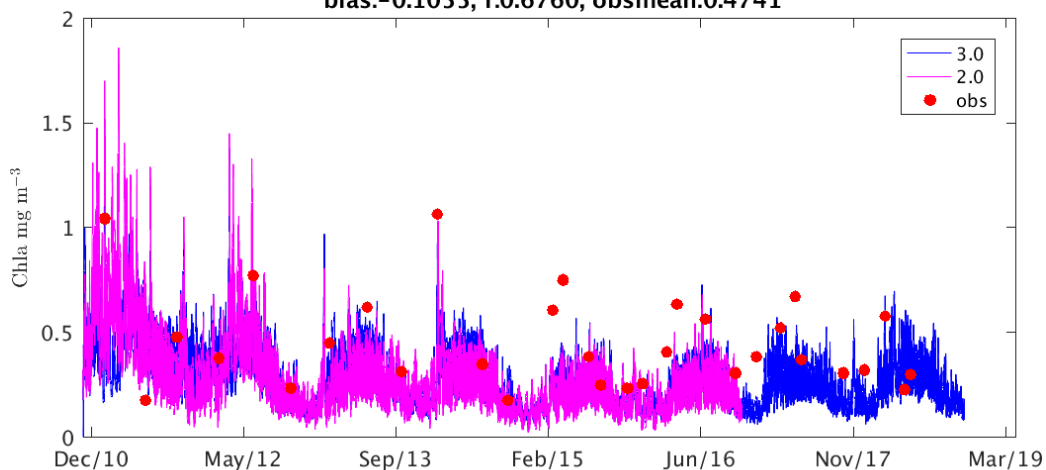
Pelorus686\_0m 3.0 d2:0.53, mape:49.4, rms:0.2533  
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 bias:-0.1664, r:0.5682, obsmean:0.3842



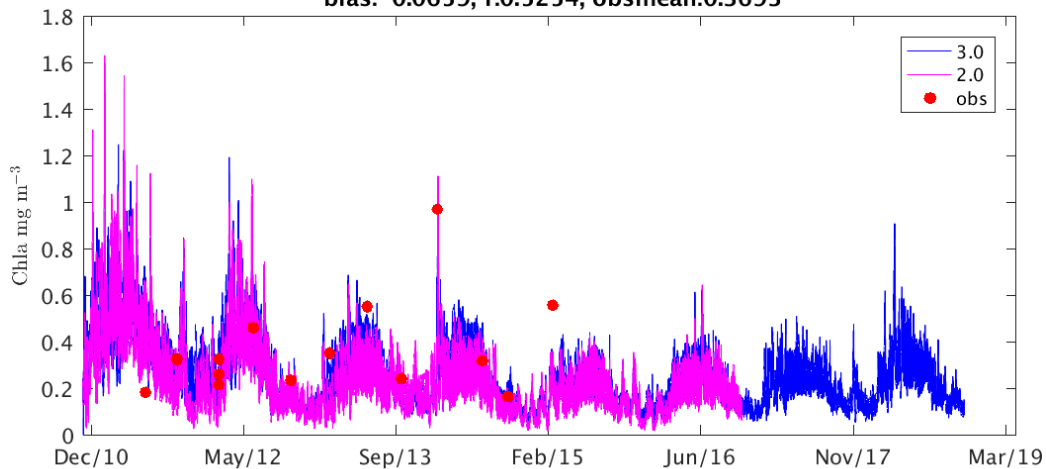
**Dunk859\_5m 3.0 d2:0.39, mape:104.4, rms:0.4133**  
**bias:-0.1841, r:0.0841, obsmean:0.5985**  
**Dunk859\_5m 2.0 d2:0.46, mape:82.8, rms:0.4714**  
**bias:-0.3172, r:0.2437, obsmean:0.5985**



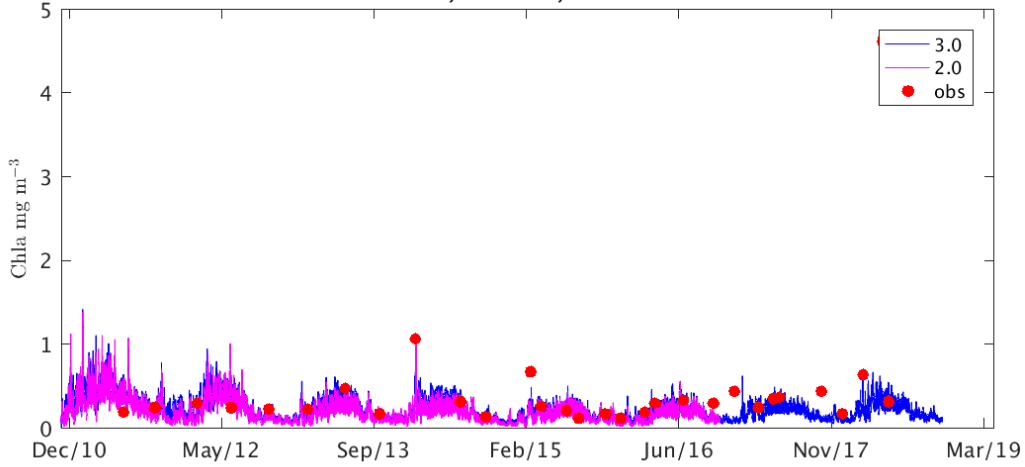
**Russell695\_20m 3.0 d2:0.78, mape:43.3, rms:0.1924**  
**bias:-0.0913, r:0.6808, obsmean:0.4548**  
**Russell695\_20m 2.0 d2:0.79, mape:49.3, rms:0.2258**  
**bias:-0.1055, r:0.6760, obsmean:0.4741**



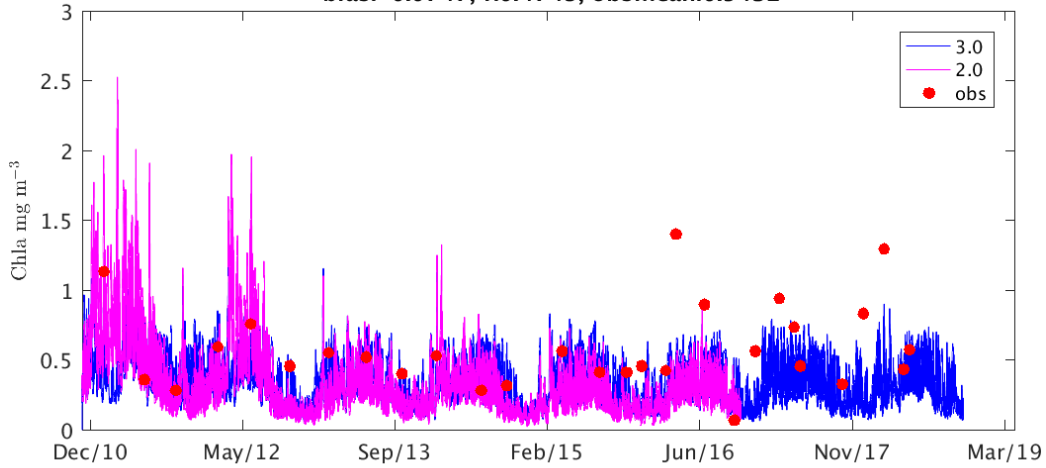
**Russell695\_10m 3.0 d2:0.81, mape:43.1, rms:0.1847**  
**bias:0.0116, r:0.6360, obsmean:0.3693**  
**Russell695\_10m 2.0 d2:0.72, mape:53.6, rms:0.2122**  
**bias:-0.0659, r:0.5254, obsmean:0.3693**



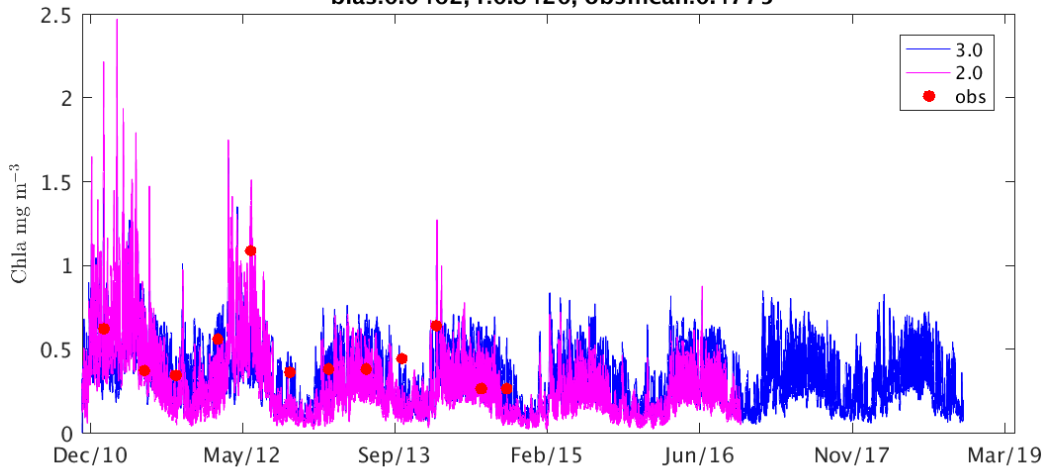
**Russell695\_0m 3.0 d2:0.24, mape:45.5, rms:0.7935**  
**bias:-0.1895, r:0.2573, obsmean:0.4599**  
**Russell695\_0m 2.0 d2:0.71, mape:56.4, rms:0.1937**  
**bias:-0.0597, r:0.5597, obsmean:0.2969**



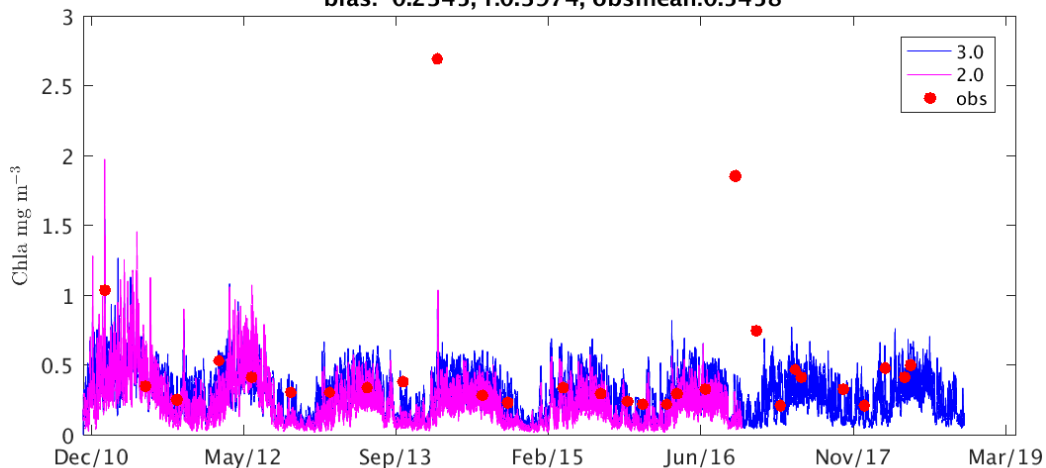
**Highl\_20m 3.0 d2:0.53, mape:44.2, rms:0.3529**  
**bias:-0.1602, r:0.2936, obsmean:0.5876**  
**Highl\_20m 2.0 d2:0.67, mape:48.1, rms:0.3618**  
**bias:-0.0747, r:0.4749, obsmean:0.5432**



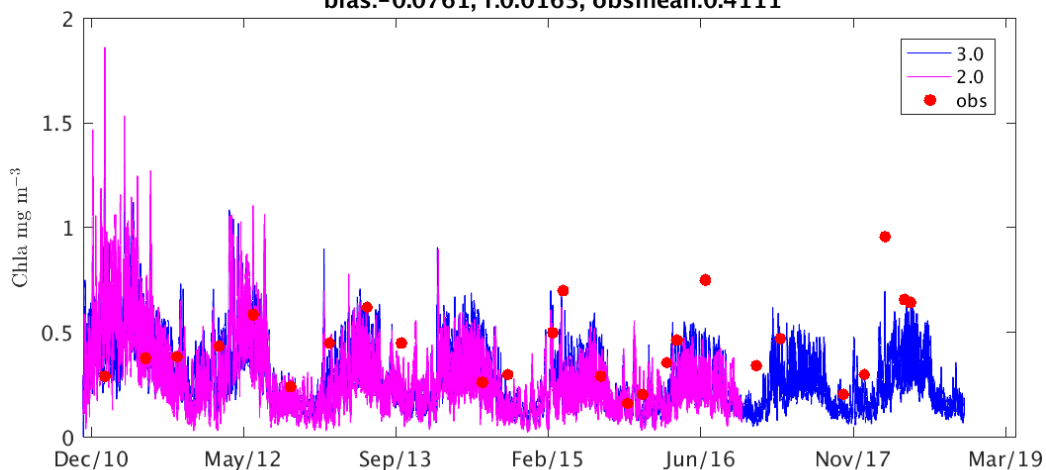
**Highl\_10m 3.0 d2:0.76, mape:40.6, rms:0.2359**  
**bias:0.0434, r:0.6409, obsmean:0.4775**  
**Highl\_10m 2.0 d2:0.81, mape:44.6, rms:0.2709**  
**bias:0.0462, r:0.8420, obsmean:0.4775**



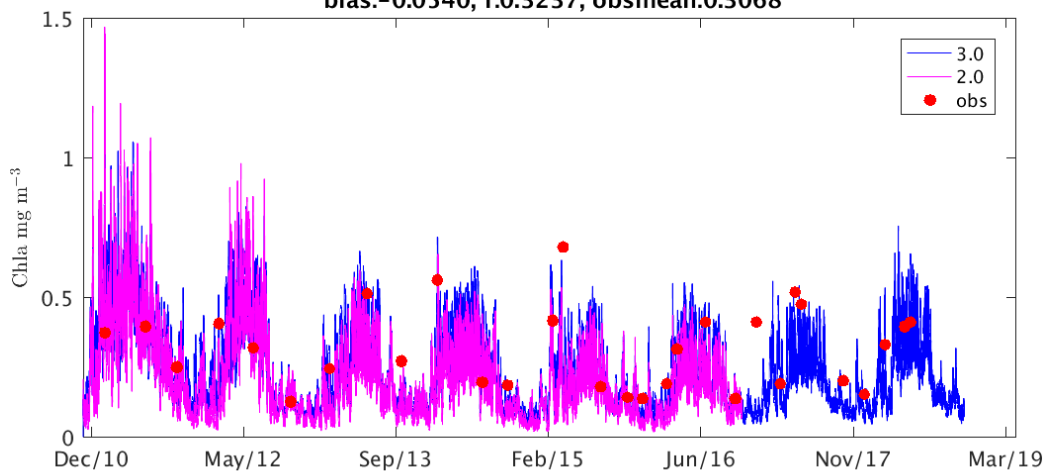
High1697\_0m 3.0 d2:0.56, mape:39.1, rms:0.4900  
 bias:-0.1606, r:0.4649, obsmean:0.5063  
 High1697\_0m 2.0 d2:0.51, mape:47.7, rms:0.6122  
 bias:-0.2345, r:0.3974, obsmean:0.5458



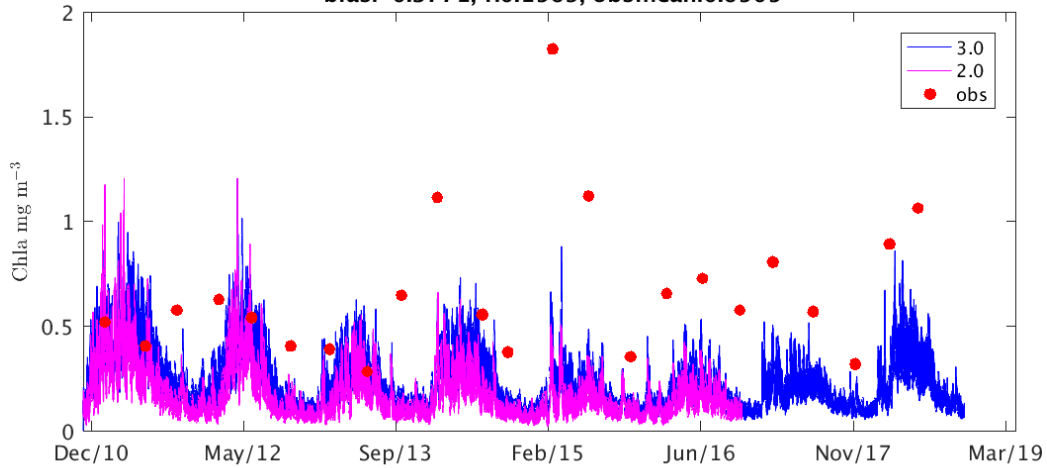
FitzCoral852\_15m 3.0 d2:0.67, mape:38.7, rms:0.2004  
 bias:-0.1040, r:0.5337, obsmean:0.4375  
 FitzCoral852\_15m 2.0 d2:0.33, mape:57.0, rms:0.3094  
 bias:-0.0761, r:0.0163, obsmean:0.4111



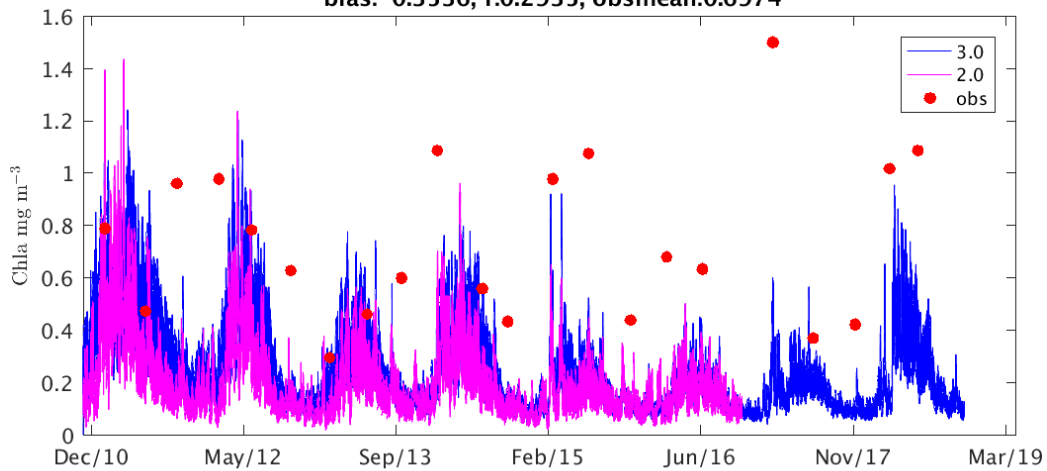
FitzCoral852\_0m 3.0 d2:0.73, mape:34.9, rms:0.1509  
 bias:-0.0408, r:0.5372, obsmean:0.3179  
 FitzCoral852\_0m 2.0 d2:0.56, mape:48.2, rms:0.2106  
 bias:-0.0540, r:0.3237, obsmean:0.3068



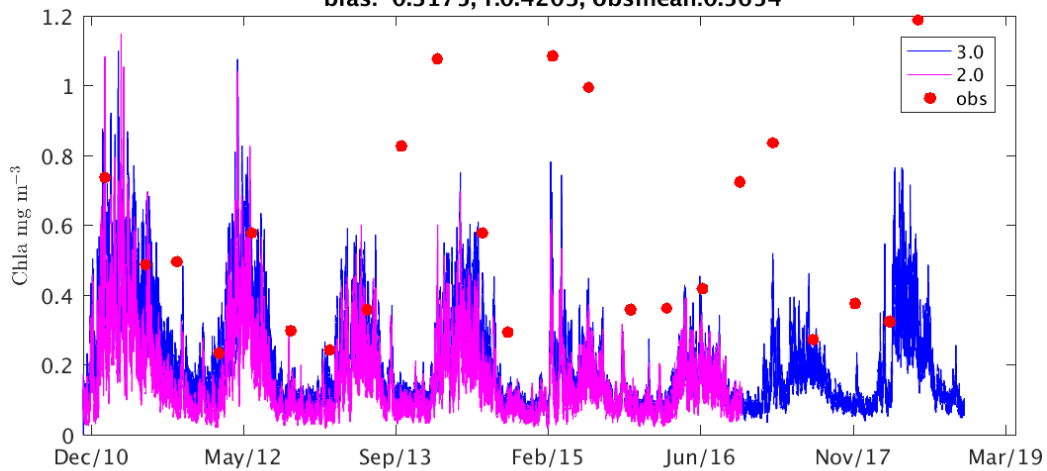
FairleadBuoy518\_0m 3.0 d2:0.45, mape:59.8, rms:0.5110  
 bias:-0.3551, r:0.2555, obsmean:0.6679  
 FairleadBuoy518\_0m 2.0 d2:0.41, mape:71.6, rms:0.5717  
 bias:-0.3771, r:0.1569, obsmean:0.6505



Yorkeys519\_8m 3.0 d2:0.49, mape:56.1, rms:0.5174  
 bias:-0.3840, r:0.2652, obsmean:0.7386  
 Yorkeys519\_8m 2.0 d2:0.46, mape:65.4, rms:0.5216  
 bias:-0.3536, r:0.2935, obsmean:0.6974

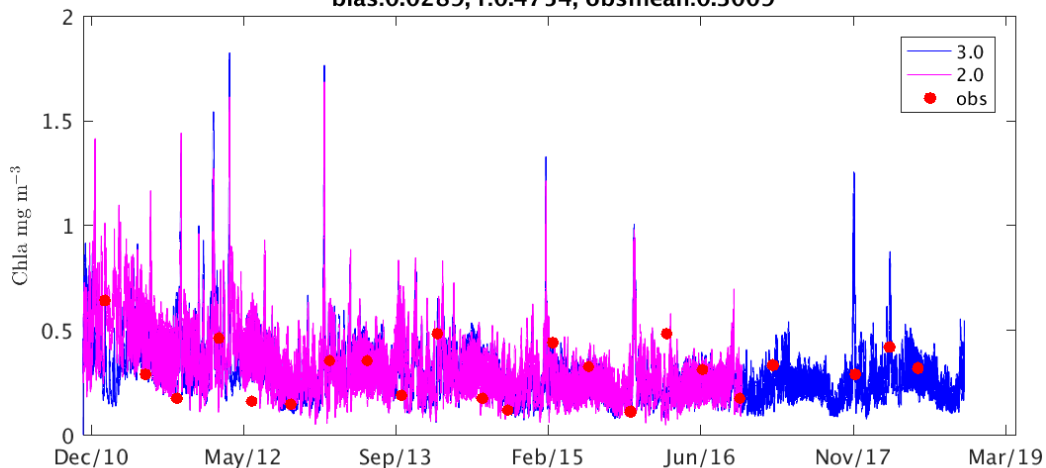


Yorkeys519\_0m 3.0 d2:0.54, mape:53.4, rms:0.4271  
 bias:-0.2961, r:0.3067, obsmean:0.5731  
 Yorkeys519\_0m 2.0 d2:0.55, mape:60.2, rms:0.4192  
 bias:-0.3175, r:0.4203, obsmean:0.5654

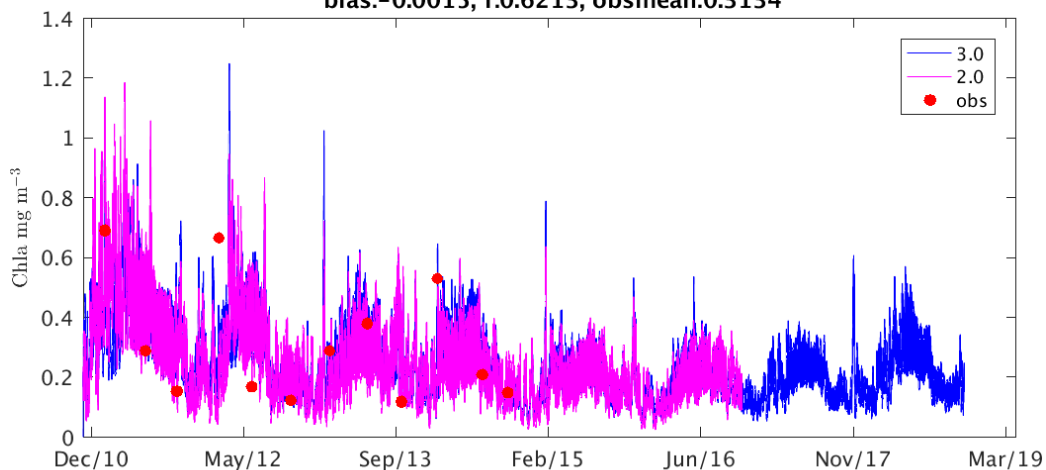




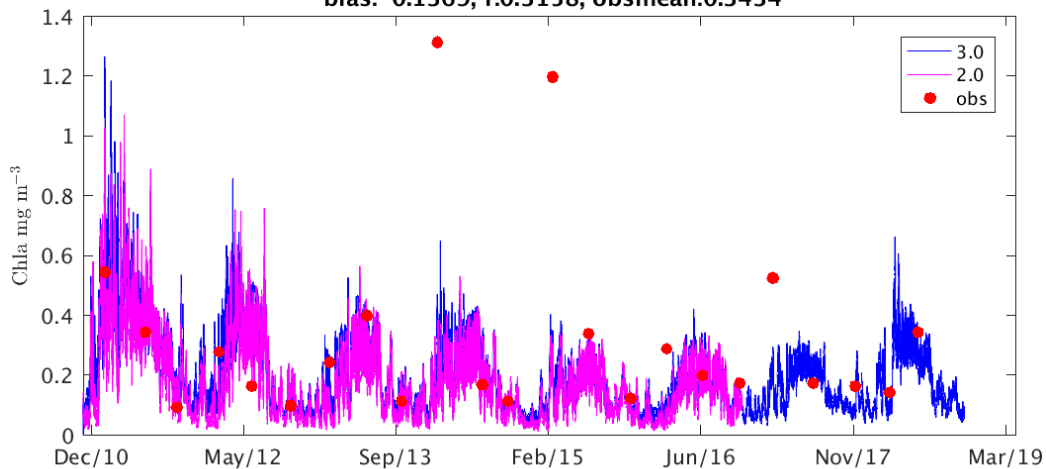
Green830\_36m 3.0 d2:0.77, mape:42.6, rms:0.1302  
bias:0.0132, r:0.5727, obsmean:0.3083  
Green830\_36m 2.0 d2:0.68, mape:59.7, rms:0.1901  
bias:0.0289, r:0.4754, obsmean:0.3009



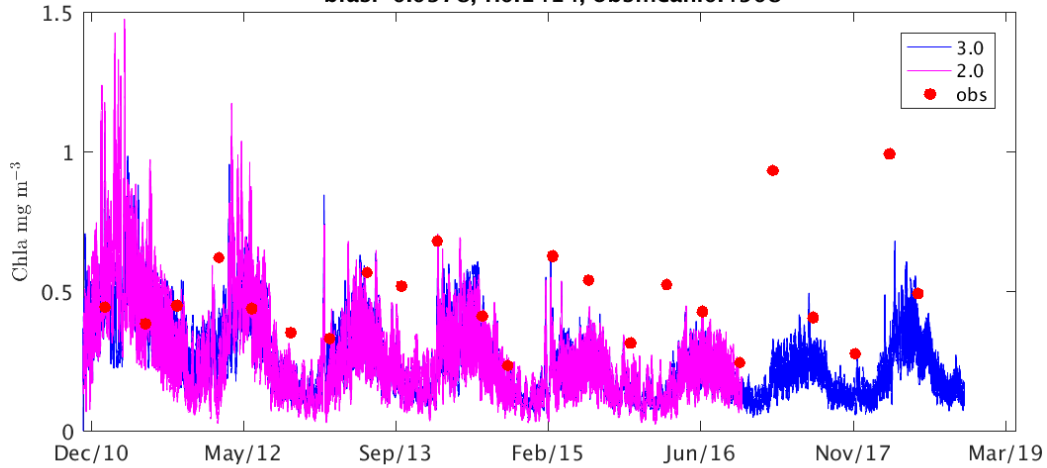
Green830\_18m 3.0 d2:0.86, mape:42.7, rms:0.1654  
bias:0.0400, r:0.7804, obsmean:0.3134  
Green830\_18m 2.0 d2:0.75, mape:47.9, rms:0.2277  
bias:-0.0015, r:0.6213, obsmean:0.3134



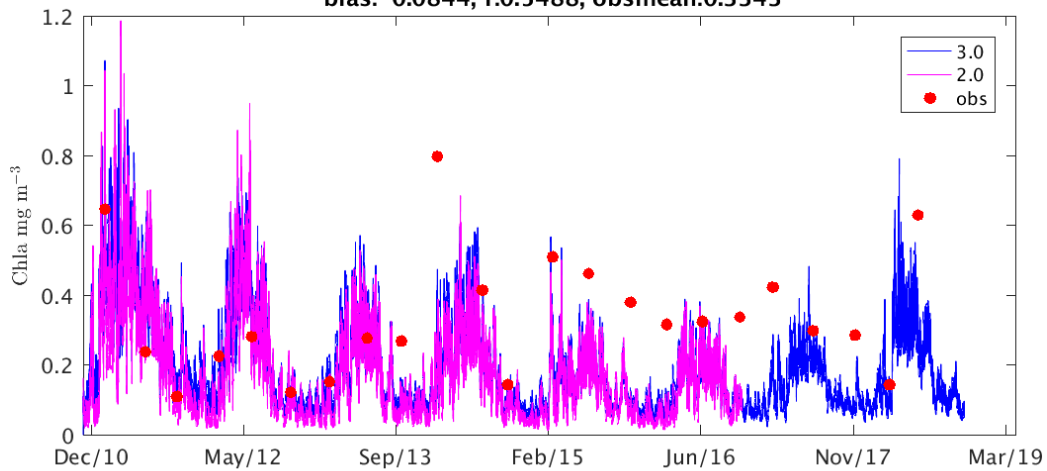
Green830\_0m 3.0 d2:0.56, mape:34.2, rms:0.2756  
bias:-0.0867, r:0.5624, obsmean:0.3272  
Green830\_0m 2.0 d2:0.49, mape:39.2, rms:0.3629  
bias:-0.1369, r:0.3158, obsmean:0.3434



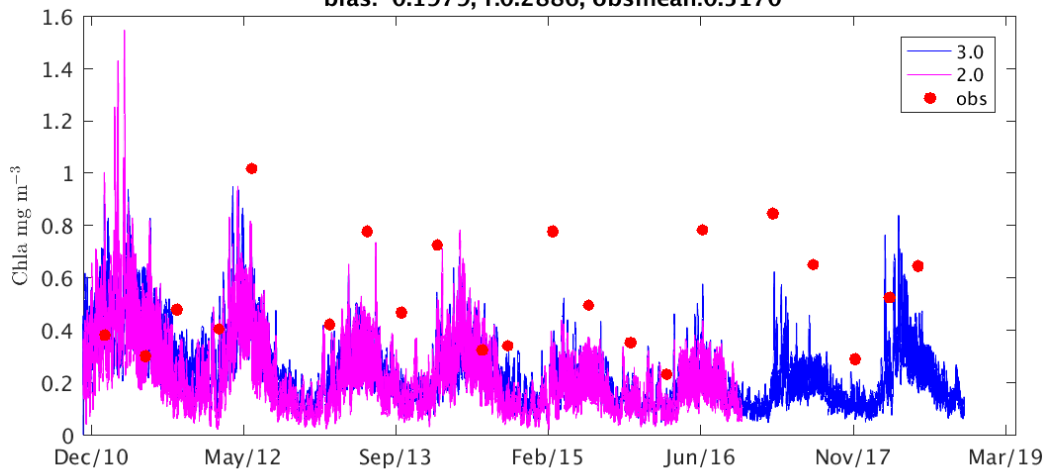
**DoubleI520\_18m 3.0 d2:0.47, mape:41.5, rms:0.2813**  
**bias:-0.1438, r:0.1947, obsmean:0.4878**  
**DoubleI520\_18m 2.0 d2:0.41, mape:42.0, rms:0.2617**  
**bias:-0.0978, r:0.1414, obsmean:0.4508**



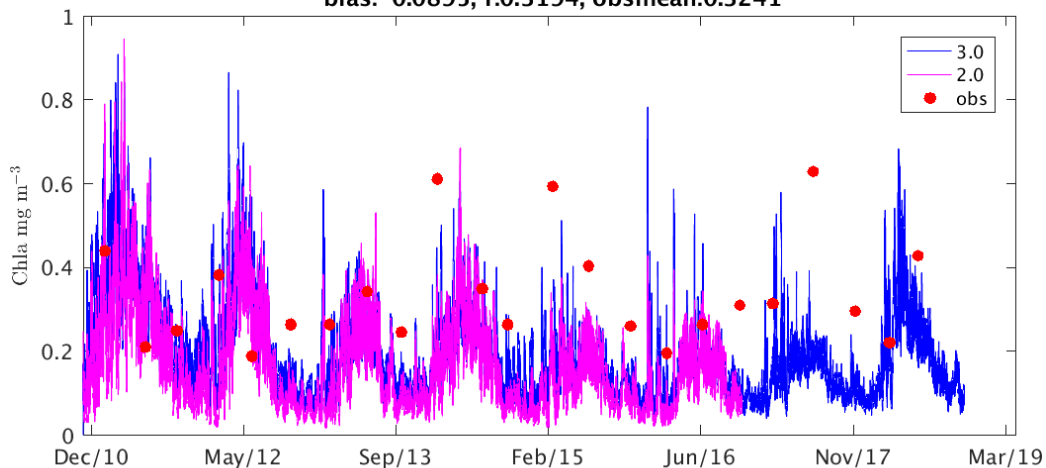
**DoubleI520\_0m 3.0 d2:0.73, mape:38.8, rms:0.1774**  
**bias:-0.0768, r:0.5786, obsmean:0.3393**  
**DoubleI520\_0m 2.0 d2:0.70, mape:38.4, rms:0.2068**  
**bias:-0.0844, r:0.5488, obsmean:0.3343**



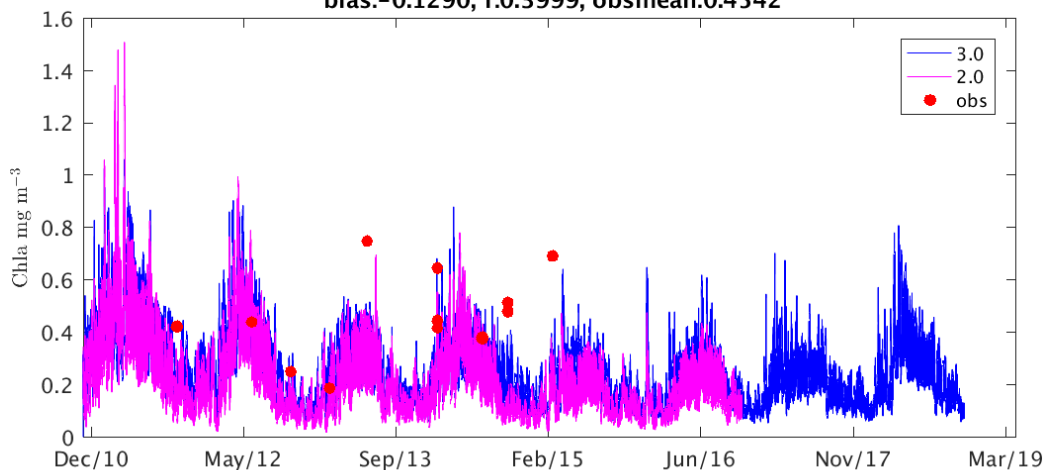
**PortD\_15m 3.0 d2:0.52, mape:49.4, rms:0.3023**  
**bias:-0.1985, r:0.2759, obsmean:0.5346**  
**PortD\_15m 2.0 d2:0.49, mape:55.9, rms:0.3097**  
**bias:-0.1979, r:0.2886, obsmean:0.5170**



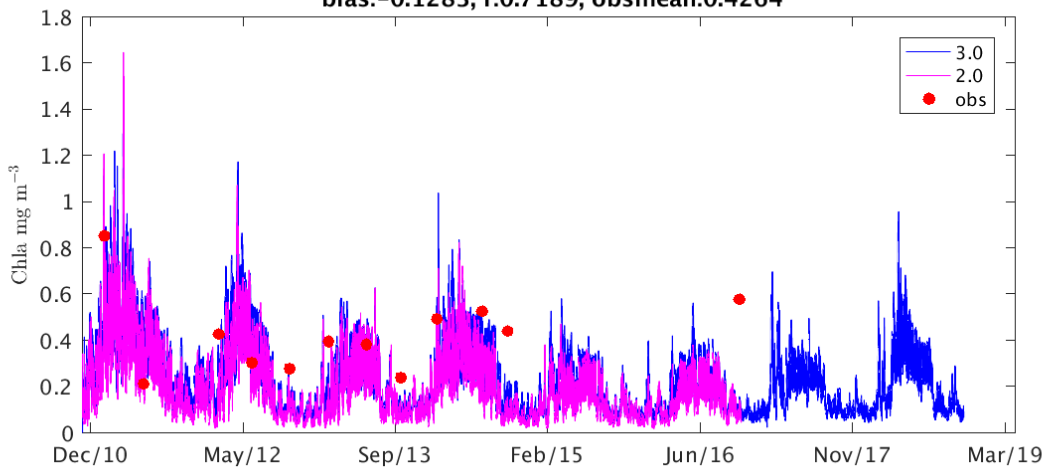
PortD\_0m 3.0 d2:0.46, mape:48.8, rms:0.1924  
 bias:-0.0837, r:0.1316, obsmean:0.3356  
 PortD\_0m 2.0 d2:0.50, mape:55.0, rms:0.2010  
 bias:-0.0895, r:0.3194, obsmean:0.3241



Snap\_10m 3.0 d2:0.65, mape:26.6, rms:0.1679  
 bias:-0.0996, r:0.5499, obsmean:0.4542  
 Snap\_10m 2.0 d2:0.56, mape:35.5, rms:0.2152  
 bias:-0.1290, r:0.3999, obsmean:0.4542



CapeTrib356\_10m 3.0 d2:0.76, mape:44.0, rms:0.1922  
 bias:-0.0840, r:0.6408, obsmean:0.4264  
 CapeTrib356\_10m 2.0 d2:0.75, mape:46.9, rms:0.2214  
 bias:-0.1283, r:0.7189, obsmean:0.4264



## 11. Simulated Secchi depth assessment against AIMS Long Term Monitoring

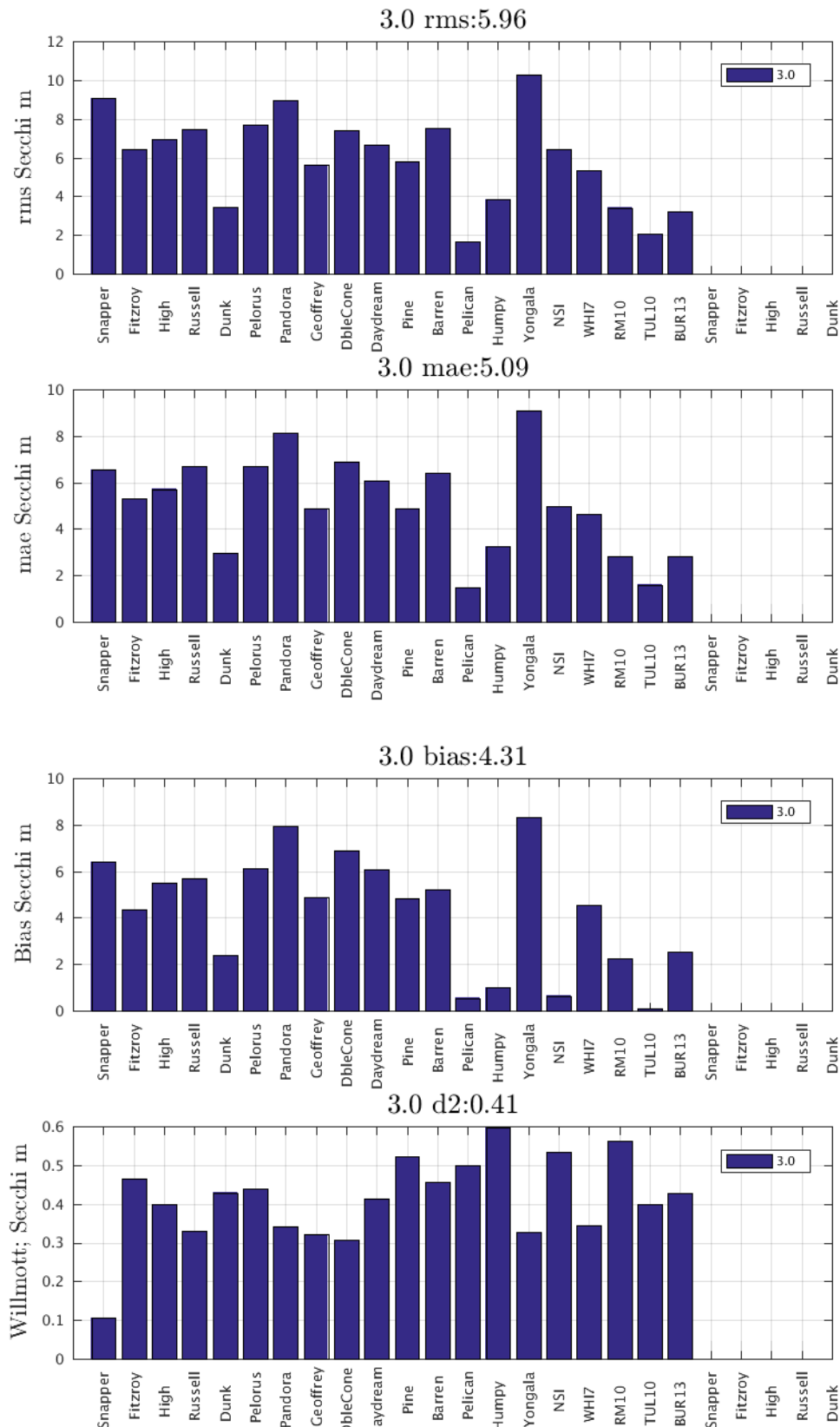
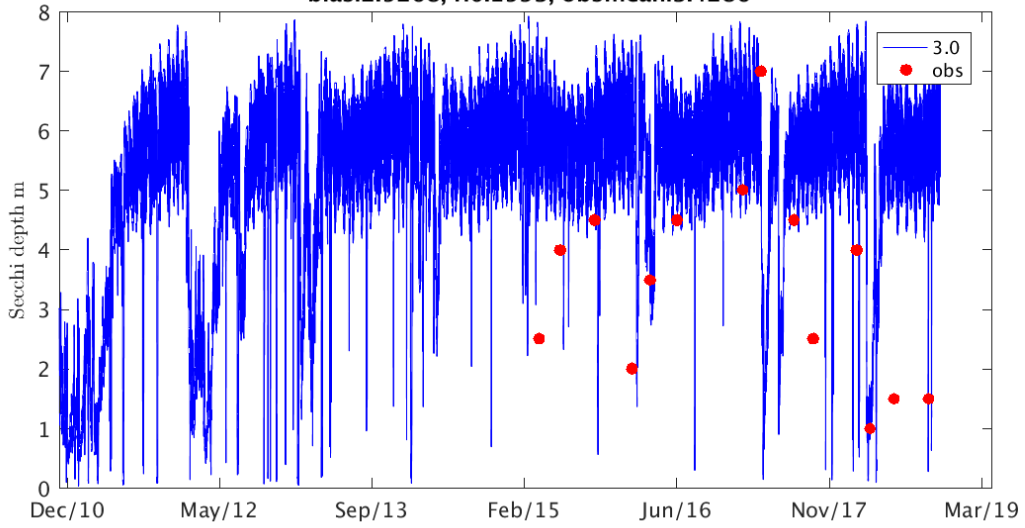
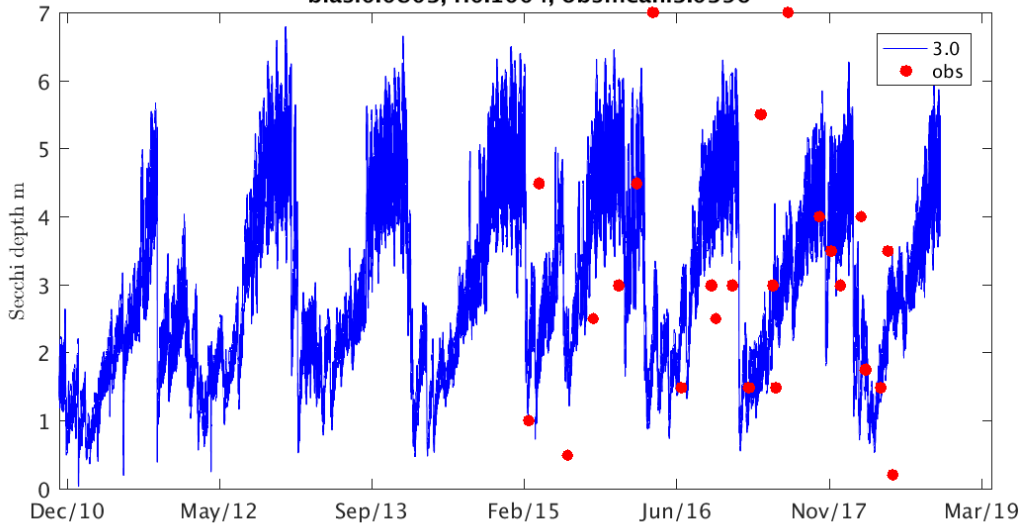


Figure 5 Metrics for Long Term Monitoring sites Secchi depth assessment against observations for model version 3p0, d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

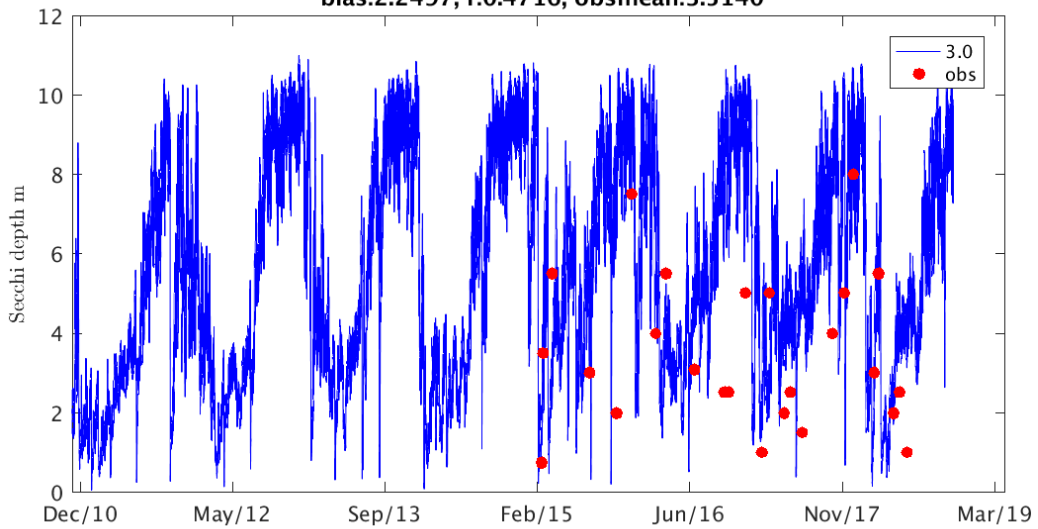
**BUR13 3.0 d2:0.43, mape:116.7, rms:3.2032  
bias:2.5268, r:0.1593, obsmean:3.4286**



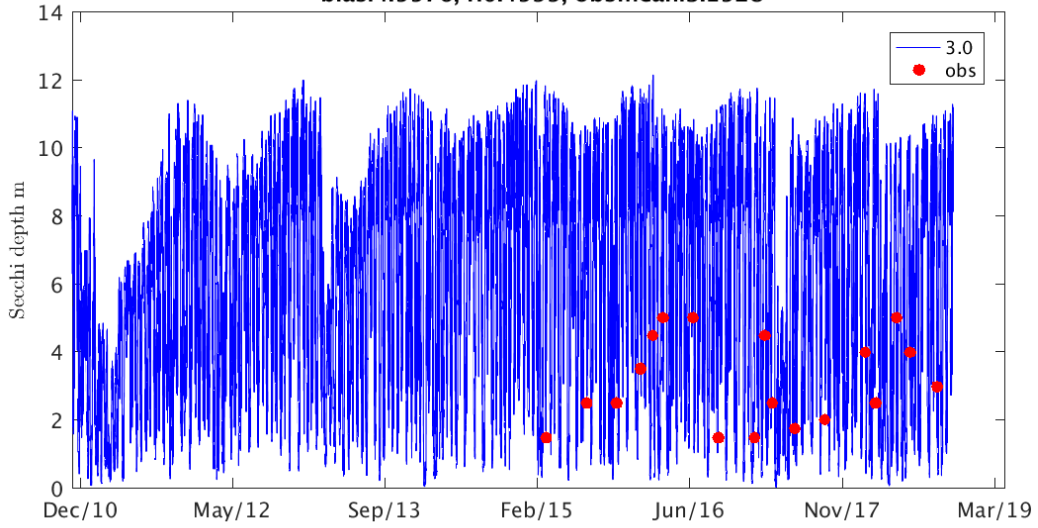
**TUL10 3.0 d2:0.40, mape:106.9, rms:2.0431  
bias:0.0803, r:0.1004, obsmean:3.0396**



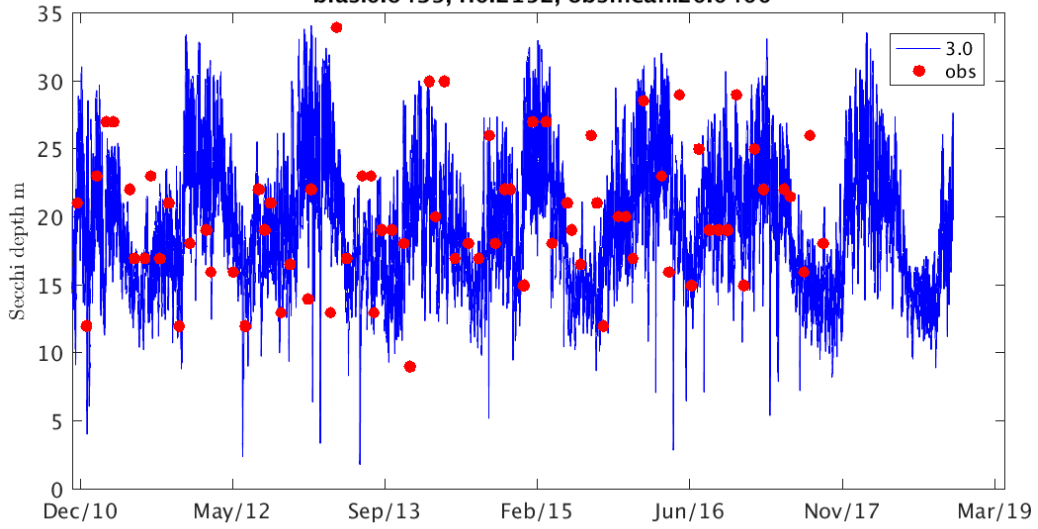
**RM10 3.0 d2:0.56, mape:109.9, rms:3.4147  
bias:2.2497, r:0.4716, obsmean:3.5140**



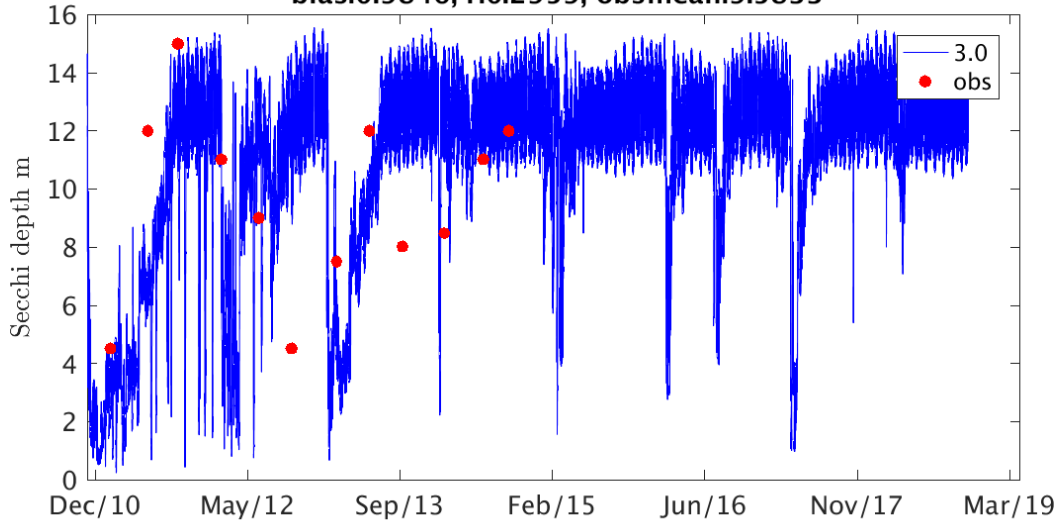
**WHI7 3.0 d2:0.34, mape:170.9, rms:5.3227  
bias:4.5576, r:0.4599, obsmean:3.1528**

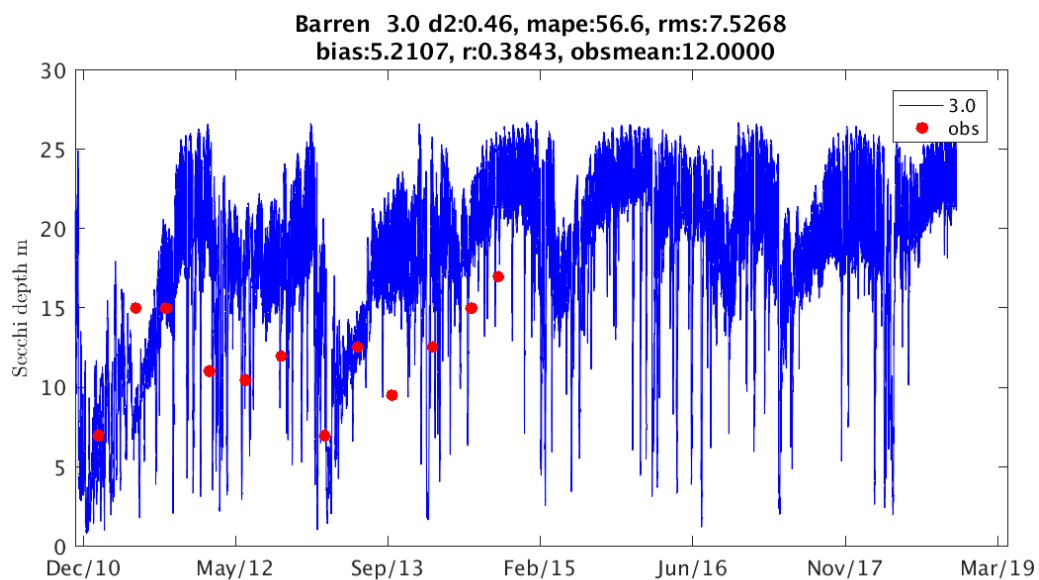
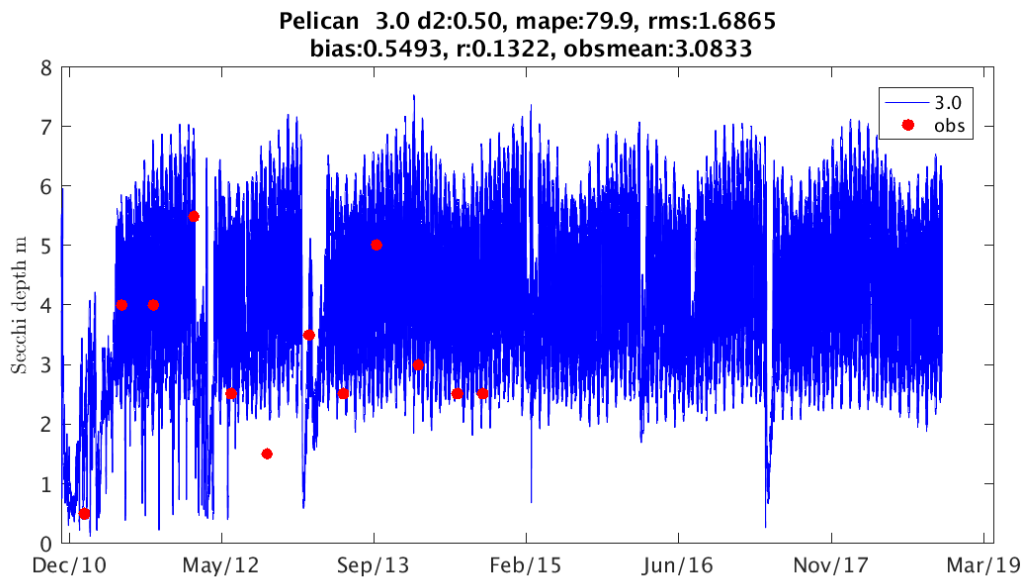
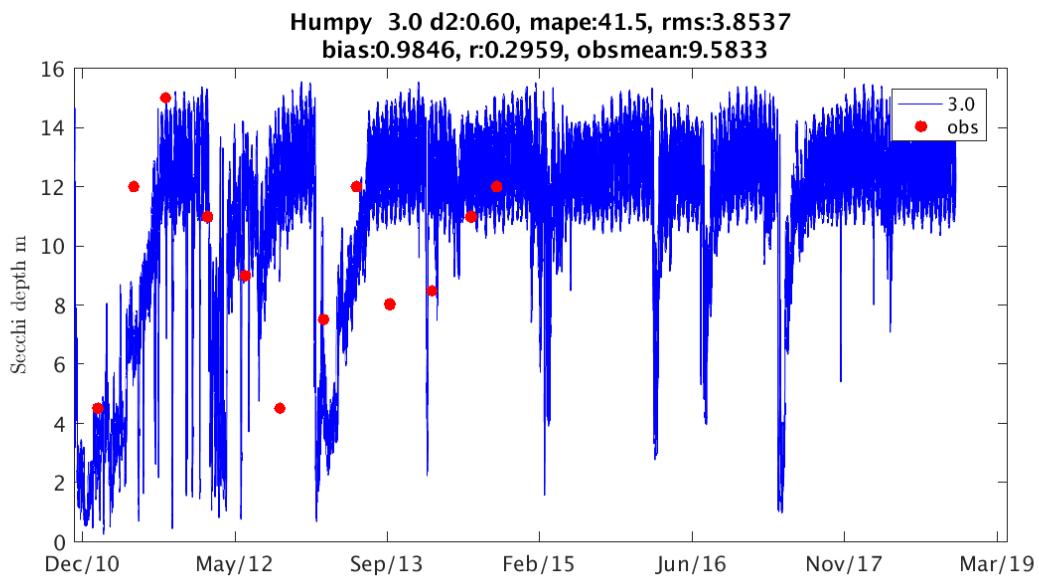


**NSI 3.0 d2:0.53, mape:26.9, rms:6.4217  
bias:0.6439, r:0.2152, obsmean:20.0400**

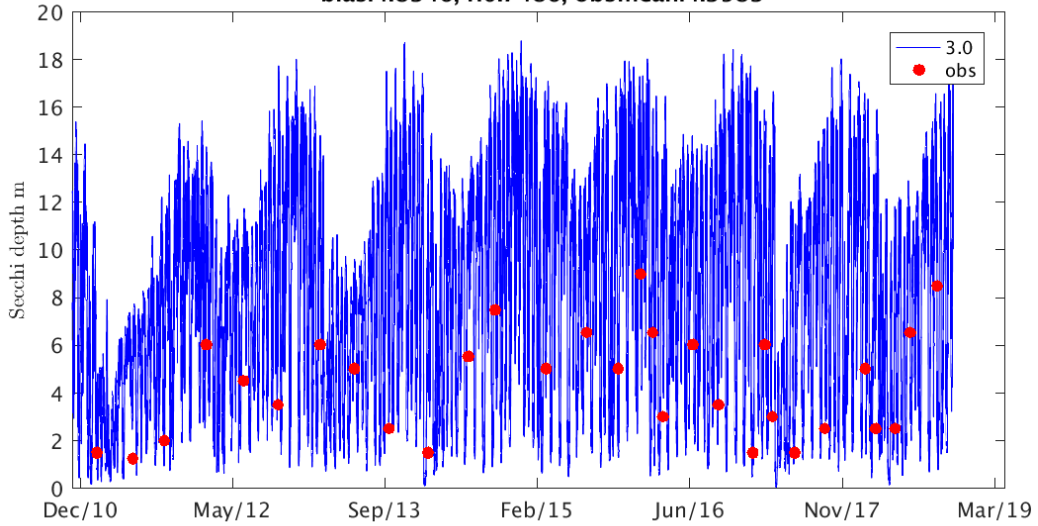


**Humpy 3.0 d2:0.60, mape:41.5, rms:3.8537  
bias:0.9846, r:0.2959, obsmean:9.5833**

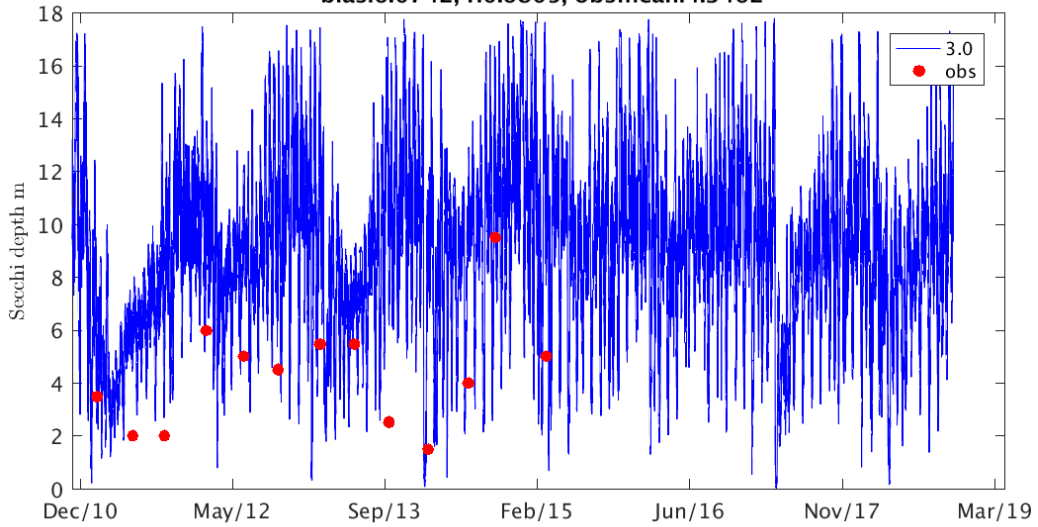




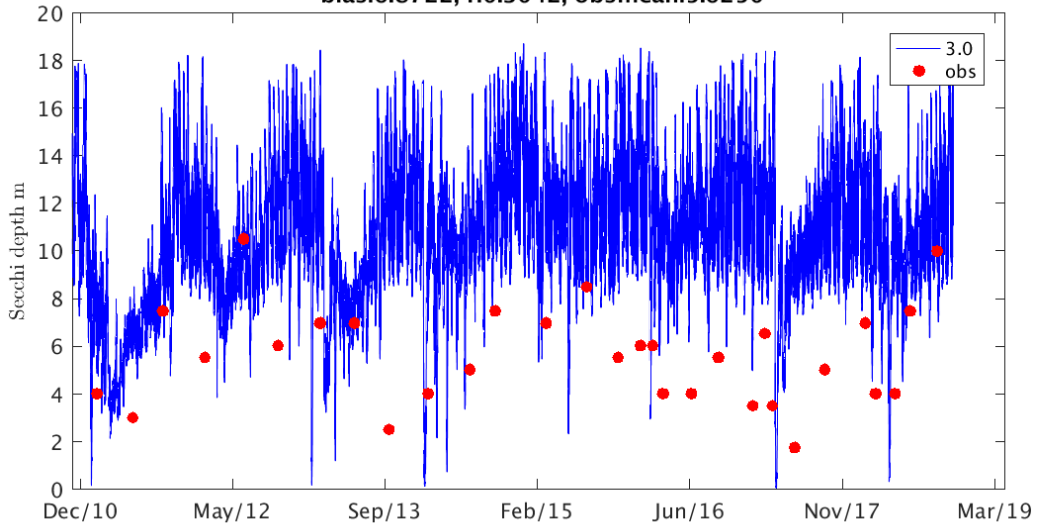
**Pine 3.0 d2:0.52, mape:125.2, rms:5.8227  
bias:4.8346, r:0.7486, obsmean:4.3583**



**Daydream 3.0 d2:0.41, mape:177.0, rms:6.6422  
bias:6.0742, r:0.6805, obsmean:4.3462**

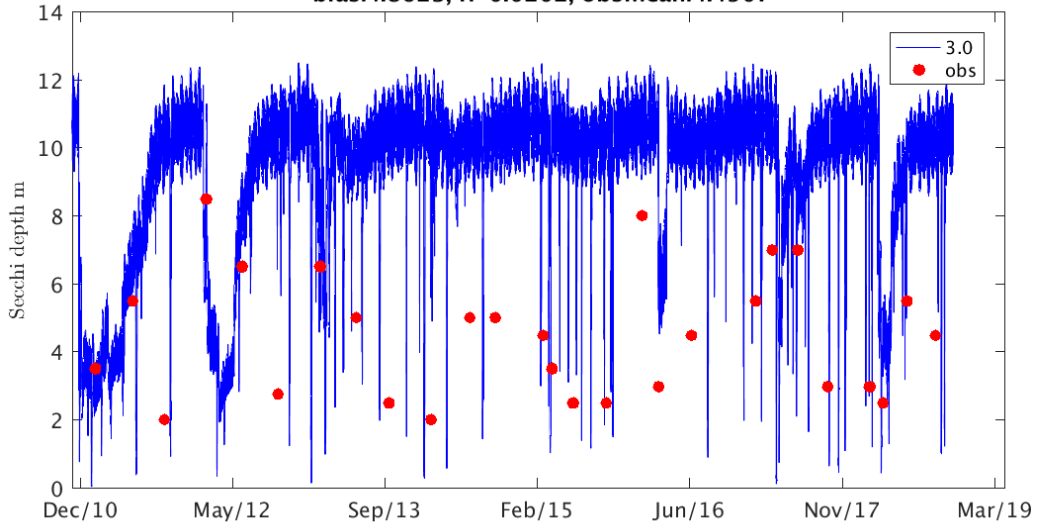


**DoubleCone 3.0 d2:0.31, mape:150.6, rms:7.3992  
bias:6.8722, r:0.3042, obsmean:5.6250**

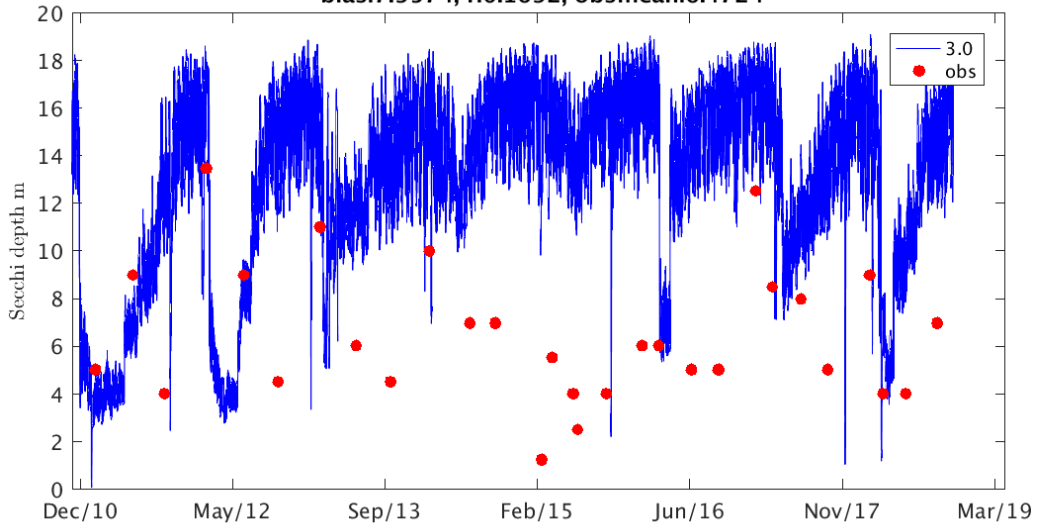




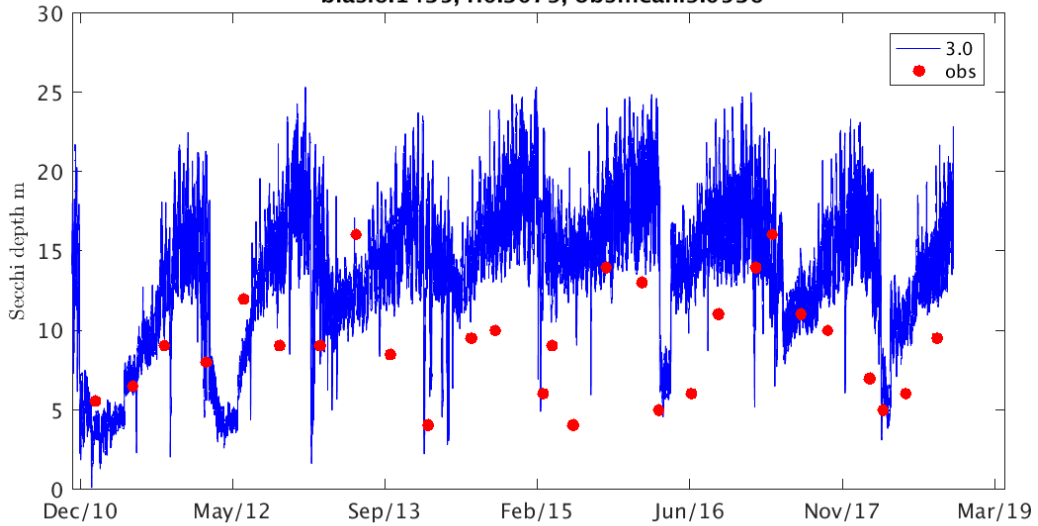
**GeoffreyBay 3.0 d2:0.32, mape:149.3, rms:5.6285  
bias:4.8623, r:-0.0202, obsmean:4.4907**

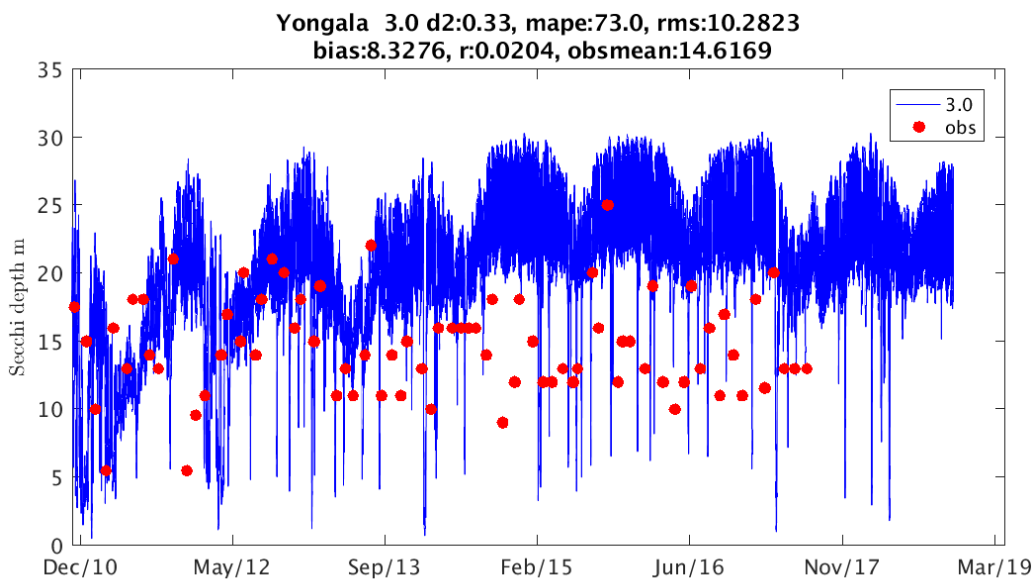
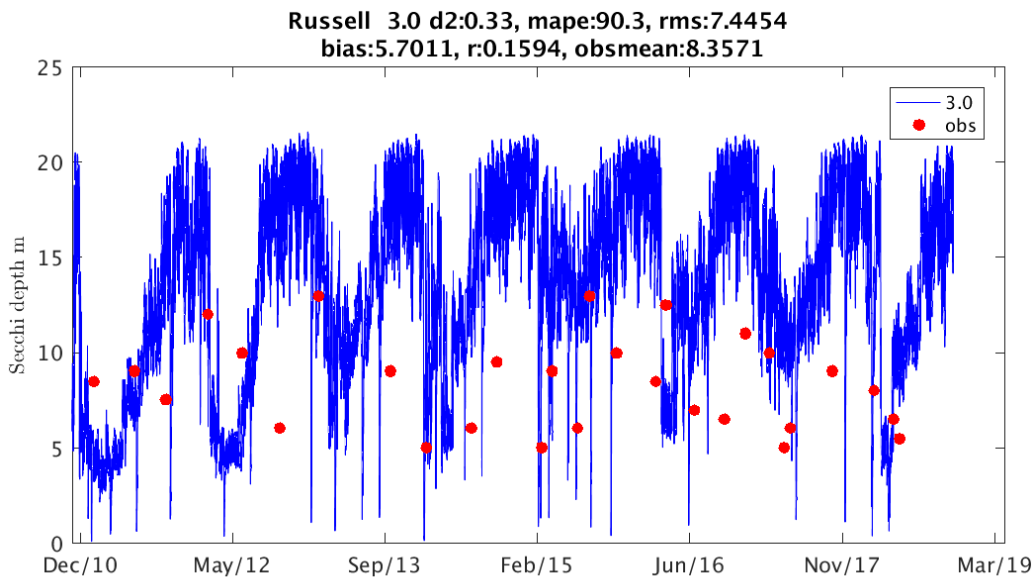
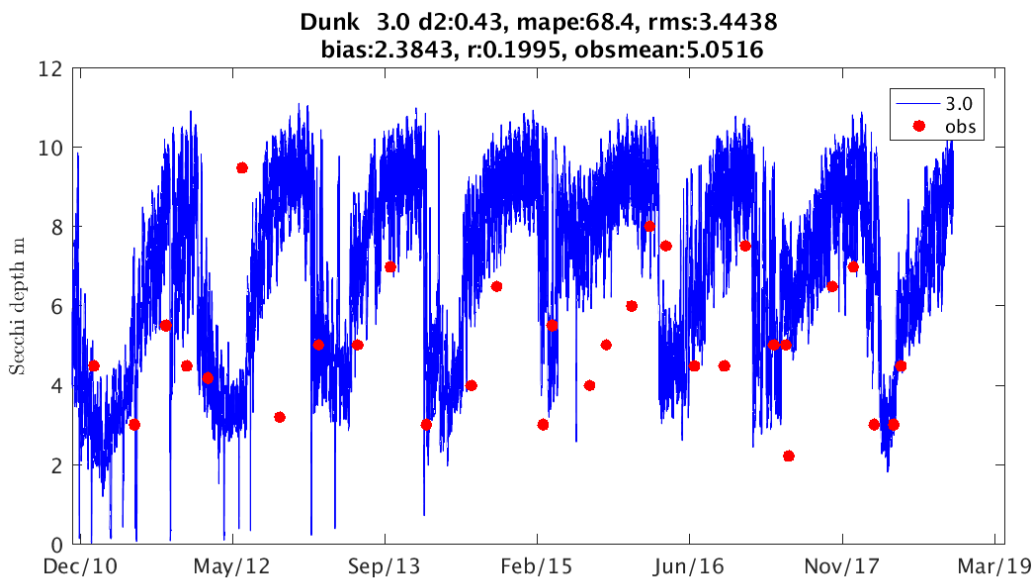


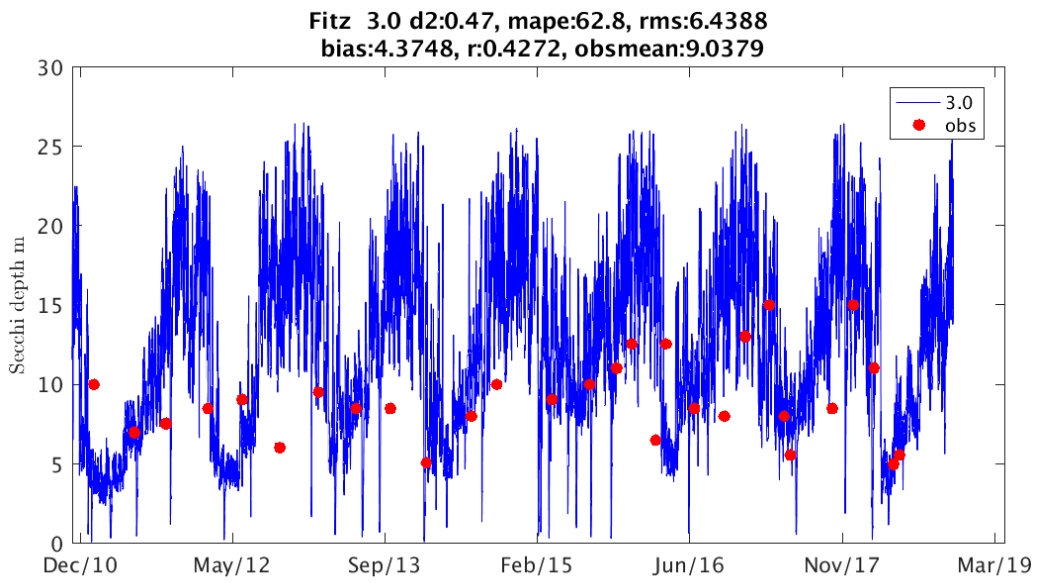
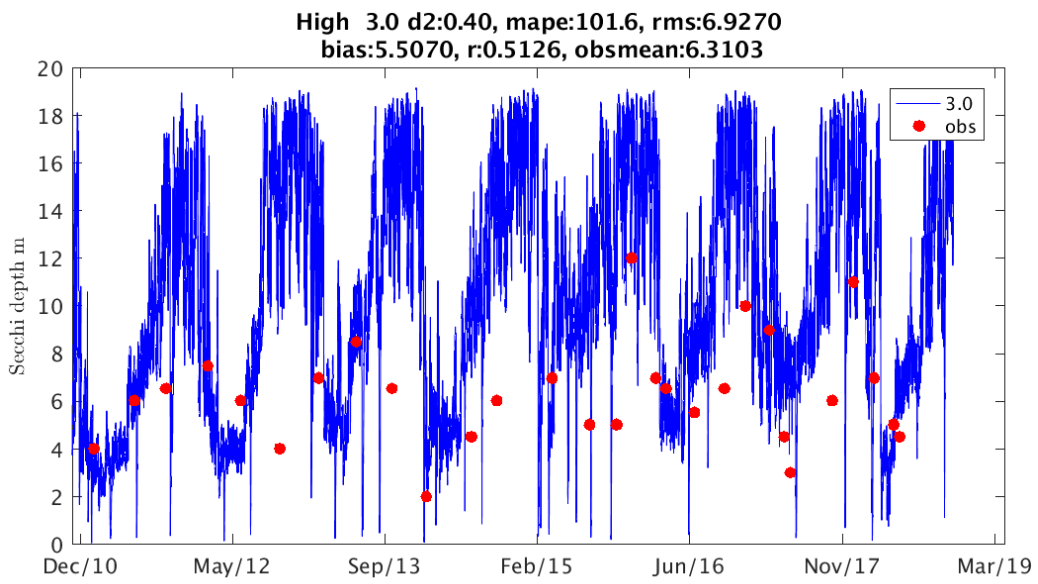
**Pandora 3.0 d2:0.34, mape:186.3, rms:8.9670  
bias:7.9574, r:0.1692, obsmean:6.4724**



**Pelorus 3.0 d2:0.44, mape:93.7, rms:7.7045  
bias:6.1435, r:0.3079, obsmean:9.0536**







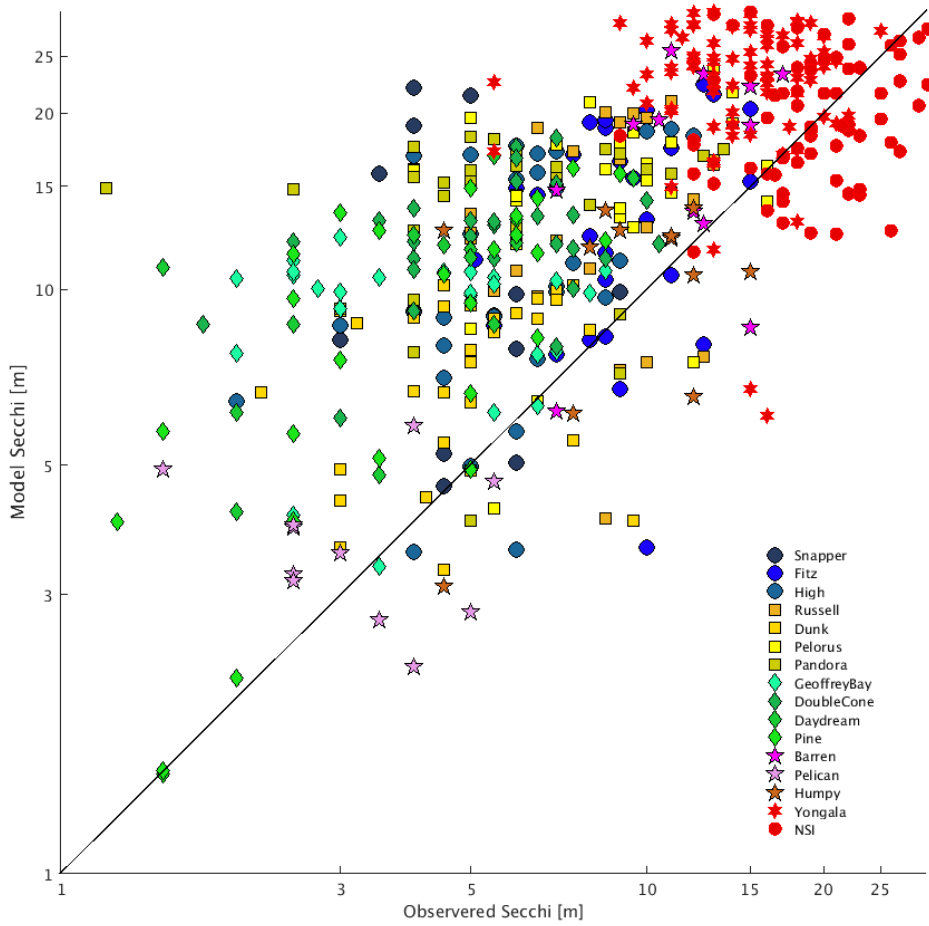


Figure 6 Scatter plot of observed Secchi for long Term Monitoring sites and NRS sites (Yongala and North Stradbroke) assessment against simulated Secchi for model version 3p0

## 12. Simulated DIP assessment against AIMS Long Term Monitoring

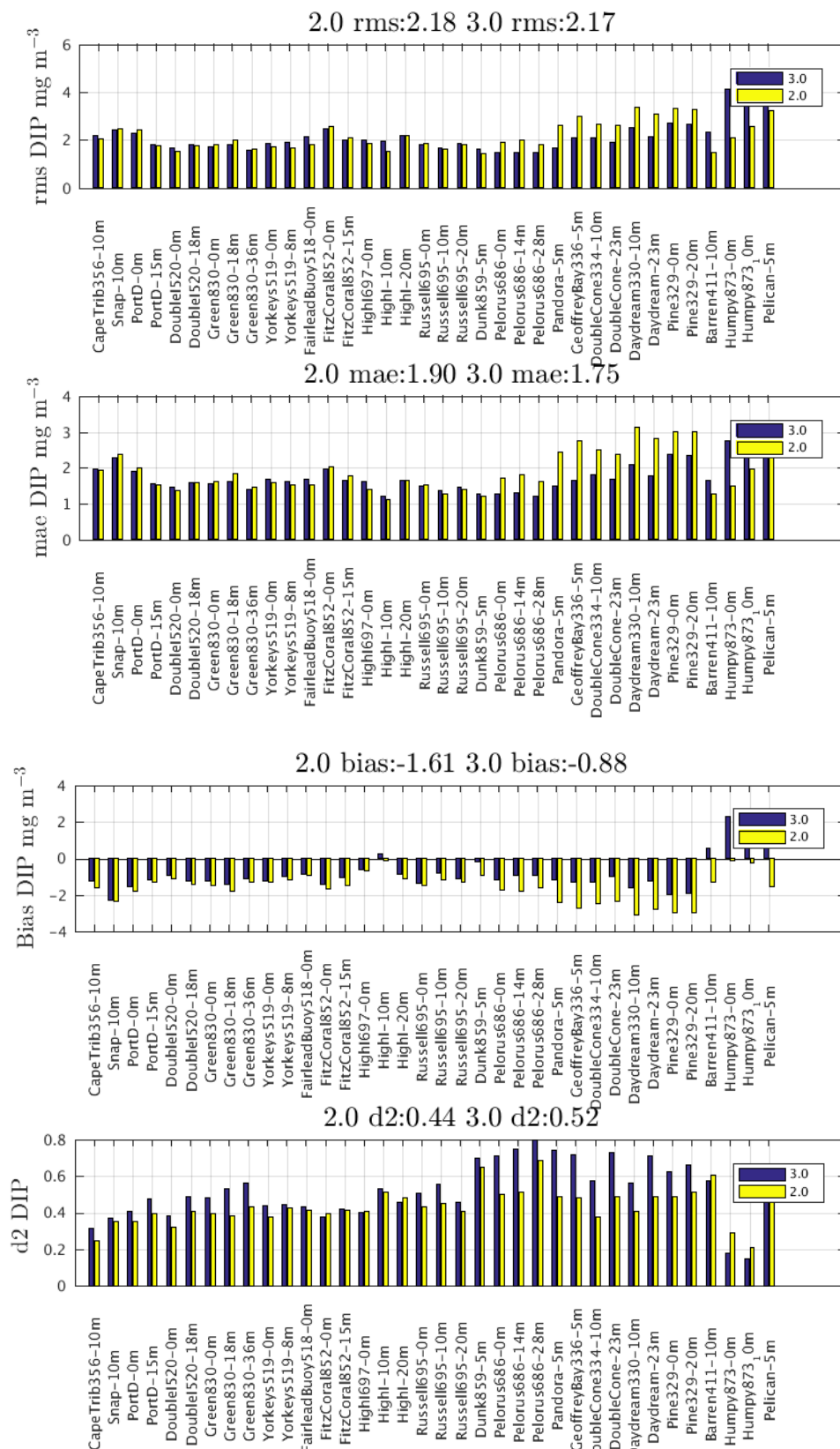
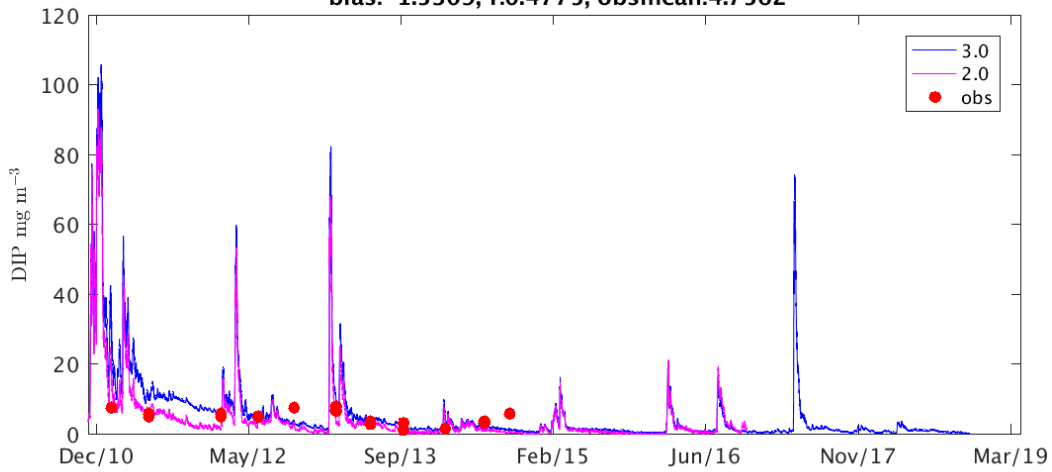
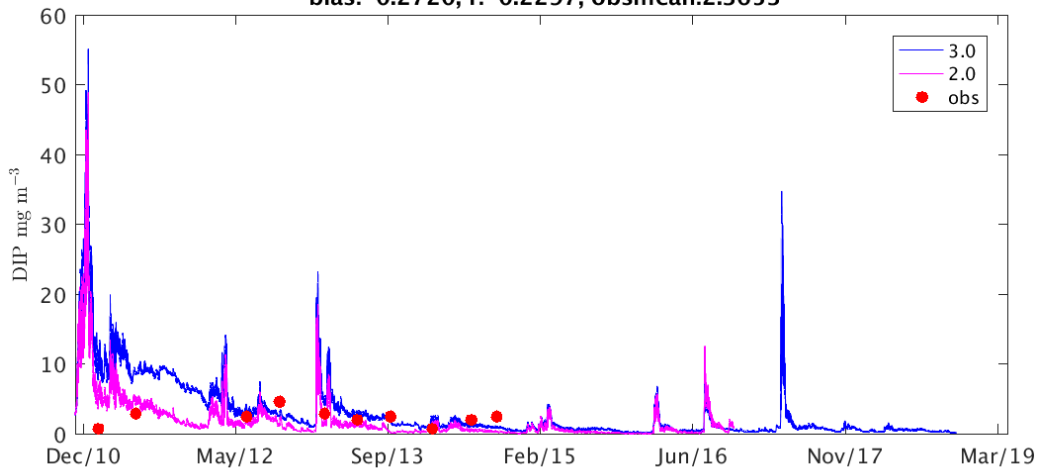


Figure 7 Metrics for Long Term Monitoring sites DIP assessment against observations for model version 3p0 and 2p0  
*d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square*

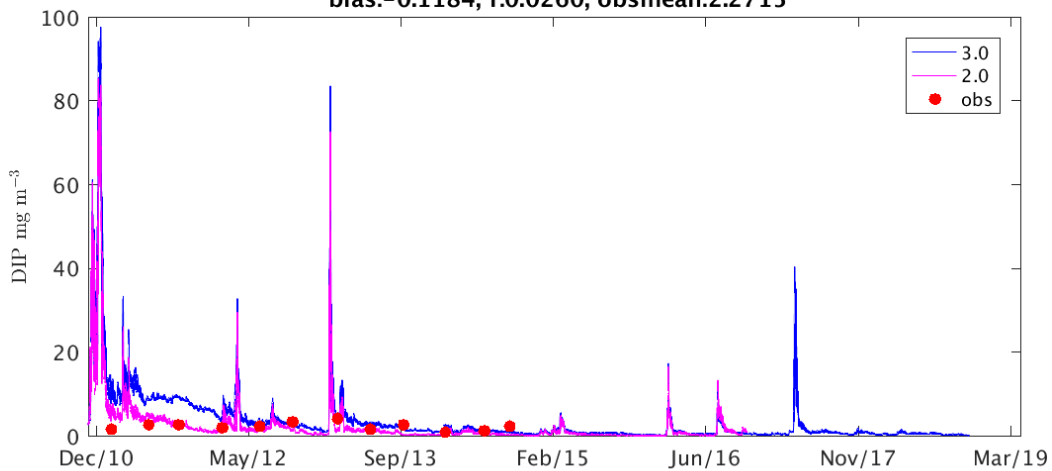
Pelican\_5m 3.0 d2:0.52, mape:60.1, rms:4.4336  
bias:0.9543, r:0.5008, obsmean:4.7562  
Pelican\_5m 2.0 d2:0.62, mape:57.9, rms:3.2174  
bias:-1.5309, r:0.4775, obsmean:4.7562



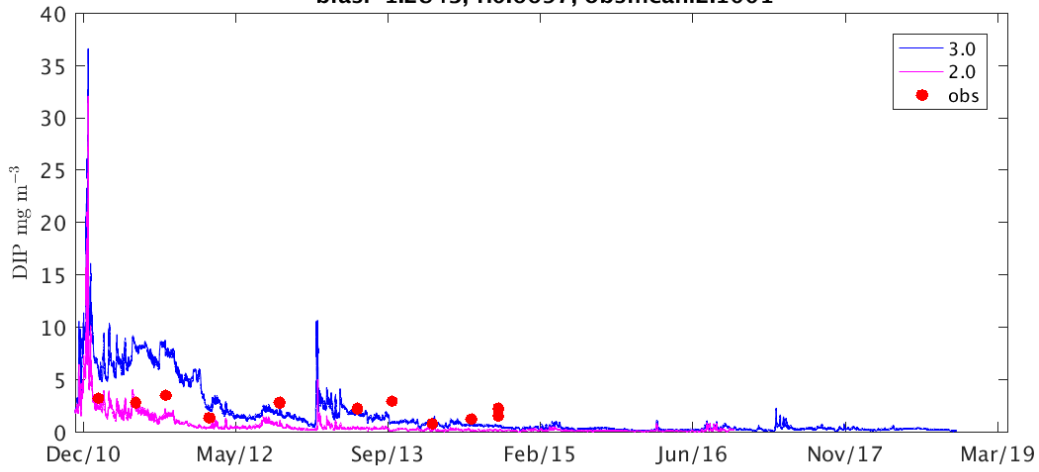
Humpy873\_10m 3.0 d2:0.15, mape:220.4, rms:4.2733  
bias:1.7741, r:-0.2305, obsmean:2.3653  
Humpy873\_10m 2.0 d2:0.20, mape:136.1, rms:2.5691  
bias:-0.2720, r:-0.2297, obsmean:2.3653



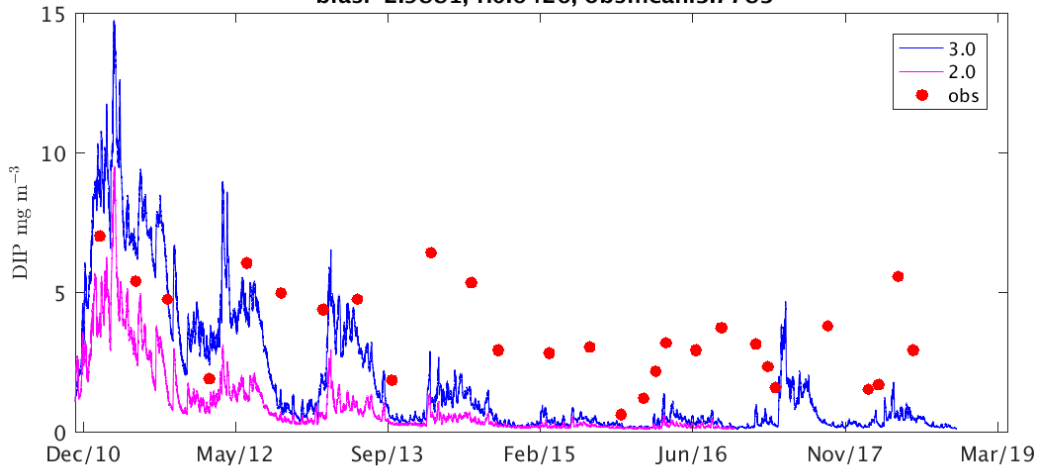
Humpy873\_0m 3.0 d2:0.18, mape:136.5, rms:4.1244  
bias:2.2803, r:0.1179, obsmean:2.2715  
Humpy873\_0m 2.0 d2:0.29, mape:68.9, rms:2.1009  
bias:-0.1184, r:0.0260, obsmean:2.2715



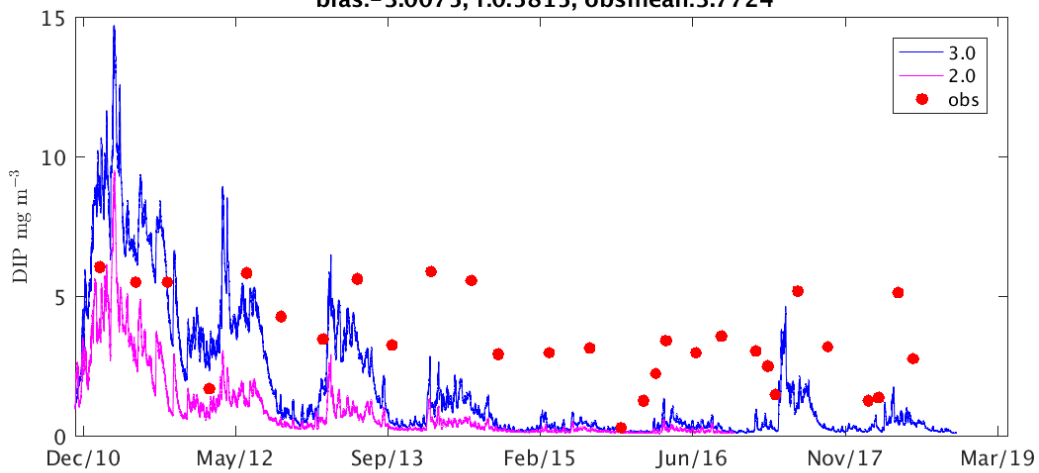
Barren411\_10m 3.0 d2:0.58, mape:67.9, rms:2.3439  
bias:0.5380, r:0.6883, obsmean:2.1001  
Barren411\_10m 2.0 d2:0.61, mape:67.6, rms:1.4913  
bias:-1.2843, r:0.6697, obsmean:2.1001



Pine329\_20m 3.0 d2:0.66, mape:71.0, rms:2.6551  
bias:-1.9380, r:0.6373, obsmean:3.5062  
Pine329\_20m 2.0 d2:0.51, mape:81.7, rms:3.2758  
bias:-2.9881, r:0.6426, obsmean:3.7783



Pine329\_0m 3.0 d2:0.63, mape:71.6, rms:2.6900  
bias:-1.9750, r:0.6078, obsmean:3.4935  
Pine329\_0m 2.0 d2:0.48, mape:80.9, rms:3.2962  
bias:-3.0075, r:0.5815, obsmean:3.7724

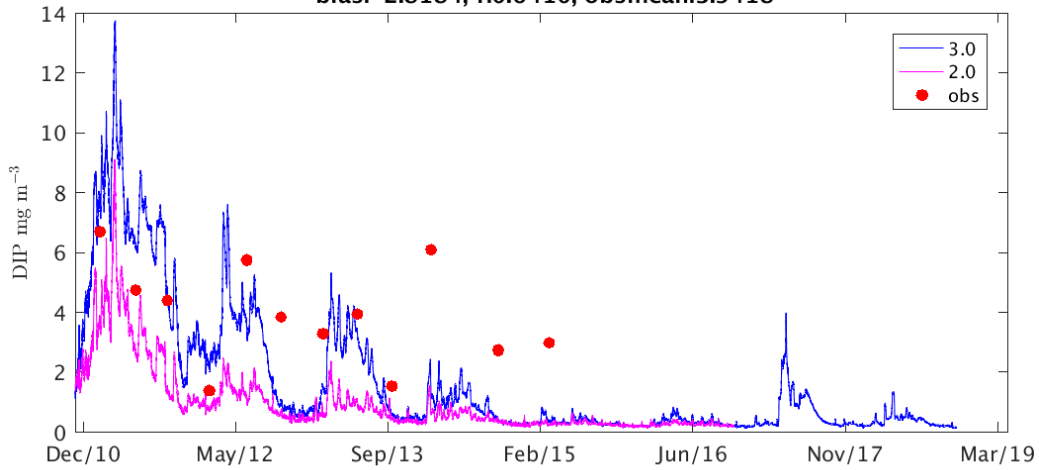


Daydream\_23m 3.0 d2:0.71, mape:49.9, rms:2.1620

bias:-1.2492, r:0.6306, obsmean:3.9418

Daydream\_23m 2.0 d2:0.49, mape:71.8, rms:3.0820

bias:-2.8184, r:0.6410, obsmean:3.9418

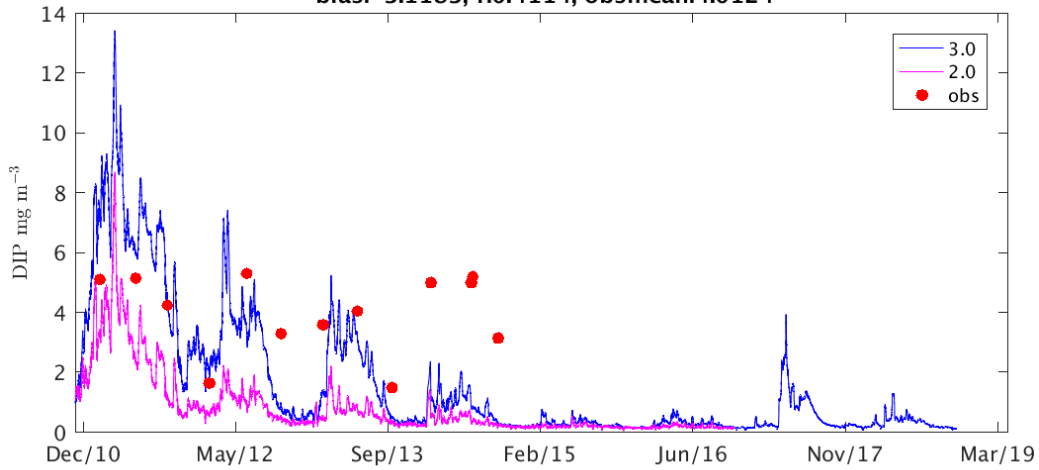


Daydream330\_10m 3.0 d2:0.56, mape:52.1, rms:2.5075

bias:-1.5843, r:0.4367, obsmean:4.0124

Daydream330\_10m 2.0 d2:0.41, mape:78.0, rms:3.3453

bias:-3.1183, r:0.4114, obsmean:4.0124

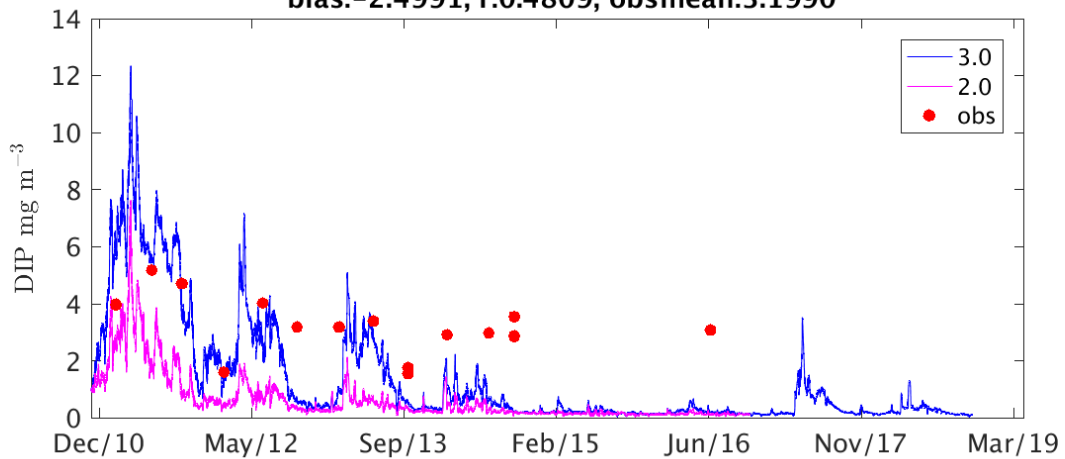


DoubleCone334\_10m 3.0 d2:0.57, mape:59.0, rms:2.0945

bias:-1.2781, r:0.6372, obsmean:3.1990

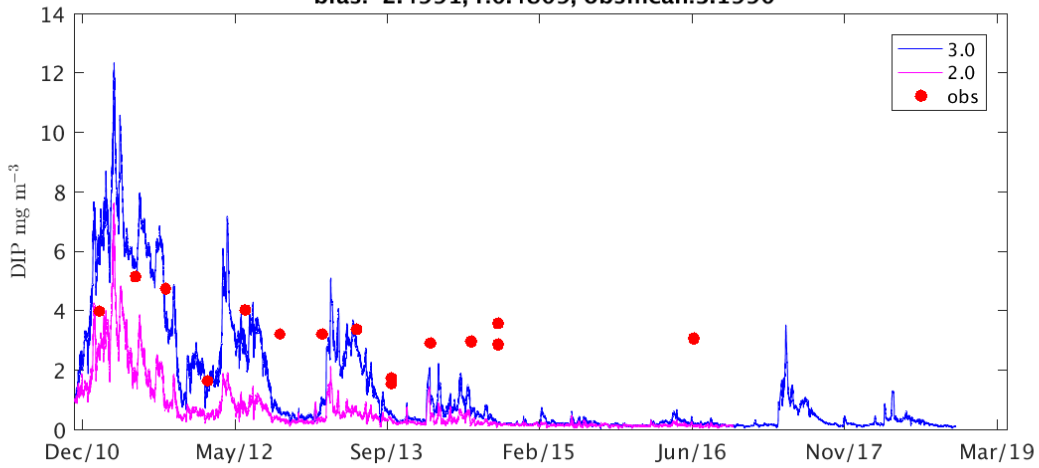
DoubleCone334\_10m 2.0 d2:0.38, mape:79.5, rms:2.6785

bias:-2.4991, r:0.4809, obsmean:3.1990

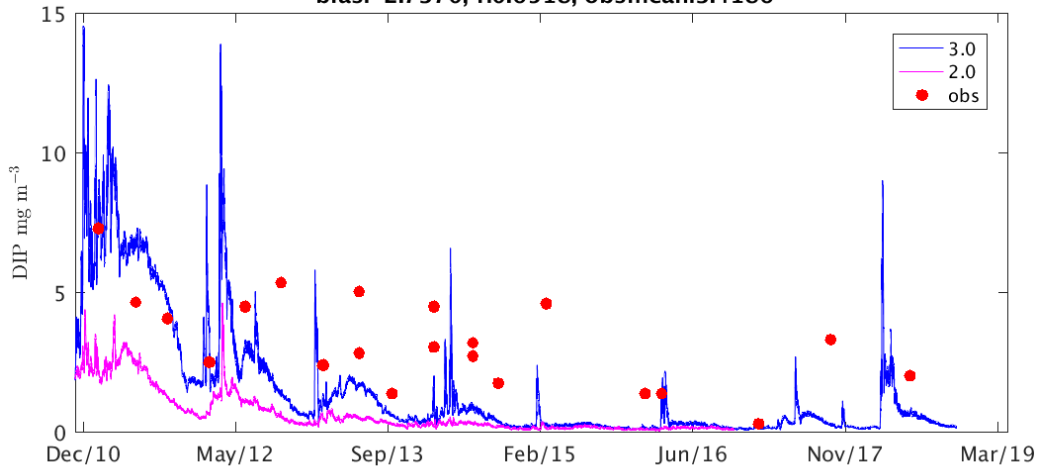




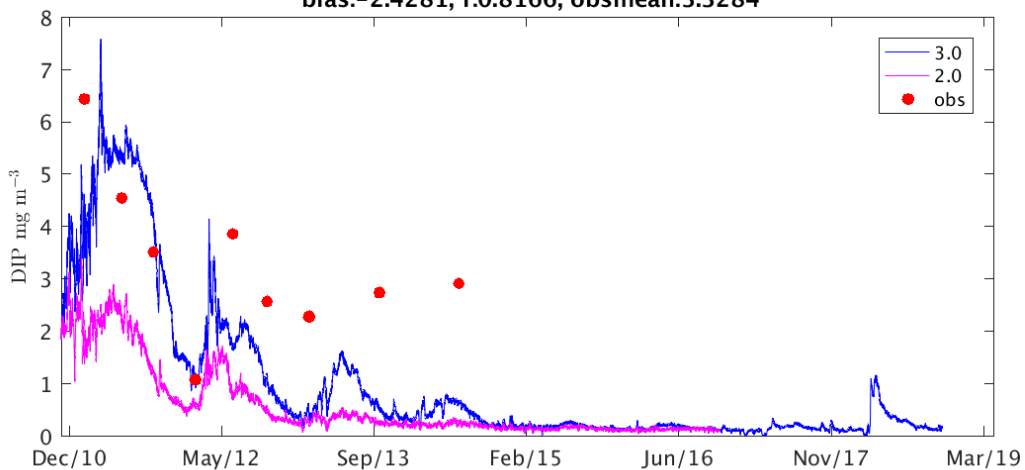
**DoubleCone334\_10m 3.0 d2:0.57, mape:59.0, rms:2.0945**  
**bias:-1.2781, r:0.6372, obsmean:3.1990**  
**DoubleCone334\_10m 2.0 d2:0.38, mape:79.5, rms:2.6785**  
**bias:-2.4991, r:0.4809, obsmean:3.1990**



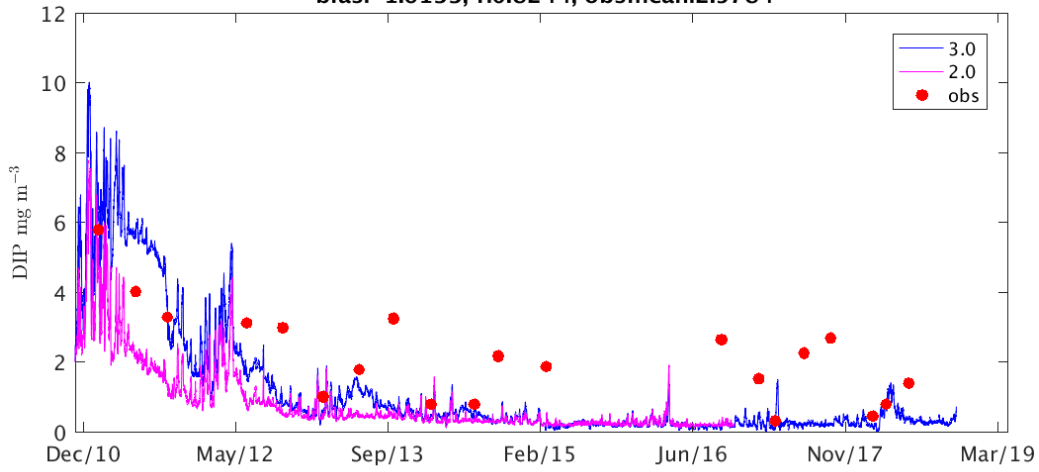
**GeoffreyBay336\_5m 3.0 d2:0.71, mape:51.1, rms:2.0757**  
**bias:-1.2867, r:0.6263, obsmean:3.2645**  
**GeoffreyBay336\_5m 2.0 d2:0.48, mape:81.8, rms:2.9963**  
**bias:-2.7370, r:0.6518, obsmean:3.4186**



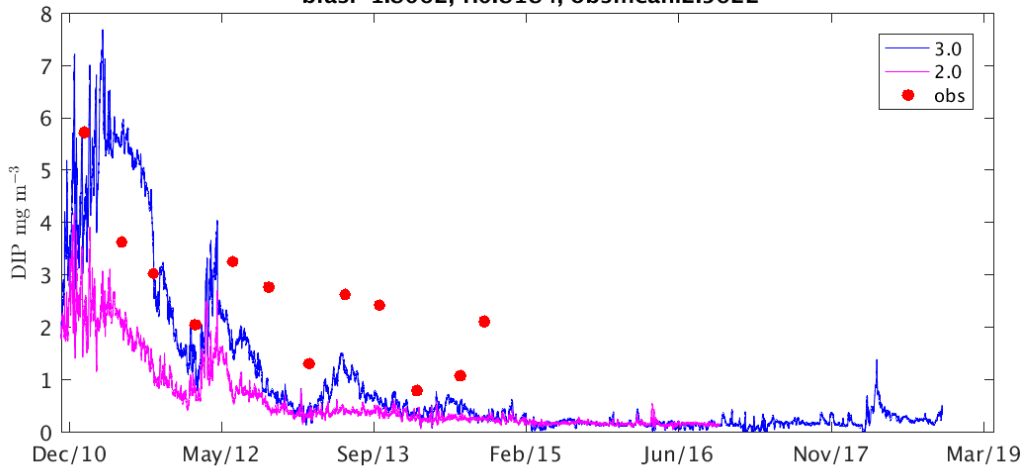
**Pandora\_5m 3.0 d2:0.74, mape:47.5, rms:1.6856**  
**bias:-1.1941, r:0.7463, obsmean:3.3284**  
**Pandora\_5m 2.0 d2:0.49, mape:73.8, rms:2.6102**  
**bias:-2.4281, r:0.8166, obsmean:3.3284**



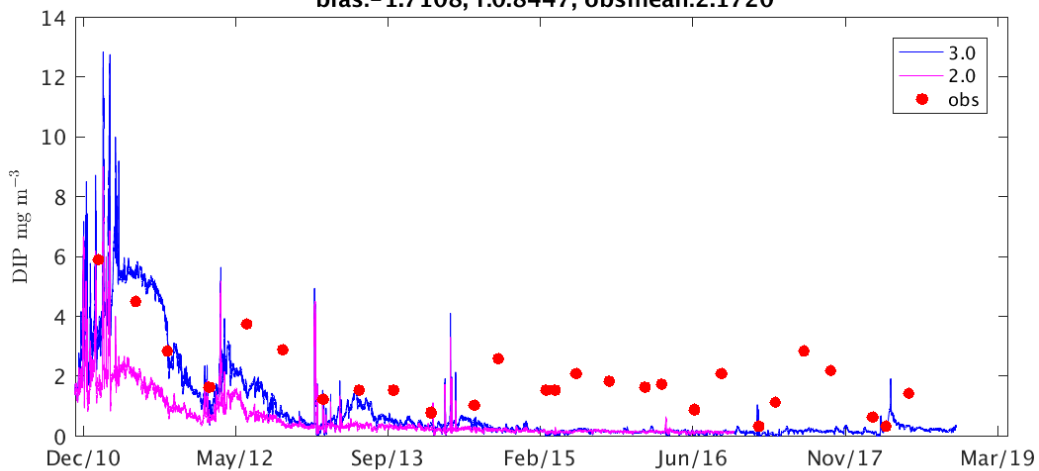
**Pelorus686\_28m 3.0 d2:0.79, mape:56.4, rms:1.4723**  
**bias:-0.9280, r:0.7673, obsmean:2.1467**  
**Pelorus686\_28m 2.0 d2:0.69, mape:66.9, rms:1.7906**  
**bias:-1.6133, r:0.8244, obsmean:2.5784**



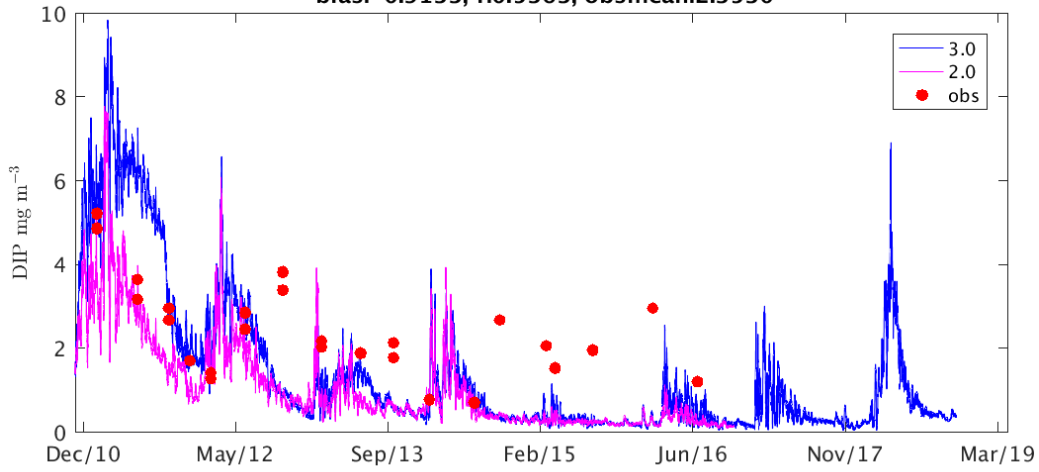
**Pelorus686\_14m 3.0 d2:0.75, mape:54.8, rms:1.4622**  
**bias:-0.9590, r:0.7311, obsmean:2.5622**  
**Pelorus686\_14m 2.0 d2:0.51, mape:72.0, rms:1.9891**  
**bias:-1.8062, r:0.8184, obsmean:2.5622**



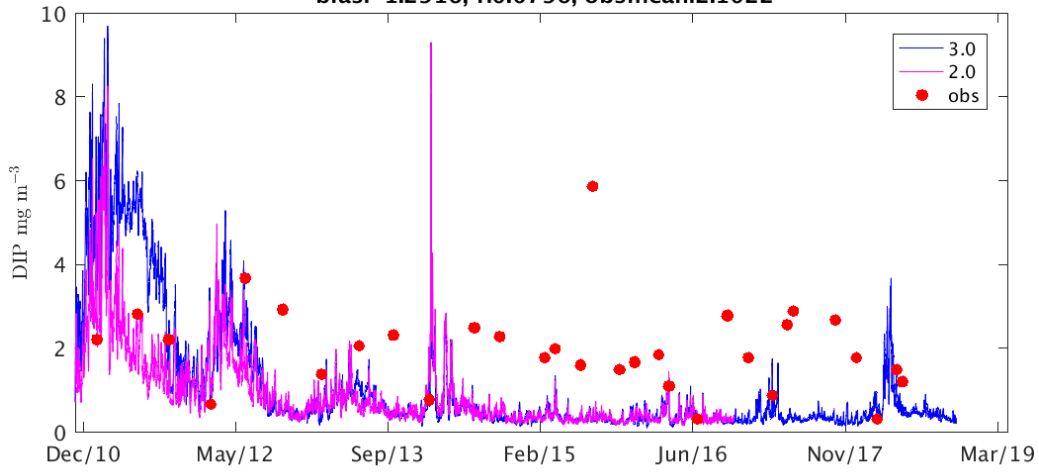
**Pelorus686\_0m 3.0 d2:0.71, mape:72.1, rms:1.4860**  
**bias:-1.1856, r:0.7430, obsmean:1.9342**  
**Pelorus686\_0m 2.0 d2:0.50, mape:81.2, rms:1.9110**  
**bias:-1.7108, r:0.8447, obsmean:2.1720**



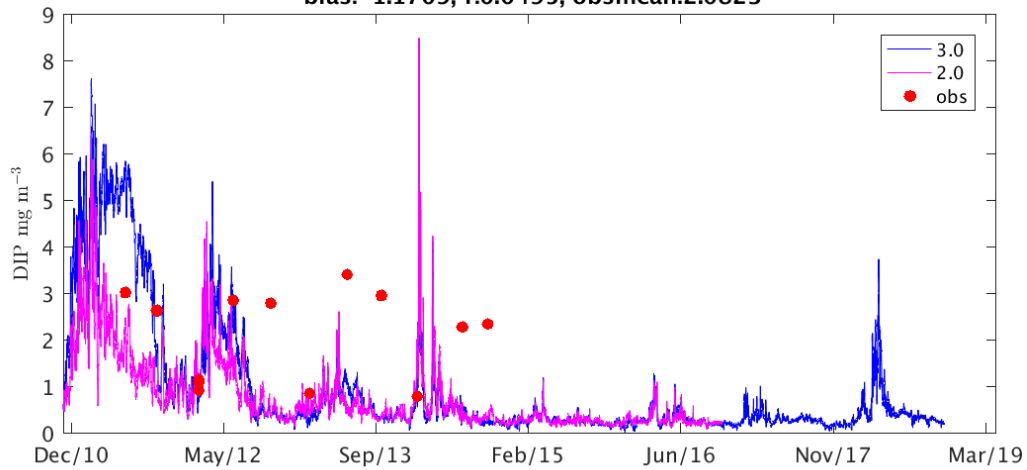
Dunk859\_5m 3.0 d2:0.70, mape:57.6, rms:1.6308  
bias:-0.1835, r:0.5943, obsmean:2.3530  
Dunk859\_5m 2.0 d2:0.65, mape:56.3, rms:1.4147  
bias:-0.9133, r:0.5363, obsmean:2.3530



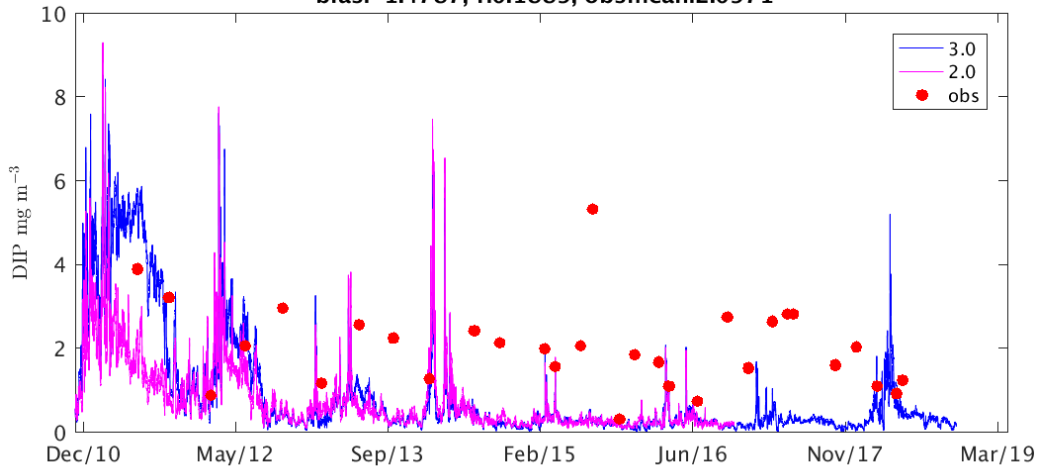
Russell695\_20m 3.0 d2:0.46, mape:64.6, rms:1.8396  
bias:-1.0928, r:0.1808, obsmean:1.9928  
Russell695\_20m 2.0 d2:0.40, mape:62.9, rms:1.8190  
bias:-1.2916, r:0.0796, obsmean:2.1022



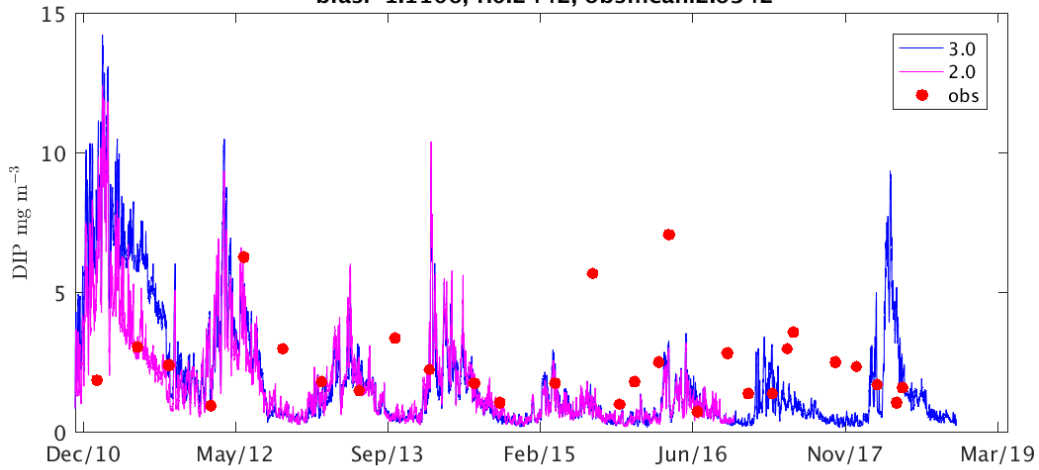
Russell695\_10m 3.0 d2:0.56, mape:62.3, rms:1.6678  
bias:-0.8214, r:0.3468, obsmean:2.0823  
Russell695\_10m 2.0 d2:0.45, mape:56.8, rms:1.5992  
bias:-1.1709, r:0.0495, obsmean:2.0823



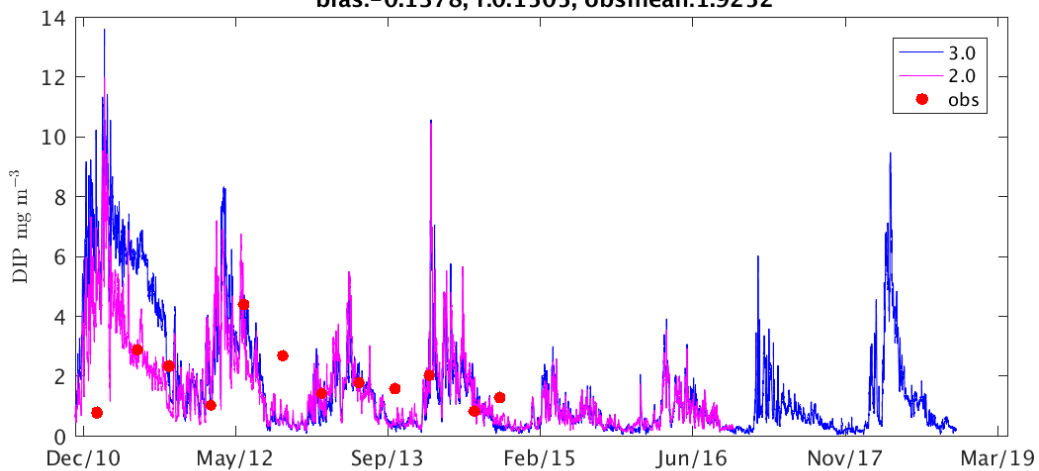
Russell695\_0m 3.0 d2:0.50, mape:69.6, rms:1.8138  
bias:-1.3396, r:0.3225, obsmean:2.0215  
Russell695\_0m 2.0 d2:0.43, mape:67.5, rms:1.8771  
bias:-1.4787, r:0.1889, obsmean:2.0971



Highl\_20m 3.0 d2:0.46, mape:67.9, rms:2.1781  
bias:-0.8446, r:0.1746, obsmean:2.4529  
Highl\_20m 2.0 d2:0.48, mape:59.6, rms:2.1851  
bias:-1.1106, r:0.2442, obsmean:2.6342



Highl\_10m 3.0 d2:0.53, mape:95.9, rms:1.9546  
bias:0.2291, r:0.2843, obsmean:1.9252  
Highl\_10m 2.0 d2:0.51, mape:85.6, rms:1.5082  
bias:-0.1378, r:0.1505, obsmean:1.9252

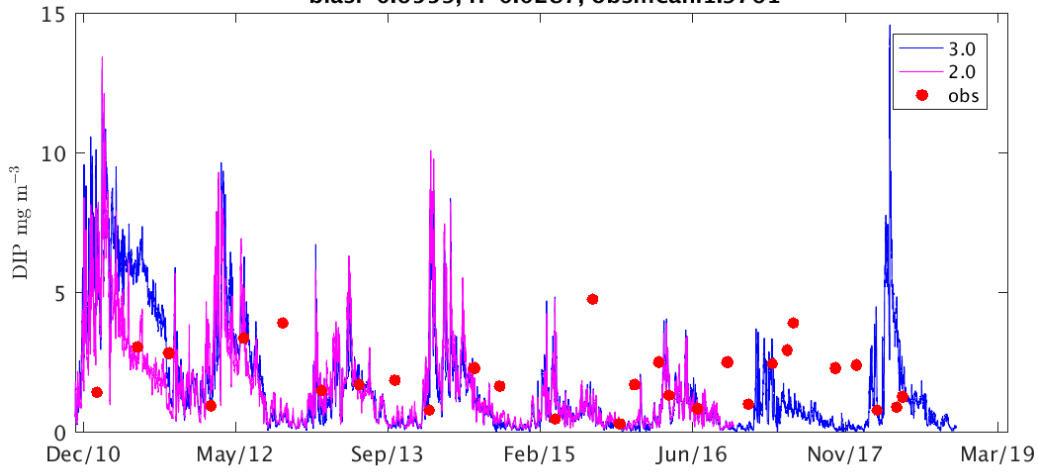


High697\_0m 3.0 d2:0.40, mape:84.1, rms:2.0173

bias:-0.6394, r:0.0219, obsmean:1.9810

High697\_0m 2.0 d2:0.40, mape:75.5, rms:1.8426

bias:-0.6559, r:-0.0287, obsmean:1.9761

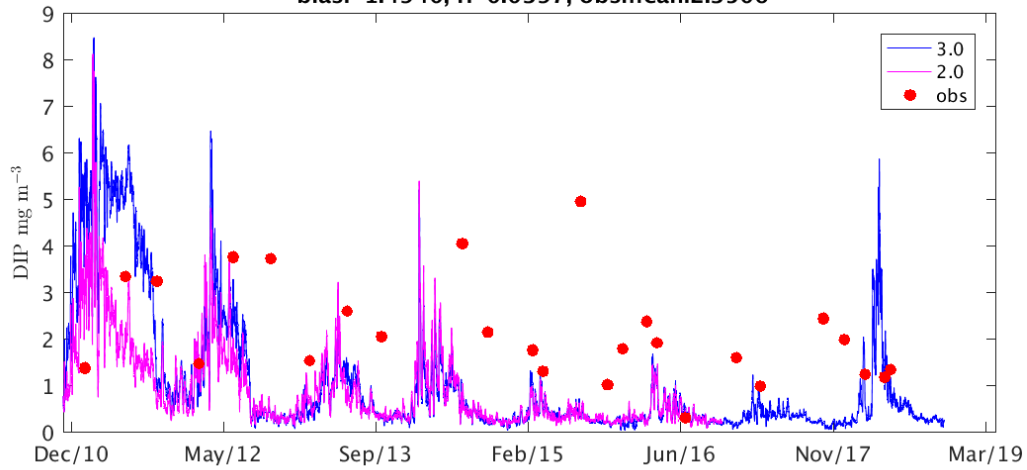


FitzCoral852\_15m 3.0 d2:0.42, mape:76.2, rms:2.0131

bias:-1.0795, r:0.0756, obsmean:2.1317

FitzCoral852\_15m 2.0 d2:0.41, mape:72.4, rms:2.1002

bias:-1.4940, r:-0.0397, obsmean:2.3506

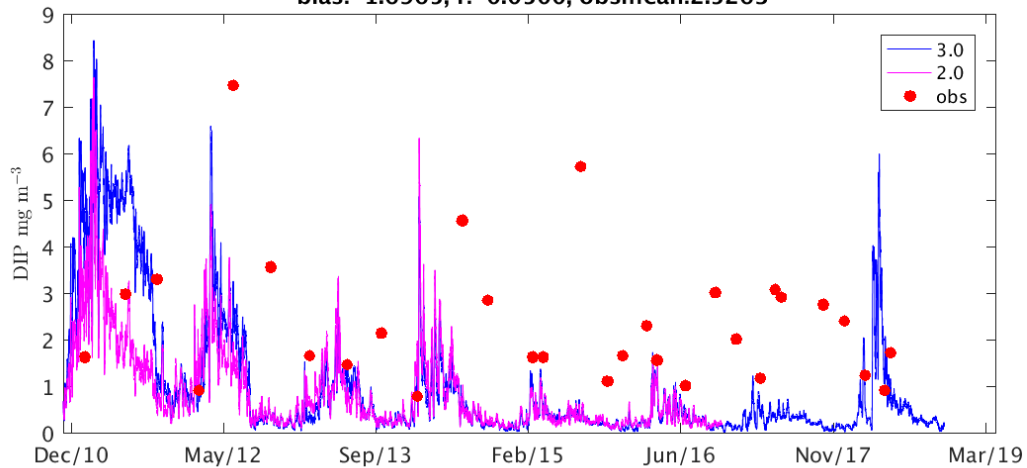


FitzCoral852\_0m 3.0 d2:0.37, mape:79.3, rms:2.4476

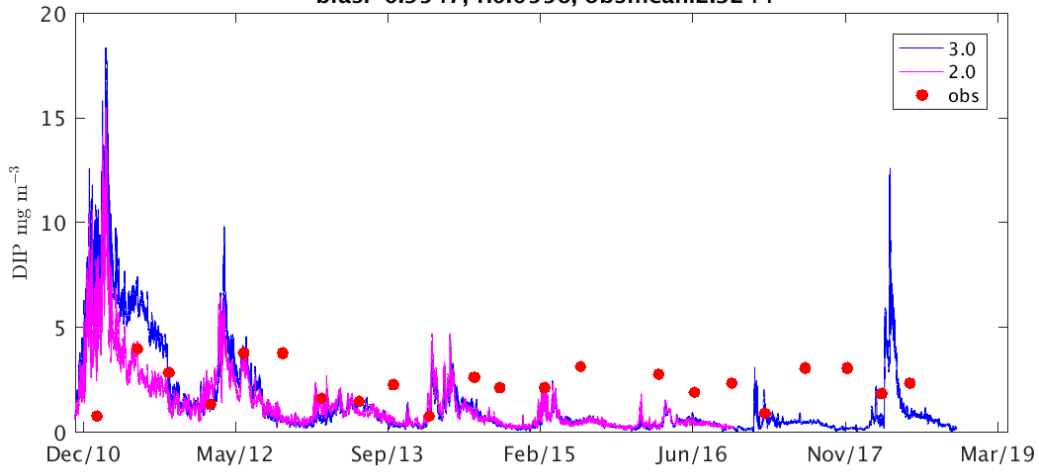
bias:-1.4403, r:0.0394, obsmean:2.3769

FitzCoral852\_0m 2.0 d2:0.39, mape:76.0, rms:2.5651

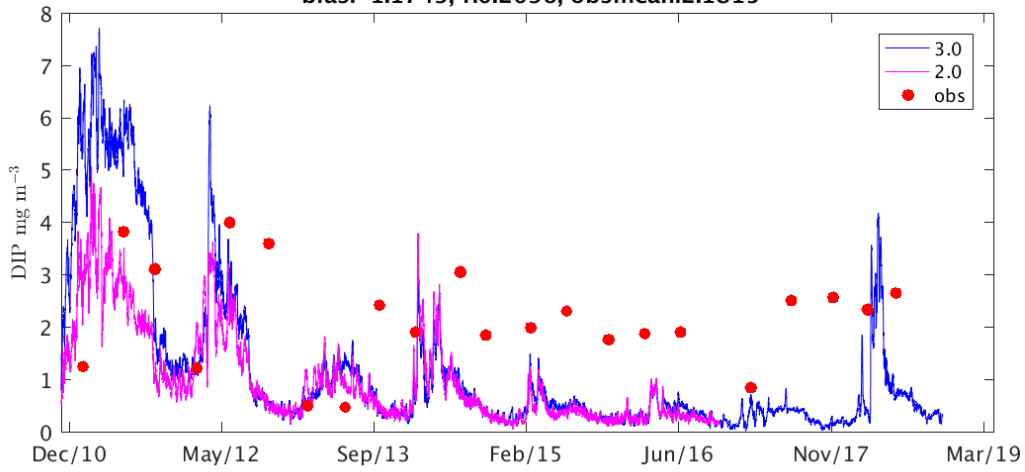
bias:-1.6965, r:-0.0500, obsmean:2.5263



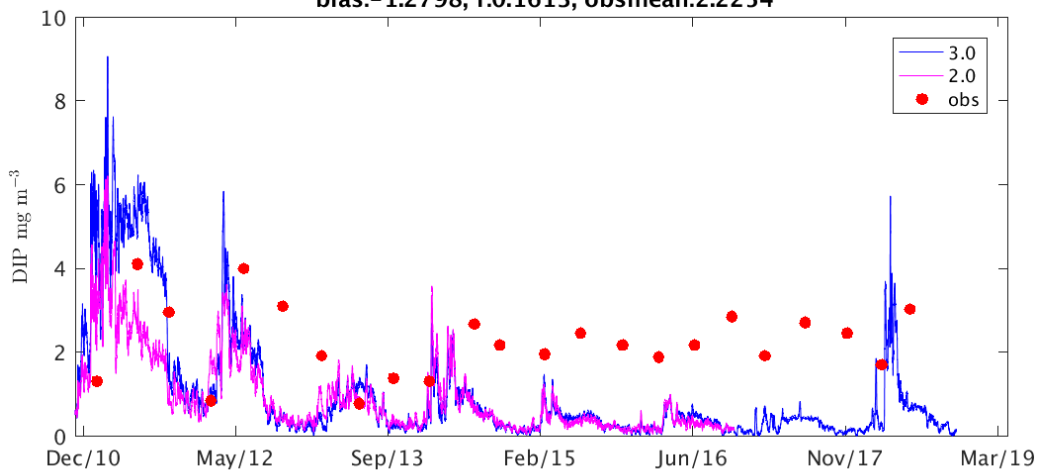
FairleadBuoy518\_0m 3.0 d2:0.43, mape:88.5, rms:2.1537  
 bias:-0.8519, r:0.1135, obsmean:2.3035  
 FairleadBuoy518\_0m 2.0 d2:0.42, mape:82.8, rms:1.7984  
 bias:-0.9547, r:0.0556, obsmean:2.3244



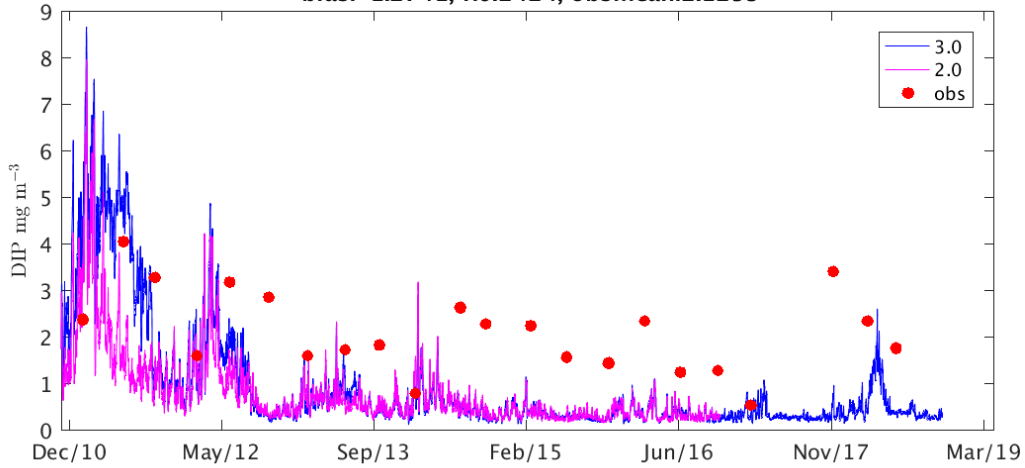
Yorkeys519\_8m 3.0 d2:0.44, mape:82.3, rms:1.9025  
 bias:-0.9954, r:0.1730, obsmean:2.1810  
 Yorkeys519\_8m 2.0 d2:0.43, mape:75.1, rms:1.6567  
 bias:-1.1749, r:0.2096, obsmean:2.1815



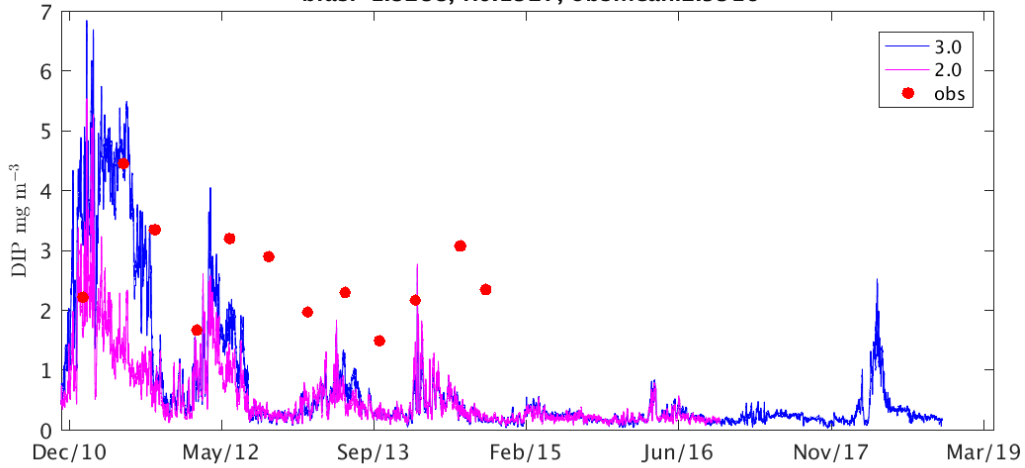
Yorkeys519\_0m 3.0 d2:0.44, mape:79.9, rms:1.8592  
 bias:-1.2355, r:0.2365, obsmean:2.2547  
 Yorkeys519\_0m 2.0 d2:0.37, mape:73.2, rms:1.7175  
 bias:-1.2798, r:0.1613, obsmean:2.2254



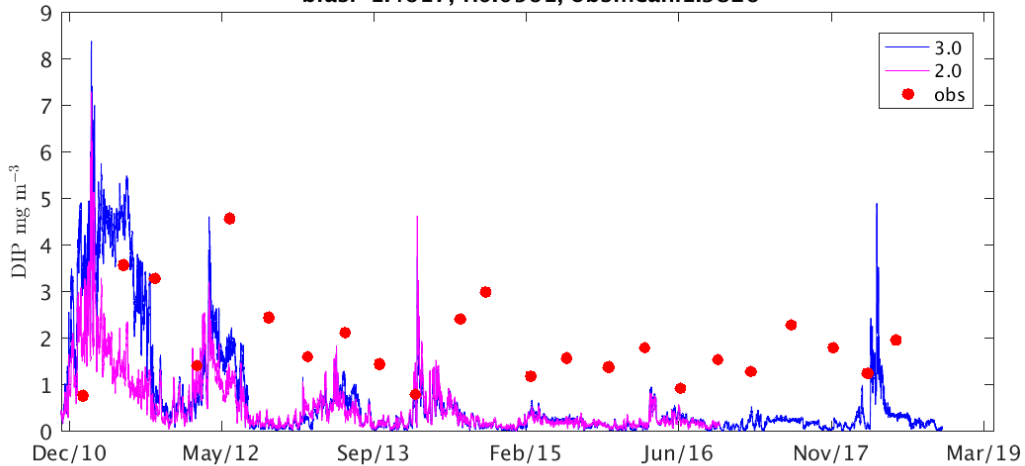
**Green830\_36m 3.0 d2:0.56, mape:65.1, rms:1.5962**  
**bias:-1.1311, r:0.4758, obsmean:2.1052**  
**Green830\_36m 2.0 d2:0.43, mape:69.4, rms:1.6013**  
**bias:-1.2741, r:0.2424, obsmean:2.1259**



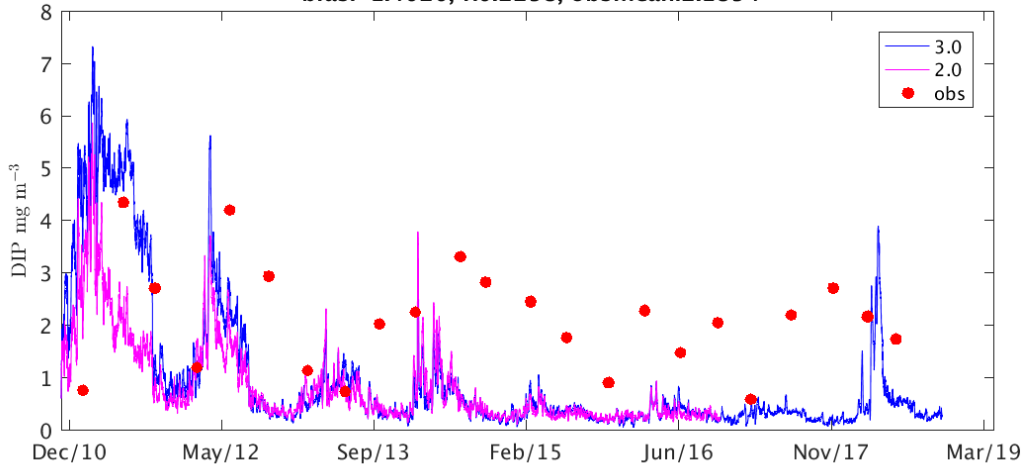
**Green830\_18m 3.0 d2:0.53, mape:66.2, rms:1.8024**  
**bias:-1.4328, r:0.5535, obsmean:2.5916**  
**Green830\_18m 2.0 d2:0.38, mape:68.8, rms:2.0202**  
**bias:-1.8288, r:0.1927, obsmean:2.5916**



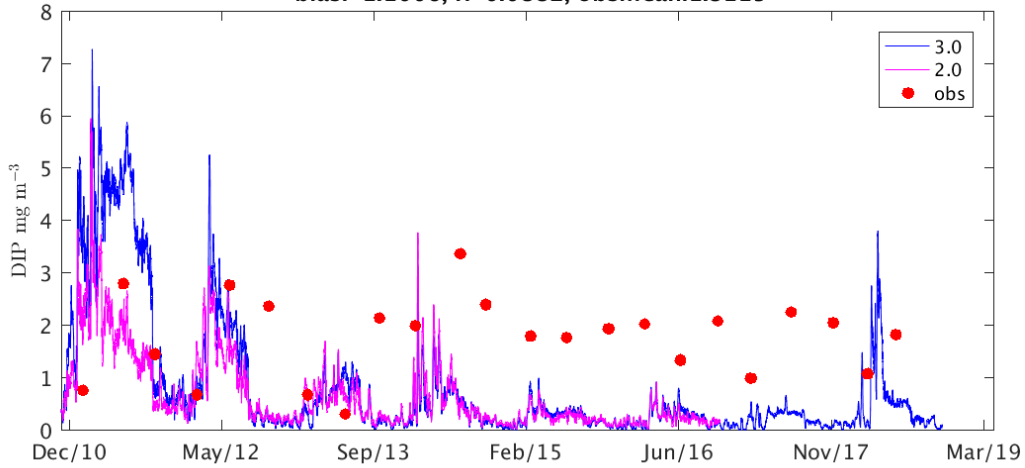
**Green830\_0m 3.0 d2:0.48, mape:87.5, rms:1.7146**  
**bias:-1.2327, r:0.2975, obsmean:1.9229**  
**Green830\_0m 2.0 d2:0.39, mape:81.9, rms:1.8257**  
**bias:-1.4617, r:0.0561, obsmean:1.9826**



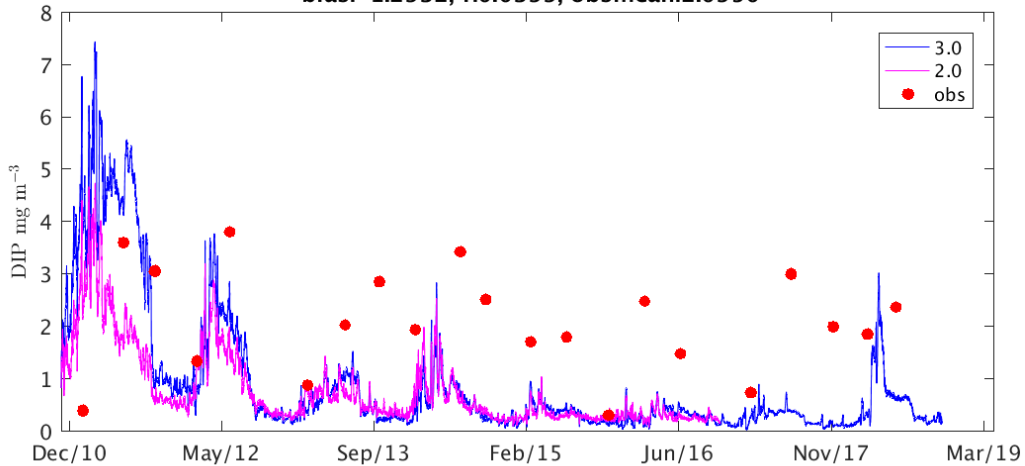
**DoubleI520\_18m 3.0 d2:0.49, mape:83.0, rms:1.7888**  
**bias:-1.2322, r:0.2824, obsmean:2.1176**  
**DoubleI520\_18m 2.0 d2:0.41, mape:72.2, rms:1.7771**  
**bias:-1.4020, r:0.2258, obsmean:2.1854**



**DoubleI520\_0m 3.0 d2:0.38, mape:96.1, rms:1.6505**  
**bias:-0.9586, r:0.0324, obsmean:1.7727**  
**DoubleI520\_0m 2.0 d2:0.32, mape:79.7, rms:1.5164**  
**bias:-1.1006, r:-0.0882, obsmean:1.8115**



**PortD\_15m 3.0 d2:0.48, mape:108.5, rms:1.7973**  
**bias:-1.1596, r:0.1849, obsmean:2.0684**  
**PortD\_15m 2.0 d2:0.39, mape:88.4, rms:1.7539**  
**bias:-1.2932, r:0.0399, obsmean:2.0950**



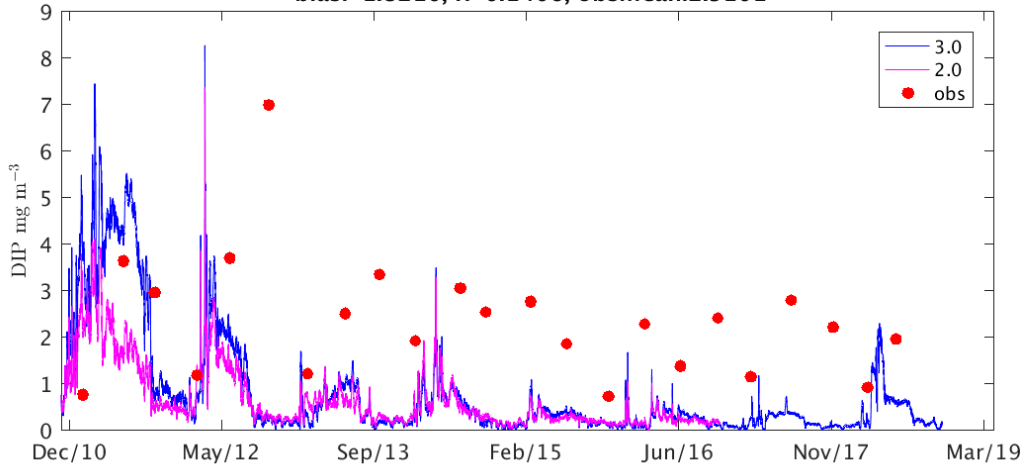


PortD\_0m 3.0 d2:0.41, mape:89.7, rms:2.2945

bias:-1.5586, r:0.0518, obsmean:2.3577

PortD\_0m 2.0 d2:0.35, mape:80.9, rms:2.4268

bias:-1.8210, r:-0.1406, obsmean:2.5101

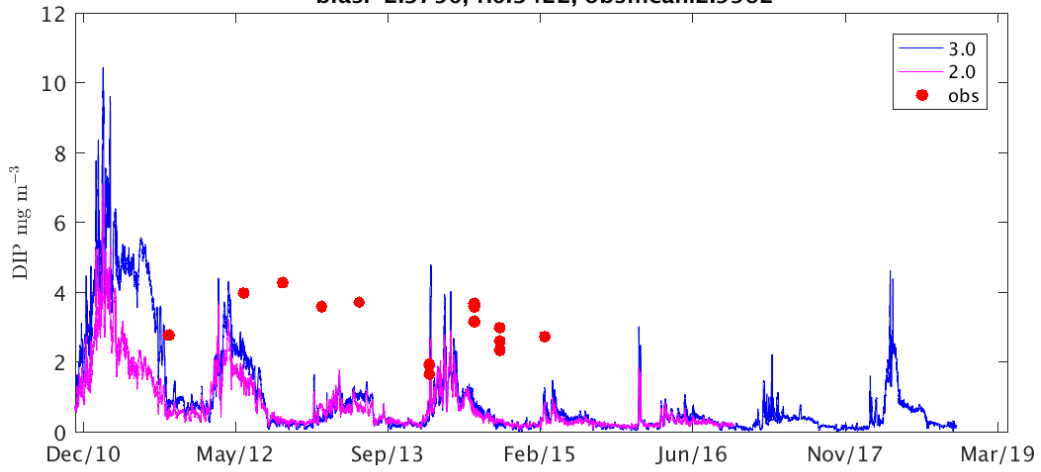


Snap\_10m 3.0 d2:0.37, mape:76.4, rms:2.4100

bias:-2.2861, r:0.3779, obsmean:2.9962

Snap\_10m 2.0 d2:0.35, mape:78.5, rms:2.4860

bias:-2.3750, r:0.3422, obsmean:2.9962



### 13. Simulated NOx assessment against AIMS Long Term Monitoring

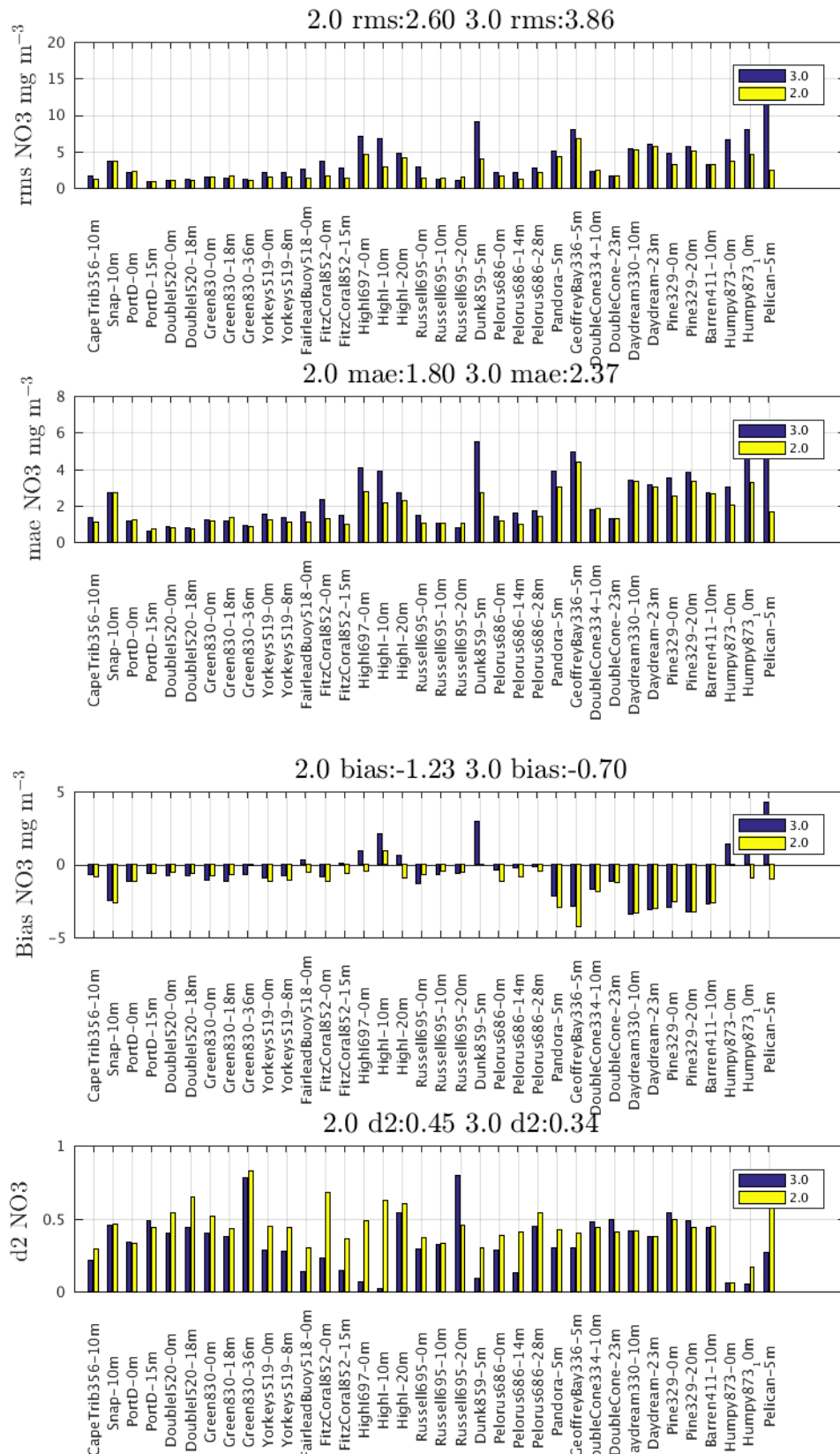
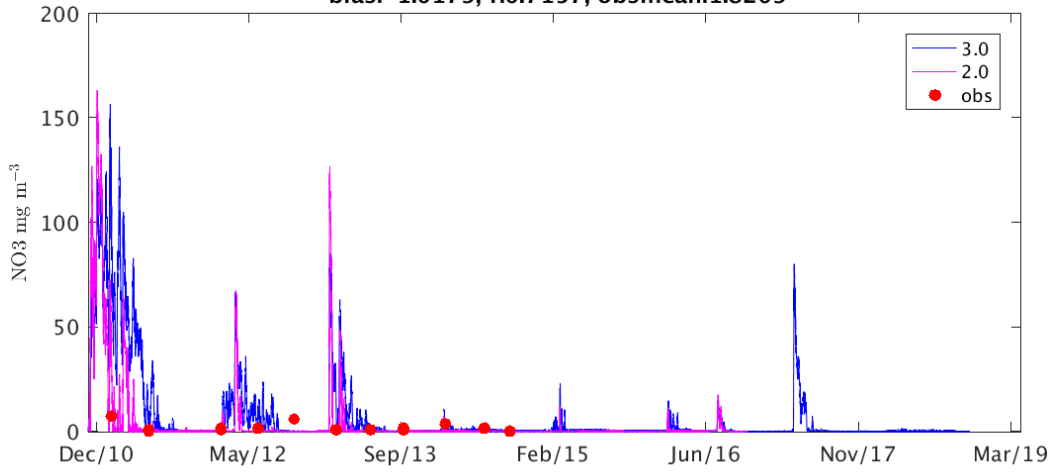
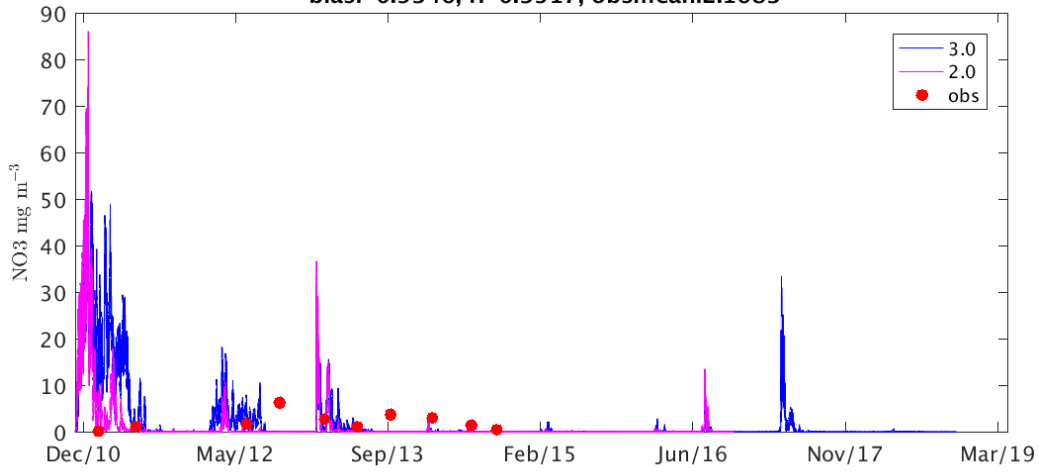


Figure 8 Metrics for Long Term Monitoring sites NO<sub>3</sub> assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

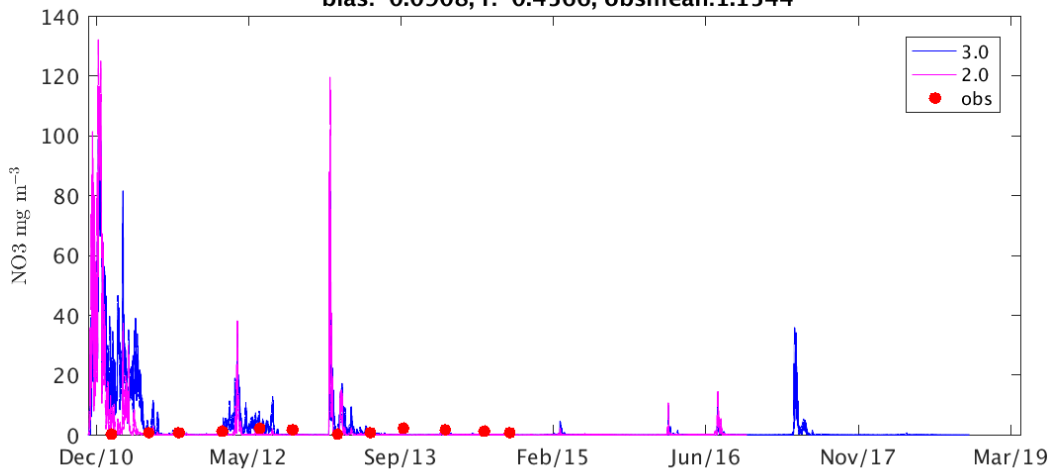
Pelican\_5m 3.0 d2:0.27, mape:463.2, rms:15.8783  
 bias:4.2269, r:0.6679, obsmean:1.8209  
 Pelican\_5m 2.0 d2:0.78, mape:91.0, rms:2.3327  
 bias:-1.0179, r:0.7157, obsmean:1.8209



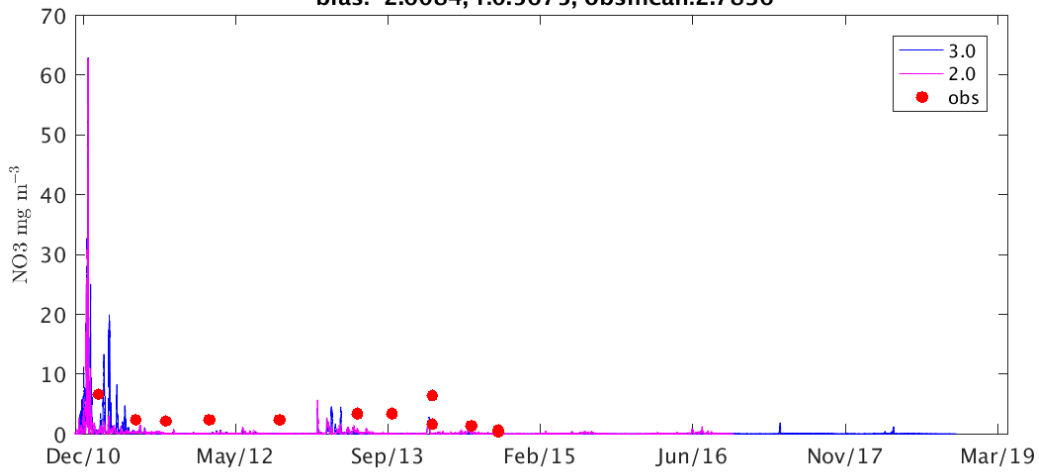
Humpy873\_10m 3.0 d2:0.05, mape:1749.5, rms:7.9106  
 bias:0.9358, r:-0.4230, obsmean:2.1683  
 Humpy873\_10m 2.0 d2:0.17, mape:906.1, rms:4.5475  
 bias:-0.9346, r:-0.3917, obsmean:2.1683



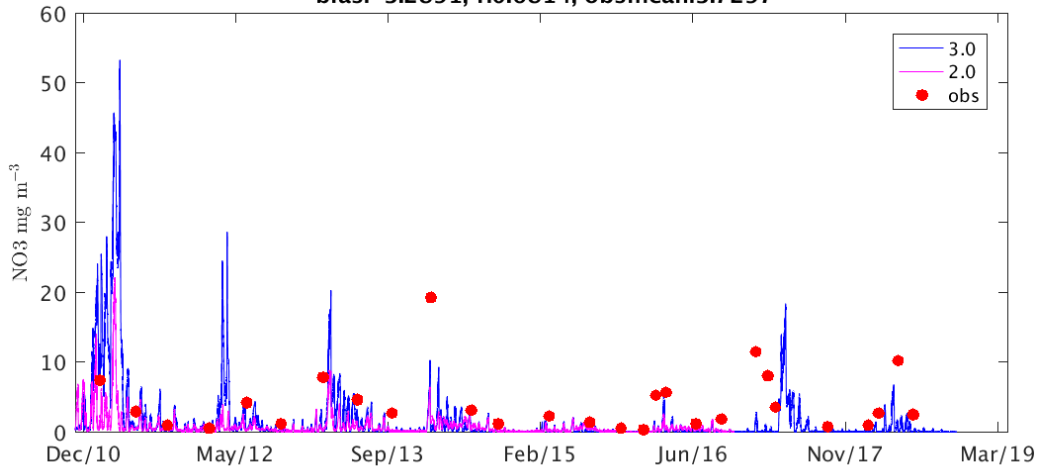
Humpy873\_0m 3.0 d2:0.06, mape:1394.5, rms:6.5672  
 bias:1.3937, r:-0.2983, obsmean:1.1544  
 Humpy873\_0m 2.0 d2:0.06, mape:768.7, rms:3.5890  
 bias:-0.0908, r:-0.4566, obsmean:1.1544



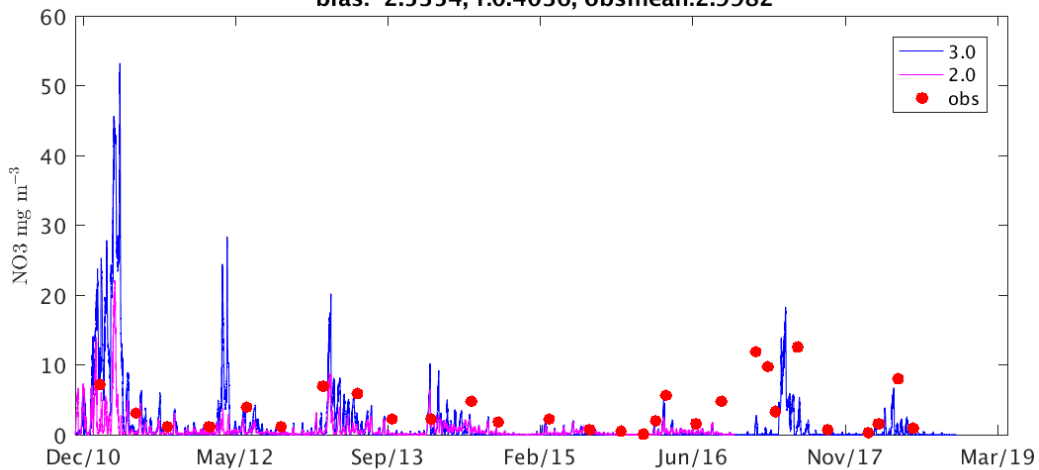
Barren411\_10m 3.0 d2:0.44, mape:96.7, rms:3.2380  
bias:-2.6796, r:0.5995, obsmean:2.7836  
Barren411\_10m 2.0 d2:0.45, mape:94.2, rms:3.1538  
bias:-2.6084, r:0.5675, obsmean:2.7836



Pine329\_20m 3.0 d2:0.49, mape:87.2, rms:5.6015  
bias:-3.2316, r:0.2042, obsmean:4.1014  
Pine329\_20m 2.0 d2:0.44, mape:85.1, rms:5.0701  
bias:-3.2891, r:0.6814, obsmean:3.7297



Pine329\_0m 3.0 d2:0.54, mape:91.2, rms:4.7214  
bias:-2.9330, r:0.3001, obsmean:3.7608  
Pine329\_0m 2.0 d2:0.49, mape:78.8, rms:3.2404  
bias:-2.5354, r:0.4036, obsmean:2.9982

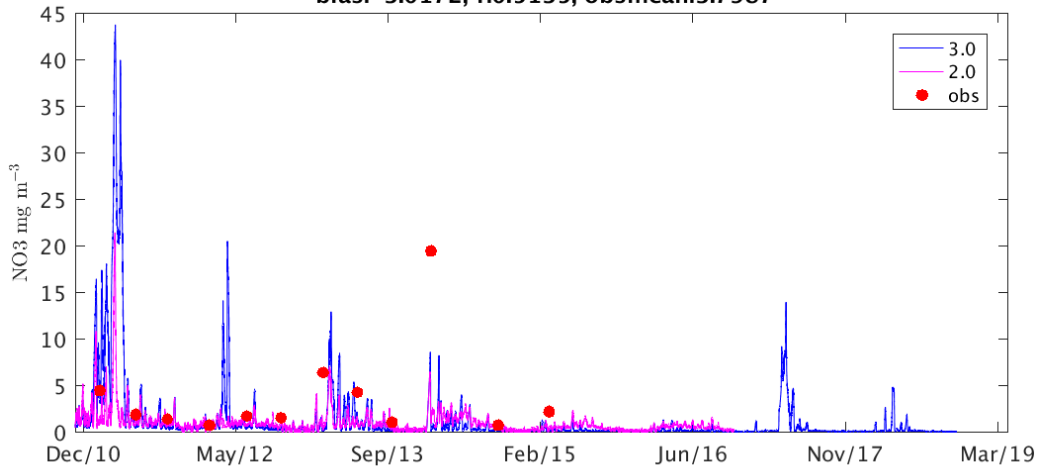


**Daydream\_23m 3.0 d2:0.38, mape:70.0, rms:5.9701**

**bias:-3.1180, r:-0.0331, obsmean:3.7987**

**Daydream\_23m 2.0 d2:0.38, mape:56.5, rms:5.7215**

**bias:-3.0172, r:0.5135, obsmean:3.7987**

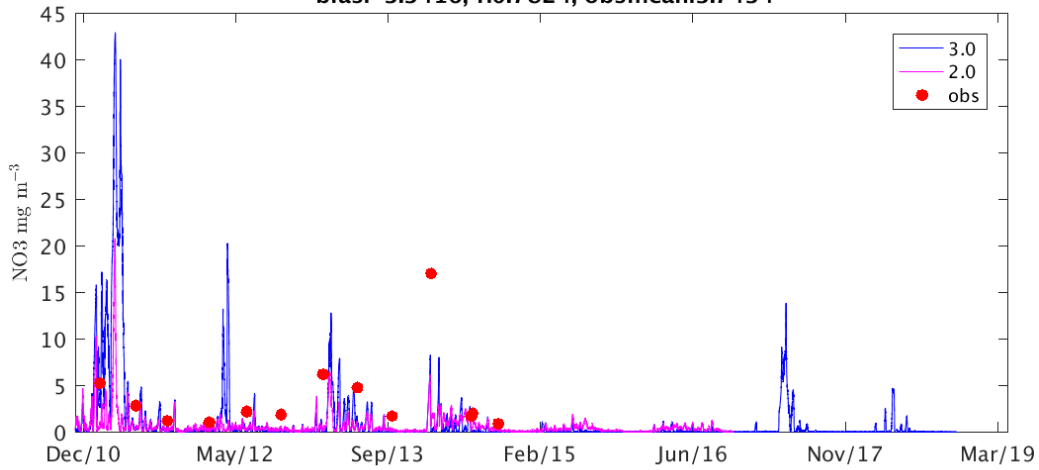


**Daydream330\_10m 3.0 d2:0.41, mape:88.8, rms:5.3704**

**bias:-3.3853, r:0.0920, obsmean:3.7434**

**Daydream330\_10m 2.0 d2:0.41, mape:83.4, rms:5.2331**

**bias:-3.3416, r:0.7824, obsmean:3.7434**

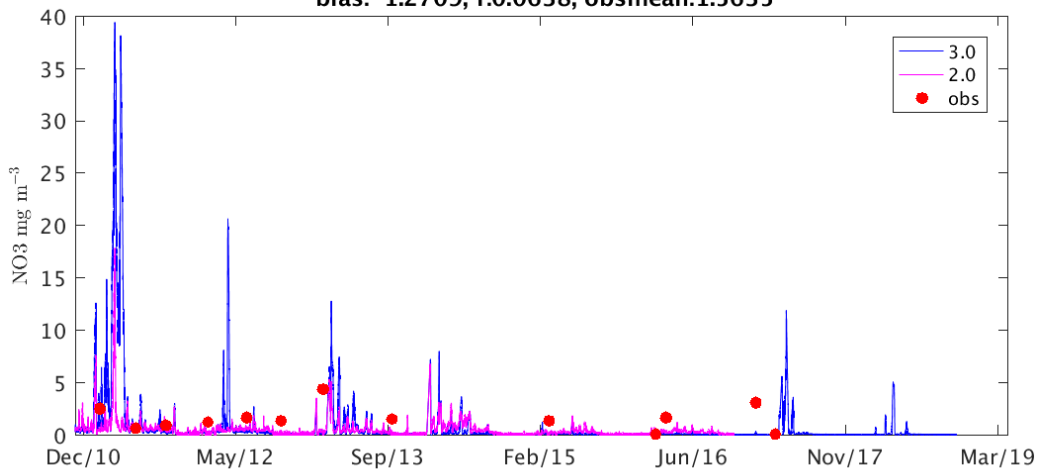


**DoubleCone\_23m 3.0 d2:0.49, mape:78.3, rms:1.6977**

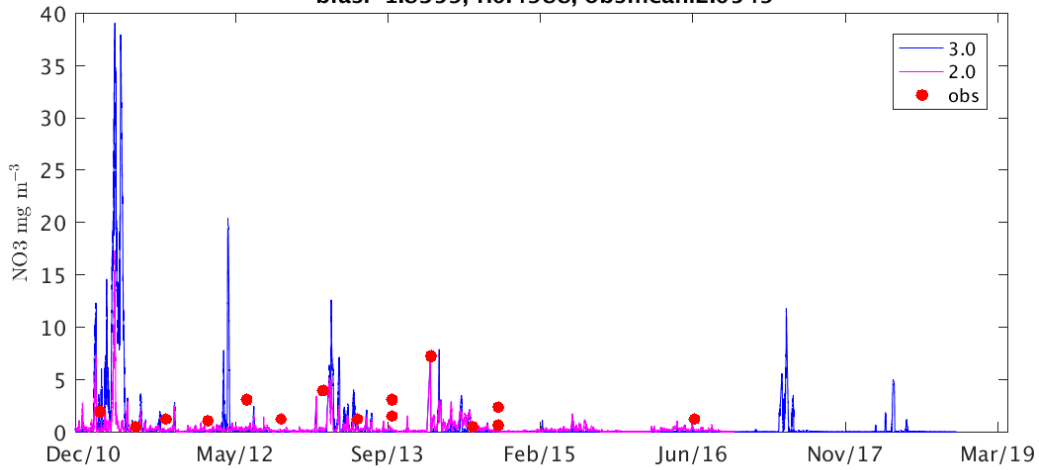
**bias:-1.1957, r:0.2328, obsmean:1.5676**

**DoubleCone\_23m 2.0 d2:0.41, mape:76.9, rms:1.6603**

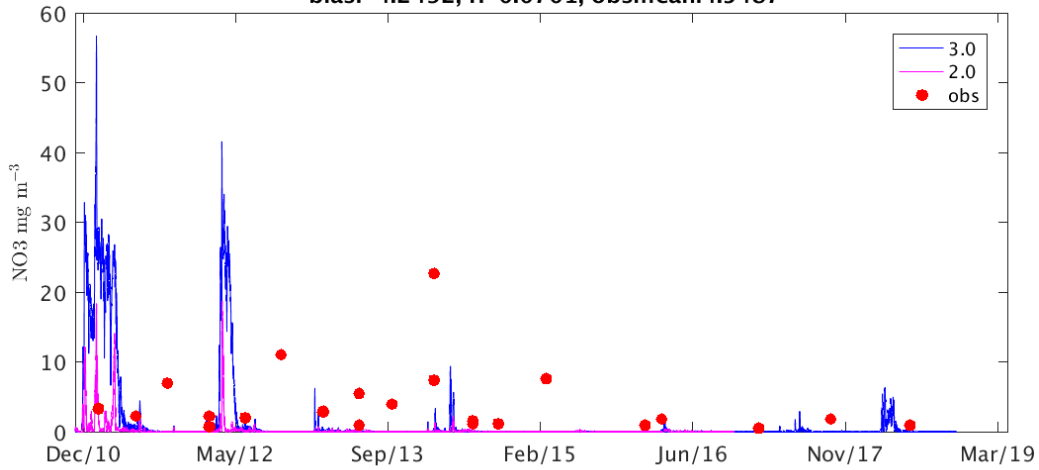
**bias:-1.2709, r:0.0638, obsmean:1.5635**



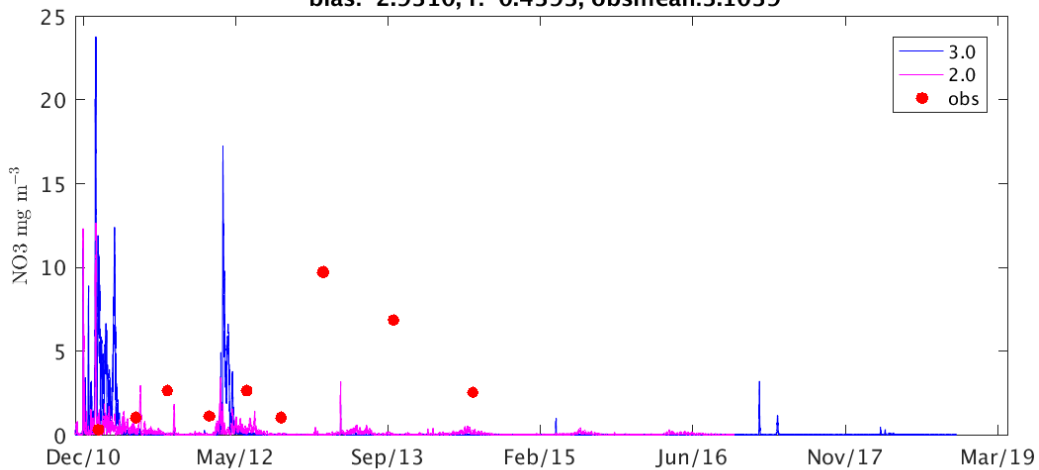
**DoubleCone334\_10m 3.0 d2:0.48, mape:86.2, rms:2.3105**  
**bias:-1.7163, r:0.4151, obsmean:2.0549**  
**DoubleCone334\_10m 2.0 d2:0.44, mape:83.3, rms:2.4648**  
**bias:-1.8359, r:0.4988, obsmean:2.0549**



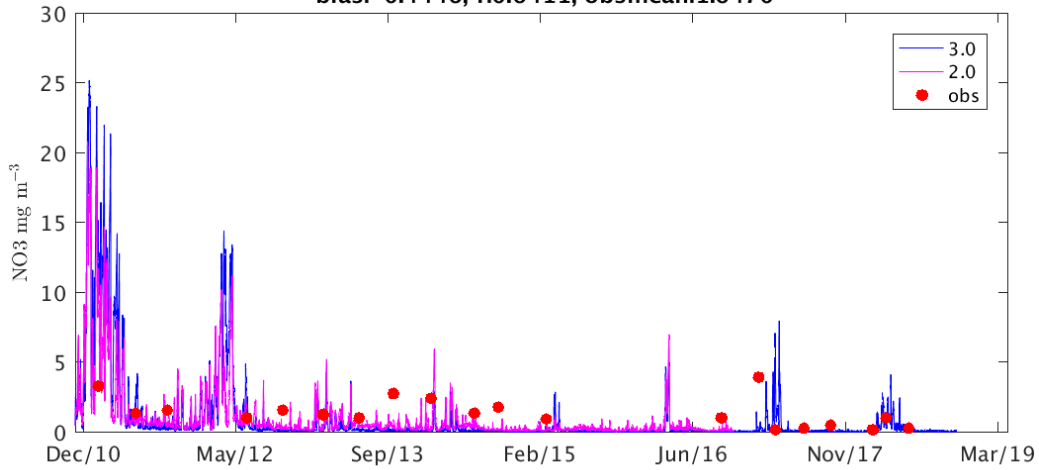
**GeoffreyBay336\_5m 3.0 d2:0.30, mape:119.3, rms:7.9536**  
**bias:-2.8808, r:-0.0450, obsmean:4.2282**  
**GeoffreyBay336\_5m 2.0 d2:0.40, mape:92.5, rms:6.7874**  
**bias:-4.2492, r:-0.0701, obsmean:4.5487**



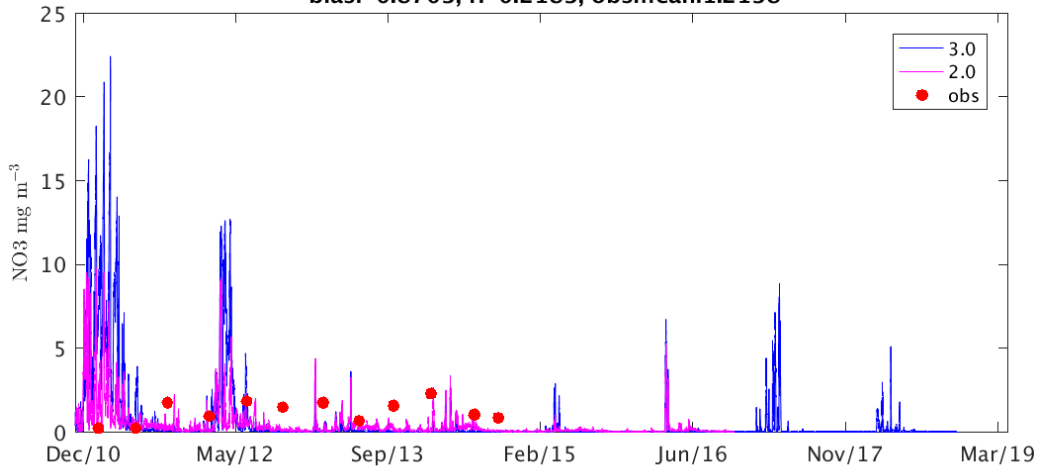
**Pandora\_5m 3.0 d2:0.30, mape:342.3, rms:4.9838**  
**bias:-2.1844, r:-0.3308, obsmean:3.1039**  
**Pandora\_5m 2.0 d2:0.42, mape:93.3, rms:4.2381**  
**bias:-2.9310, r:-0.4393, obsmean:3.1039**



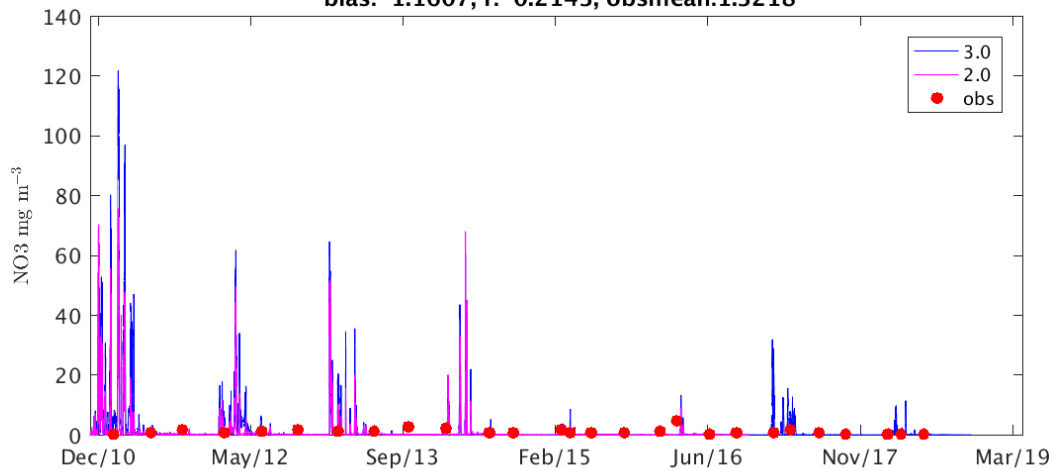
Pelorus686\_28m 3.0 d2:0.45, mape:199.3, rms:2.7353  
 bias:-0.1555, r:0.3491, obsmean:1.3843  
 Pelorus686\_28m 2.0 d2:0.54, mape:72.8, rms:2.1121  
 bias:-0.4446, r:0.6411, obsmean:1.6470



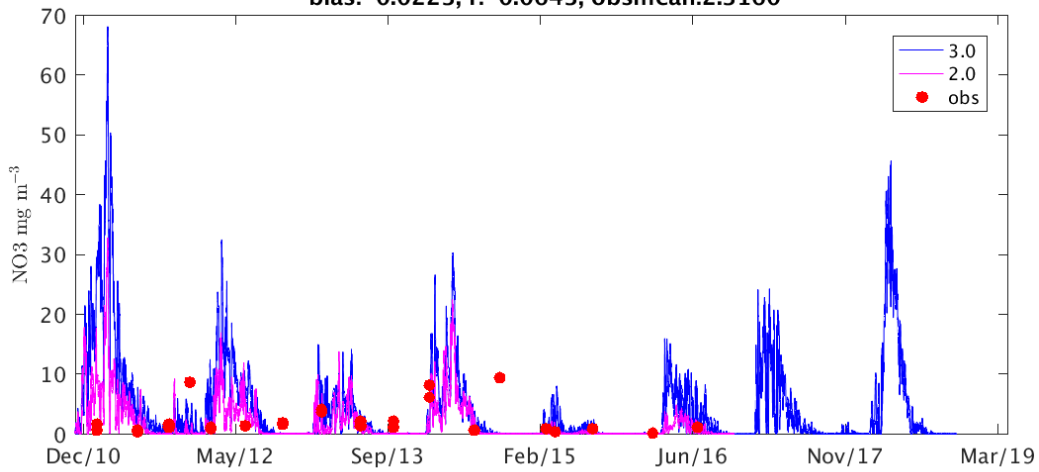
Pelorus686\_14m 3.0 d2:0.12, mape:384.5, rms:2.1355  
 bias:-0.2636, r:-0.5484, obsmean:1.2138  
 Pelorus686\_14m 2.0 d2:0.41, mape:84.2, rms:1.1510  
 bias:-0.8703, r:-0.2183, obsmean:1.2138



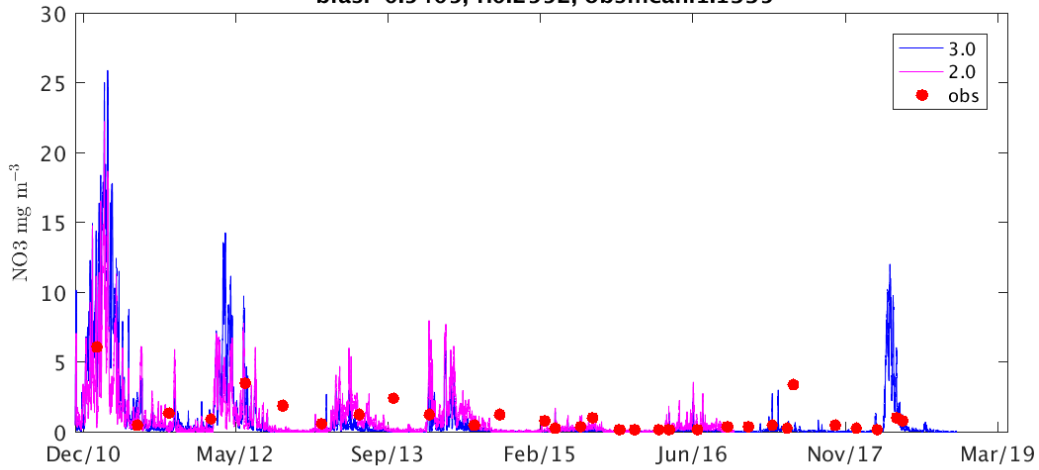
Pelorus686\_0m 3.0 d2:0.28, mape:136.0, rms:2.0423  
 bias:-0.3503, r:-0.0325, obsmean:1.1362  
 Pelorus686\_0m 2.0 d2:0.38, mape:80.0, rms:1.5936  
 bias:-1.1607, r:-0.2143, obsmean:1.3218



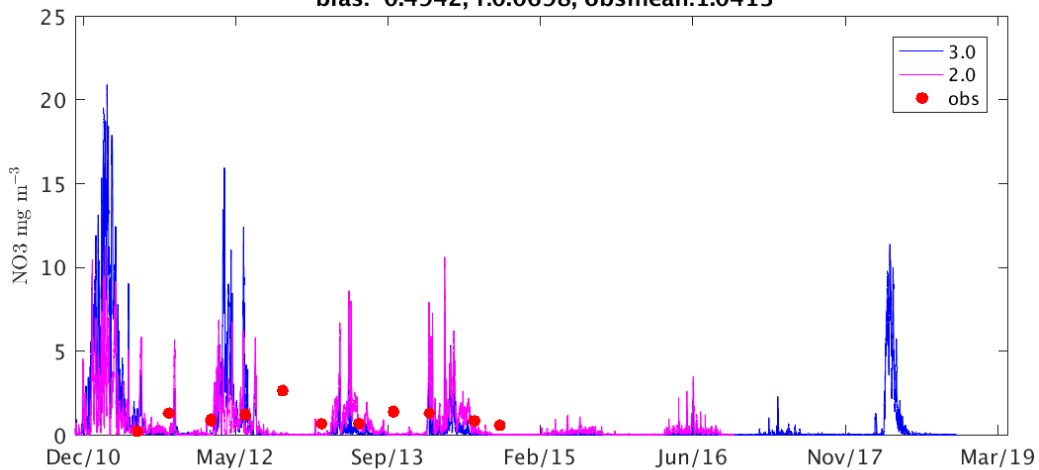
Dunk859\_5m 3.0 d2:0.09, mape:513.9, rms:9.0890  
bias:2.9842, r:-0.1698, obsmean:2.3160  
Dunk859\_5m 2.0 d2:0.30, mape:198.9, rms:3.9263  
bias:-0.0223, r:-0.0643, obsmean:2.3160



Russell695\_20m 3.0 d2:0.80, mape:90.9, rms:1.0418  
bias:-0.5843, r:0.7304, obsmean:1.0395  
Russell695\_20m 2.0 d2:0.45, mape:118.0, rms:1.5485  
bias:-0.5405, r:0.2552, obsmean:1.1335

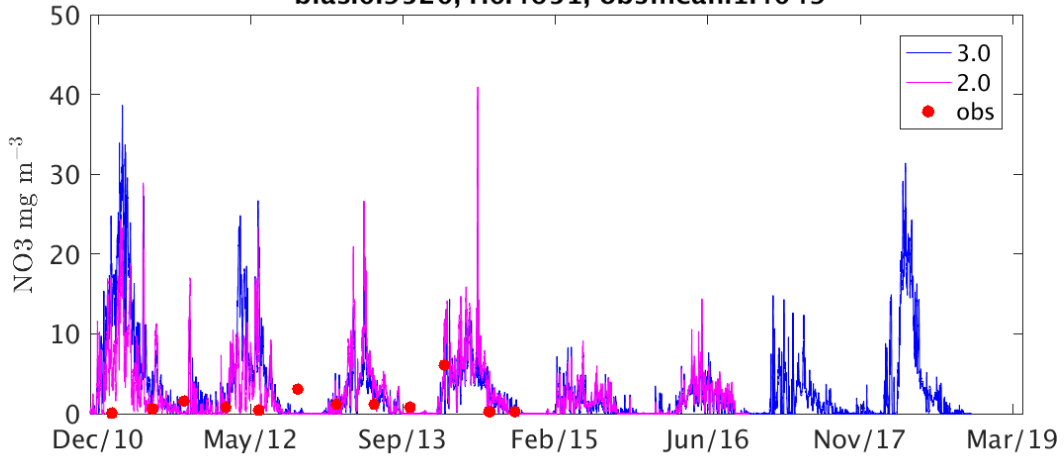


Russell695\_10m 3.0 d2:0.32, mape:134.6, rms:1.1518  
bias:-0.6778, r:-0.1952, obsmean:1.0413  
Russell695\_10m 2.0 d2:0.33, mape:97.1, rms:1.3502  
bias:-0.4942, r:0.0698, obsmean:1.0413

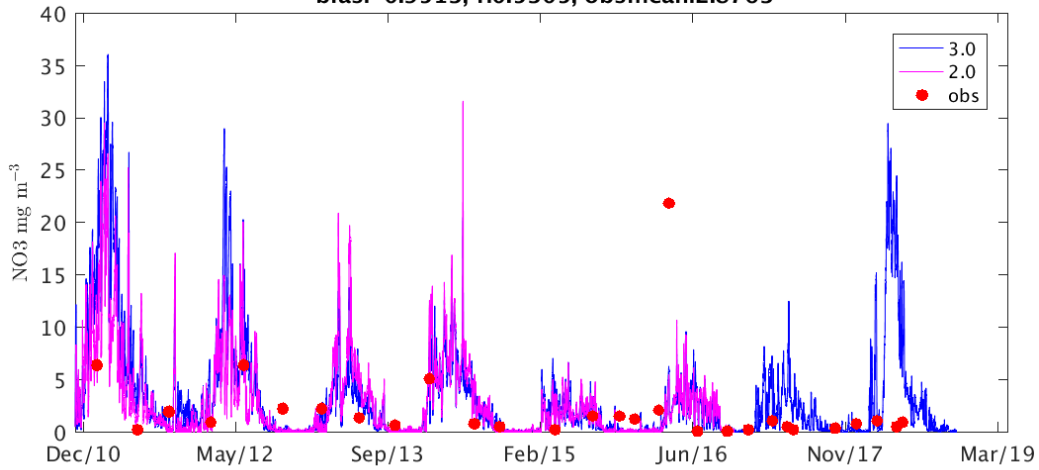




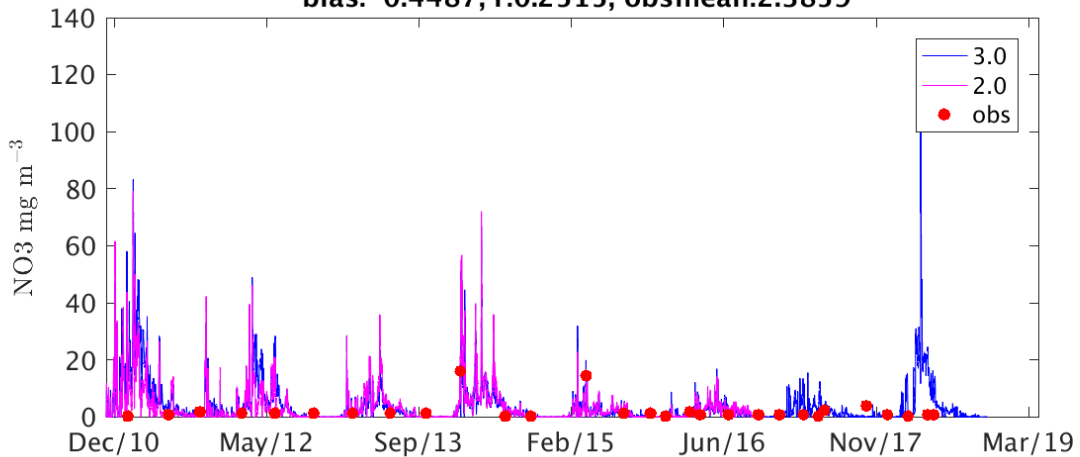
**Highl\_10m 3.0 d2:0.02, mape:1080.1, rms:6.7554**  
**bias:2.0861, r:-0.2585, obsmean:1.4049**  
**Highl\_10m 2.0 d2:0.62, mape:475.3, rms:2.8124**  
**bias:0.9520, r:0.4651, obsmean:1.4049**



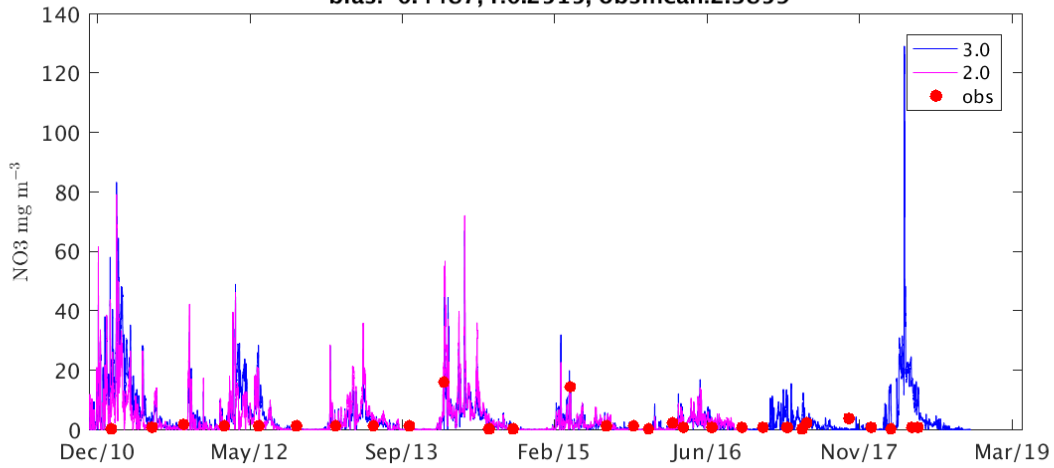
**Highl\_20m 3.0 d2:0.54, mape:330.6, rms:4.7201**  
**bias:0.6523, r:0.3286, obsmean:2.1869**  
**Highl\_20m 2.0 d2:0.60, mape:211.4, rms:4.1357**  
**bias:-0.9513, r:0.5305, obsmean:2.8763**



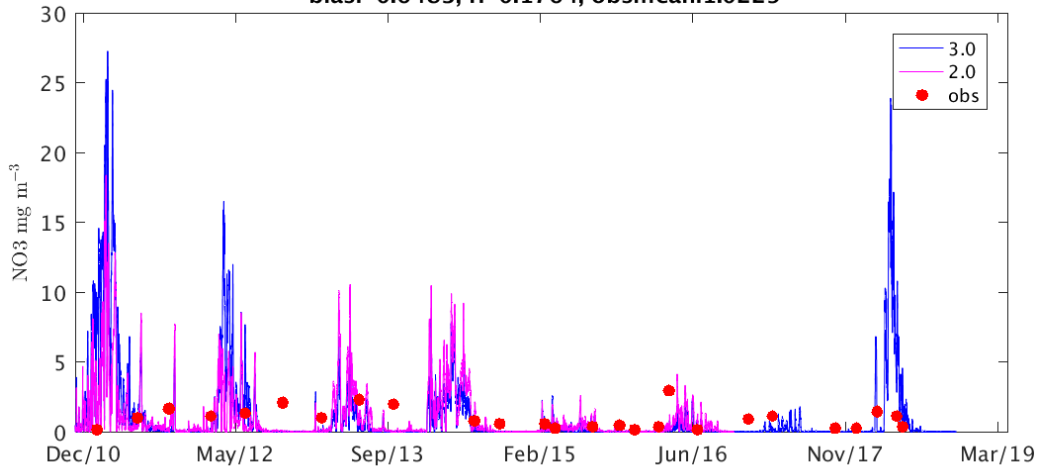
**Highl697\_0m 3.0 d2:0.07, mape:767.3, rms:6.9776**  
**bias:0.9008, r:-0.1369, obsmean:1.9928**  
**Highl697\_0m 2.0 d2:0.49, mape:379.6, rms:4.5492**  
**bias:-0.4487, r:0.2515, obsmean:2.3859**



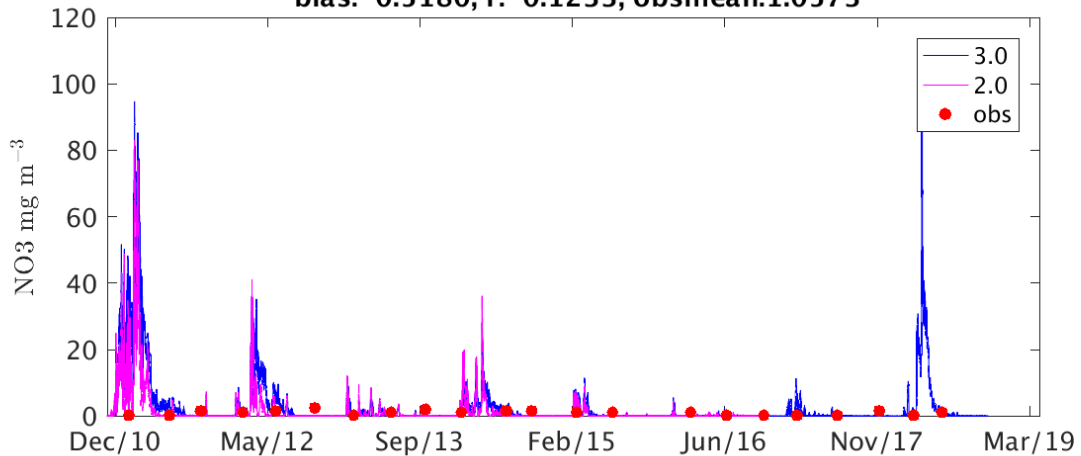
High1697\_0m 3.0 d2:0.07, mape:767.3, rms:6.9776  
 bias:0.9008, r:-0.1369, obsmean:1.9928  
 High1697\_0m 2.0 d2:0.49, mape:379.6, rms:4.5492  
 bias:-0.4487, r:0.2515, obsmean:2.3859



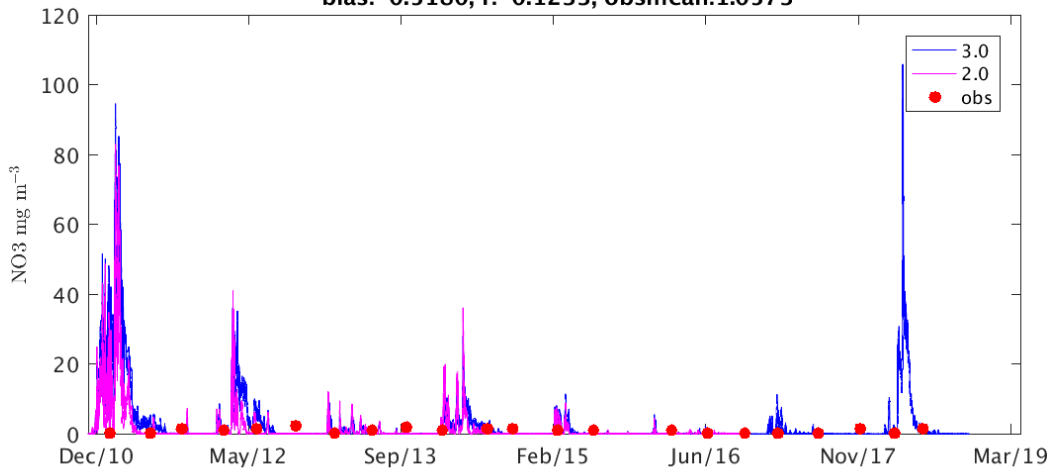
FitzCoral852\_15m 3.0 d2:0.15, mape:339.3, rms:2.6590  
 bias:0.0909, r:-0.0821, obsmean:0.9622  
 FitzCoral852\_15m 2.0 d2:0.36, mape:174.2, rms:1.2471  
 bias:-0.6483, r:-0.1764, obsmean:1.0229



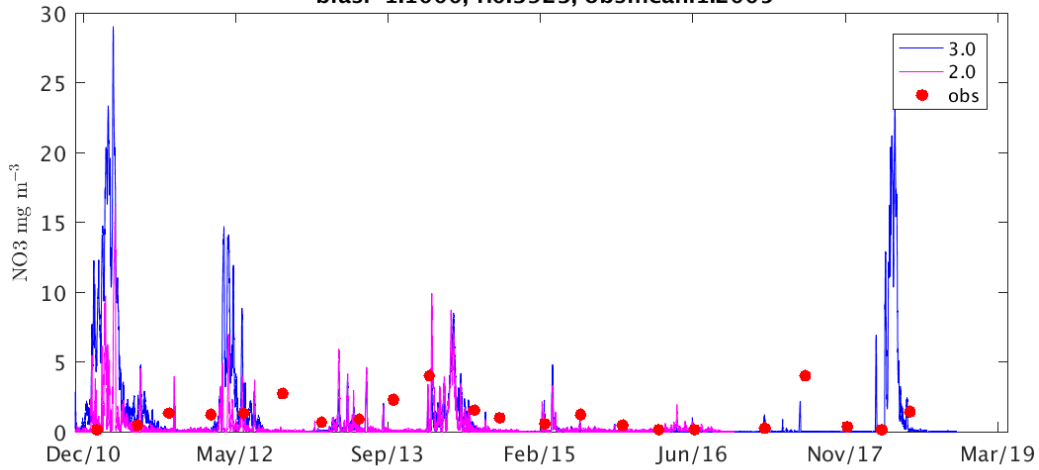
FairleadBuoy518\_0m 3.0 d2:0.14, mape:287.7, rms:2.5812  
 bias:0.3047, r:-0.2208, obsmean:0.9832  
 FairleadBuoy518\_0m 2.0 d2:0.30, mape:114.4, rms:1.2965  
 bias:-0.5180, r:-0.1233, obsmean:1.0573



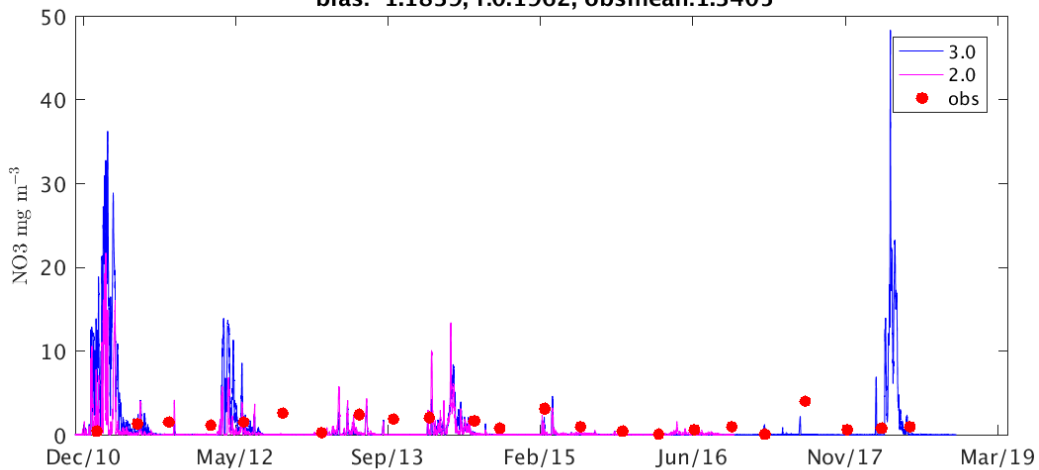
FairleadBuoy518\_0m 3.0 d2:0.14, mape:287.7, rms:2.5812  
bias:0.3047, r:-0.2208, obsmean:0.9832  
FairleadBuoy518\_0m 2.0 d2:0.30, mape:114.4, rms:1.2965  
bias:-0.5180, r:-0.1233, obsmean:1.0573



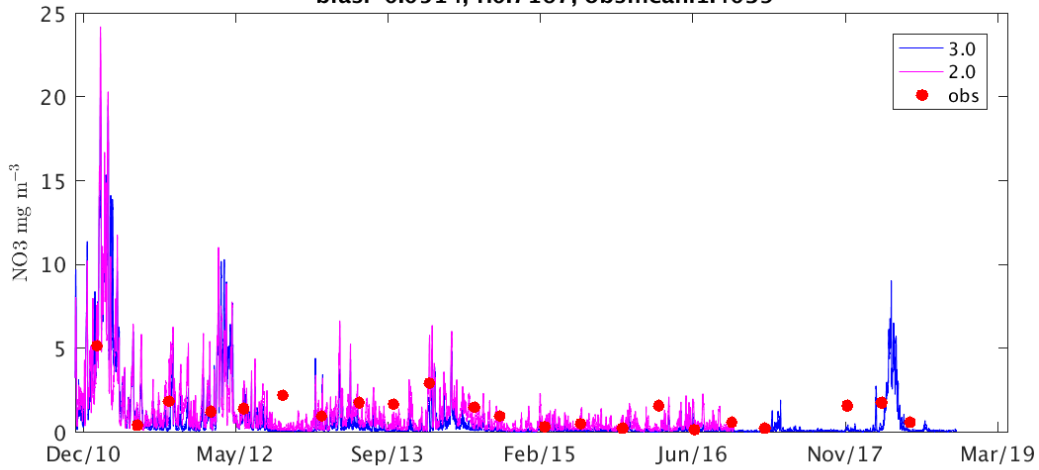
Yorkeys519\_8m 3.0 d2:0.27, mape:275.7, rms:2.0435  
bias:-0.7598, r:-0.2275, obsmean:1.2110  
Yorkeys519\_8m 2.0 d2:0.44, mape:85.2, rms:1.4456  
bias:-1.1000, r:0.3923, obsmean:1.2005



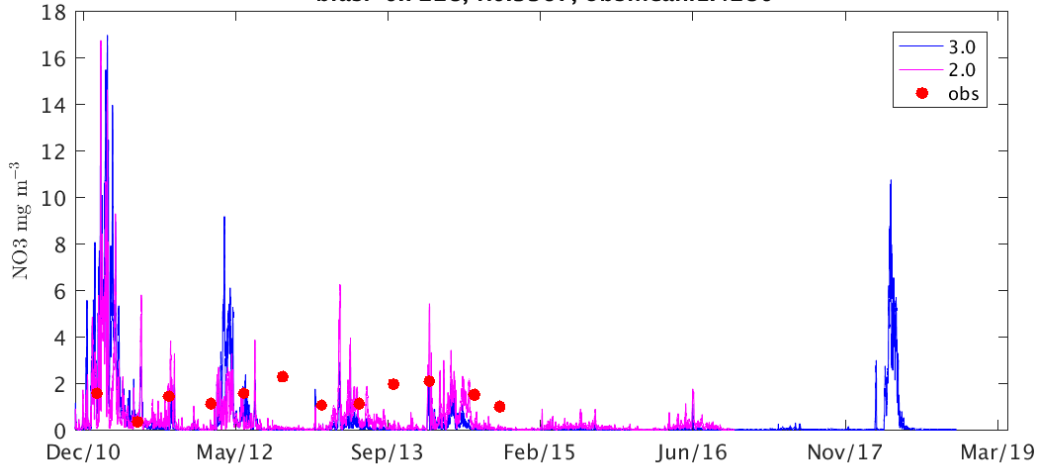
Yorkeys519\_0m 3.0 d2:0.28, mape:161.5, rms:2.1247  
bias:-0.9196, r:-0.1978, obsmean:1.3327  
Yorkeys519\_0m 2.0 d2:0.45, mape:83.6, rms:1.4347  
bias:-1.1839, r:0.1962, obsmean:1.3405



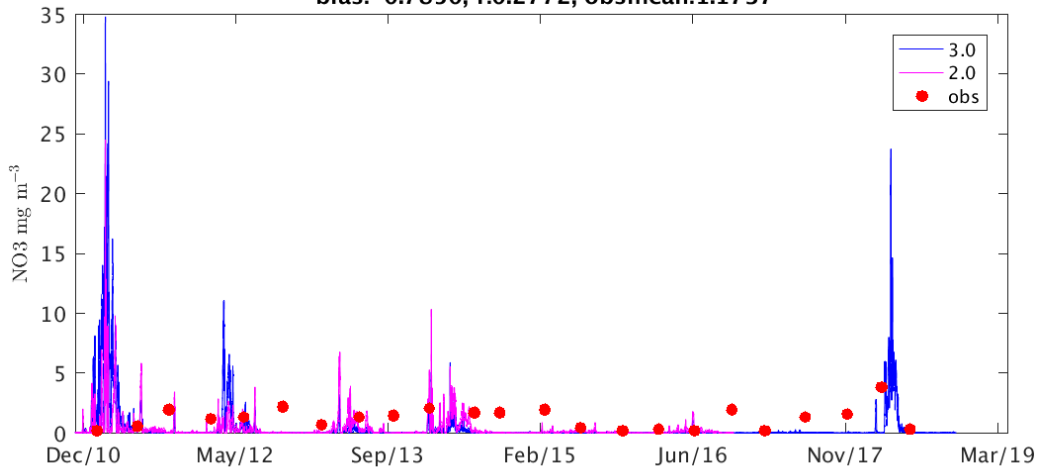
**Green830\_36m 3.0 d2:0.78, mape:79.5, rms:1.0963**  
**bias:-0.7076, r:0.7112, obsmean:1.3384**  
**Green830\_36m 2.0 d2:0.83, mape:83.3, rms:1.0803**  
**bias:-0.0514, r:0.7167, obsmean:1.4039**



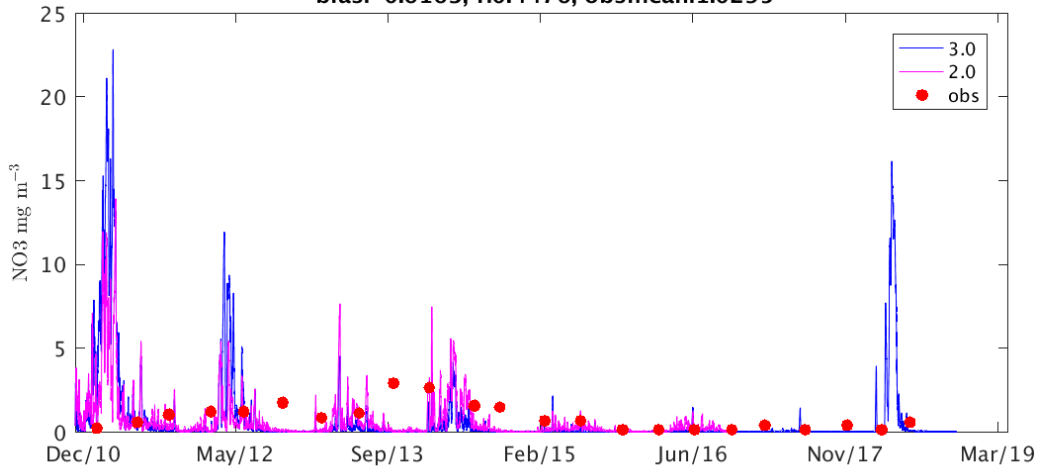
**Green830\_18m 3.0 d2:0.37, mape:77.3, rms:1.3029**  
**bias:-1.1600, r:0.1396, obsmean:1.4280**  
**Green830\_18m 2.0 d2:0.43, mape:84.4, rms:1.5618**  
**bias:-0.7228, r:0.3367, obsmean:1.4280**



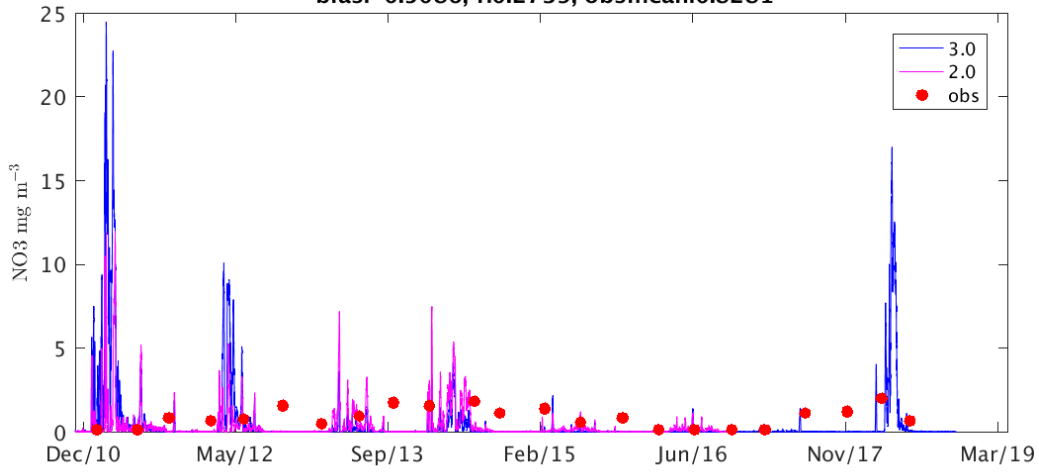
**Green830\_0m 3.0 d2:0.40, mape:125.6, rms:1.4871**  
**bias:-1.1001, r:-0.2343, obsmean:1.2316**  
**Green830\_0m 2.0 d2:0.52, mape:86.4, rms:1.3991**  
**bias:-0.7850, r:0.2772, obsmean:1.1737**



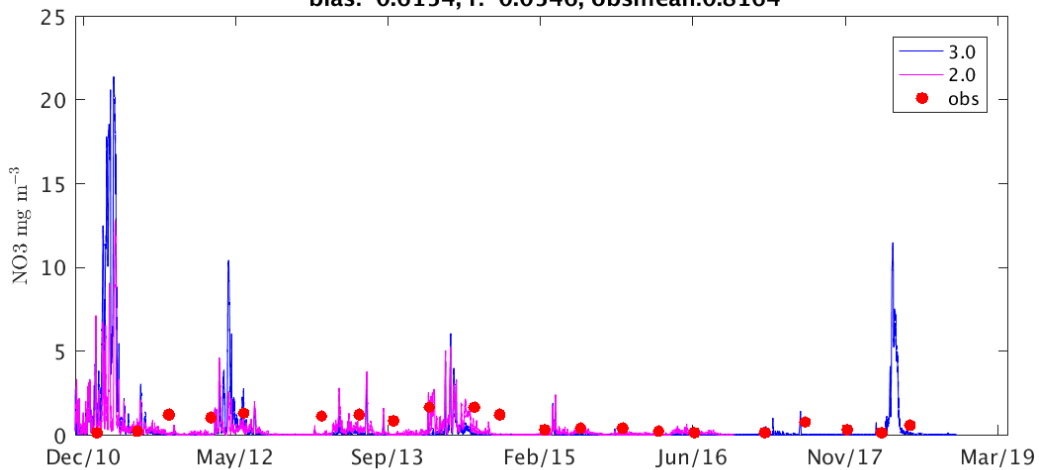
**DoubleI520\_18m 3.0 d2:0.44, mape:88.8, rms:1.0965**  
**bias:-0.7440, r:-0.0741, obsmean:0.8782**  
**DoubleI520\_18m 2.0 d2:0.64, mape:70.8, rms:1.0140**  
**bias:-0.6163, r:0.4476, obsmean:1.0295**



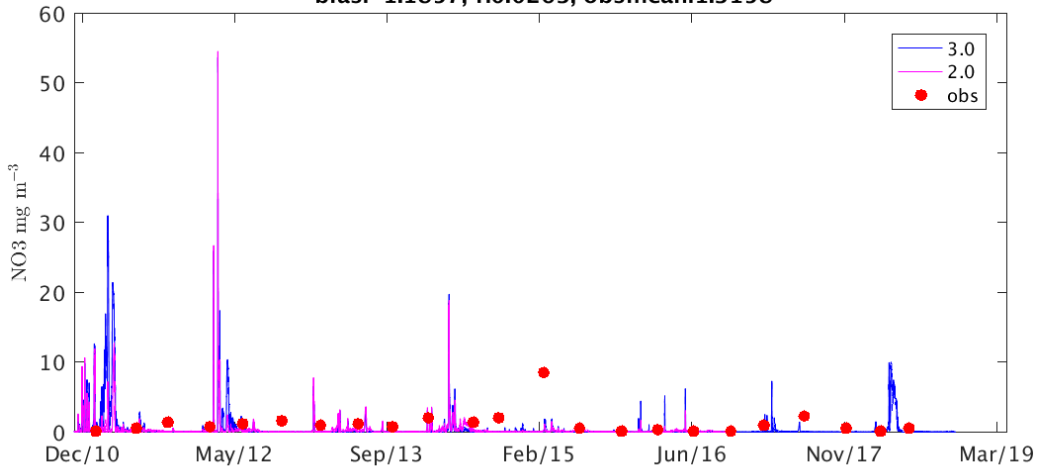
**DoubleI520\_0m 3.0 d2:0.40, mape:109.8, rms:1.0354**  
**bias:-0.7818, r:-0.3071, obsmean:0.8739**  
**DoubleI520\_0m 2.0 d2:0.54, mape:92.8, rms:0.9328**  
**bias:-0.5086, r:0.2739, obsmean:0.8281**



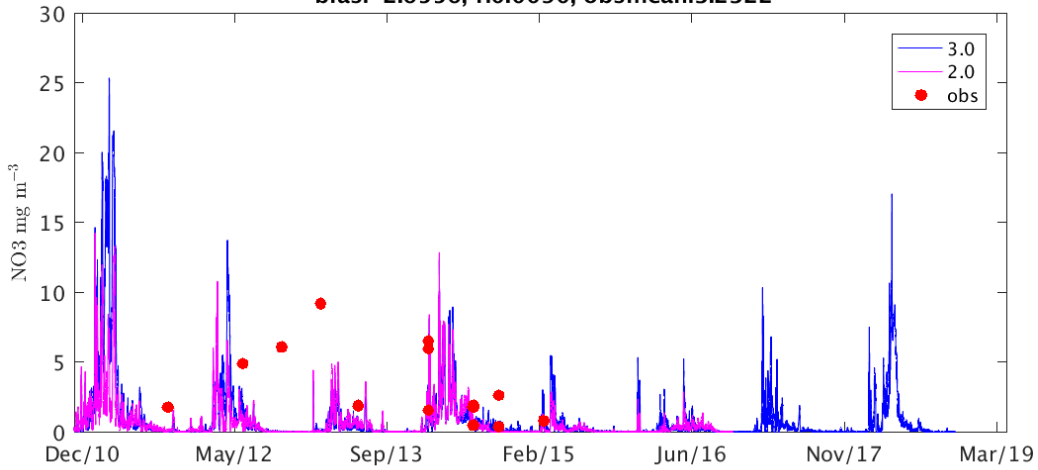
**PortD\_15m 3.0 d2:0.48, mape:78.9, rms:0.7965**  
**bias:-0.6062, r:0.1459, obsmean:0.7116**  
**PortD\_15m 2.0 d2:0.44, mape:87.8, rms:0.8419**  
**bias:-0.6154, r:-0.0546, obsmean:0.8164**



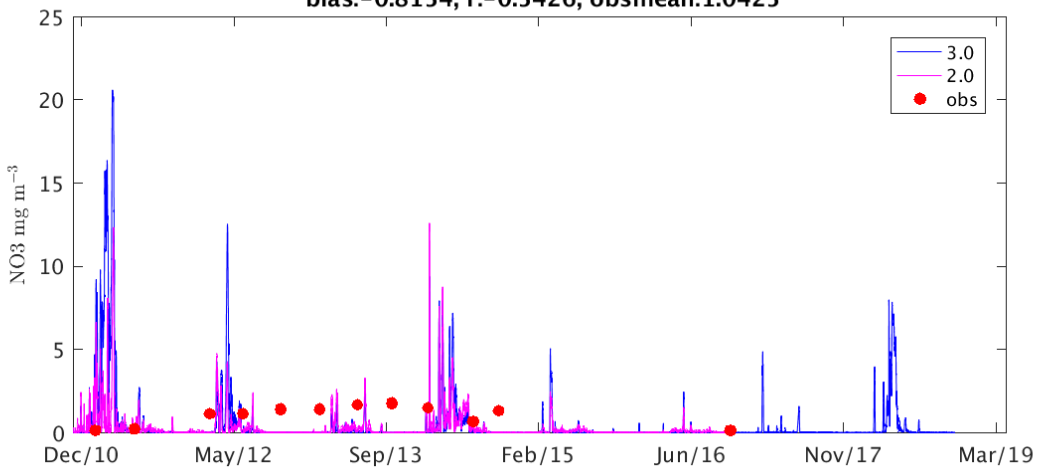
**PortD\_0m 3.0 d2:0.34, mape:87.0, rms:2.0542**  
**bias:-1.1574, r:-0.0697, obsmean:1.2266**  
**PortD\_0m 2.0 d2:0.33, mape:79.9, rms:2.2013**  
**bias:-1.1857, r:0.0263, obsmean:1.3158**



**Snap\_10m 3.0 d2:0.45, mape:74.2, rms:3.6532**  
**bias:-2.5124, r:-0.0263, obsmean:3.2322**  
**Snap\_10m 2.0 d2:0.46, mape:72.4, rms:3.7206**  
**bias:-2.6556, r:0.0090, obsmean:3.2322**



**CapeTrib356\_10m 3.0 d2:0.21, mape:311.3, rms:1.5911**  
**bias:-0.6762, r:-0.4876, obsmean:1.0425**  
**CapeTrib356\_10m 2.0 d2:0.29, mape:163.9, rms:1.2029**  
**bias:-0.8154, r:-0.5426, obsmean:1.0425**



# 14. Simulated NH4 assessment against AIMS Long Term Monitoring

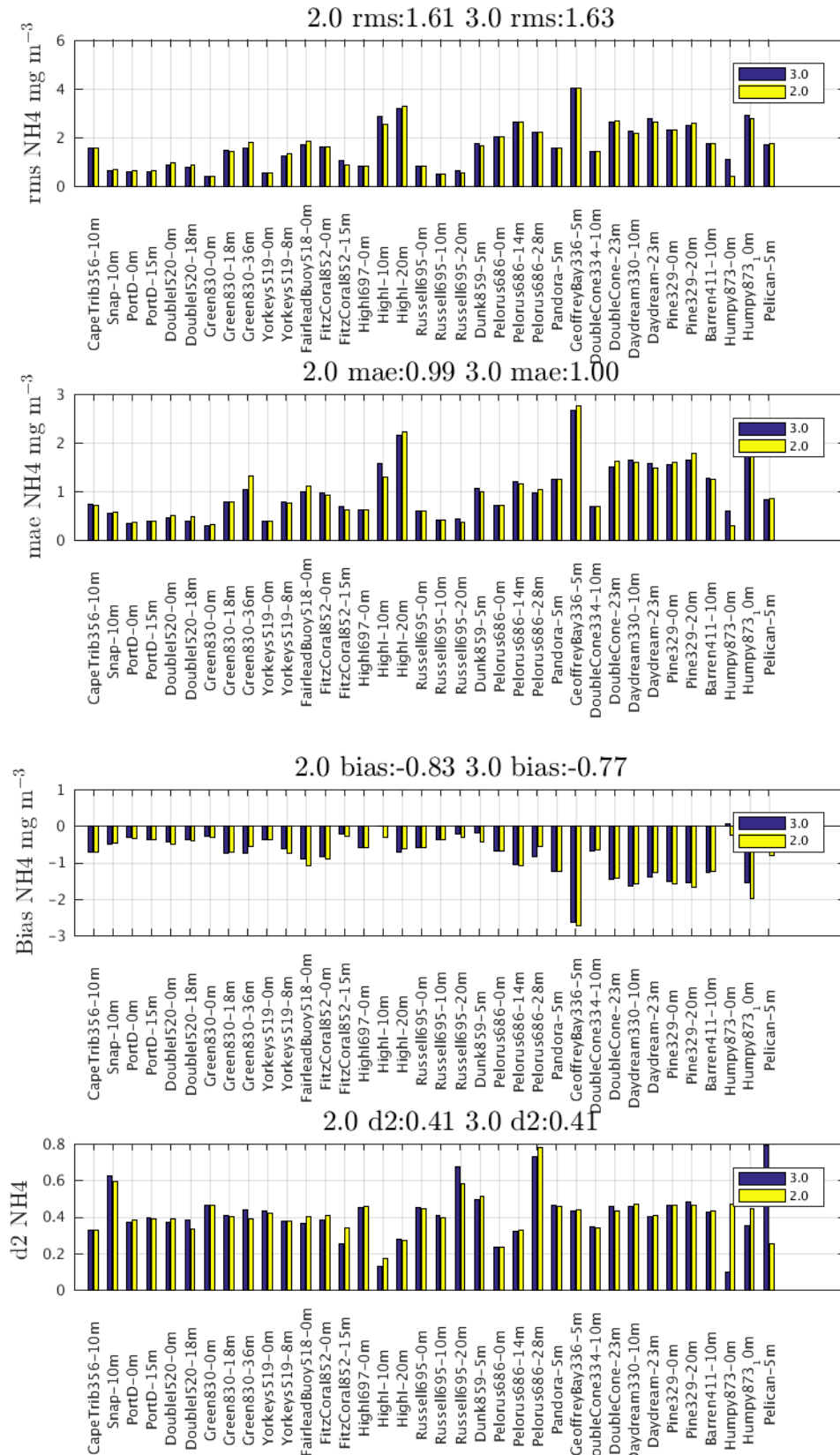
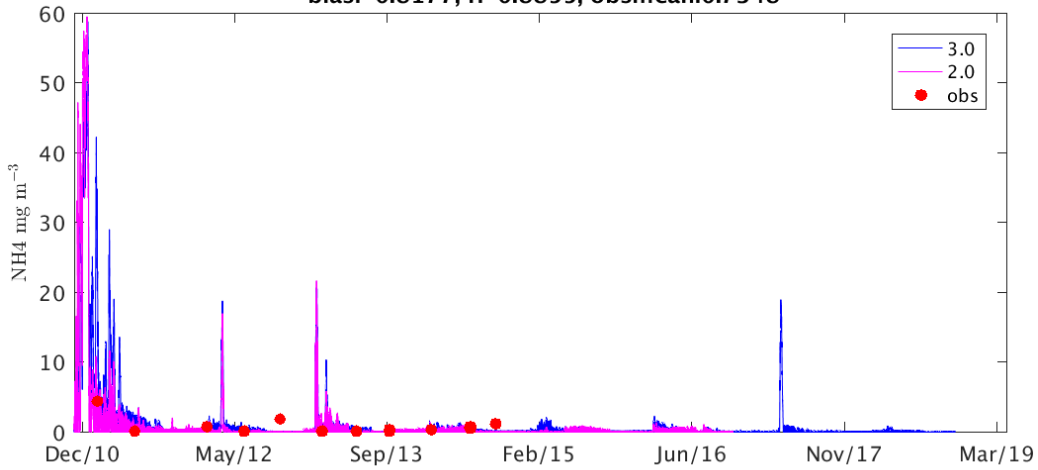
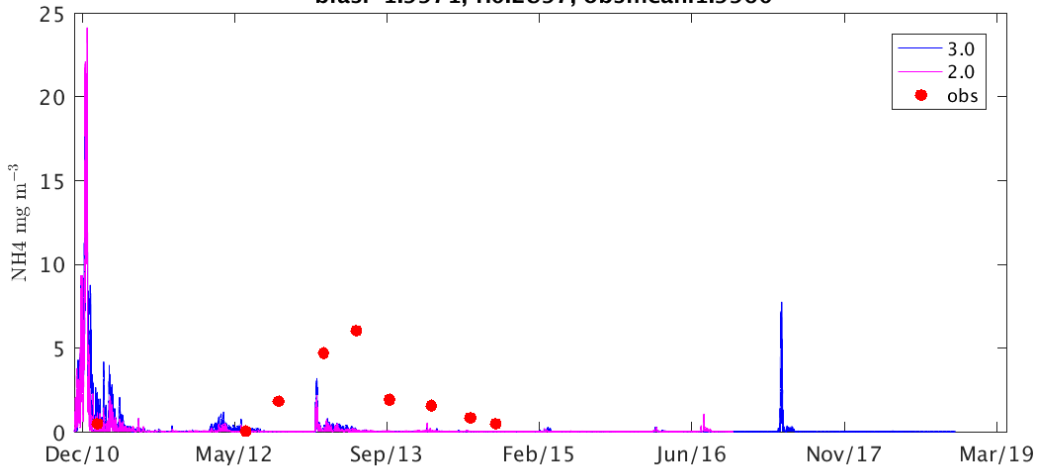


Figure 9 Metrics for Long Term Monitoring sites NH4 assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

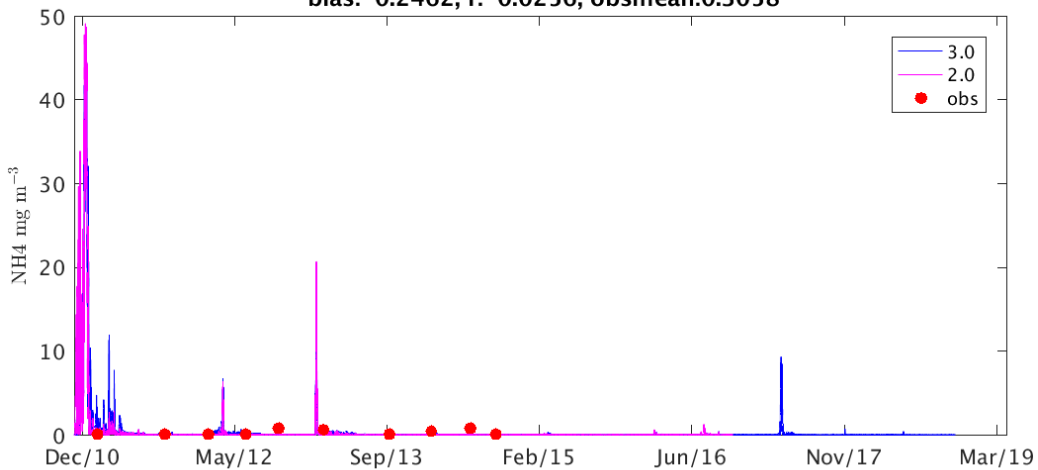
**Pelican\_5m 3.0 d2:0.79, mape:89.0, rms:1.6907**  
**bias:0.0103, r:0.8810, obsmean:0.7348**  
**Pelican\_5m 2.0 d2:0.25, mape:94.7, rms:1.7502**  
**bias:-0.8177, r:-0.8855, obsmean:0.7348**



**Humpy873\_10m 3.0 d2:0.35, mape:237.6, rms:2.8912**  
**bias:-1.5584, r:-0.2555, obsmean:1.9960**  
**Humpy873\_10m 2.0 d2:0.44, mape:127.5, rms:2.7663**  
**bias:-1.9971, r:0.2897, obsmean:1.9960**

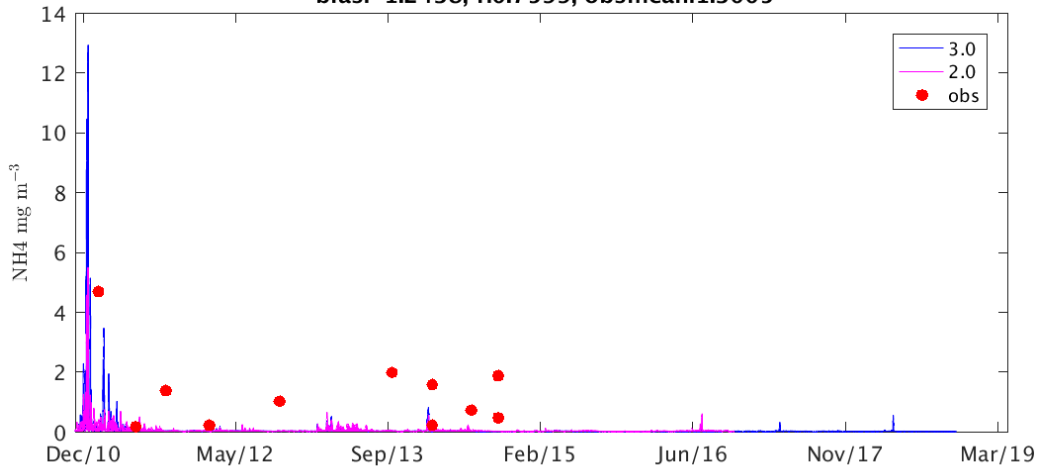


**Humpy873\_0m 3.0 d2:0.10, mape:220.2, rms:1.0706**  
**bias:0.0604, r:-0.3076, obsmean:0.3058**  
**Humpy873\_0m 2.0 d2:0.47, mape:150.5, rms:0.4175**  
**bias:-0.2462, r:-0.0256, obsmean:0.3058**

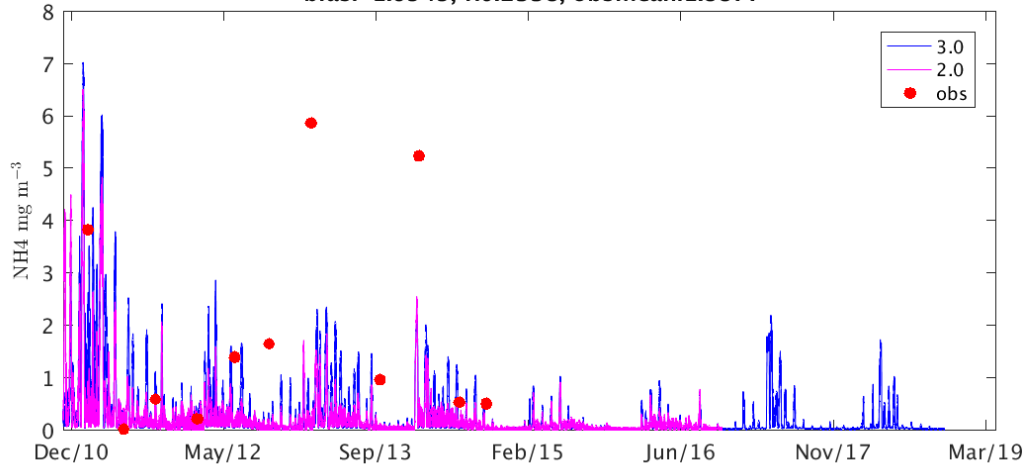




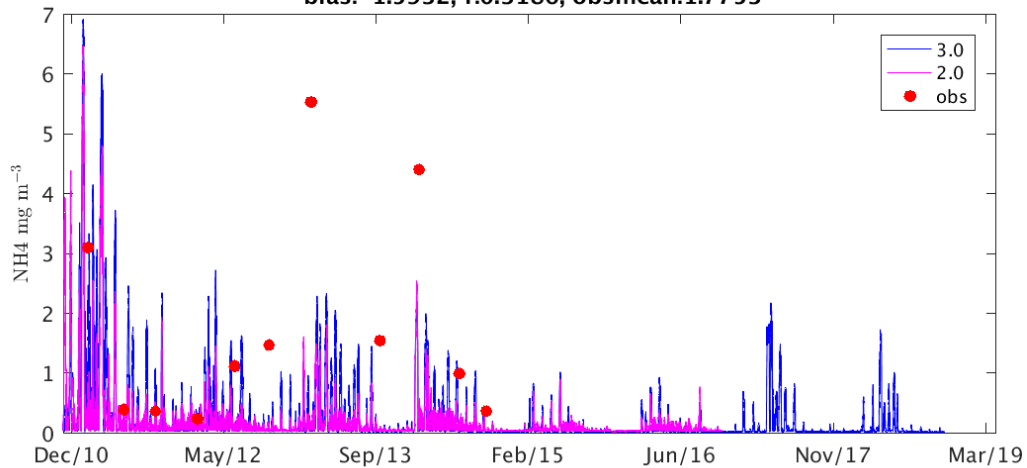
Barren411\_10m 3.0 d2:0.42, mape:94.3, rms:1.7634  
bias:-1.2681, r:0.8369, obsmean:1.3005  
Barren411\_10m 2.0 d2:0.43, mape:89.4, rms:1.7239  
bias:-1.2438, r:0.7599, obsmean:1.3005



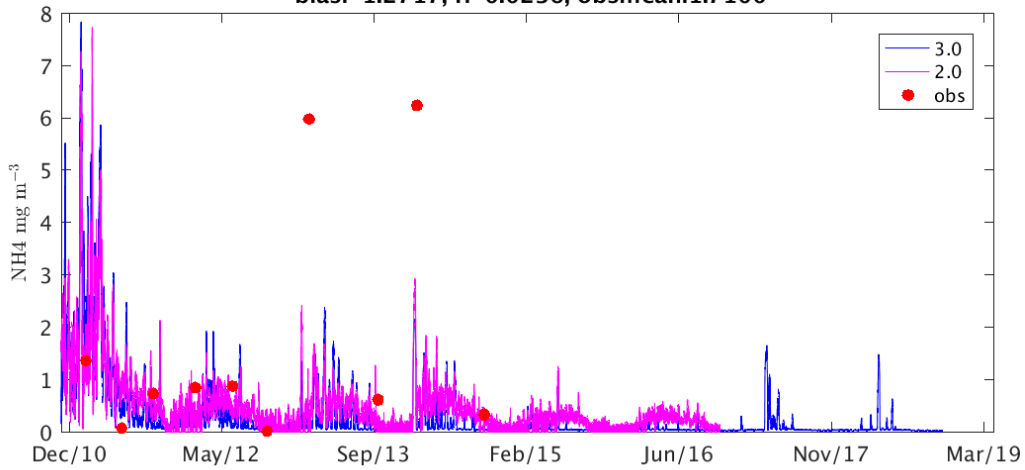
Pine329\_20m 3.0 d2:0.48, mape:79.9, rms:2.5048  
bias:-1.5693, r:0.2186, obsmean:1.8877  
Pine329\_20m 2.0 d2:0.46, mape:86.9, rms:2.5896  
bias:-1.6949, r:0.2338, obsmean:1.8877



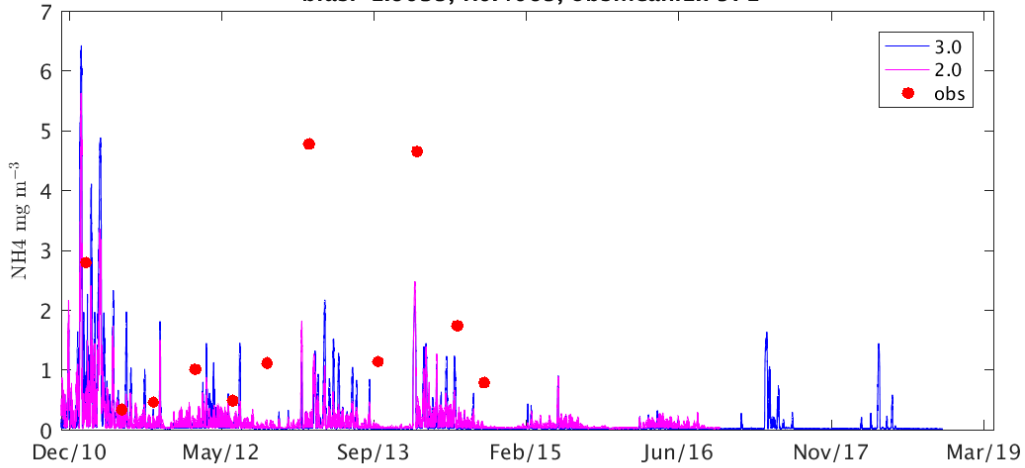
Pine329\_0m 3.0 d2:0.46, mape:80.5, rms:2.2893  
bias:-1.5255, r:0.1459, obsmean:1.7753  
Pine329\_0m 2.0 d2:0.46, mape:77.7, rms:2.3135  
bias:-1.5932, r:0.3186, obsmean:1.7753



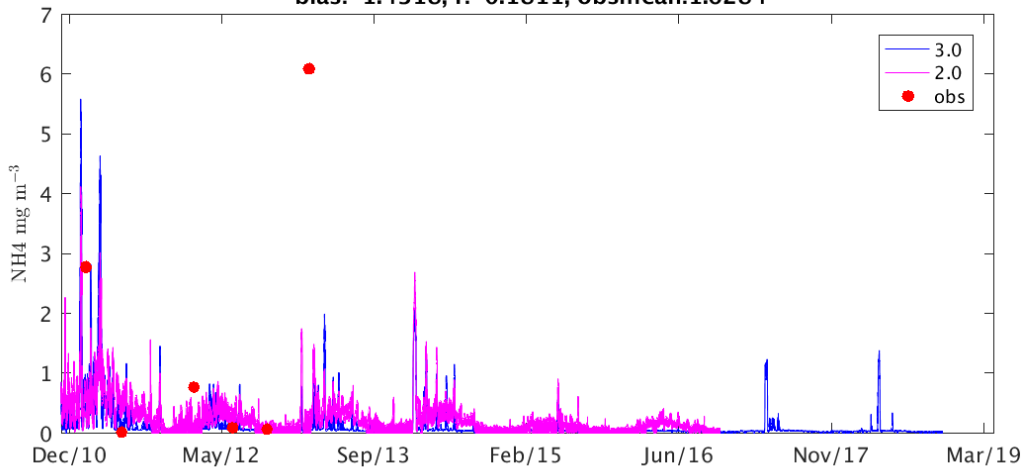
Daydream\_23m 3.0 d2:0.40, mape:156.4, rms:2.7555  
 bias:-1.3964, r:-0.1885, obsmean:1.7100  
 Daydream\_23m 2.0 d2:0.40, mape:202.2, rms:2.6217  
 bias:-1.2717, r:-0.0236, obsmean:1.7100



Daydream330\_10m 3.0 d2:0.46, mape:87.4, rms:2.2432  
 bias:-1.6369, r:0.0997, obsmean:1.7571  
 Daydream330\_10m 2.0 d2:0.47, mape:84.3, rms:2.1857  
 bias:-1.6039, r:0.4069, obsmean:1.7571



DoubleCone\_23m 3.0 d2:0.46, mape:69.5, rms:2.6340  
 bias:-1.4751, r:0.1709, obsmean:1.6284  
 DoubleCone\_23m 2.0 d2:0.43, mape:124.8, rms:2.6627  
 bias:-1.4318, r:-0.1811, obsmean:1.6284

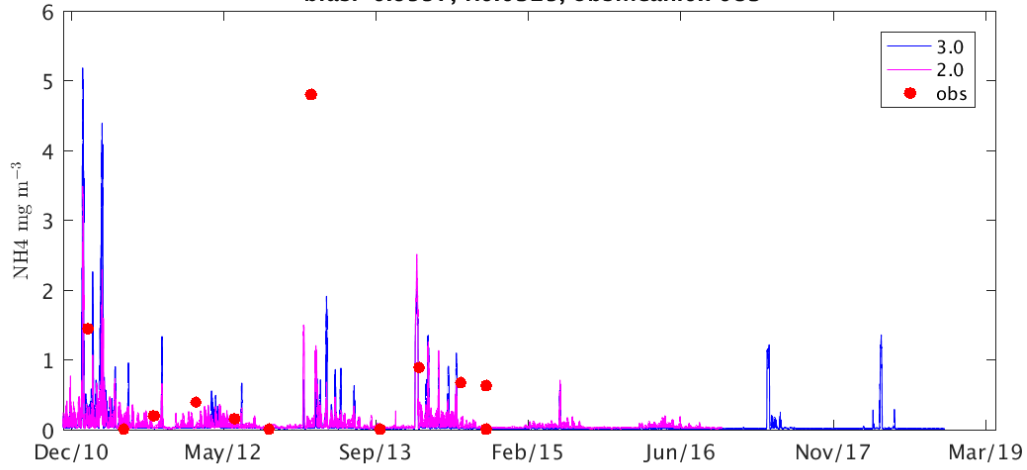


DoubleCone334\_10m 3.0 d2:0.34, mape:91.1, rms:1.4248

bias:-0.6778, r:0.2137, obsmean:0.7083

DoubleCone334\_10m 2.0 d2:0.34, mape:98.6, rms:1.4186

bias:-0.6597, r:0.0325, obsmean:0.7083

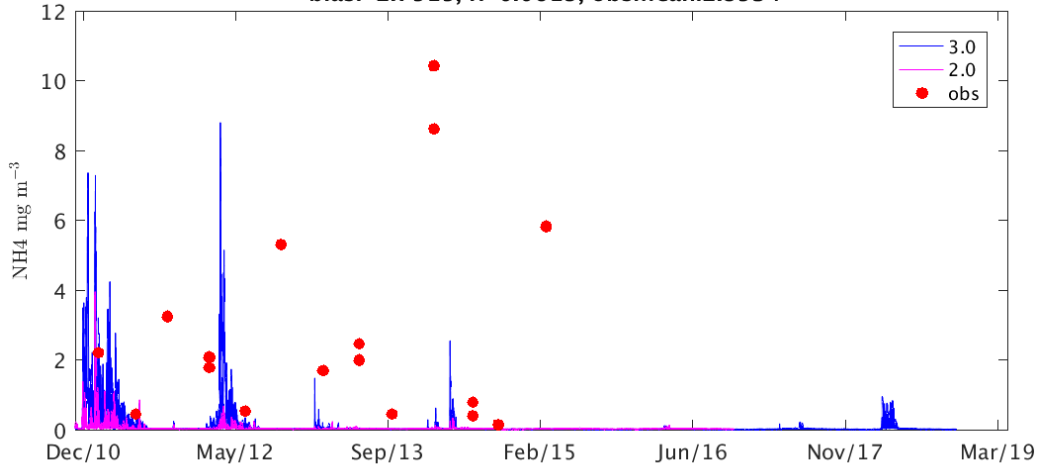


GeoffreyBay336\_5m 3.0 d2:0.43, mape:84.7, rms:4.0163

bias:-2.6494, r:-0.1036, obsmean:2.8534

GeoffreyBay336\_5m 2.0 d2:0.44, mape:92.7, rms:4.0303

bias:-2.7515, r:-0.0619, obsmean:2.8534

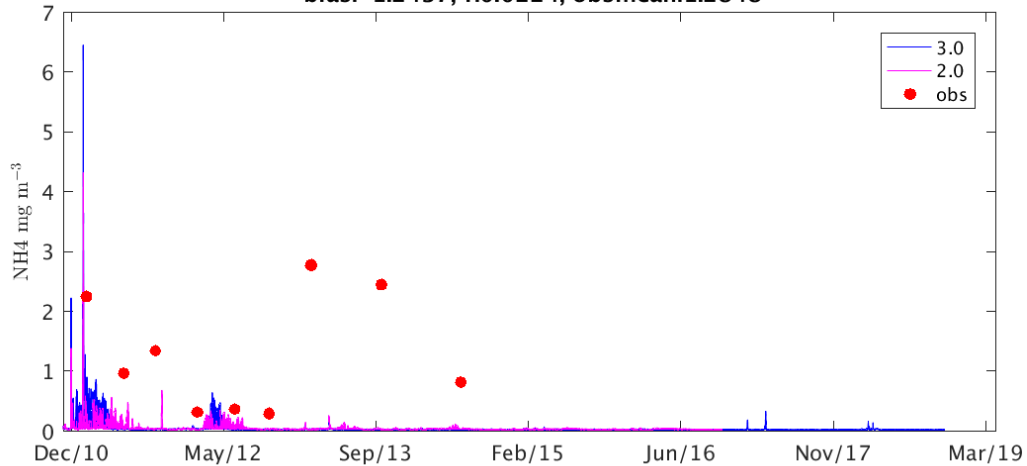


Pandora\_5m 3.0 d2:0.46, mape:95.1, rms:1.5375

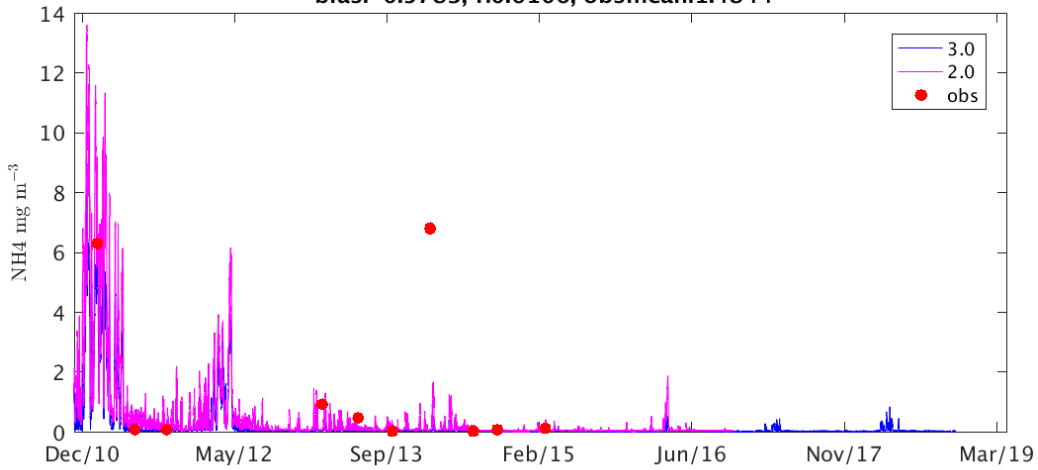
bias:-1.2436, r:0.3630, obsmean:1.2848

Pandora\_5m 2.0 d2:0.46, mape:94.1, rms:1.5451

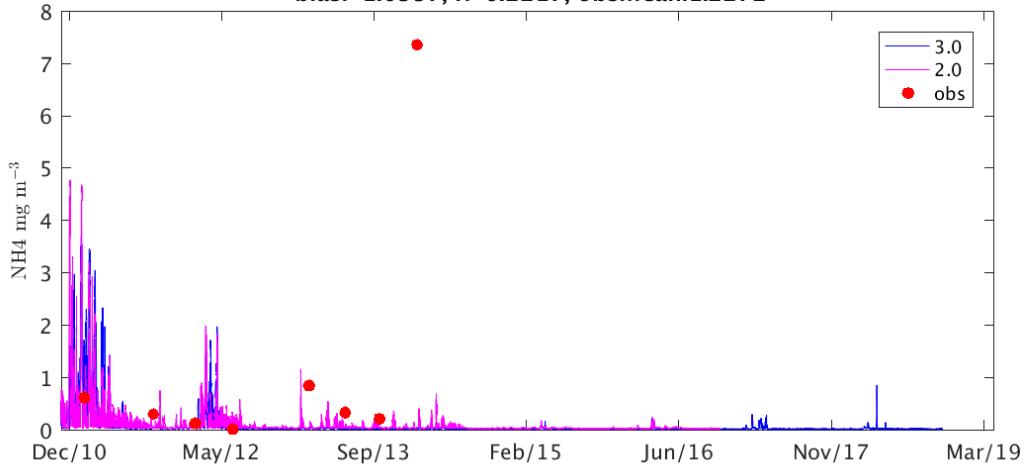
bias:-1.2437, r:0.0224, obsmean:1.2848



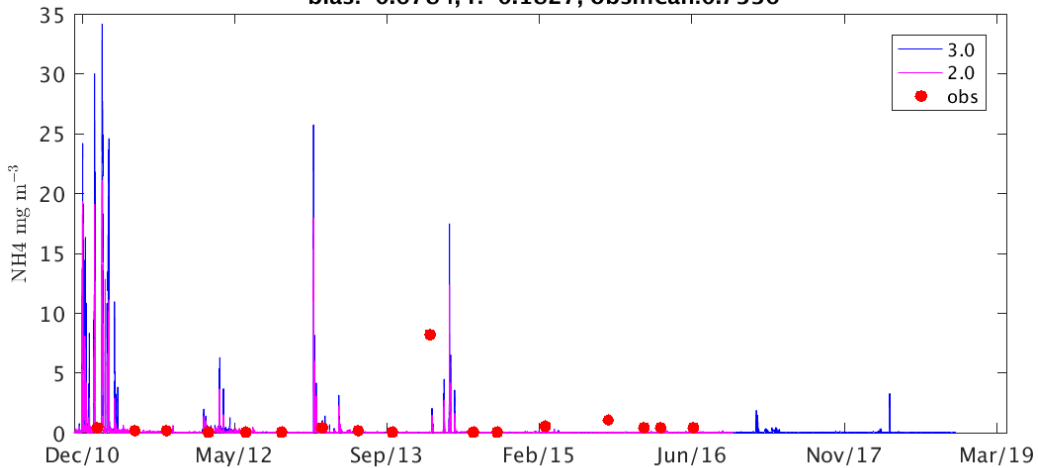
Pelorus686\_28m 3.0 d2:0.73, mape:200.4, rms:2.1900  
 bias:-0.8486, r:0.6116, obsmean:1.4844  
 Pelorus686\_28m 2.0 d2:0.78, mape:456.6, rms:2.1931  
 bias:-0.5783, r:0.6106, obsmean:1.4844



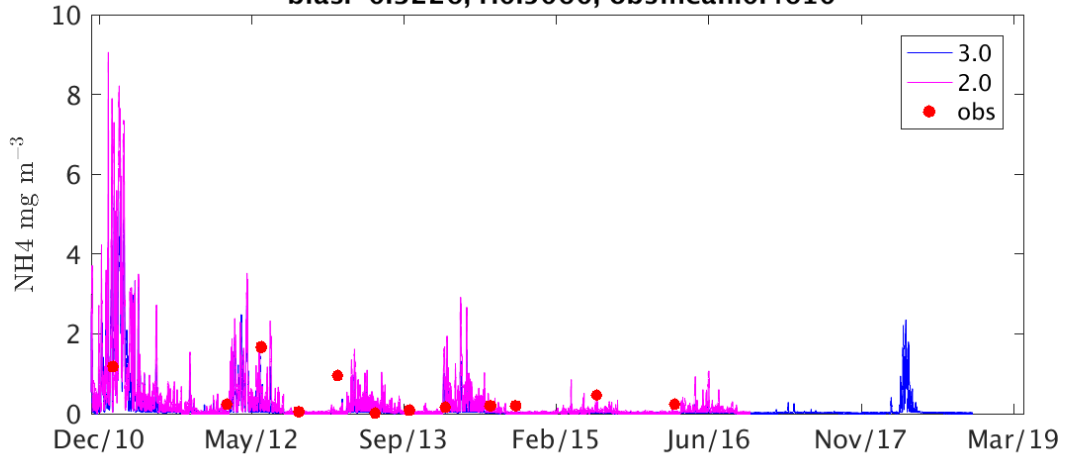
Pelorus686\_14m 3.0 d2:0.32, mape:149.6, rms:2.6190  
 bias:-1.0504, r:-0.1395, obsmean:1.2272  
 Pelorus686\_14m 2.0 d2:0.33, mape:168.4, rms:2.6108  
 bias:-1.0957, r:-0.2217, obsmean:1.2272



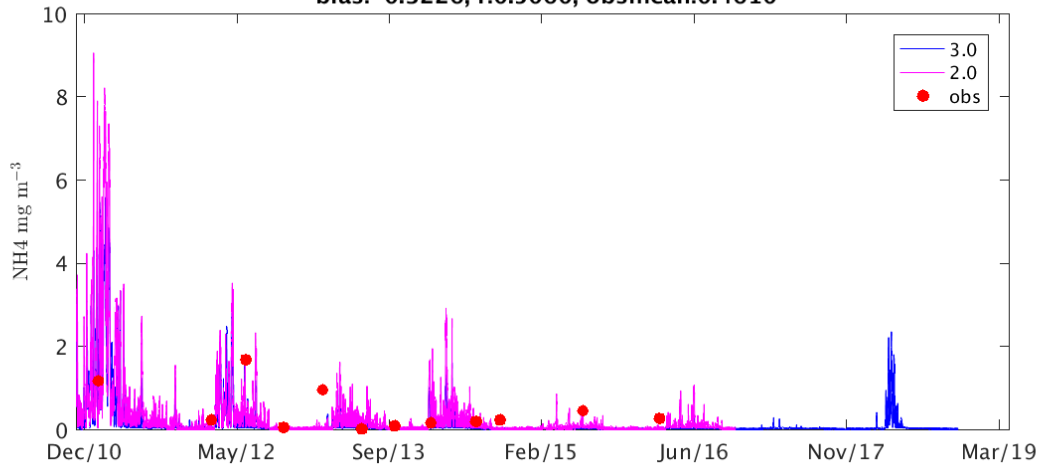
Pelorus686\_0m 3.0 d2:0.23, mape:86.6, rms:2.0129  
 bias:-0.6792, r:-0.1596, obsmean:0.7336  
 Pelorus686\_0m 2.0 d2:0.23, mape:93.8, rms:2.0119  
 bias:-0.6784, r:-0.1827, obsmean:0.7336



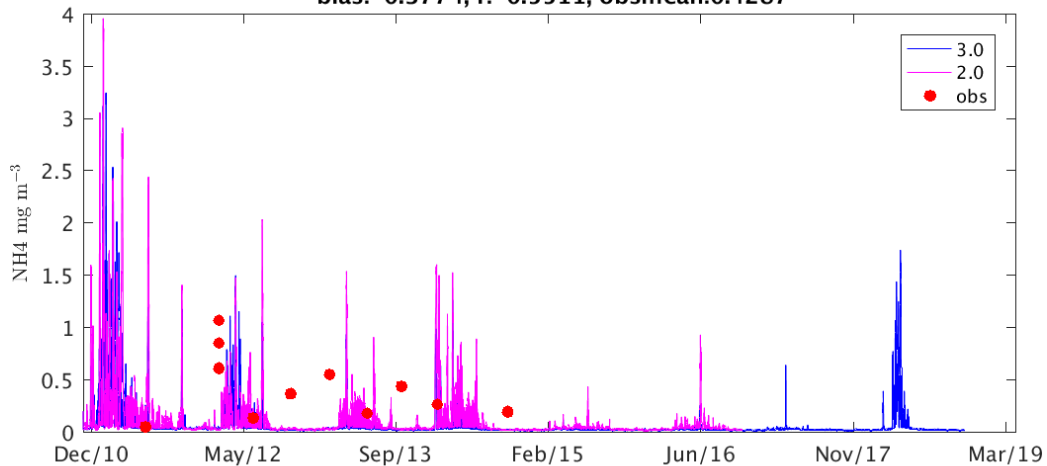
**Russell695\_20m 3.0 d2:0.67, mape:87.2, rms:0.6295**  
**bias:-0.2208, r:0.4974, obsmean:0.4610**  
**Russell695\_20m 2.0 d2:0.58, mape:112.0, rms:0.5415**  
**bias:-0.3226, r:0.5060, obsmean:0.4610**



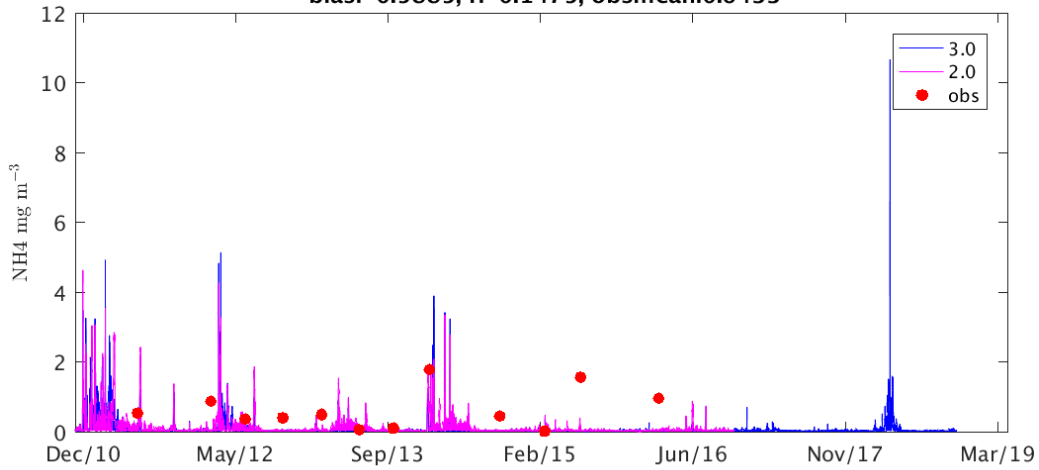
**Russell695\_20m 3.0 d2:0.67, mape:87.2, rms:0.6295**  
**bias:-0.2208, r:0.4974, obsmean:0.4610**  
**Russell695\_20m 2.0 d2:0.58, mape:112.0, rms:0.5415**  
**bias:-0.3226, r:0.5060, obsmean:0.4610**



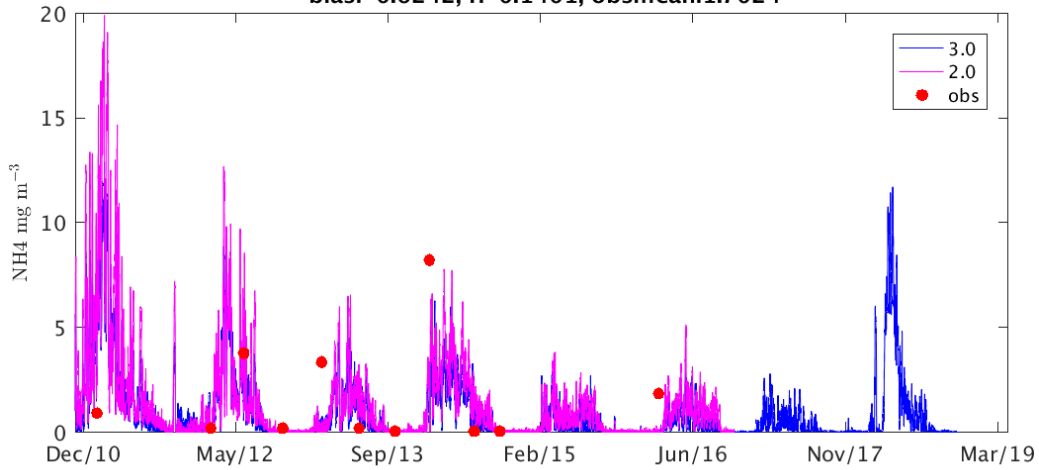
**Russell695\_10m 3.0 d2:0.40, mape:117.4, rms:0.5050**  
**bias:-0.3828, r:-0.4052, obsmean:0.4287**  
**Russell695\_10m 2.0 d2:0.39, mape:112.8, rms:0.5058**  
**bias:-0.3774, r:-0.5511, obsmean:0.4287**



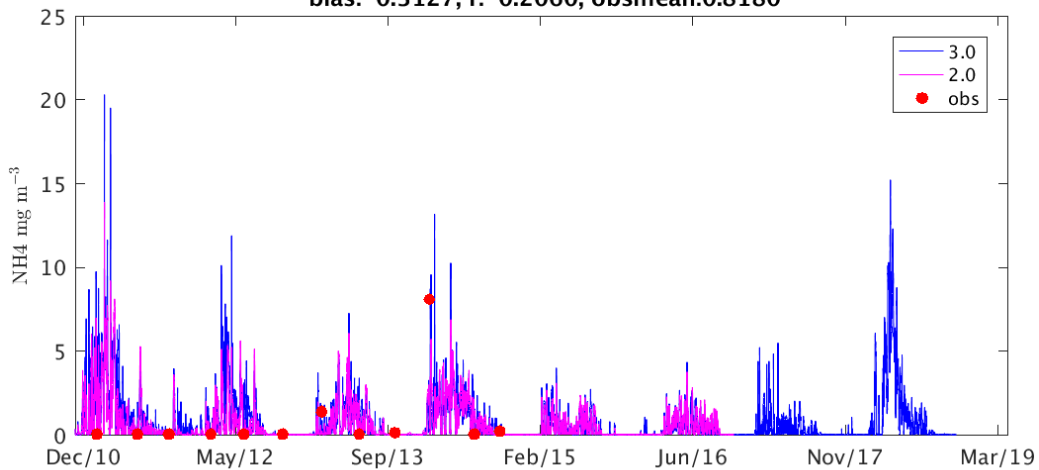
**Russell695\_0m 3.0 d2:0.45, mape:79.9, rms:0.8126**  
**bias:-0.6032, r:-0.1053, obsmean:0.6433**  
**Russell695\_0m 2.0 d2:0.45, mape:82.2, rms:0.8045**  
**bias:-0.5885, r:-0.1475, obsmean:0.6433**



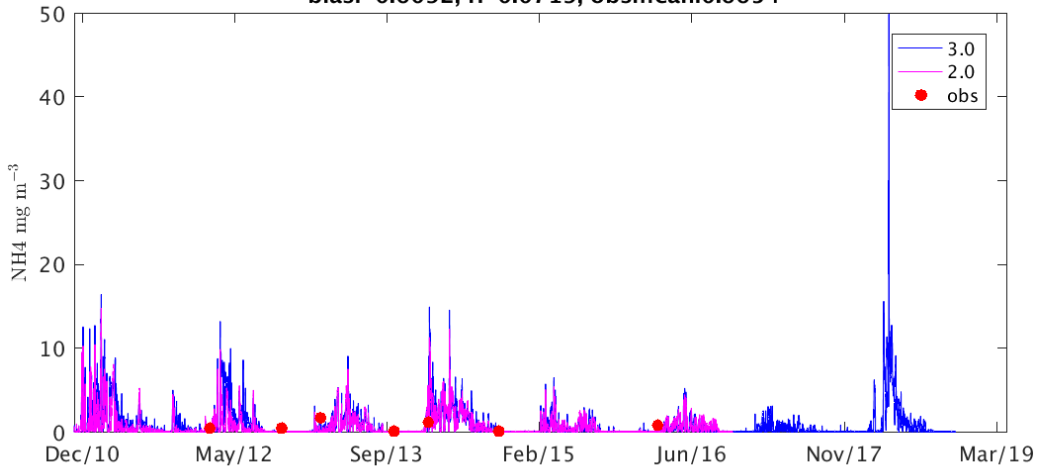
**Highl\_20m 3.0 d2:0.28, mape:440.4, rms:3.1876**  
**bias:-0.7305, r:-0.1468, obsmean:1.7024**  
**Highl\_20m 2.0 d2:0.27, mape:472.2, rms:3.2901**  
**bias:-0.6242, r:-0.1401, obsmean:1.7024**



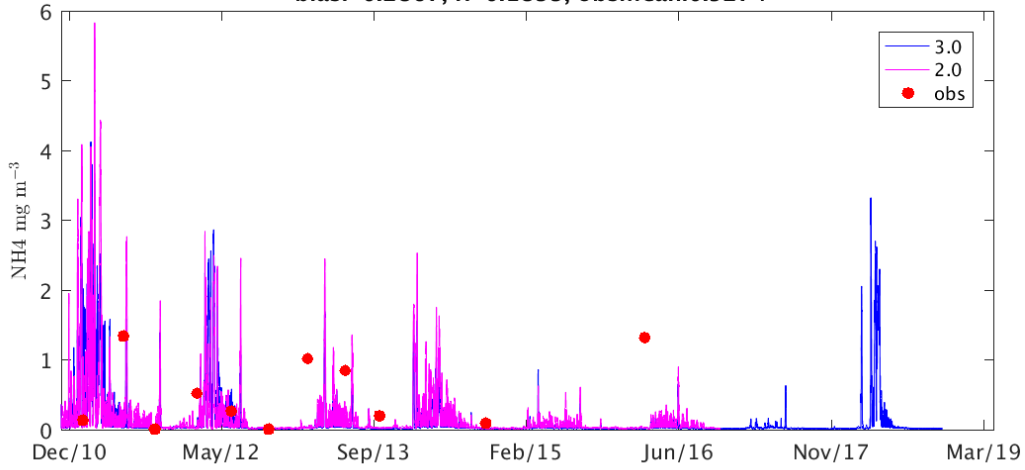
**Highl\_10m 3.0 d2:0.12, mape:74.1, rms:2.8698**  
**bias:-0.0183, r:-0.1929, obsmean:0.8180**  
**Highl\_10m 2.0 d2:0.17, mape:91.2, rms:2.5441**  
**bias:-0.3127, r:-0.2060, obsmean:0.8180**



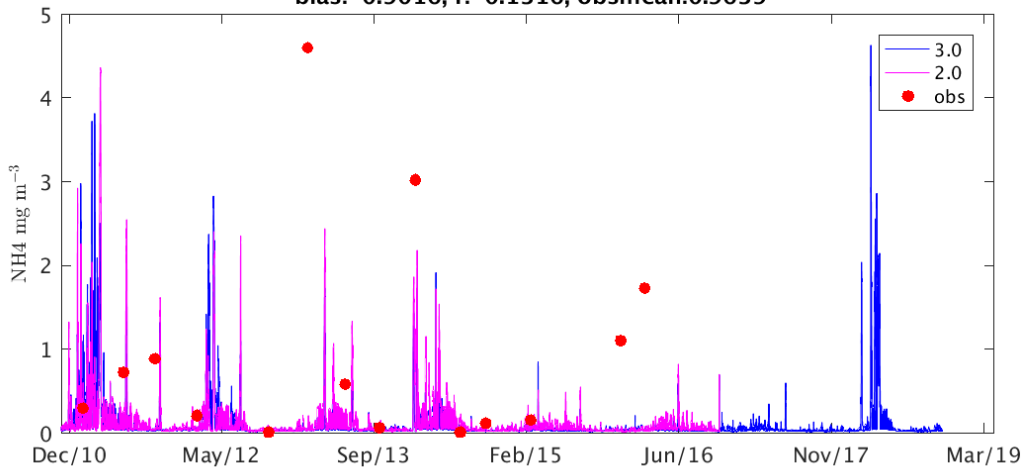
High1697\_0m 3.0 d2:0.45, mape:107.1, rms:0.8318  
 bias:-0.6026, r:-0.4427, obsmean:0.6654  
 High1697\_0m 2.0 d2:0.46, mape:121.9, rms:0.8326  
 bias:-0.6092, r:-0.0719, obsmean:0.6654



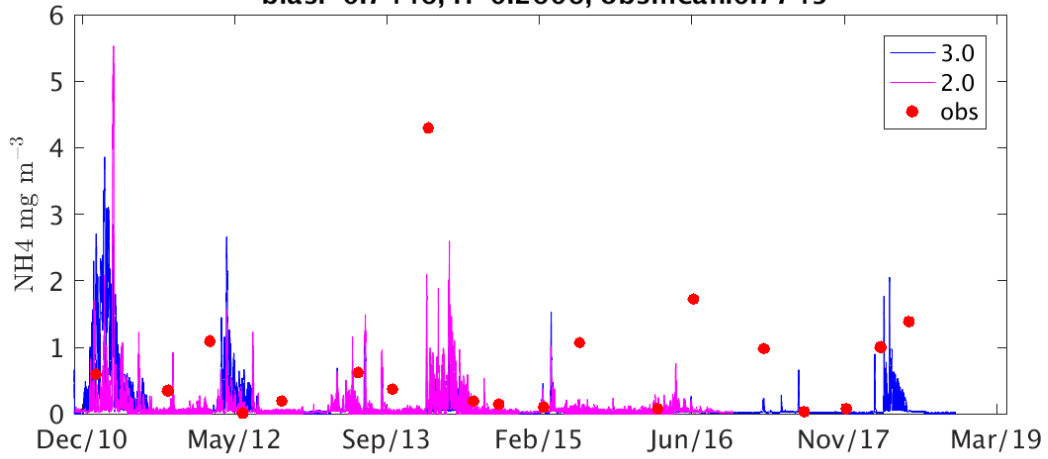
FitzCoral852\_15m 3.0 d2:0.25, mape:246.1, rms:1.0254  
 bias:-0.2191, r:-0.2335, obsmean:0.5274  
 FitzCoral852\_15m 2.0 d2:0.34, mape:203.5, rms:0.8421  
 bias:-0.2867, r:-0.1899, obsmean:0.5274



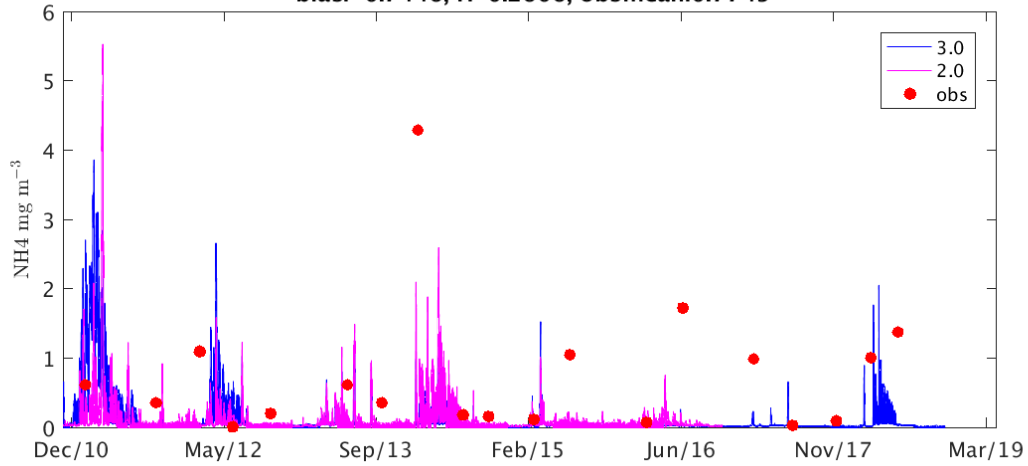
FitzCoral852\_0m 3.0 d2:0.38, mape:102.3, rms:1.6010  
 bias:-0.8564, r:-0.1490, obsmean:0.9639  
 FitzCoral852\_0m 2.0 d2:0.40, mape:82.5, rms:1.5815  
 bias:-0.9016, r:-0.1316, obsmean:0.9639



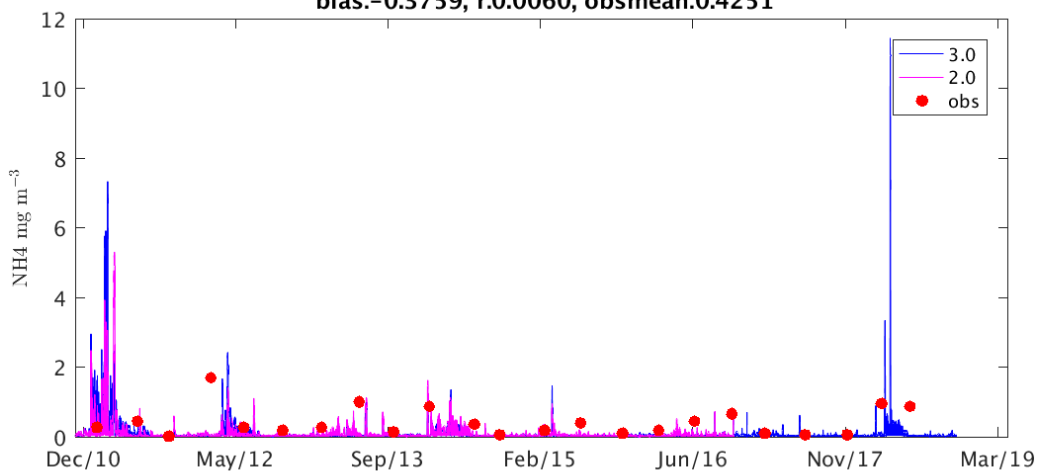
**Yorkeys519\_8m 3.0 d2:0.37, mape:284.1, rms:1.2314**  
**bias:-0.6240, r:-0.0555, obsmean:0.7553**  
**Yorkeys519\_8m 2.0 d2:0.38, mape:181.6, rms:1.3230**  
**bias:-0.7446, r:-0.2606, obsmean:0.7745**



**Yorkeys519\_8m 3.0 d2:0.37, mape:284.1, rms:1.2314**  
**bias:-0.6240, r:-0.0555, obsmean:0.7553**  
**Yorkeys519\_8m 2.0 d2:0.38, mape:181.6, rms:1.3230**  
**bias:-0.7446, r:-0.2606, obsmean:0.7745**

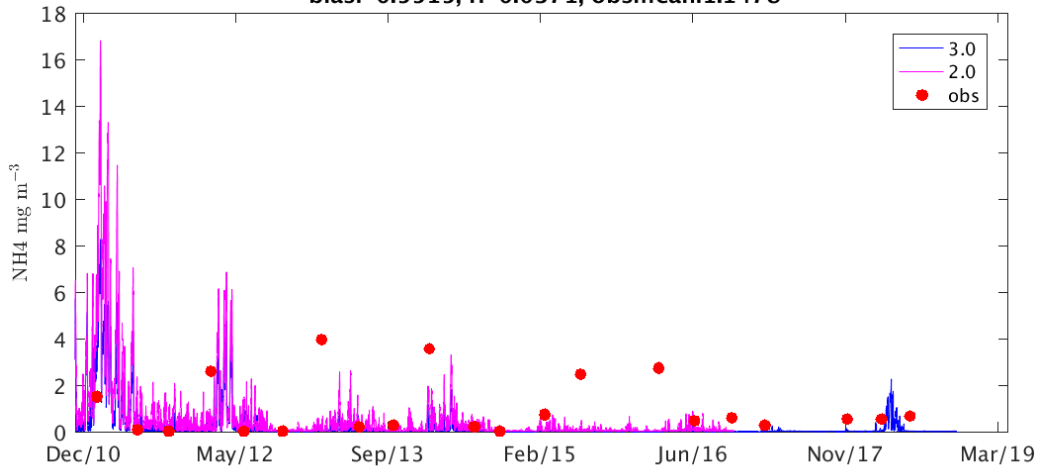


**Yorkeys519\_0m 3.0 d2:0.43, mape:84.5, rms:0.5556**  
**bias:-0.3711, r:-0.0683, obsmean:0.4225**  
**Yorkeys519\_0m 2.0 d2:0.42, mape:93.7, rms:0.5498**  
**bias:-0.3759, r:0.0060, obsmean:0.4251**

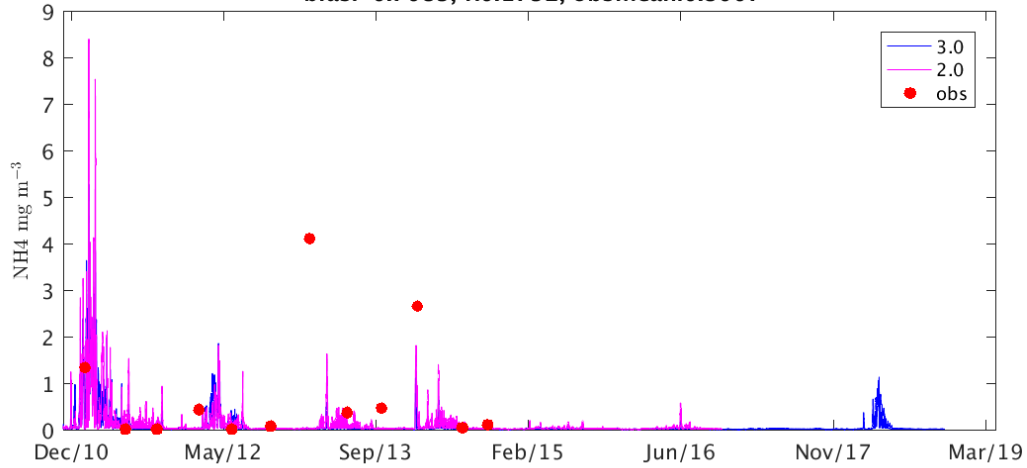




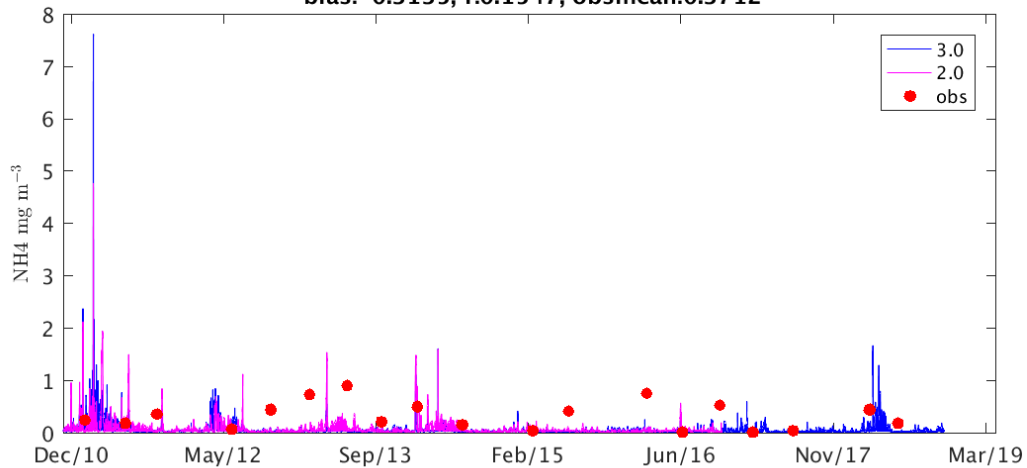
Green830\_36m 3.0 d2:0.44, mape:109.7, rms:1.5635  
bias:-0.7596, r:0.0206, obsmean:1.0298  
Green830\_36m 2.0 d2:0.39, mape:211.8, rms:1.8060  
bias:-0.5515, r:-0.0371, obsmean:1.1478



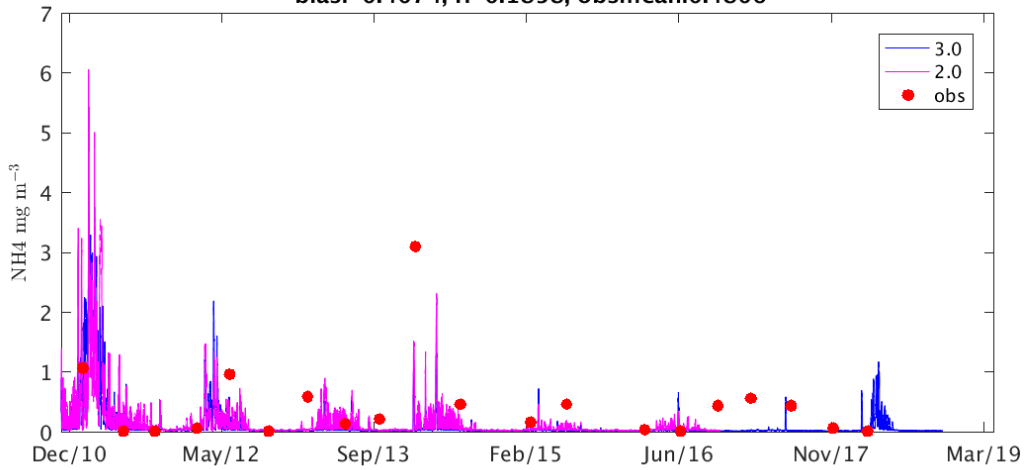
Green830\_18m 3.0 d2:0.41, mape:85.3, rms:1.4584  
bias:-0.7597, r:0.0662, obsmean:0.8007  
Green830\_18m 2.0 d2:0.40, mape:75.8, rms:1.4221  
bias:-0.7089, r:0.1792, obsmean:0.8007



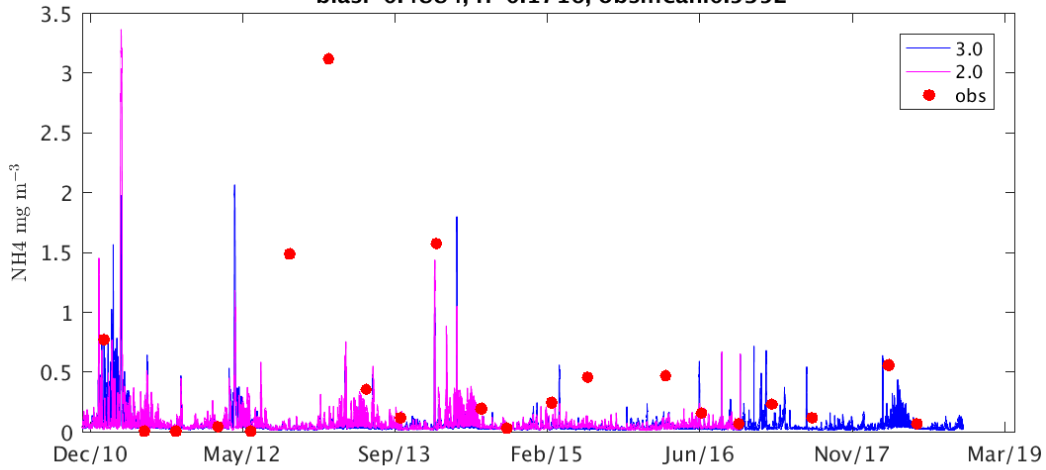
Green830\_0m 3.0 d2:0.46, mape:376.2, rms:0.3936  
bias:-0.2920, r:-0.0007, obsmean:0.3296  
Green830\_0m 2.0 d2:0.46, mape:533.1, rms:0.4101  
bias:-0.3135, r:0.1547, obsmean:0.3712



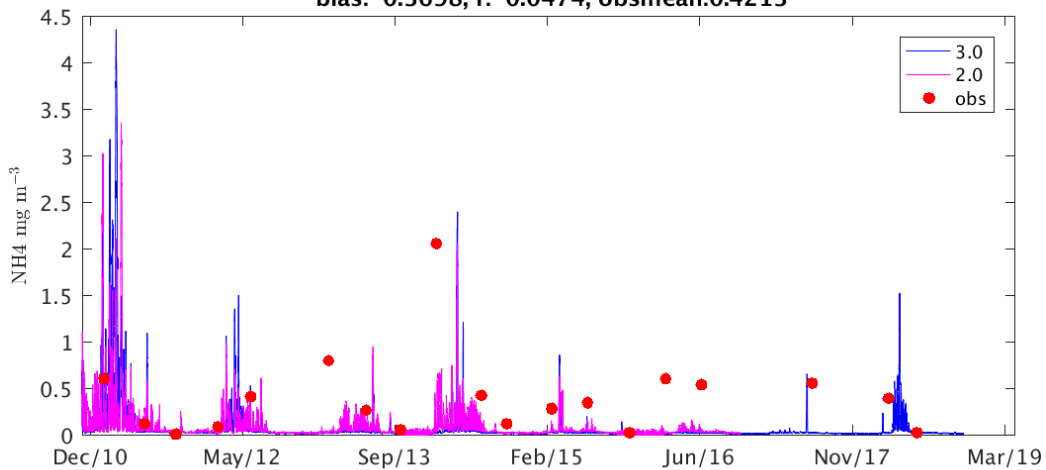
**Doublel520\_18m 3.0 d2:0.38, mape:184.1, rms:0.7741**  
**bias:-0.3811, r:0.2004, obsmean:0.4387**  
**Doublel520\_18m 2.0 d2:0.33, mape:310.0, rms:0.8726**  
**bias:-0.4074, r:-0.1858, obsmean:0.4806**



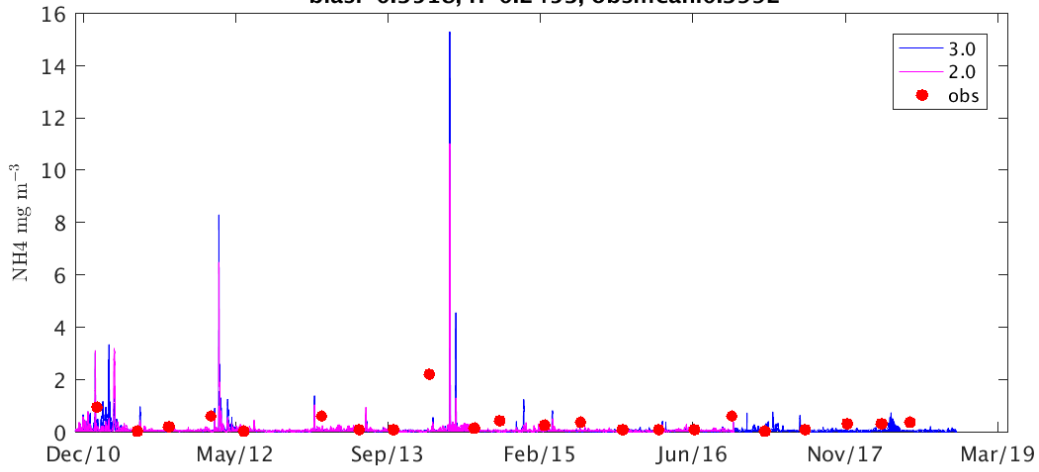
**Doublel520\_0m 3.0 d2:0.37, mape:76.4, rms:0.8572**  
**bias:-0.4441, r:-0.0343, obsmean:0.4800**  
**Doublel520\_0m 2.0 d2:0.39, mape:73.3, rms:0.9400**  
**bias:-0.4884, r:-0.1716, obsmean:0.5352**



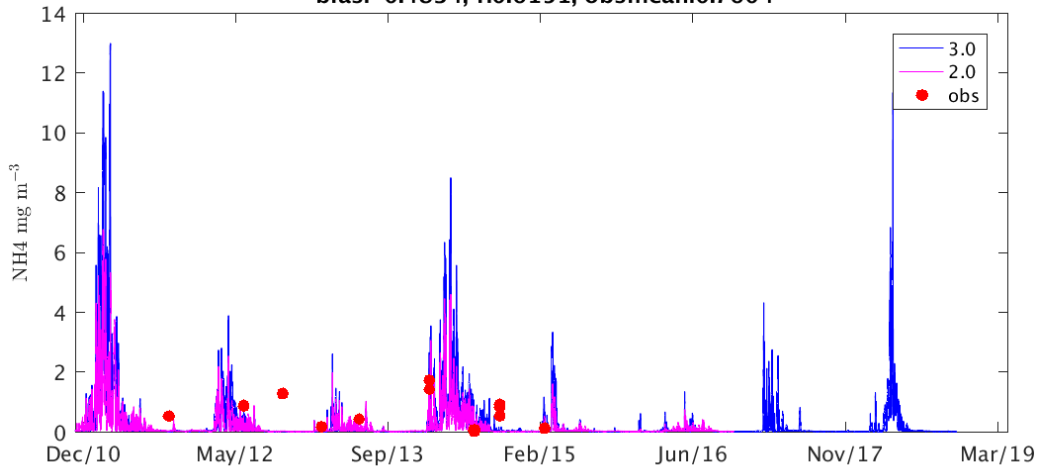
**PortD\_15m 3.0 d2:0.39, mape:81.6, rms:0.5820**  
**bias:-0.3682, r:0.0638, obsmean:0.4063**  
**PortD\_15m 2.0 d2:0.39, mape:79.5, rms:0.6096**  
**bias:-0.3698, r:-0.0474, obsmean:0.4213**



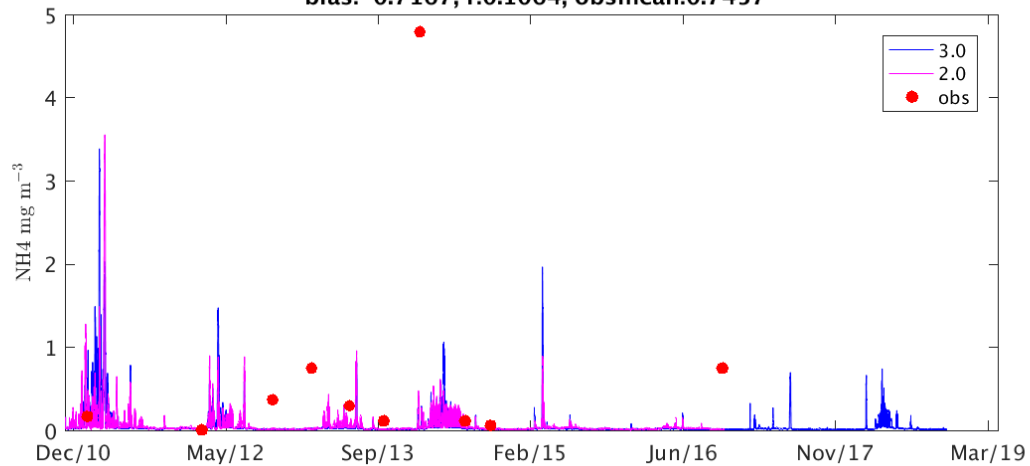
PortD\_0m 3.0 d2:0.37, mape:78.7, rms:0.5723  
 bias:-0.3190, r:-0.2731, obsmean:0.3559  
 PortD\_0m 2.0 d2:0.38, mape:74.0, rms:0.6351  
 bias:-0.3518, r:-0.2453, obsmean:0.3992



Snap\_10m 3.0 d2:0.62, mape:112.4, rms:0.6452  
 bias:-0.4901, r:0.7052, obsmean:0.7604  
 Snap\_10m 2.0 d2:0.59, mape:153.0, rms:0.6650  
 bias:-0.4834, r:0.6151, obsmean:0.7604



CapeTrib356\_10m 3.0 d2:0.33, mape:81.7, rms:1.5471  
 bias:-0.7215, r:0.1180, obsmean:0.7457  
 CapeTrib356\_10m 2.0 d2:0.33, mape:78.3, rms:1.5444  
 bias:-0.7167, r:0.1064, obsmean:0.7457



## 15. Simulated DON assessment against Long Term Monitoring

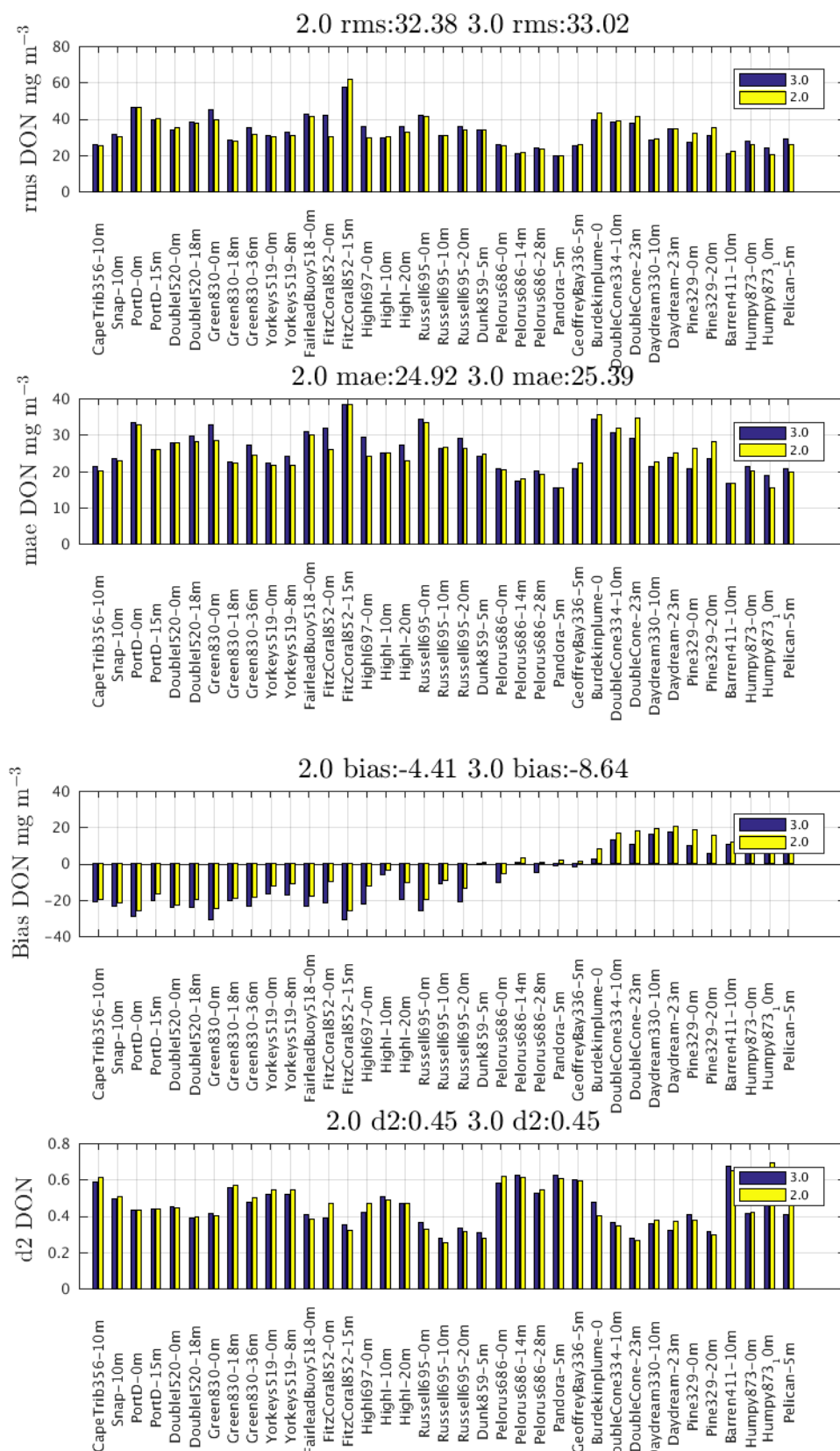
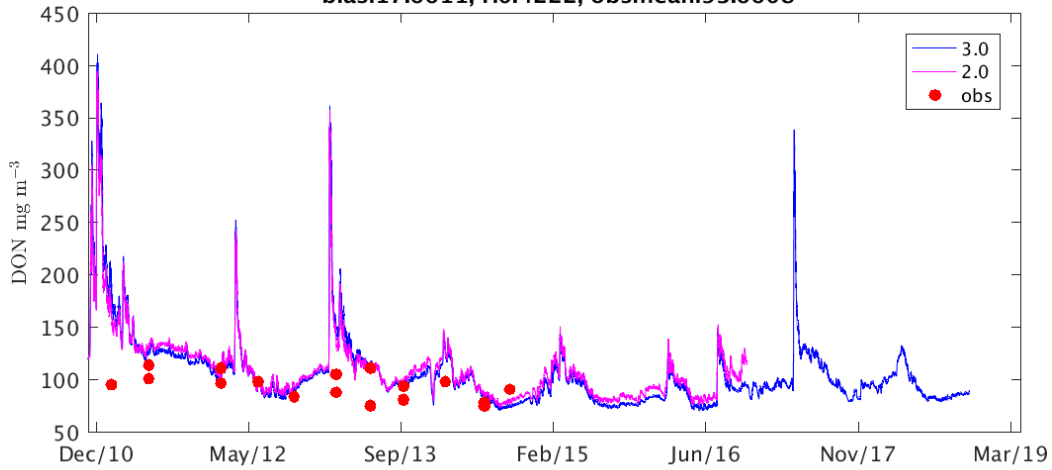
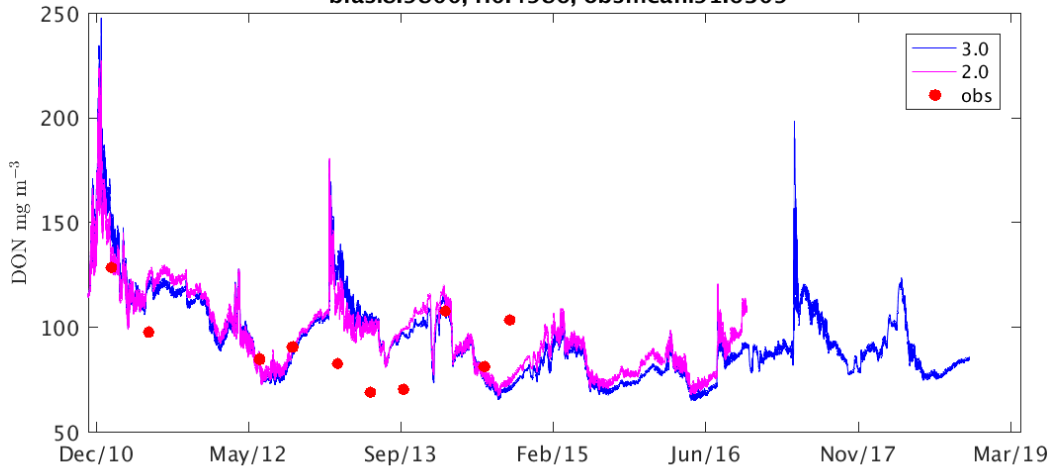


Figure 10 Metrics for Long Term Monitoring sites DON assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

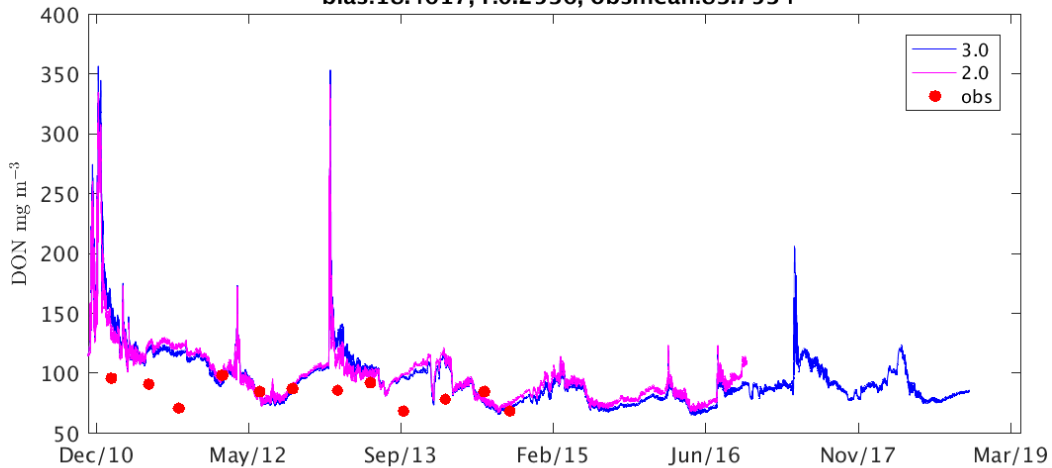
**Pelican\_5m 3.0 d2:0.41, mape:22.5, rms:28.8852**  
**bias:17.3420, r:0.3556, obsmean:93.6608**  
**Pelican\_5m 2.0 d2:0.46, mape:21.7, rms:25.9921**  
**bias:17.6611, r:0.4222, obsmean:93.6608**



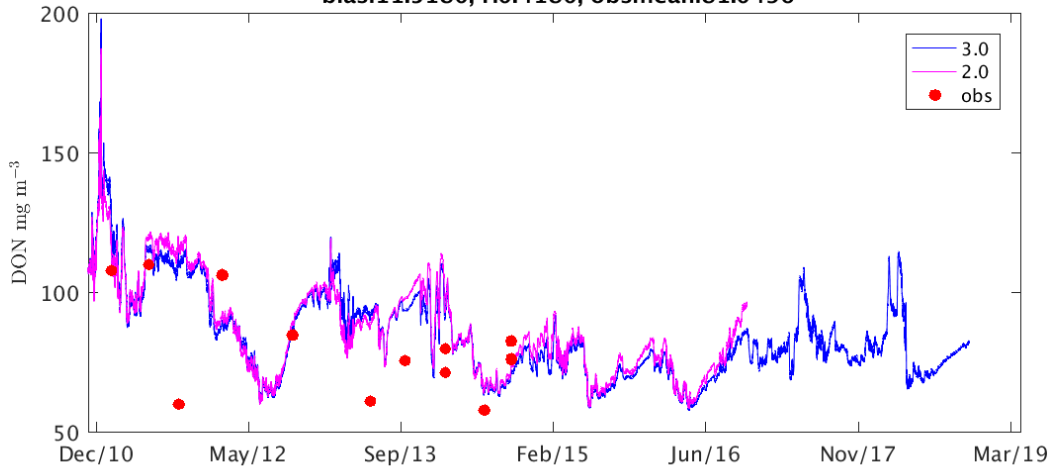
**Humpy873\_10m 3.0 d2:0.67, mape:22.0, rms:23.8206**  
**bias:10.7781, r:0.4829, obsmean:91.6309**  
**Humpy873\_10m 2.0 d2:0.69, mape:18.5, rms:20.0697**  
**bias:8.9800, r:0.4986, obsmean:91.6309**



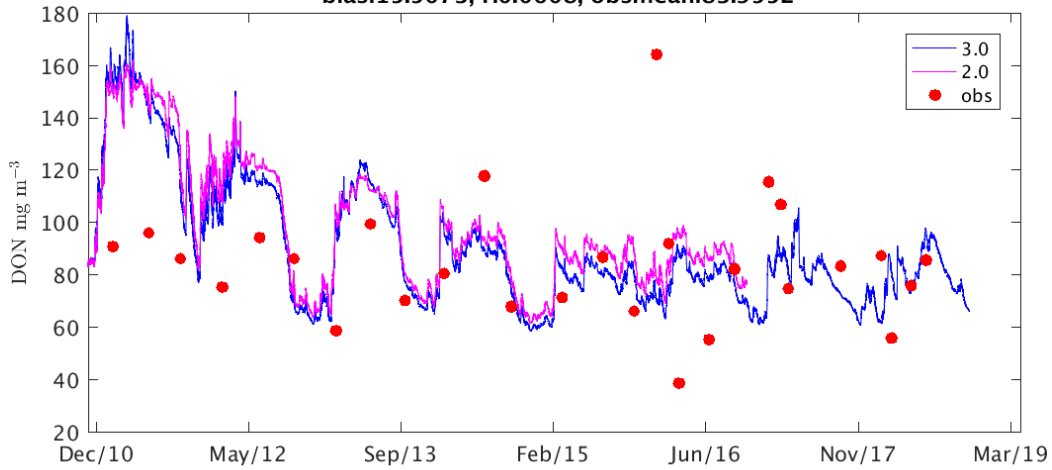
**Humpy873\_0m 3.0 d2:0.41, mape:26.1, rms:27.8723**  
**bias:19.1030, r:0.3453, obsmean:83.7534**  
**Humpy873\_0m 2.0 d2:0.42, mape:24.9, rms:25.8009**  
**bias:18.4617, r:0.2536, obsmean:83.7534**



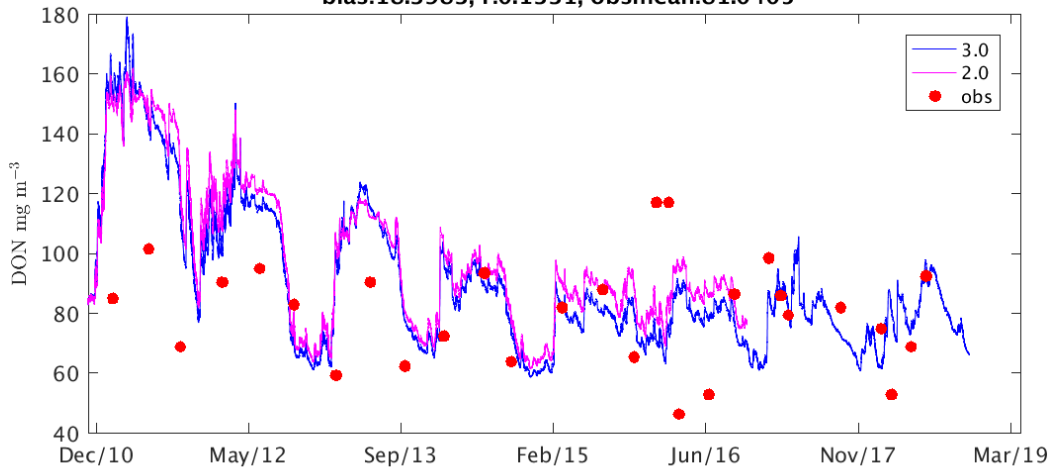
Barren411\_10m 3.0 d2:0.67, mape:23.4, rms:21.0593  
 bias:10.4258, r:0.4532, obsmean:81.0496  
 Barren411\_10m 2.0 d2:0.65, mape:23.7, rms:21.9006  
 bias:11.5180, r:0.4180, obsmean:81.0496



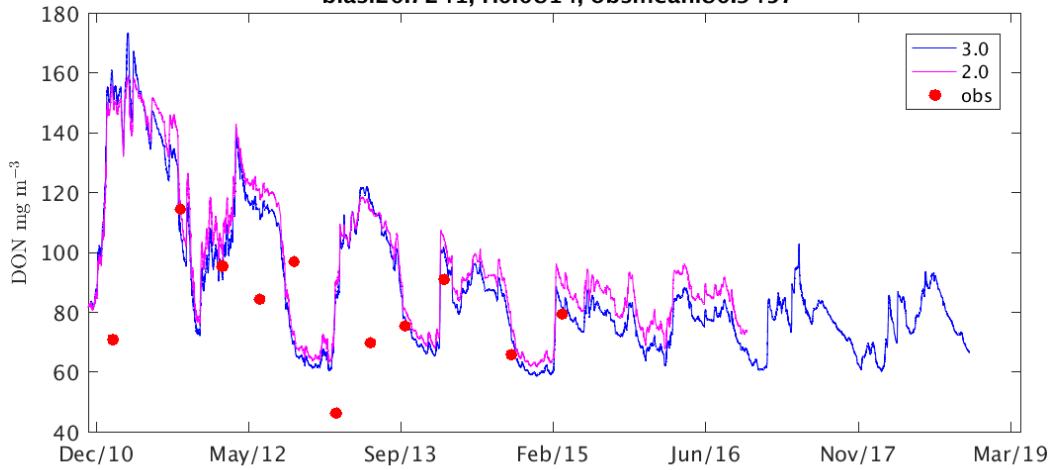
Pine329\_20m 3.0 d2:0.32, mape:29.1, rms:30.6085  
 bias:5.7444, r:0.0798, obsmean:84.4370  
 Pine329\_20m 2.0 d2:0.29, mape:36.8, rms:35.2578  
 bias:15.5073, r:0.0608, obsmean:83.9552



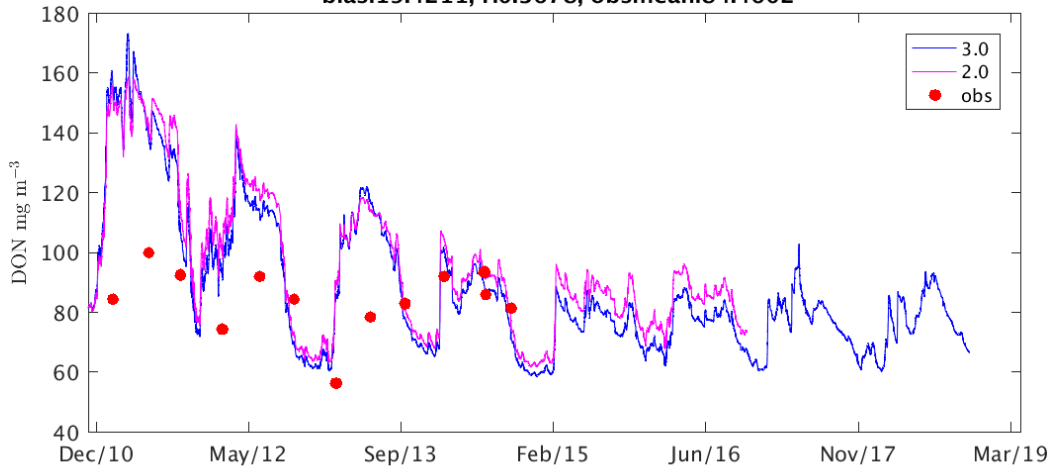
Pine329\_0m 3.0 d2:0.41, mape:27.6, rms:26.7687  
 bias:9.6345, r:0.1666, obsmean:80.5243  
 Pine329\_0m 2.0 d2:0.37, mape:36.1, rms:31.9446  
 bias:18.3983, r:0.1331, obsmean:81.0405



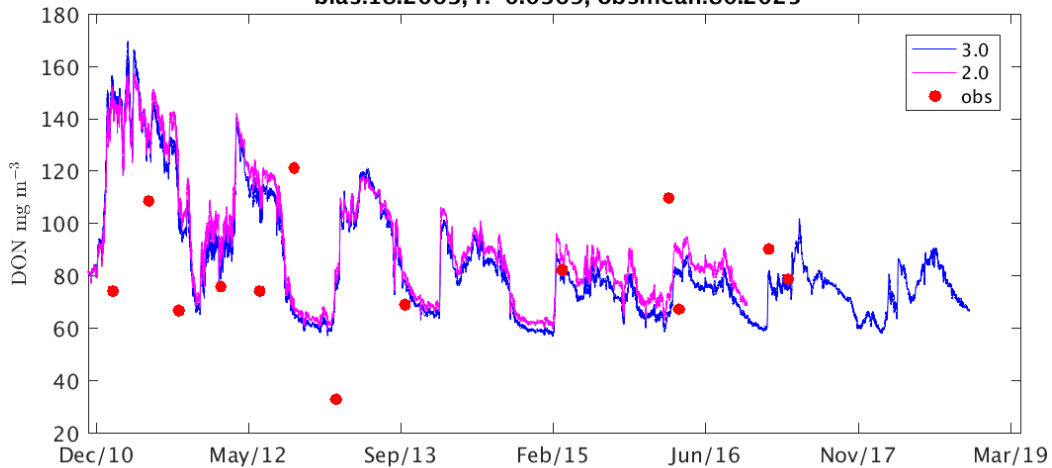
Daydream\_23m 3.0 d2:0.32, mape:33.9, rms:34.3948  
 bias:17.1074, r:0.0127, obsmean:80.9457  
 Daydream\_23m 2.0 d2:0.37, mape:36.1, rms:34.2327  
 bias:20.7241, r:0.0814, obsmean:80.9457



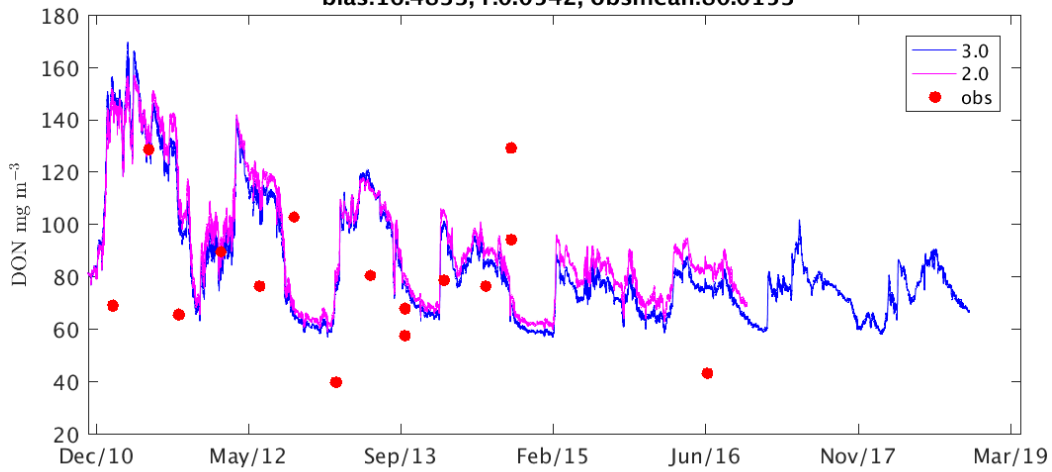
Daydream330\_10m 3.0 d2:0.35, mape:26.1, rms:28.4454  
 bias:16.1303, r:0.3373, obsmean:84.4602  
 Daydream330\_10m 2.0 d2:0.37, mape:27.5, rms:29.0659  
 bias:19.4211, r:0.3678, obsmean:84.4602



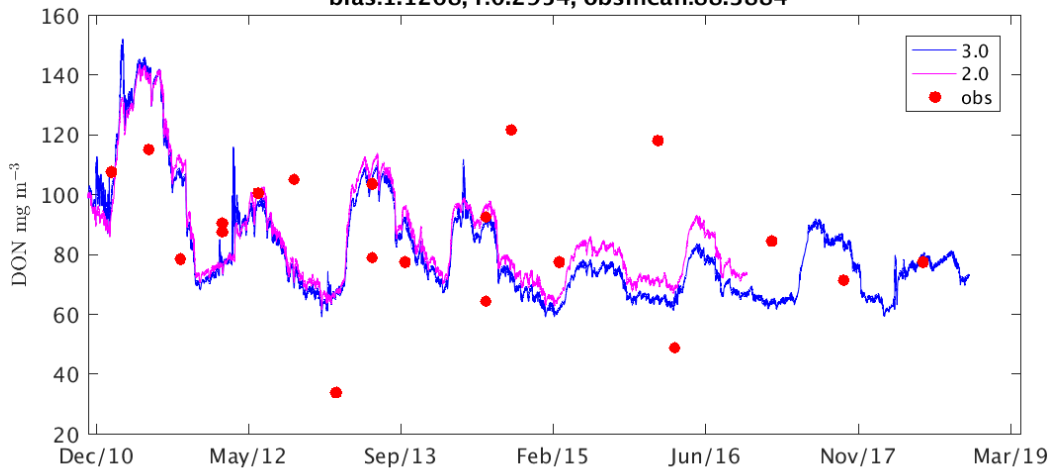
DoubleCone\_23m 3.0 d2:0.28, mape:40.1, rms:37.7251  
 bias:10.4776, r:-0.0423, obsmean:80.8608  
 DoubleCone\_23m 2.0 d2:0.27, mape:49.4, rms:41.0062  
 bias:18.2063, r:-0.0369, obsmean:80.2025



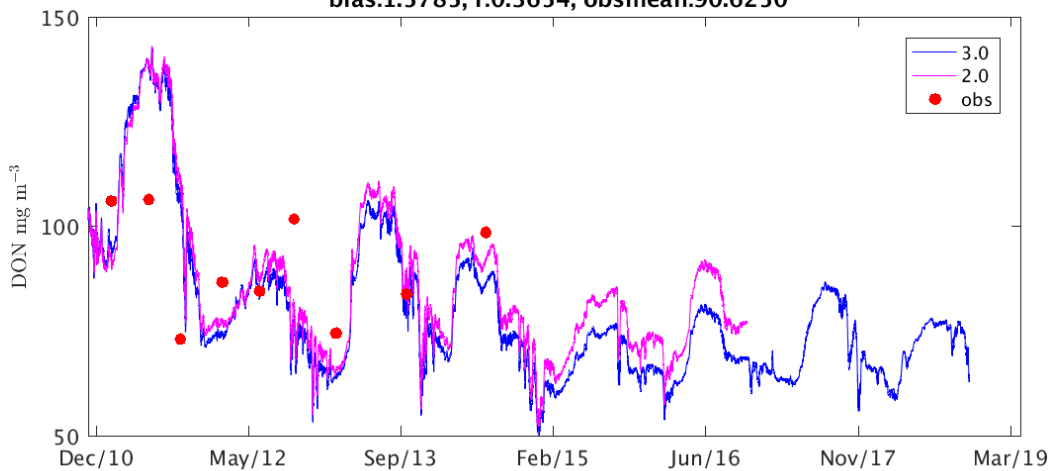
**DoubleCone334\_10m 3.0 d2:0.36, mape:43.1, rms:38.1129**  
**bias:13.2573, r:0.0655, obsmean:80.0153**  
**DoubleCone334\_10m 2.0 d2:0.34, mape:46.1, rms:38.4647**  
**bias:16.4833, r:0.0542, obsmean:80.0153**



**GeoffreyBay336\_5m 3.0 d2:0.60, mape:26.5, rms:25.0887**  
**bias:-1.7775, r:0.3018, obsmean:87.2797**  
**GeoffreyBay336\_5m 2.0 d2:0.59, mape:28.7, rms:25.7535**  
**bias:1.1268, r:0.2954, obsmean:88.3884**

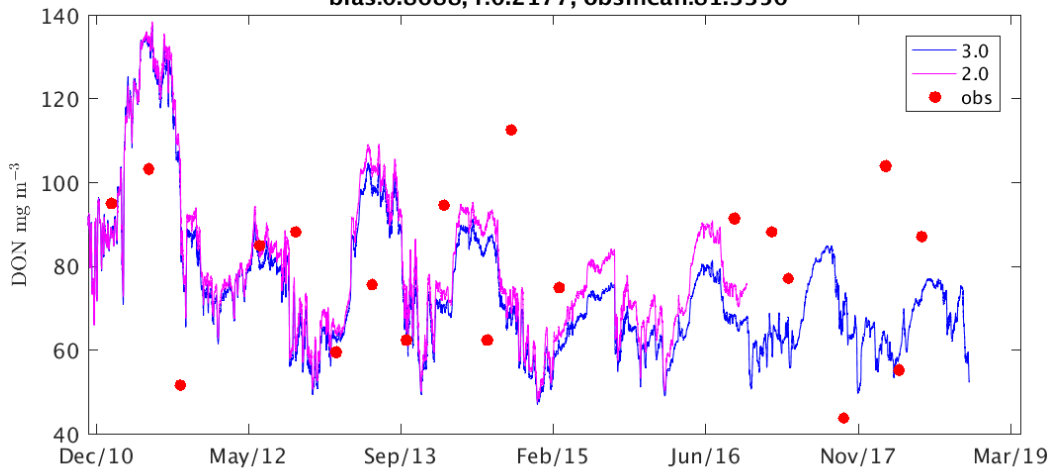


**Pandora\_5m 3.0 d2:0.63, mape:17.0, rms:19.3077**  
**bias:-0.9496, r:0.4027, obsmean:90.6250**  
**Pandora\_5m 2.0 d2:0.60, mape:17.3, rms:19.5210**  
**bias:1.5785, r:0.3654, obsmean:90.6250**

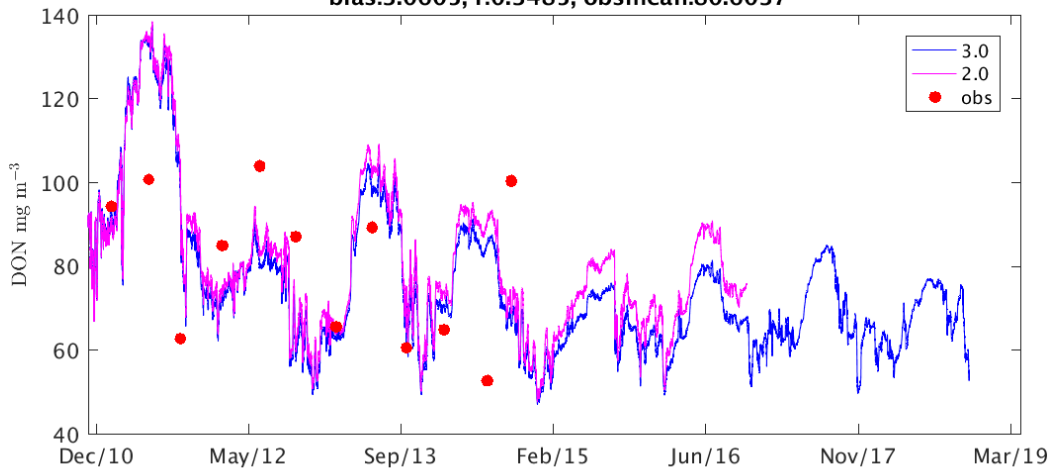




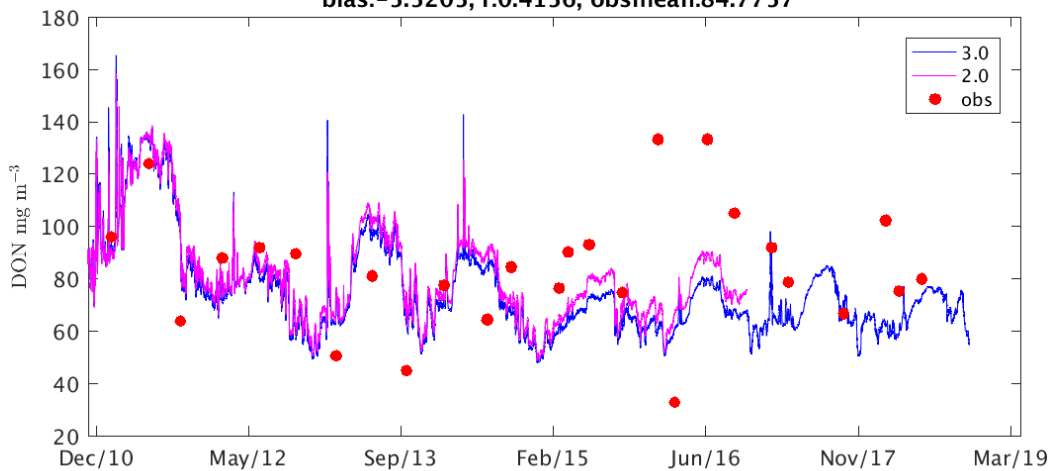
**Pelorus686\_28m 3.0 d2:0.53, mape:25.8, rms:23.7764**  
**bias:-4.7773, r:0.1881, obsmean:79.6139**  
**Pelorus686\_28m 2.0 d2:0.54, mape:24.4, rms:23.1611**  
**bias:0.8688, r:0.2177, obsmean:81.3356**



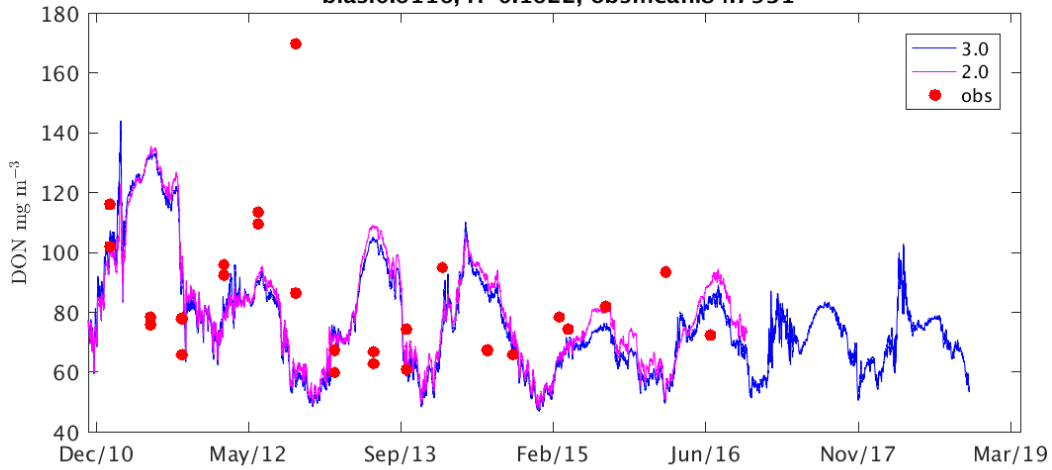
**Pelorus686\_14m 3.0 d2:0.62, mape:21.6, rms:20.8488**  
**bias:0.5789, r:0.3669, obsmean:80.6037**  
**Pelorus686\_14m 2.0 d2:0.61, mape:23.0, rms:21.1986**  
**bias:3.0605, r:0.3485, obsmean:80.6037**



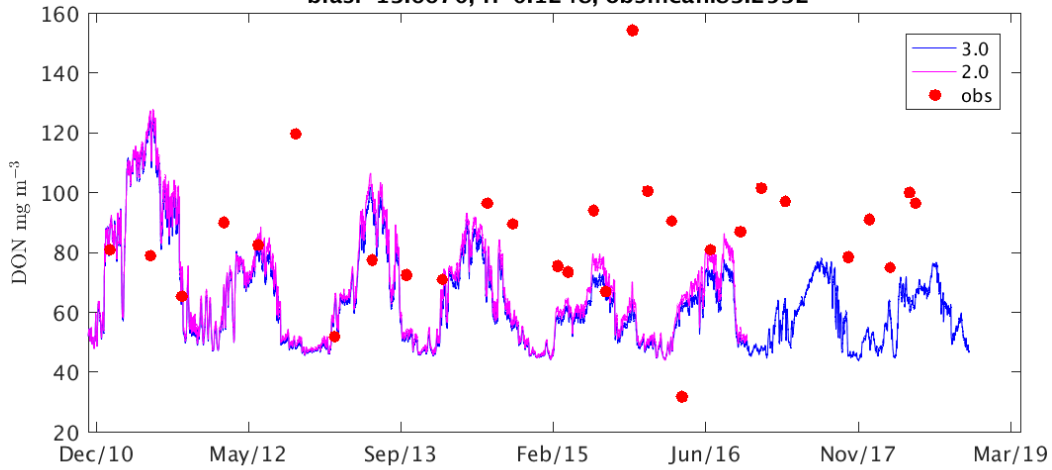
**Pelorus686\_0m 3.0 d2:0.58, mape:25.4, rms:25.6501**  
**bias:-10.7214, r:0.3393, obsmean:84.2641**  
**Pelorus686\_0m 2.0 d2:0.62, mape:26.7, rms:24.8950**  
**bias:-5.5205, r:0.4156, obsmean:84.7757**



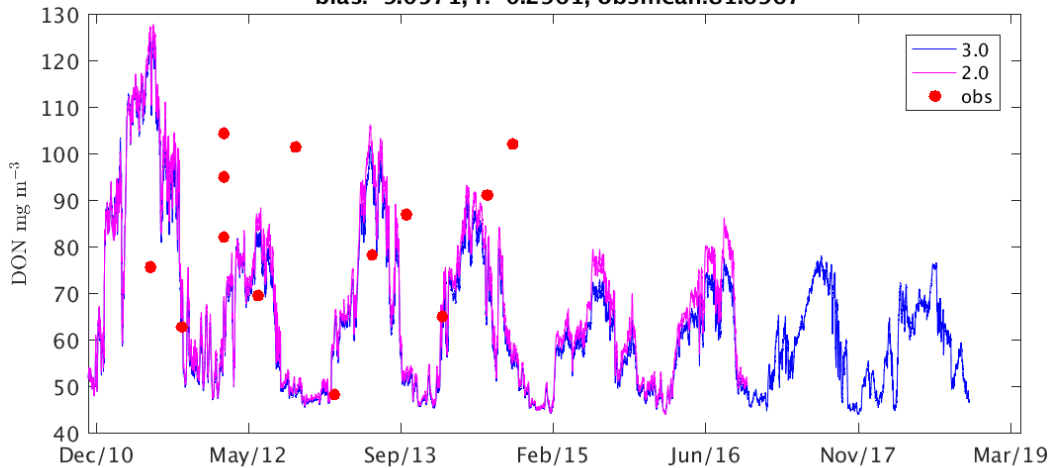
**Dunk859\_5m 3.0 d2:0.31, mape:27.7, rms:33.5612**  
**bias:-0.7276, r:-0.1129, obsmean:84.7931**  
**Dunk859\_5m 2.0 d2:0.28, mape:28.7, rms:33.9572**  
**bias:0.6116, r:-0.1622, obsmean:84.7931**



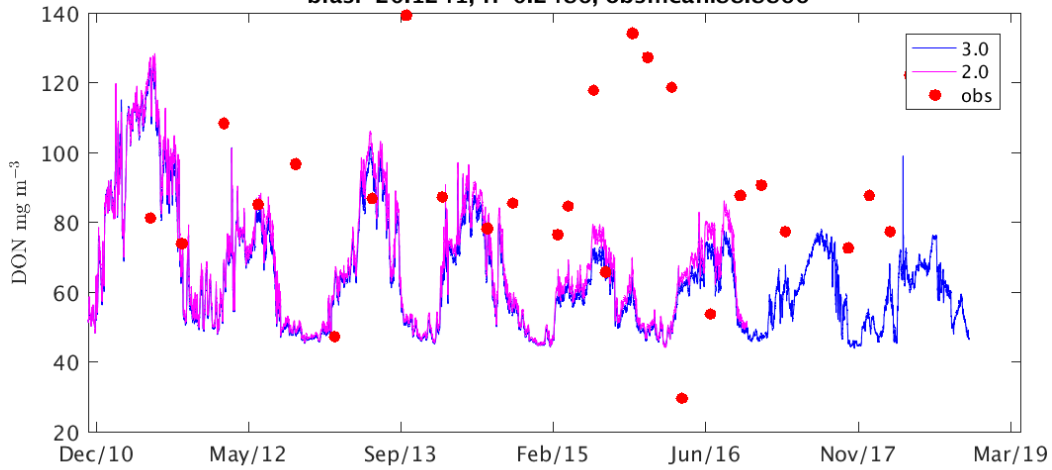
**Russell695\_20m 3.0 d2:0.33, mape:33.2, rms:35.5381**  
**bias:-20.9920, r:-0.1649, obsmean:85.1977**  
**Russell695\_20m 2.0 d2:0.31, mape:31.1, rms:34.0428**  
**bias:-13.6670, r:-0.1248, obsmean:83.2532**



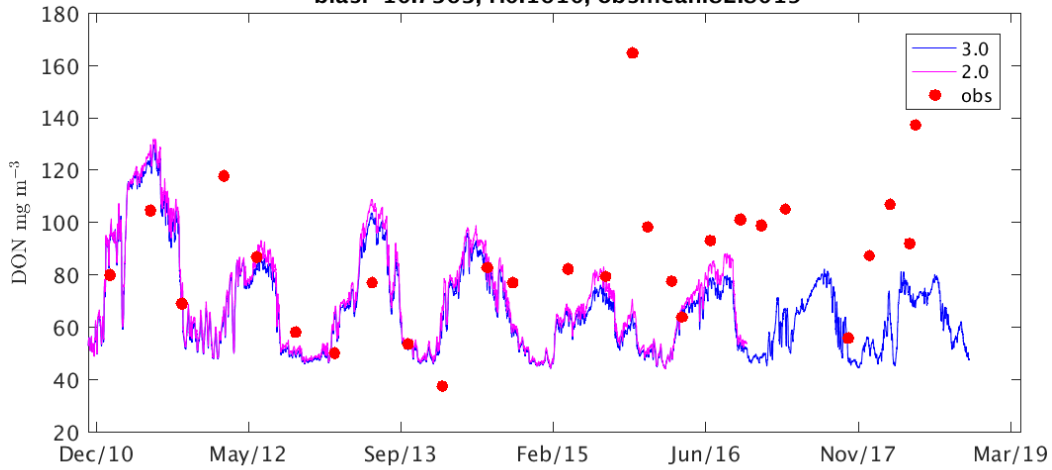
**Russell695\_10m 3.0 d2:0.28, mape:30.4, rms:30.8196**  
**bias:-11.0818, r:-0.2844, obsmean:81.6967**  
**Russell695\_10m 2.0 d2:0.25, mape:31.2, rms:30.9039**  
**bias:-9.0571, r:-0.2961, obsmean:81.6967**



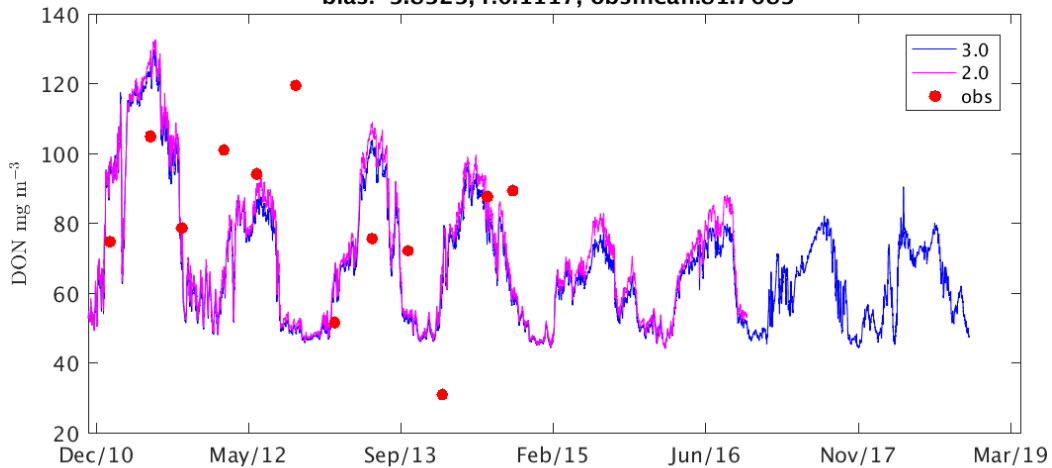
Russell695\_0m 3.0 d2:0.36, mape:36.9, rms:41.8686  
bias:-25.9955, r:-0.1984, obsmean:90.0550  
Russell695\_0m 2.0 d2:0.32, mape:37.5, rms:41.4331  
bias:-20.1241, r:-0.2486, obsmean:88.8866



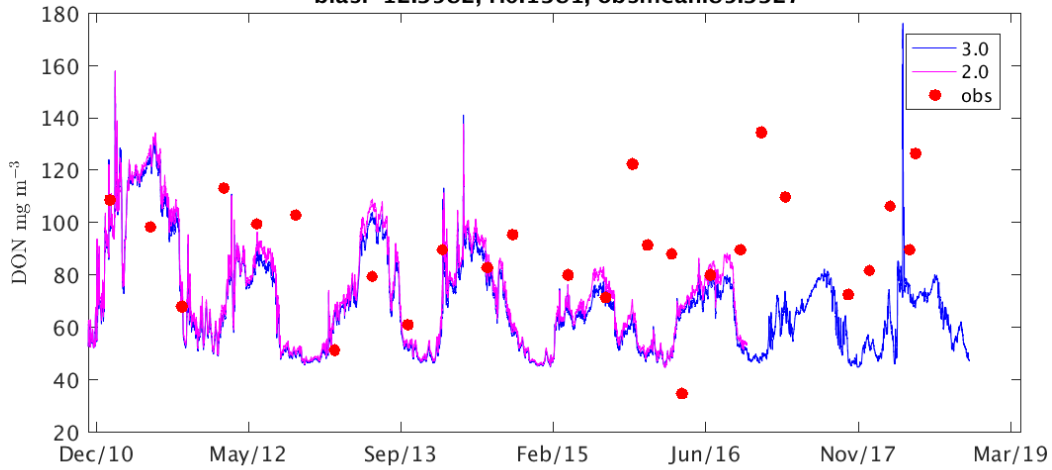
Highl\_20m 3.0 d2:0.47, mape:28.8, rms:35.7884  
bias:-19.9281, r:0.1298, obsmean:86.6509  
Highl\_20m 2.0 d2:0.47, mape:25.8, rms:32.3114  
bias:-10.7363, r:0.1610, obsmean:82.8019



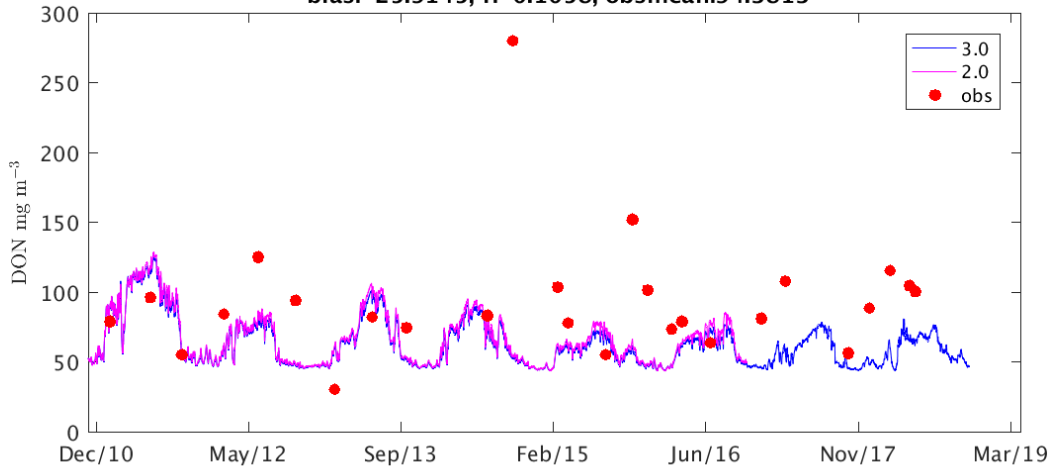
Highl\_10m 3.0 d2:0.51, mape:33.5, rms:29.7411  
bias:-6.4812, r:0.1271, obsmean:81.7683  
Highl\_10m 2.0 d2:0.49, mape:34.4, rms:30.0727  
bias:-3.8323, r:0.1117, obsmean:81.7683



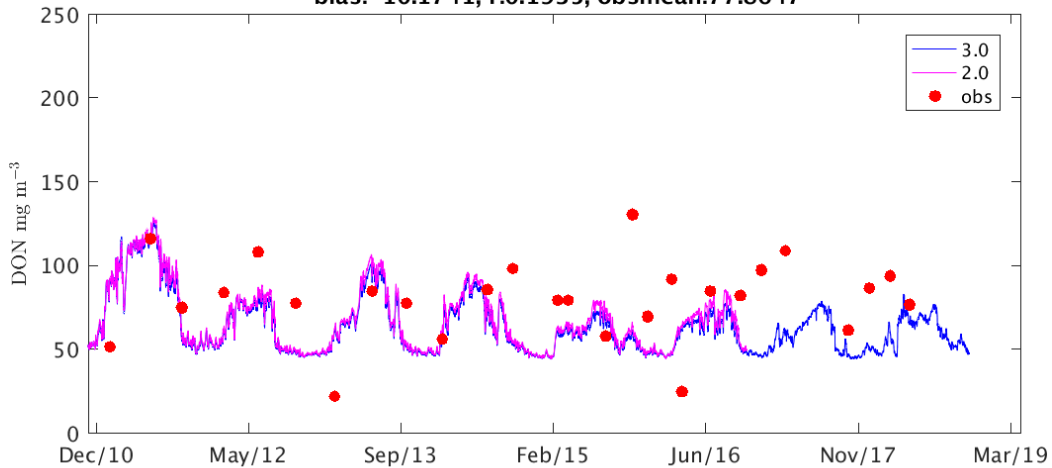
High1697\_0m 3.0 d2:0.42, mape:31.8, rms:35.4615  
 bias:-22.1480, r:0.0380, obsmean:89.8974  
 High1697\_0m 2.0 d2:0.47, mape:29.1, rms:29.2704  
 bias:-12.3582, r:0.1381, obsmean:85.3327



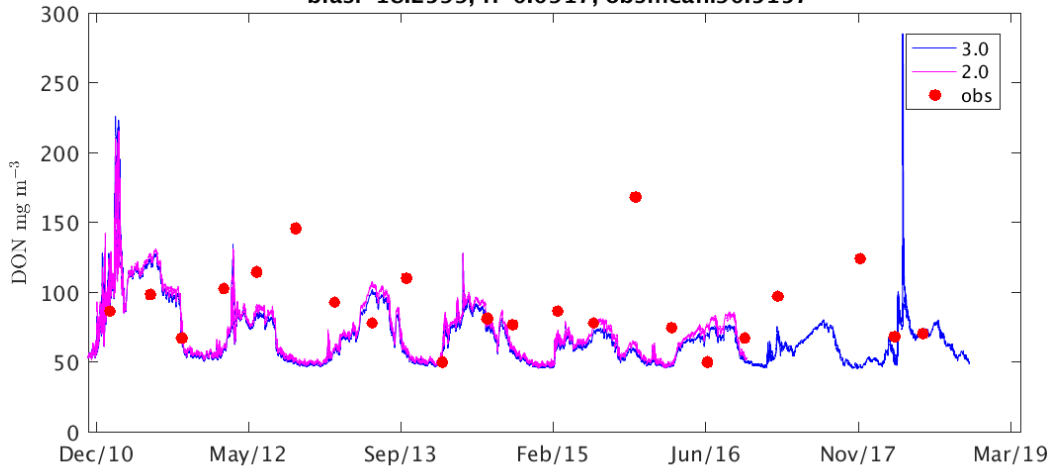
FitzCoral852\_15m 3.0 d2:0.35, mape:36.0, rms:57.0856  
 bias:-30.8132, r:-0.0485, obsmean:94.2140  
 FitzCoral852\_15m 2.0 d2:0.32, mape:35.7, rms:61.4915  
 bias:-25.9145, r:-0.1058, obsmean:94.3813



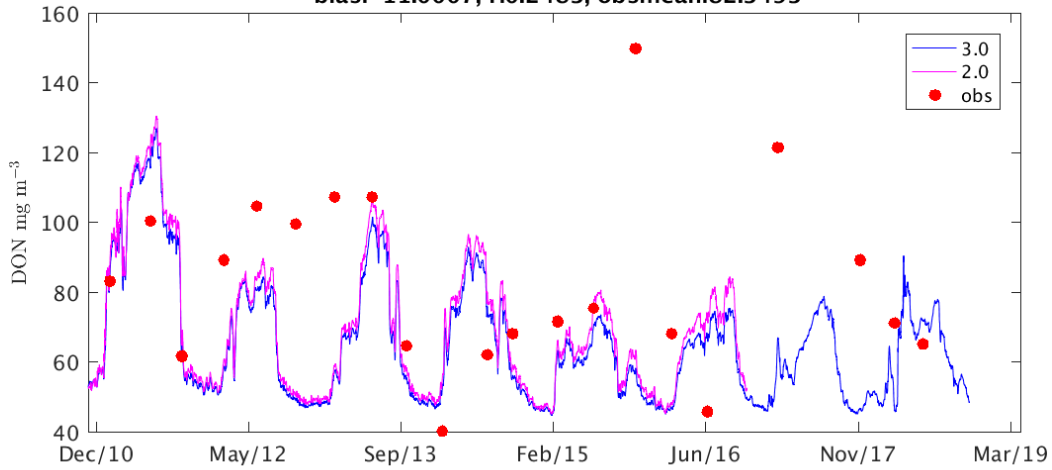
FitzCoral852\_0m 3.0 d2:0.39, mape:42.1, rms:41.9004  
 bias:-21.4908, r:0.1234, obsmean:84.7774  
 FitzCoral852\_0m 2.0 d2:0.47, mape:43.4, rms:30.0624  
 bias:-10.1741, r:0.1935, obsmean:77.8647



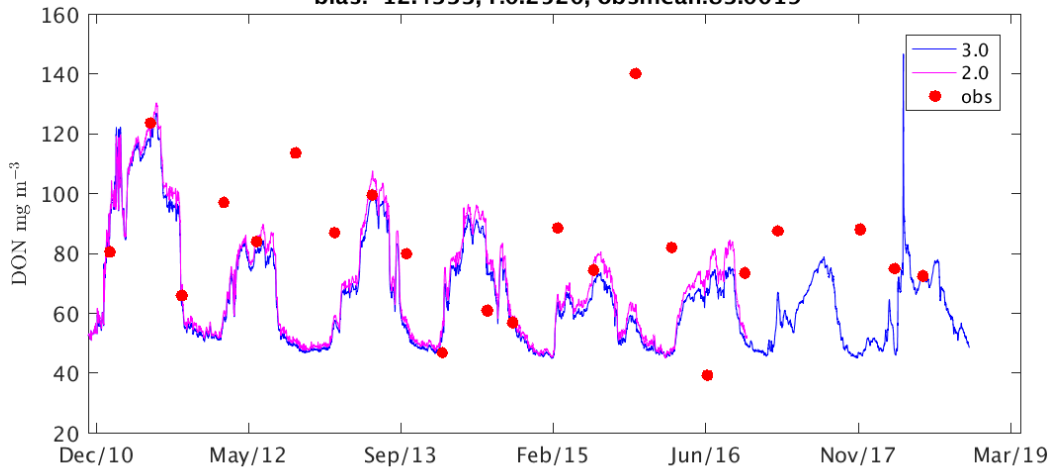
FairleadBuoy518\_0m 3.0 d2:0.40, mape:29.8, rms:42.2591  
 bias:-23.2919, r:-0.1050, obsmean:90.4248  
 FairleadBuoy518\_0m 2.0 d2:0.38, mape:29.4, rms:41.1393  
 bias:-18.2599, r:-0.0917, obsmean:90.5157



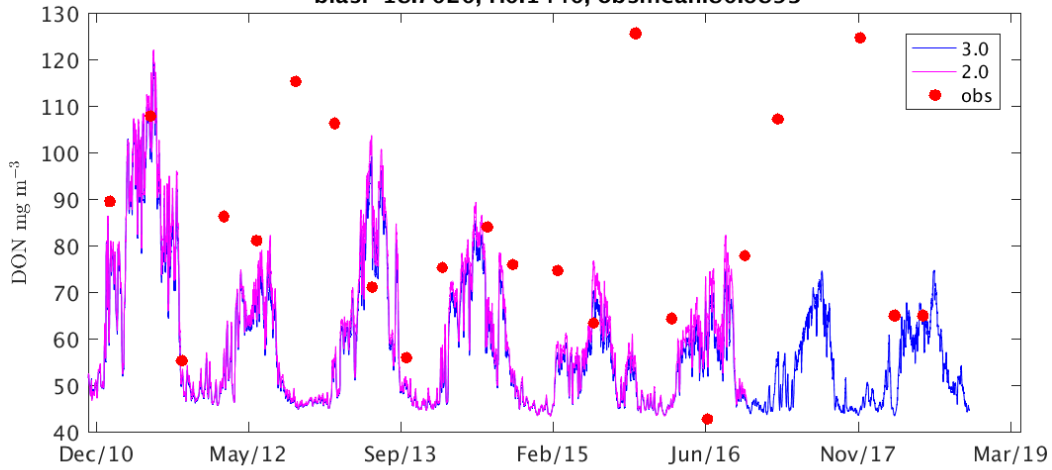
Yorkeys519\_8m 3.0 d2:0.52, mape:26.8, rms:32.6685  
 bias:-17.1162, r:0.2130, obsmean:83.1736  
 Yorkeys519\_8m 2.0 d2:0.54, mape:25.1, rms:30.4703  
 bias:-11.0007, r:0.2483, obsmean:82.3493



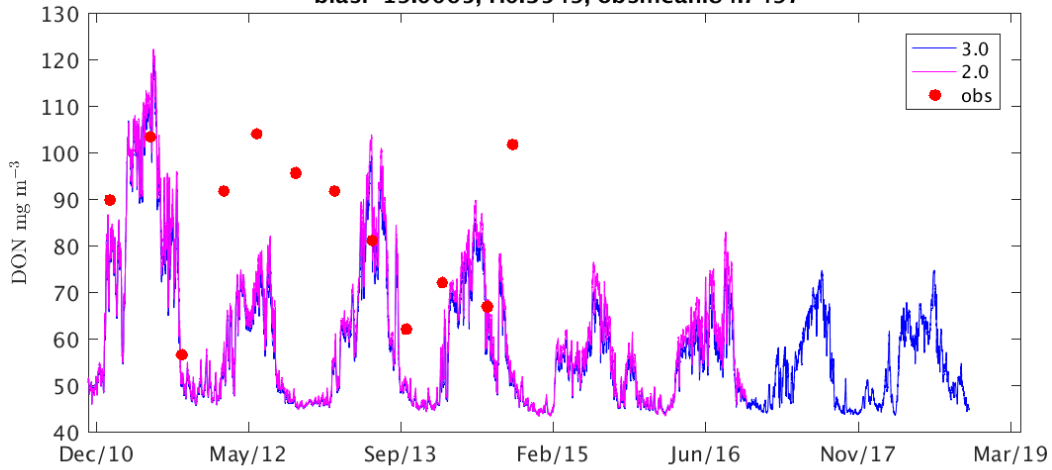
Yorkeys519\_0m 3.0 d2:0.52, mape:25.9, rms:30.4519  
 bias:-16.8809, r:0.2419, obsmean:82.5698  
 Yorkeys519\_0m 2.0 d2:0.54, mape:25.8, rms:30.0757  
 bias:-12.4333, r:0.2520, obsmean:83.0019



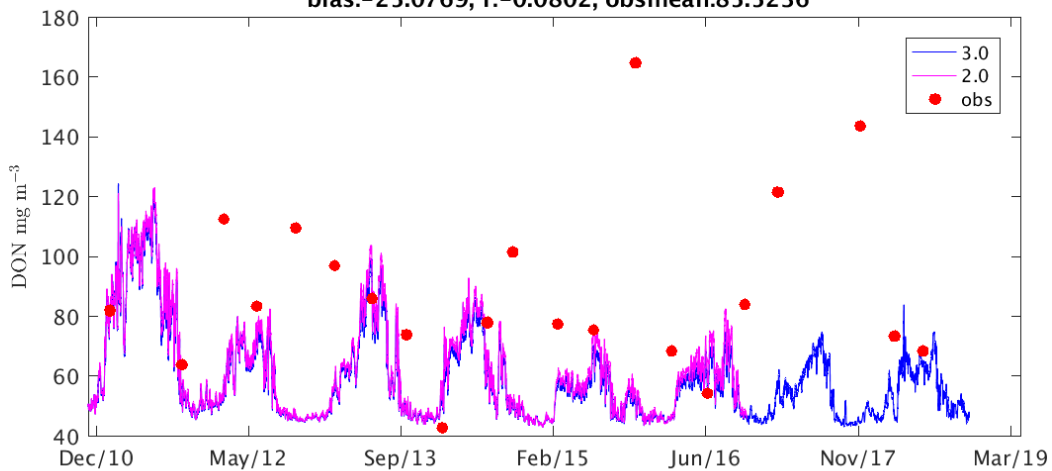
Green830\_36m 3.0 d2:0.47, mape:29.4, rms:35.1923  
 bias:-23.6051, r:0.0640, obsmean:82.4714  
 Green830\_36m 2.0 d2:0.50, mape:27.8, rms:31.0650  
 bias:-18.7020, r:0.1440, obsmean:80.6893



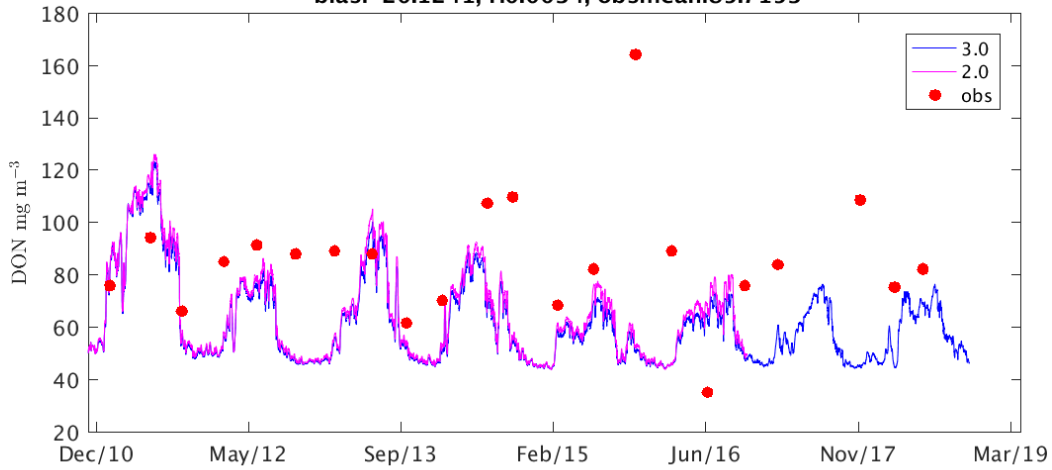
Green830\_18m 3.0 d2:0.56, mape:25.3, rms:28.0720  
 bias:-20.5235, r:0.3623, obsmean:84.7497  
 Green830\_18m 2.0 d2:0.56, mape:24.7, rms:27.4031  
 bias:-19.0065, r:0.3549, obsmean:84.7497



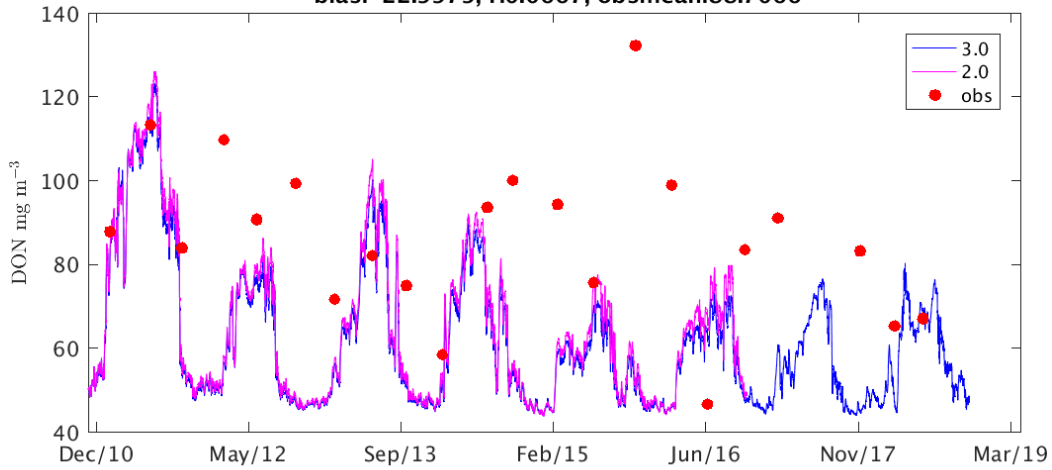
Green830\_0m 3.0 d2:0.41, mape:32.0, rms:44.9120  
 bias:-31.0471, r:-0.1659, obsmean:88.6157  
 Green830\_0m 2.0 d2:0.40, mape:29.3, rms:39.4865  
 bias:-25.0769, r:-0.0802, obsmean:85.5236



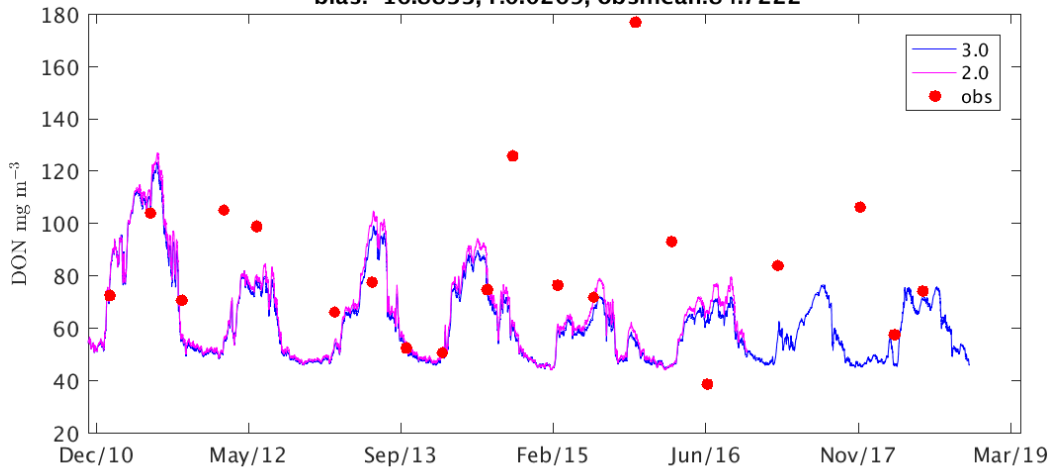
**DoubleI520\_18m 3.0 d2:0.39, mape:32.7, rms:38.0161**  
**bias:-24.1627, r:-0.0160, obsmean:86.0209**  
**DoubleI520\_18m 2.0 d2:0.39, mape:31.5, rms:37.3854**  
**bias:-20.1241, r:0.0034, obsmean:85.7153**



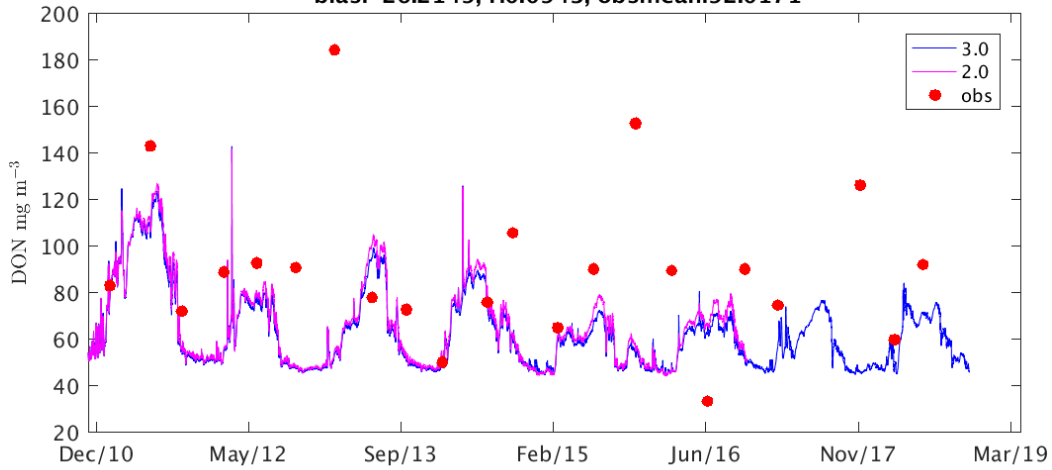
**DoubleI520\_0m 3.0 d2:0.45, mape:30.3, rms:34.1023**  
**bias:-24.4886, r:0.1262, obsmean:86.5055**  
**DoubleI520\_0m 2.0 d2:0.44, mape:30.0, rms:34.8091**  
**bias:-22.9979, r:0.0667, obsmean:88.7066**



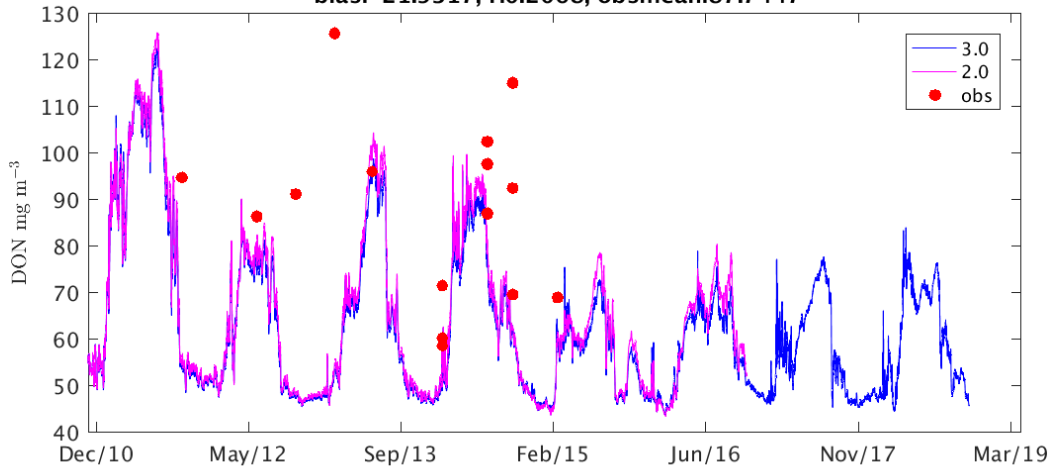
**PortD\_15m 3.0 d2:0.44, mape:26.5, rms:39.4654**  
**bias:-20.2788, r:0.0194, obsmean:83.8735**  
**PortD\_15m 2.0 d2:0.43, mape:26.3, rms:40.1281**  
**bias:-16.8833, r:0.0269, obsmean:84.7222**



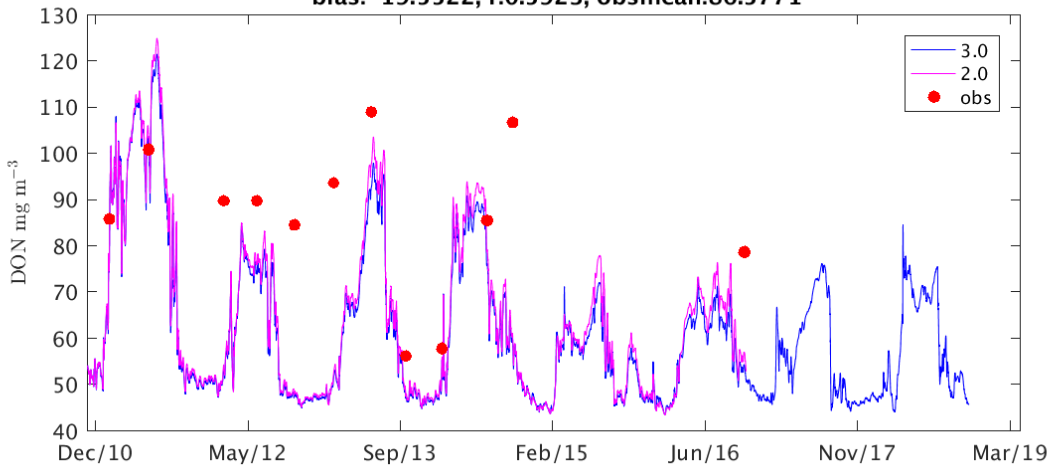
PortD\_0m 3.0 d2:0.43, mape:33.4, rms:46.2268  
 bias:-28.9889, r:0.0760, obsmean:91.2985  
 PortD\_0m 2.0 d2:0.43, mape:33.1, rms:45.9492  
 bias:-26.2149, r:0.0943, obsmean:92.0171



Snap\_10m 3.0 d2:0.49, mape:24.2, rms:31.1146  
 bias:-23.5008, r:0.1912, obsmean:87.7447  
 Snap\_10m 2.0 d2:0.50, mape:23.2, rms:30.2273  
 bias:-21.9317, r:0.2068, obsmean:87.7447



CapeTrib356\_10m 3.0 d2:0.58, mape:23.9, rms:26.0362  
 bias:-21.2193, r:0.5863, obsmean:86.5771  
 CapeTrib356\_10m 2.0 d2:0.61, mape:22.4, rms:24.9533  
 bias:-19.5522, r:0.5923, obsmean:86.5771





## 16. Simulated DOP assessment against Long Term Monitoring

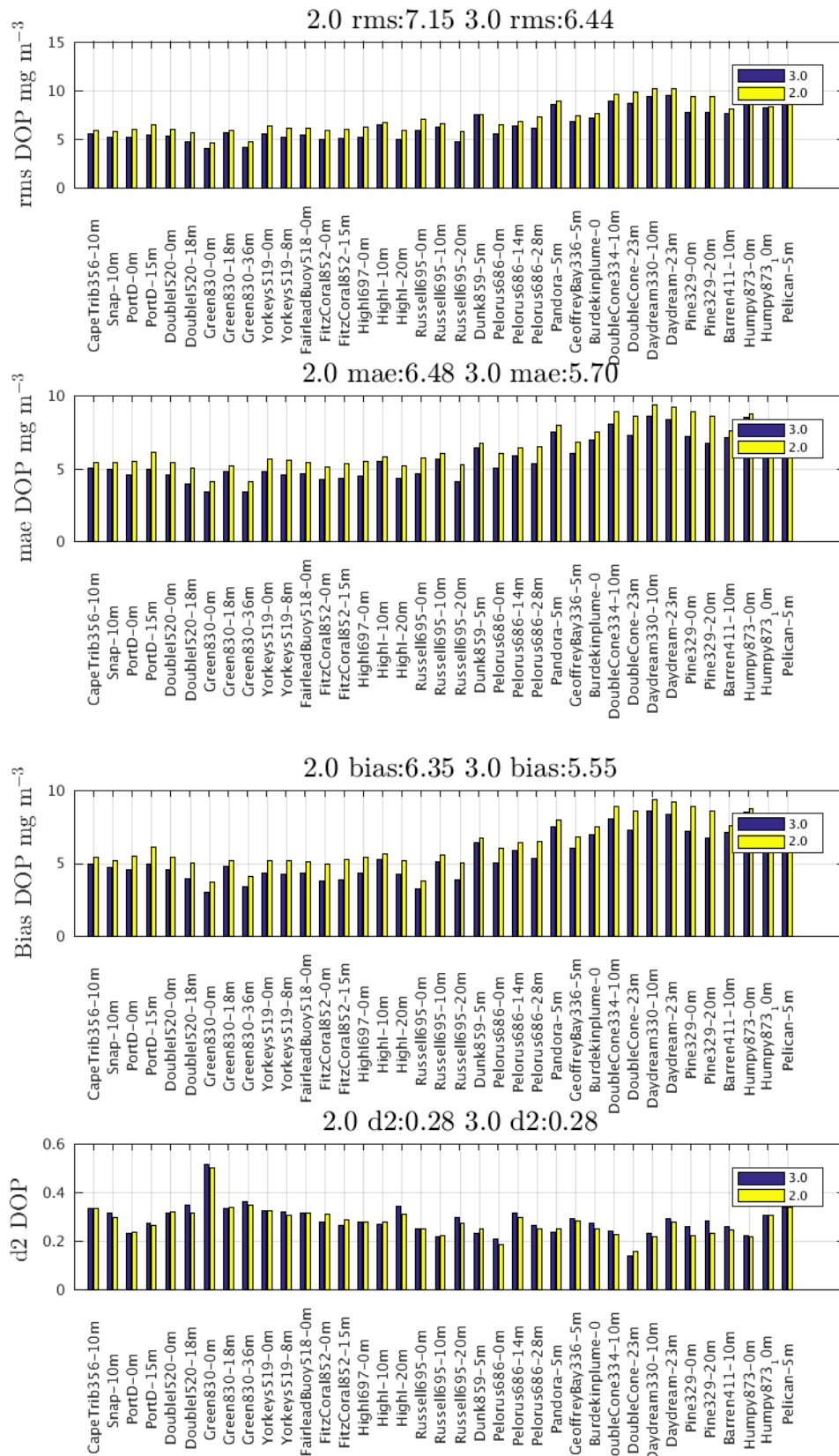
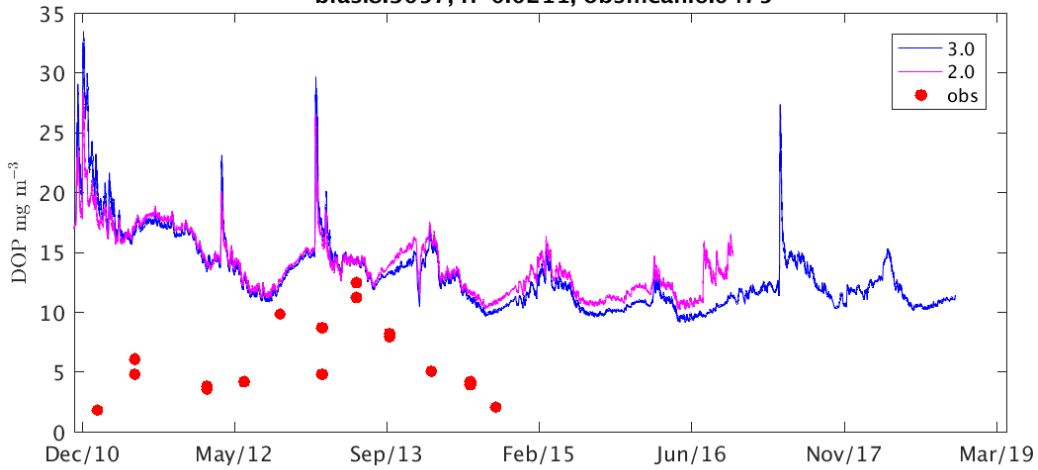
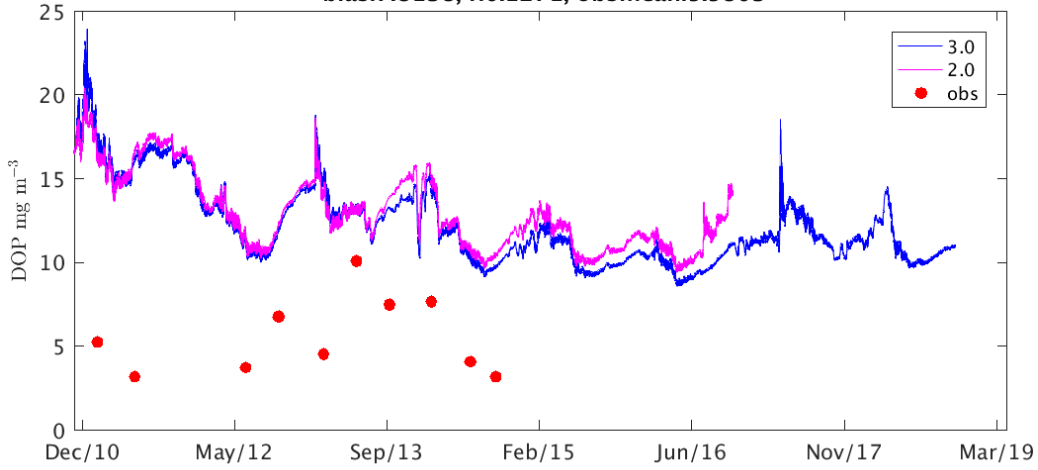


Figure 11 Metrics for Long Term Monitoring sites DOP assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

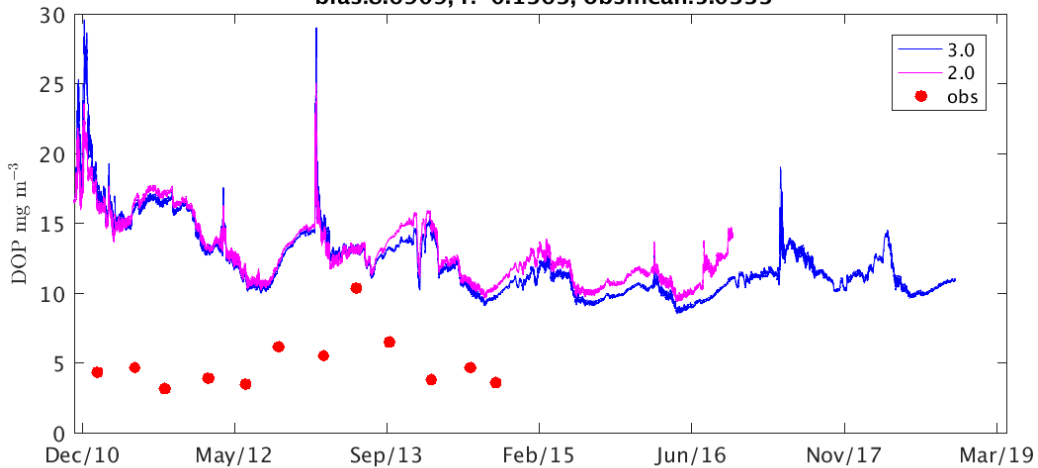
Pelican\_5m 3.0 d2:0.34, mape:213.0, rms:9.0130  
 bias:8.1407, r:-0.0260, obsmean:6.0475  
 Pelican\_5m 2.0 d2:0.34, mape:214.8, rms:9.0716  
 bias:8.3057, r:-0.0211, obsmean:6.0475



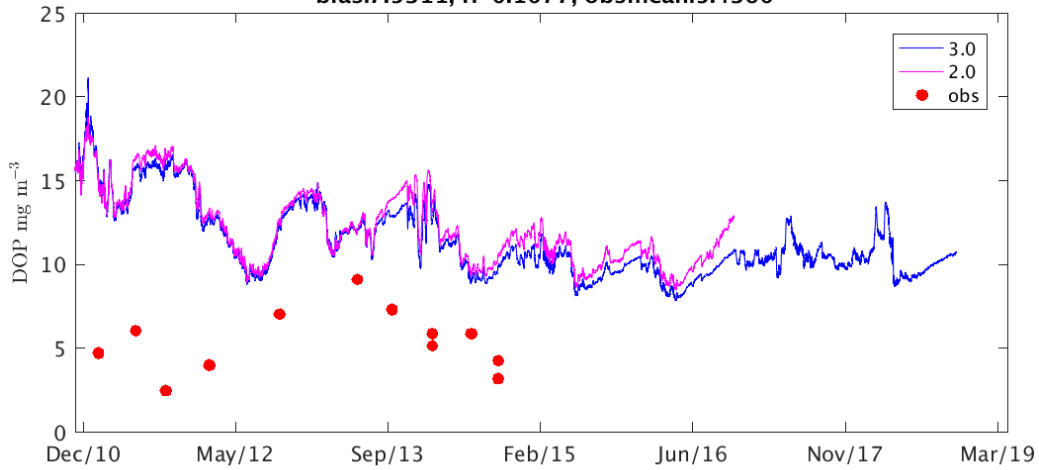
Humpy873\_10m 3.0 d2:0.30, mape:170.8, rms:8.2185  
 bias:7.6571, r:0.1190, obsmean:5.5803  
 Humpy873\_10m 2.0 d2:0.31, mape:174.7, rms:8.2907  
 bias:7.8138, r:0.1271, obsmean:5.5803



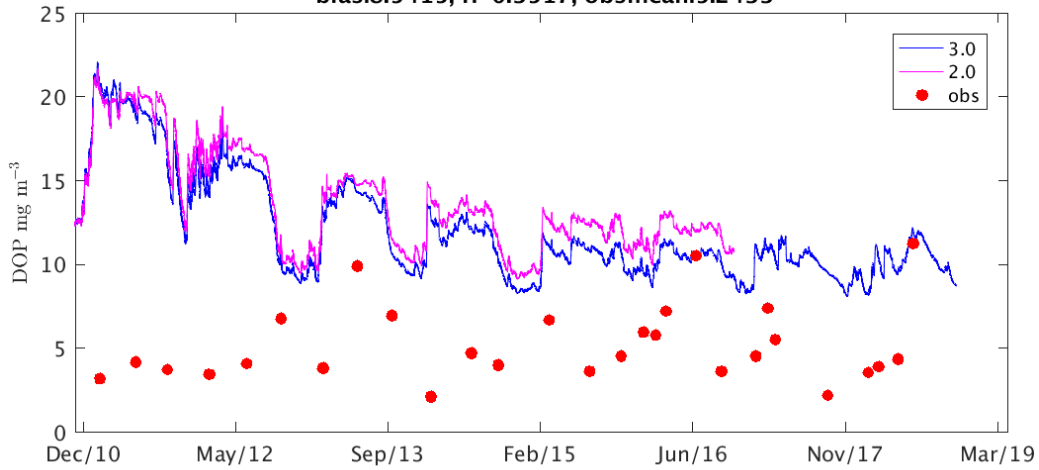
Humpy873\_0m 3.0 d2:0.22, mape:198.8, rms:9.0211  
 bias:8.4801, r:-0.0761, obsmean:5.0333  
 Humpy873\_0m 2.0 d2:0.21, mape:204.4, rms:9.1983  
 bias:8.6909, r:-0.1363, obsmean:5.0333



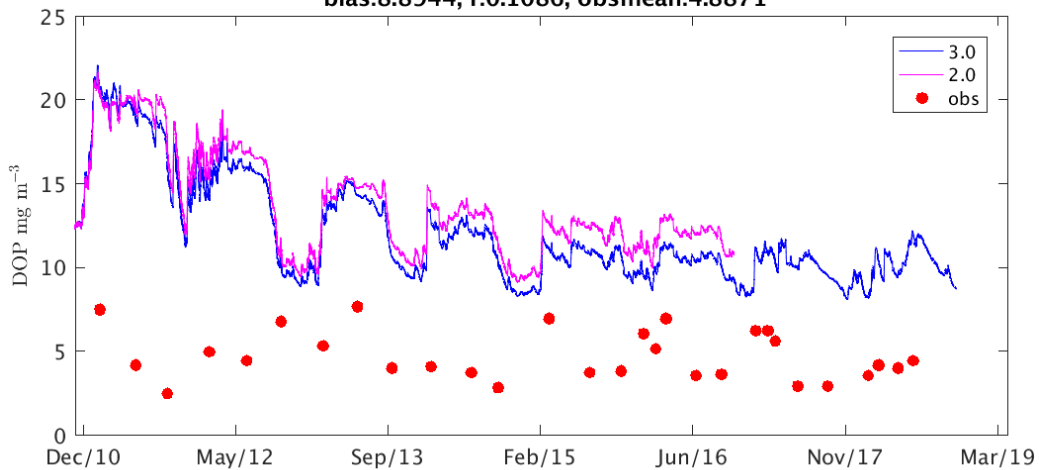
Barren411\_10m 3.0 d2:0.26, mape:163.2, rms:7.6433  
 bias:7.0674, r:-0.0790, obsmean:5.4360  
 Barren411\_10m 2.0 d2:0.25, mape:173.3, rms:8.0816  
 bias:7.5311, r:-0.1077, obsmean:5.4360



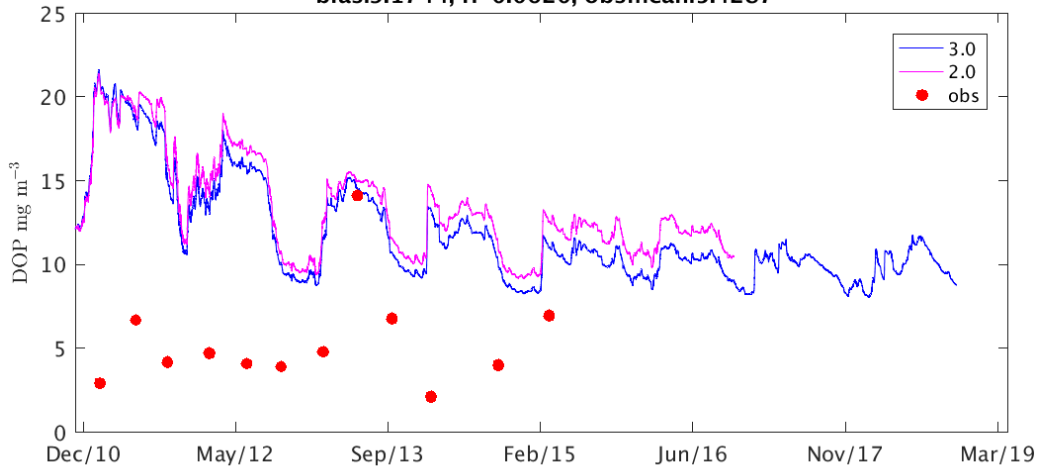
Pine329\_20m 3.0 d2:0.28, mape:172.1, rms:7.7433  
 bias:6.6951, r:-0.1454, obsmean:5.2717  
 Pine329\_20m 2.0 d2:0.23, mape:213.7, rms:9.4085  
 bias:8.5415, r:-0.3517, obsmean:5.2433



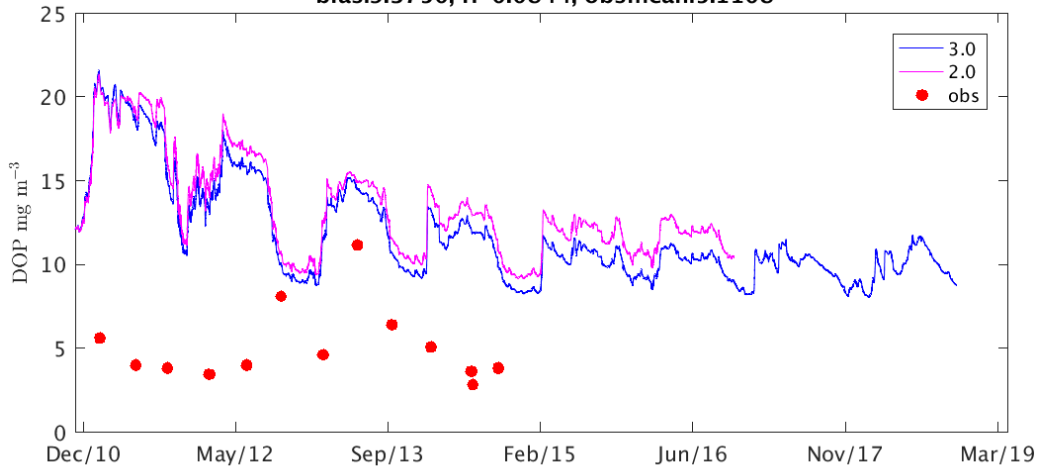
Pine329\_0m 3.0 d2:0.26, mape:172.1, rms:7.6915  
 bias:7.1480, r:0.2294, obsmean:4.7466  
 Pine329\_0m 2.0 d2:0.22, mape:210.9, rms:9.3560  
 bias:8.8944, r:0.1086, obsmean:4.8871



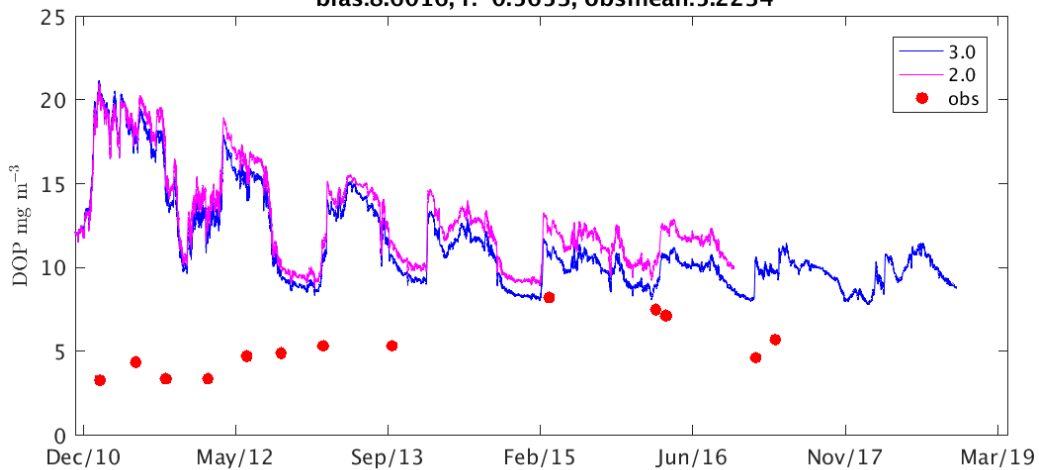
Daydream\_23m 3.0 d2:0.29, mape:219.6, rms:9.4972  
 bias:8.3270, r:-0.0435, obsmean:5.4287  
 Daydream\_23m 2.0 d2:0.28, mape:238.7, rms:10.1751  
 bias:9.1744, r:-0.0620, obsmean:5.4287



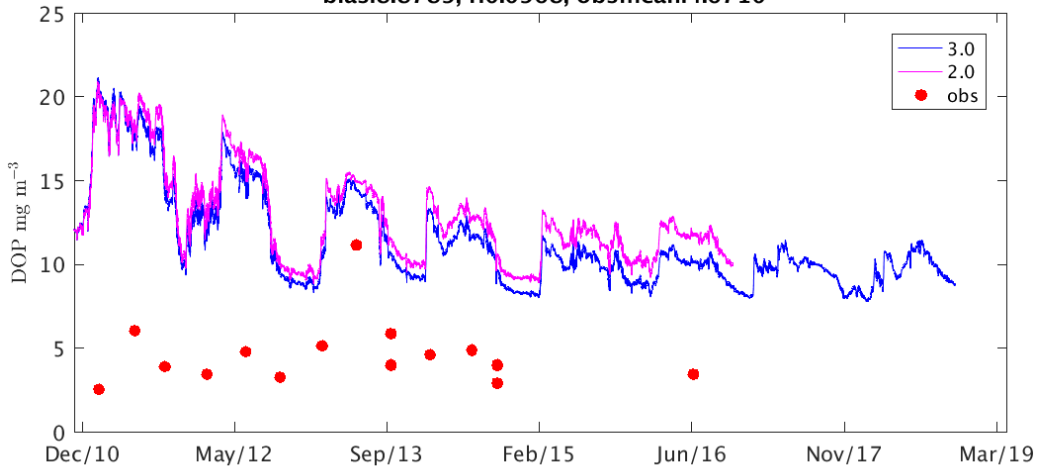
Daydream330\_10m 3.0 d2:0.23, mape:204.1, rms:9.4104  
 bias:8.5508, r:-0.0255, obsmean:5.1108  
 Daydream330\_10m 2.0 d2:0.22, mape:223.8, rms:10.1279  
 bias:9.3750, r:-0.0844, obsmean:5.1108



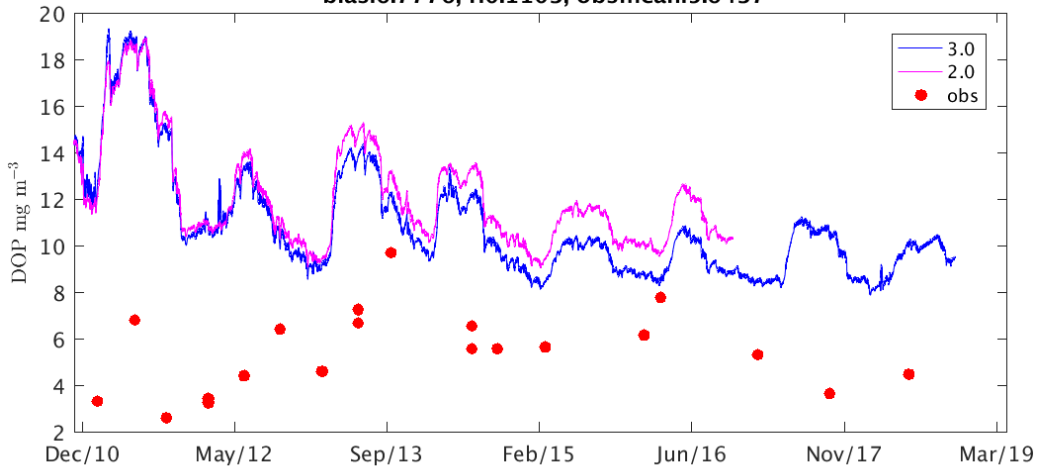
DoubleCone\_23m 3.0 d2:0.14, mape:173.9, rms:8.6765  
 bias:7.2336, r:-0.5813, obsmean:5.2107  
 DoubleCone\_23m 2.0 d2:0.15, mape:205.1, rms:9.7844  
 bias:8.6016, r:-0.5653, obsmean:5.2234



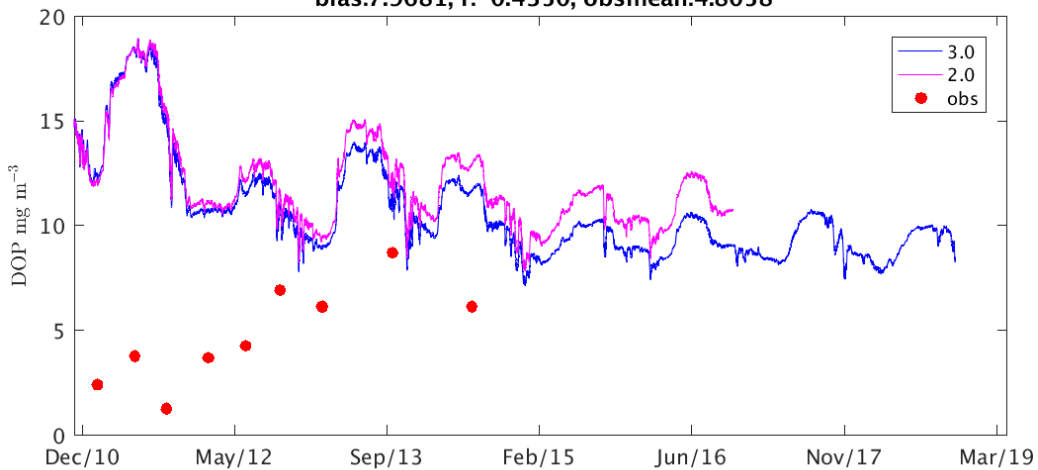
**DoubleCone334\_10m 3.0 d2:0.24, mape:209.7, rms:8.8998**  
**bias:8.0449, r:0.0996, obsmean:4.6710**  
**DoubleCone334\_10m 2.0 d2:0.22, mape:229.3, rms:9.5831**  
**bias:8.8789, r:0.0968, obsmean:4.6710**



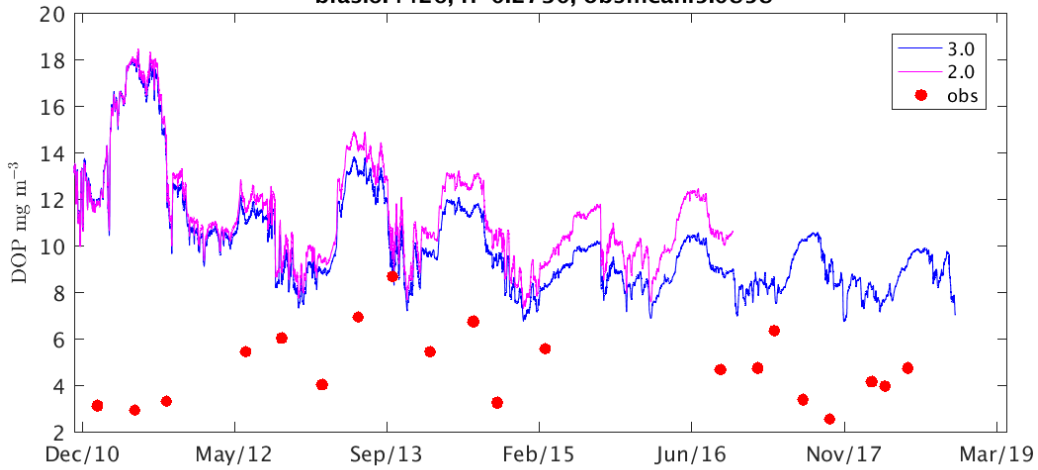
**GeoffreyBay336\_5m 3.0 d2:0.29, mape:135.0, rms:6.7514**  
**bias:6.0107, r:0.0362, obsmean:5.5183**  
**GeoffreyBay336\_5m 2.0 d2:0.28, mape:147.1, rms:7.3647**  
**bias:6.7776, r:0.1103, obsmean:5.6437**



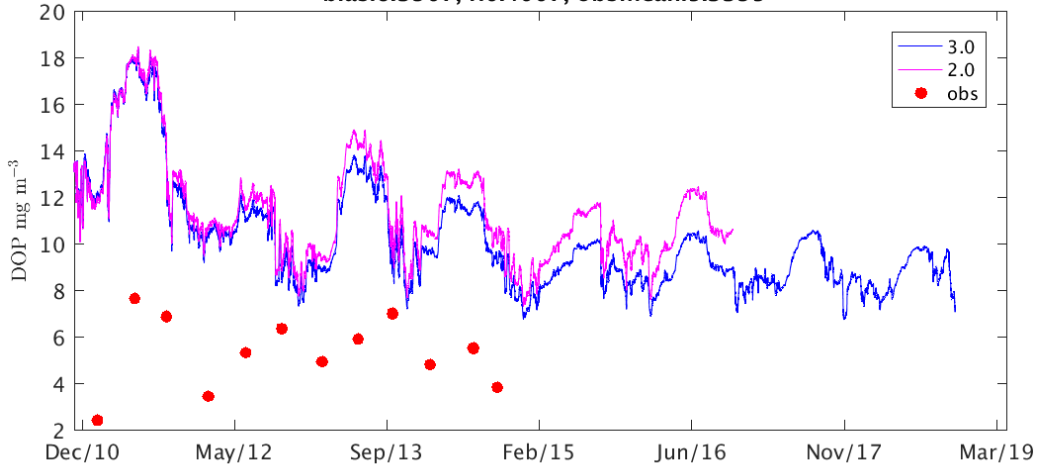
**Pandora\_5m 3.0 d2:0.24, mape:272.9, rms:8.5729**  
**bias:7.4558, r:-0.5241, obsmean:4.8058**  
**Pandora\_5m 2.0 d2:0.25, mape:284.1, rms:8.9209**  
**bias:7.9681, r:-0.4350, obsmean:4.8058**



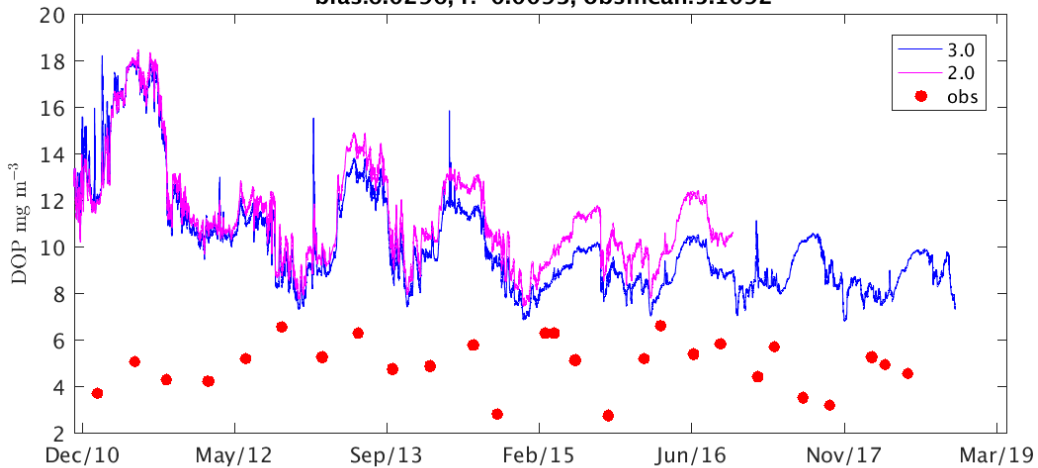
**Pelorus686\_28m 3.0 d2:0.26, mape:137.9, rms:6.1082**  
**bias:5.3106, r:-0.1849, obsmean:4.7959**  
**Pelorus686\_28m 2.0 d2:0.25, mape:159.4, rms:7.2164**  
**bias:6.4426, r:-0.2730, obsmean:5.0858**



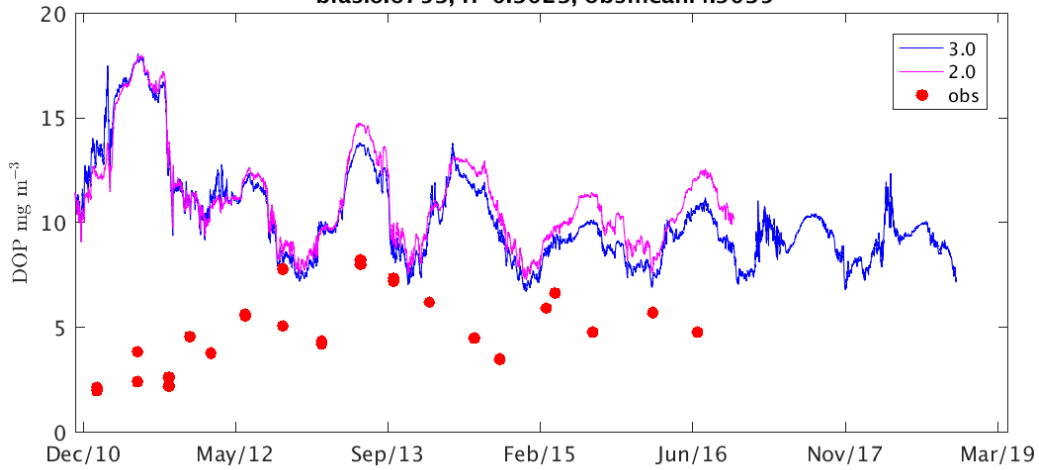
**Pelorus686\_14m 3.0 d2:0.31, mape:129.0, rms:6.2975**  
**bias:5.8324, r:0.3558, obsmean:5.3395**  
**Pelorus686\_14m 2.0 d2:0.30, mape:139.3, rms:6.7673**  
**bias:6.3907, r:0.4007, obsmean:5.3395**



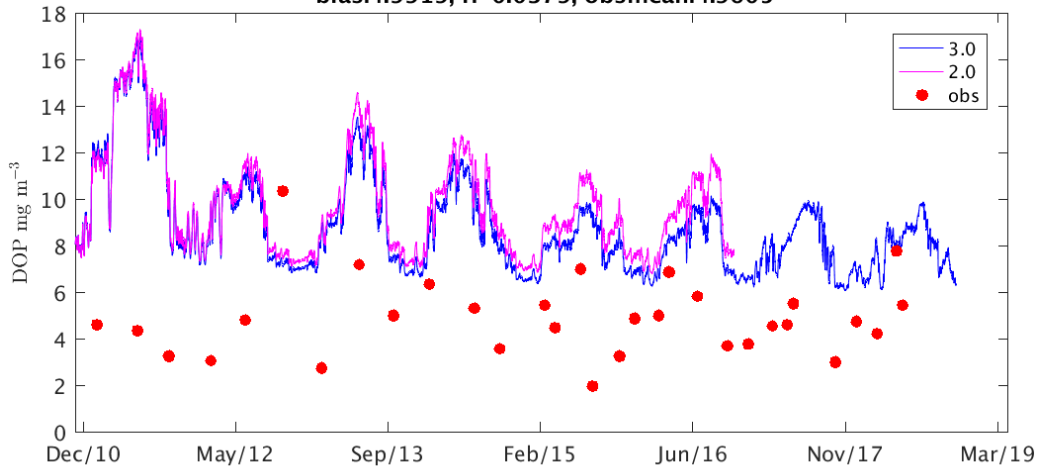
**Pelorus686\_0m 3.0 d2:0.21, mape:111.8, rms:5.4889**  
**bias:4.9645, r:-0.0405, obsmean:4.9517**  
**Pelorus686\_0m 2.0 d2:0.18, mape:130.7, rms:6.4608**  
**bias:6.0296, r:-0.0093, obsmean:5.1092**



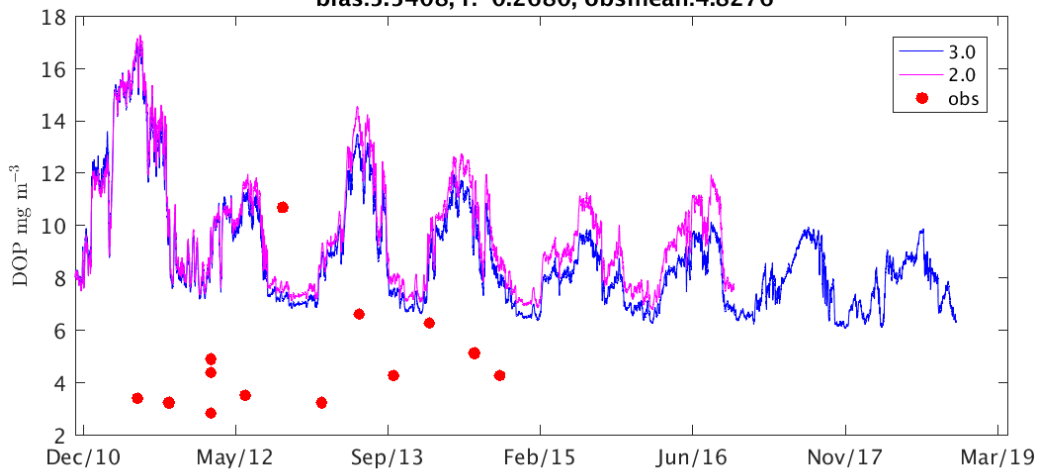
**Dunk859\_5m 3.0 d2:0.23, mape:188.2, rms:7.4690**  
**bias:6.3852, r:-0.4461, obsmean:4.9035**  
**Dunk859\_5m 2.0 d2:0.25, mape:189.8, rms:7.5541**  
**bias:6.6753, r:-0.3023, obsmean:4.9035**



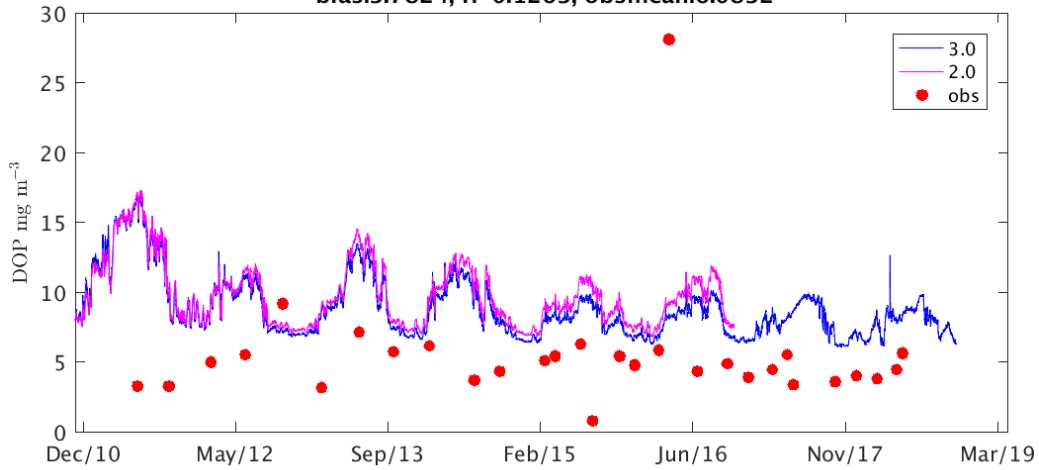
**Russell695\_20m 3.0 d2:0.30, mape:100.8, rms:4.6993**  
**bias:3.8545, r:0.0036, obsmean:4.9314**  
**Russell695\_20m 2.0 d2:0.27, mape:131.2, rms:5.7848**  
**bias:4.9919, r:-0.0379, obsmean:4.9605**



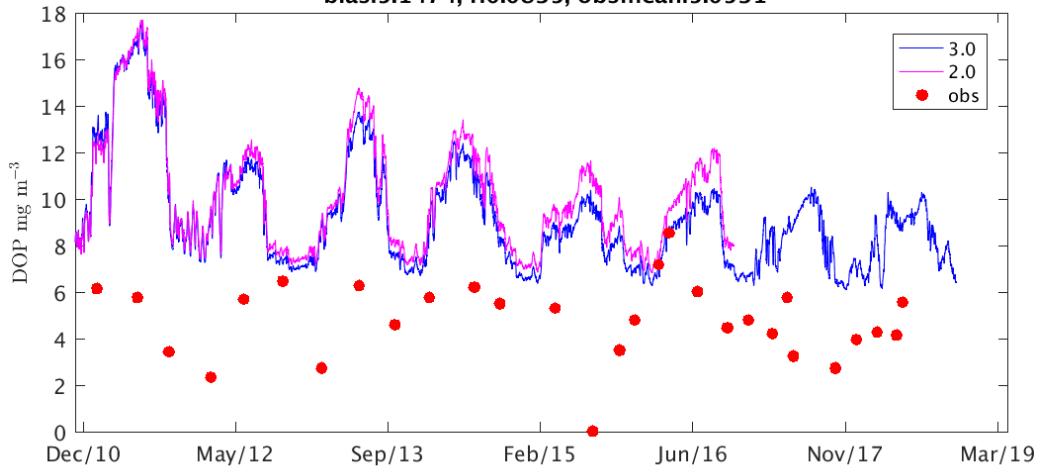
**Russell695\_10m 3.0 d2:0.22, mape:142.4, rms:6.2465**  
**bias:5.0931, r:-0.2983, obsmean:4.8276**  
**Russell695\_10m 2.0 d2:0.22, mape:151.6, rms:6.6038**  
**bias:5.5408, r:-0.2680, obsmean:4.8276**



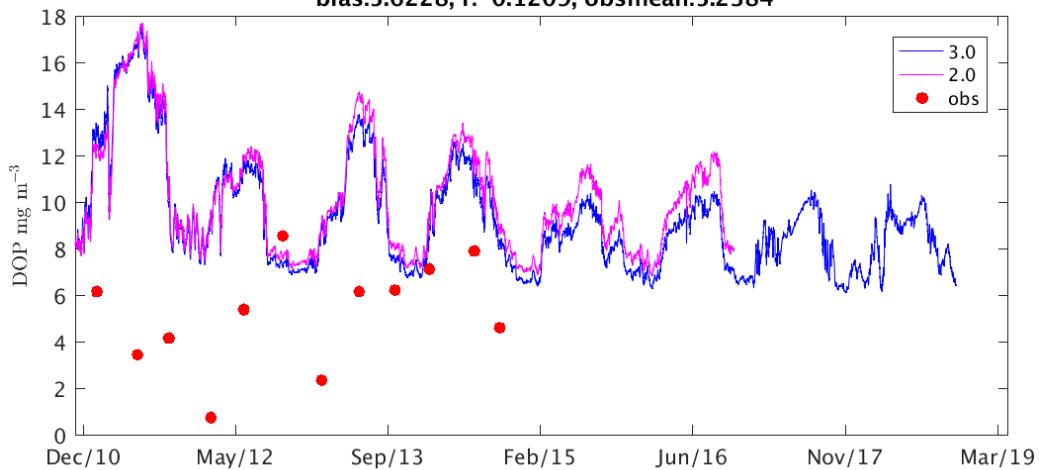
Russell695\_0m 3.0 d2:0.25, mape:122.1, rms:5.9229  
bias:3.1925, r:-0.0679, obsmean:5.5534  
Russell695\_0m 2.0 d2:0.25, mape:156.3, rms:6.9967  
bias:3.7824, r:-0.1263, obsmean:6.0832



Highl\_20m 3.0 d2:0.34, mape:850.6, rms:4.9356  
bias:4.2532, r:0.1757, obsmean:4.8275  
Highl\_20m 2.0 d2:0.31, mape:1345.5, rms:5.9000  
bias:5.1474, r:0.0835, obsmean:5.0531

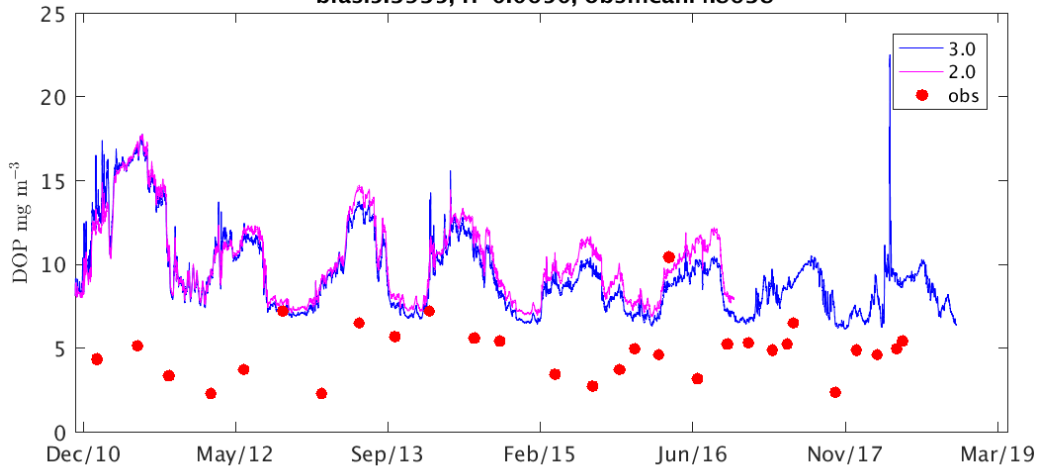


Highl\_10m 3.0 d2:0.27, mape:208.5, rms:6.4048  
bias:5.2198, r:-0.1601, obsmean:5.2384  
Highl\_10m 2.0 d2:0.27, mape:216.9, rms:6.6958  
bias:5.6228, r:-0.1209, obsmean:5.2384

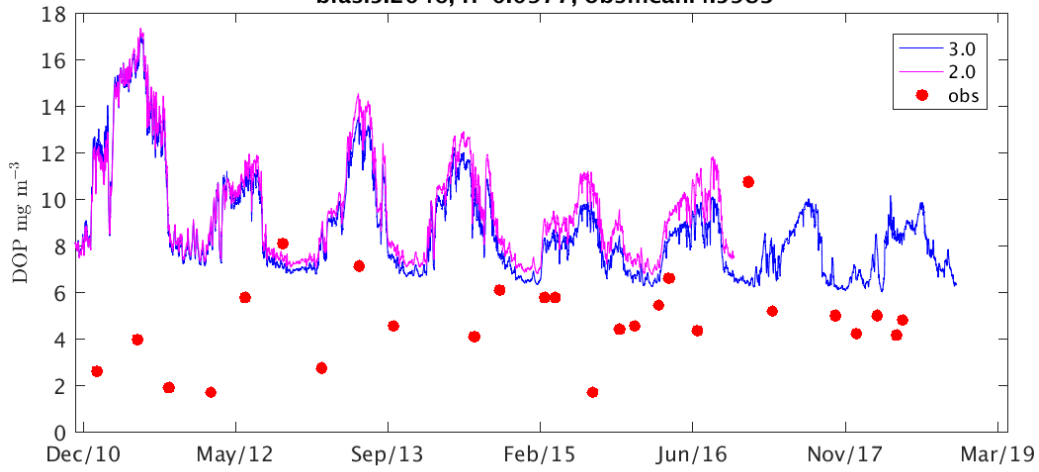




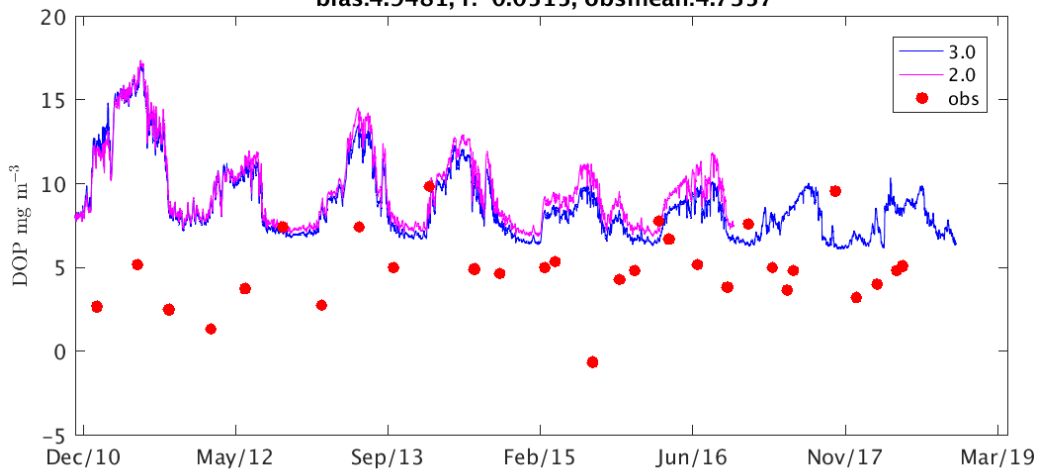
High1697\_0m 3.0 d2:0.28, mape:114.5, rms:5.1637  
bias:4.3093, r:-0.0347, obsmean:4.8786  
High1697\_0m 2.0 d2:0.28, mape:145.6, rms:6.2439  
bias:5.3935, r:-0.0650, obsmean:4.8638



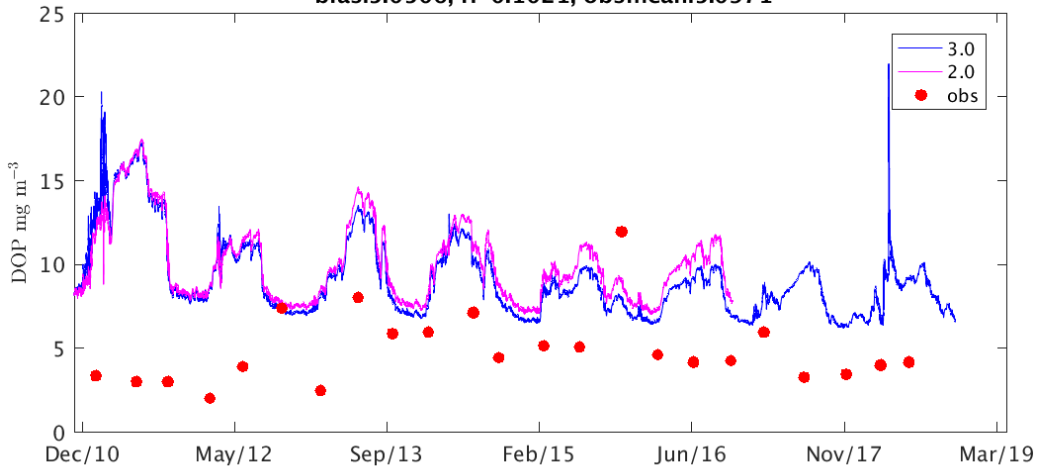
FitzCoral852\_15m 3.0 d2:0.26, mape:126.2, rms:5.0385  
bias:3.8499, r:-0.2404, obsmean:4.8643  
FitzCoral852\_15m 2.0 d2:0.29, mape:165.4, rms:6.0195  
bias:5.2046, r:-0.0977, obsmean:4.5983



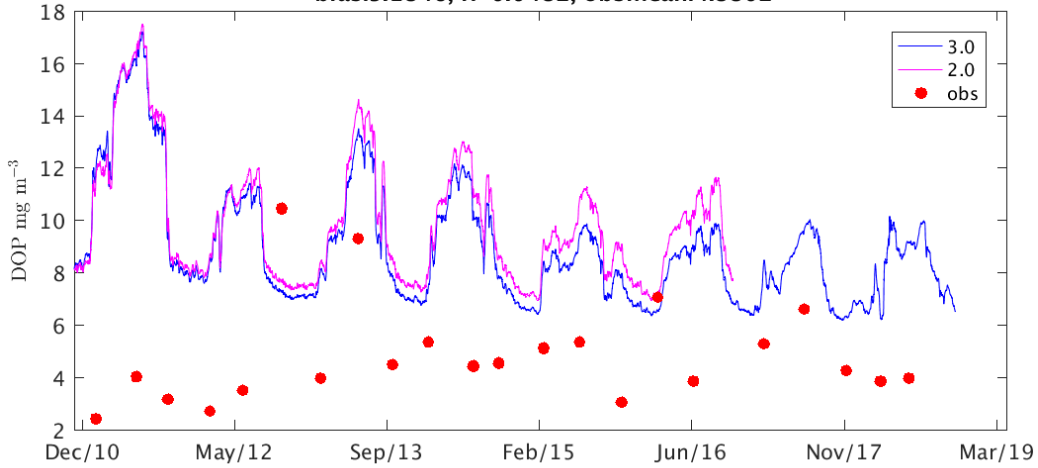
FitzCoral852\_0m 3.0 d2:0.28, mape:112.0, rms:4.9749  
bias:3.7631, r:-0.1698, obsmean:4.9073  
FitzCoral852\_0m 2.0 d2:0.31, mape:138.7, rms:5.9264  
bias:4.9481, r:-0.0515, obsmean:4.7357



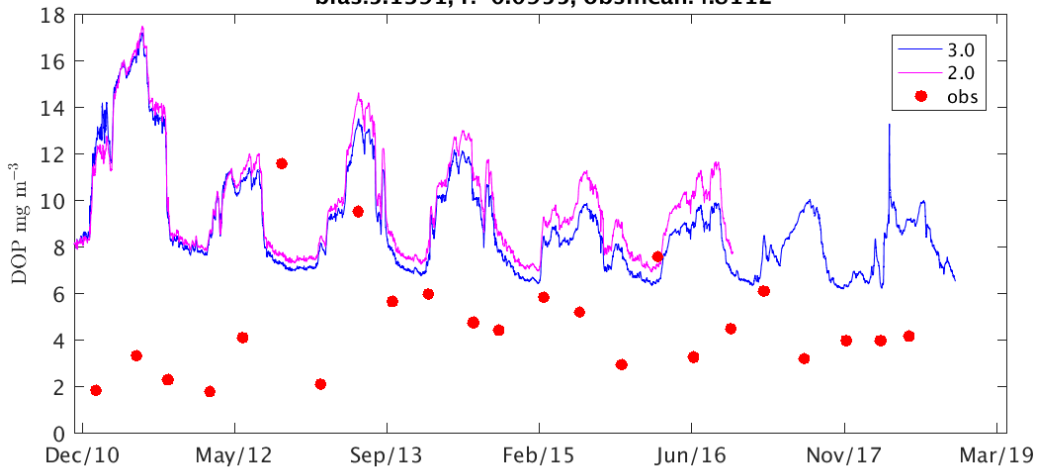
FairleadBuoy518\_0m 3.0 d2:0.31, mape:126.3, rms:5.4486  
 bias:4.2860, r:-0.1066, obsmean:4.8941  
 FairleadBuoy518\_0m 2.0 d2:0.31, mape:145.2, rms:6.1590  
 bias:5.0506, r:-0.1021, obsmean:5.0971



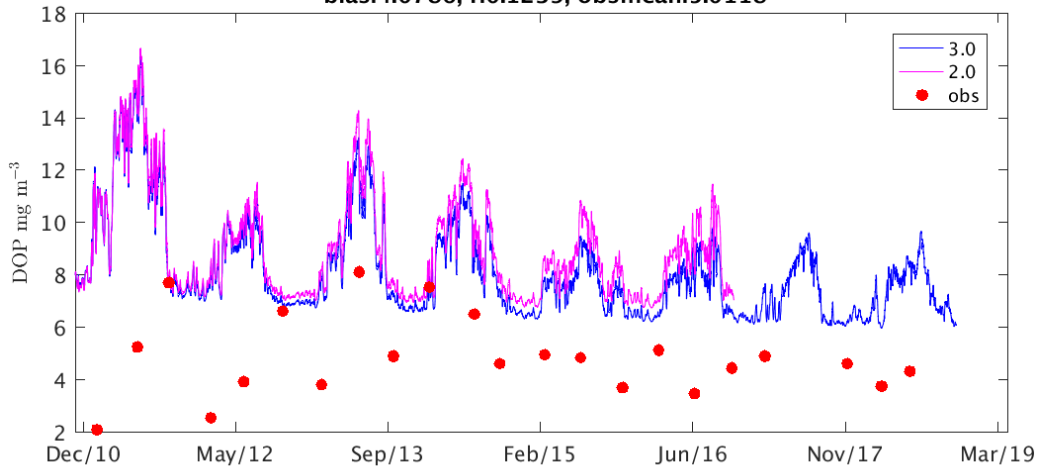
Yorkeys519\_8m 3.0 d2:0.32, mape:117.7, rms:5.2190  
 bias:4.2313, r:-0.0351, obsmean:4.8639  
 Yorkeys519\_8m 2.0 d2:0.30, mape:144.1, rms:6.1209  
 bias:5.1846, r:-0.0482, obsmean:4.8802



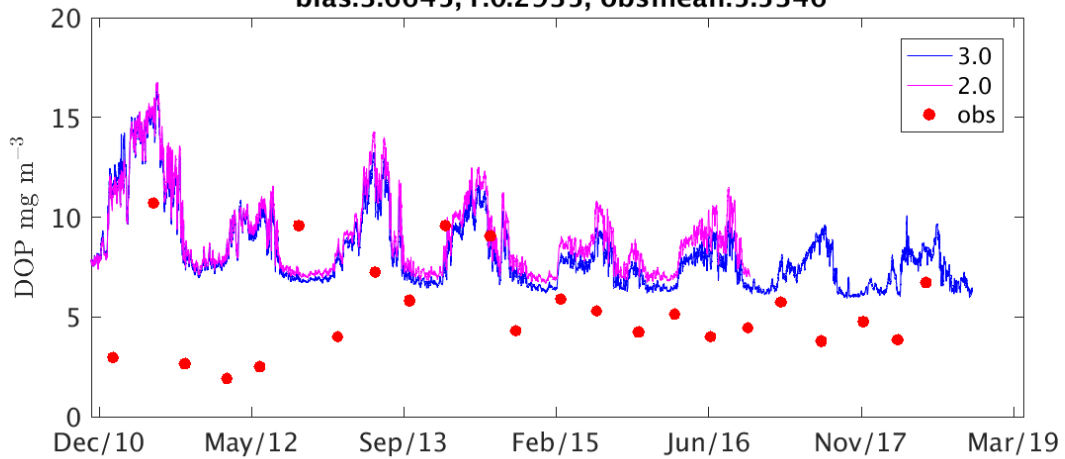
Yorkeys519\_0m 3.0 d2:0.32, mape:150.2, rms:5.5450  
 bias:4.3322, r:-0.1136, obsmean:4.6951  
 Yorkeys519\_0m 2.0 d2:0.32, mape:177.3, rms:6.2968  
 bias:5.1391, r:-0.0955, obsmean:4.8112



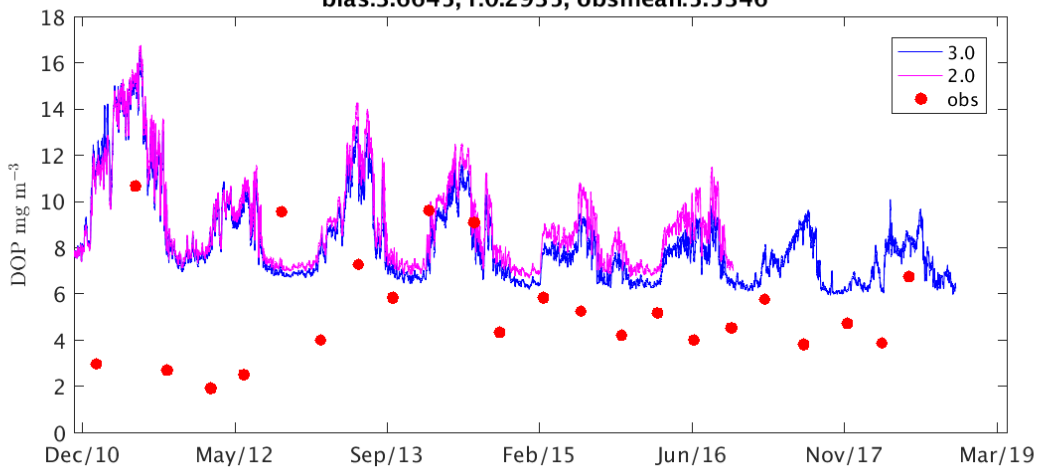
Green830\_36m 3.0 d2:0.36, mape:88.0, rms:4.0952  
bias:3.3700, r:0.1345, obsmean:4.8995  
Green830\_36m 2.0 d2:0.35, mape:105.1, rms:4.7621  
bias:4.0786, r:0.1239, obsmean:5.0118



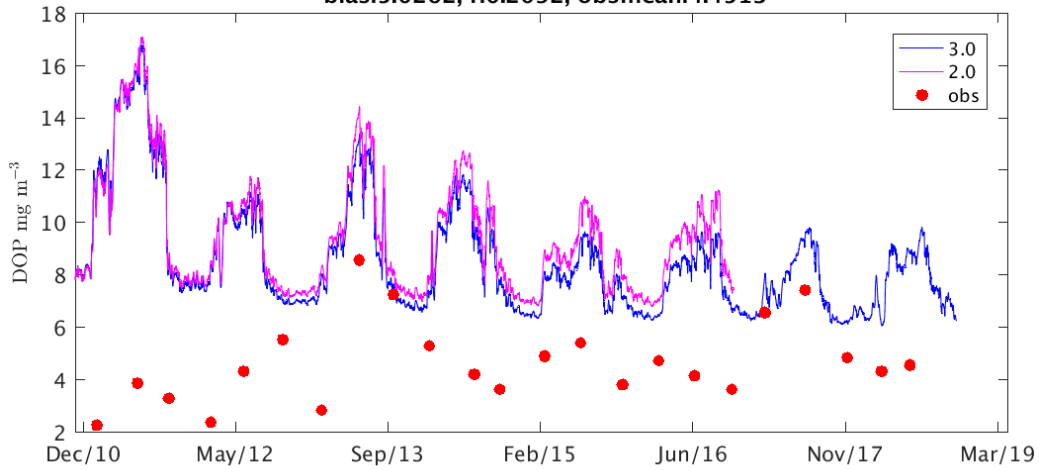
Green830\_0m 3.0 d2:0.51, mape:91.0, rms:3.9868  
bias:2.9716, r:0.2737, obsmean:5.4175  
Green830\_0m 2.0 d2:0.50, mape:109.9, rms:4.6235  
bias:3.6645, r:0.2935, obsmean:5.5346



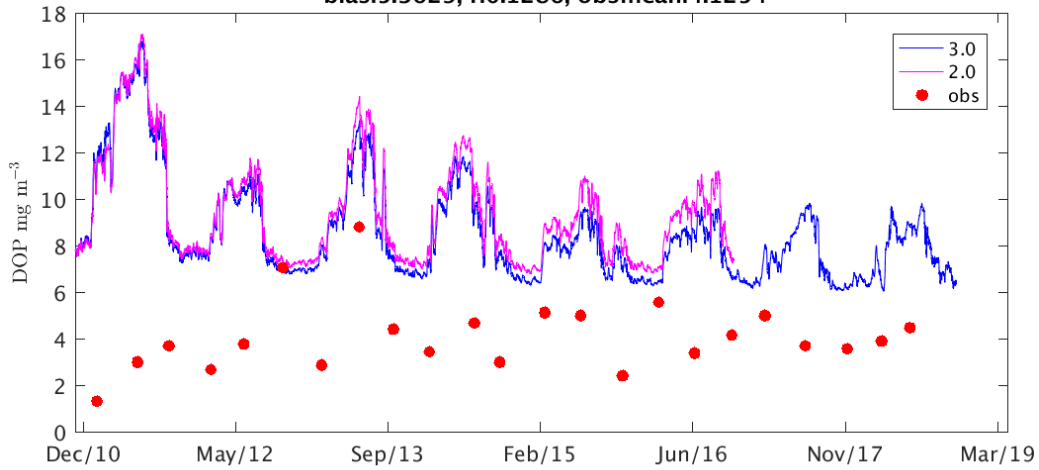
Green830\_0m 3.0 d2:0.51, mape:91.0, rms:3.9868  
bias:2.9716, r:0.2737, obsmean:5.4175  
Green830\_0m 2.0 d2:0.50, mape:109.9, rms:4.6235  
bias:3.6645, r:0.2935, obsmean:5.5346



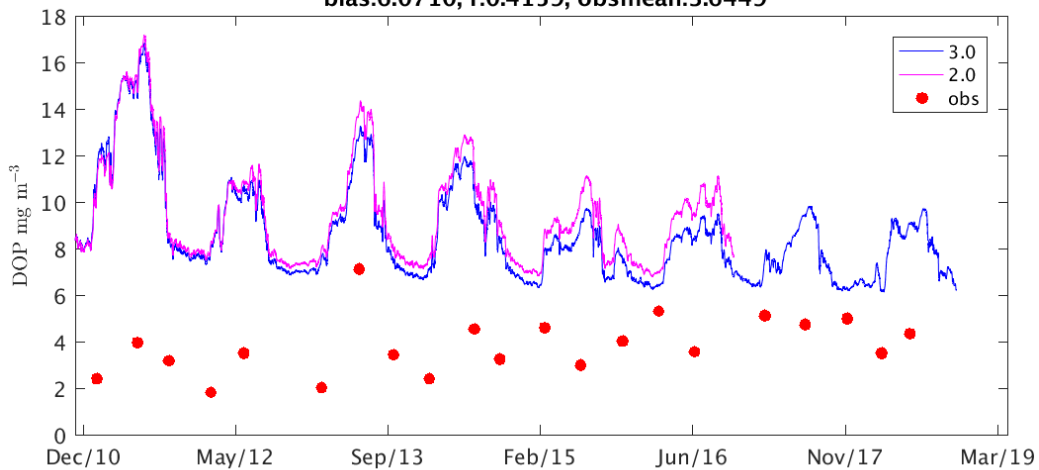
DoubleI520\_18m 3.0 d2:0.34, mape:106.3, rms:4.7207  
bias:3.9513, r:0.1004, obsmean:4.6859  
DoubleI520\_18m 2.0 d2:0.31, mape:136.4, rms:5.6207  
bias:5.0262, r:0.2092, obsmean:4.4513



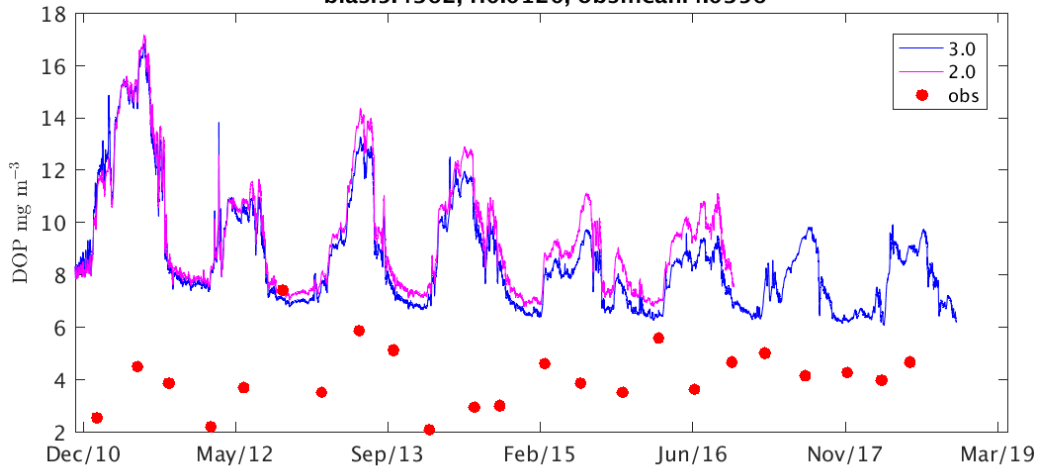
DoubleI520\_0m 3.0 d2:0.31, mape:147.8, rms:5.2335  
bias:4.5274, r:0.0605, obsmean:4.1256  
DoubleI520\_0m 2.0 d2:0.32, mape:177.5, rms:6.0089  
bias:5.3629, r:0.1286, obsmean:4.1254



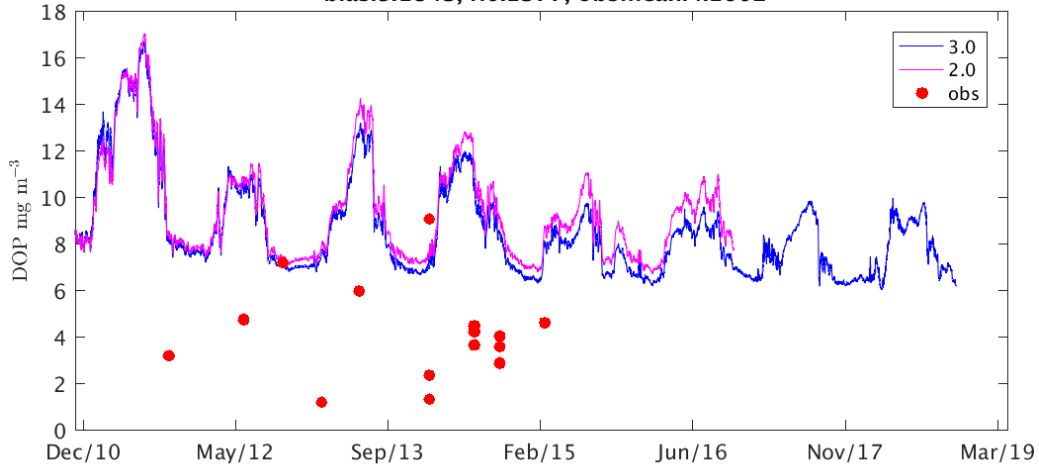
PortD\_15m 3.0 d2:0.27, mape:151.3, rms:5.4406  
bias:4.9602, r:0.2046, obsmean:3.8554  
PortD\_15m 2.0 d2:0.26, mape:191.2, rms:6.4043  
bias:6.0710, r:0.4159, obsmean:3.6449



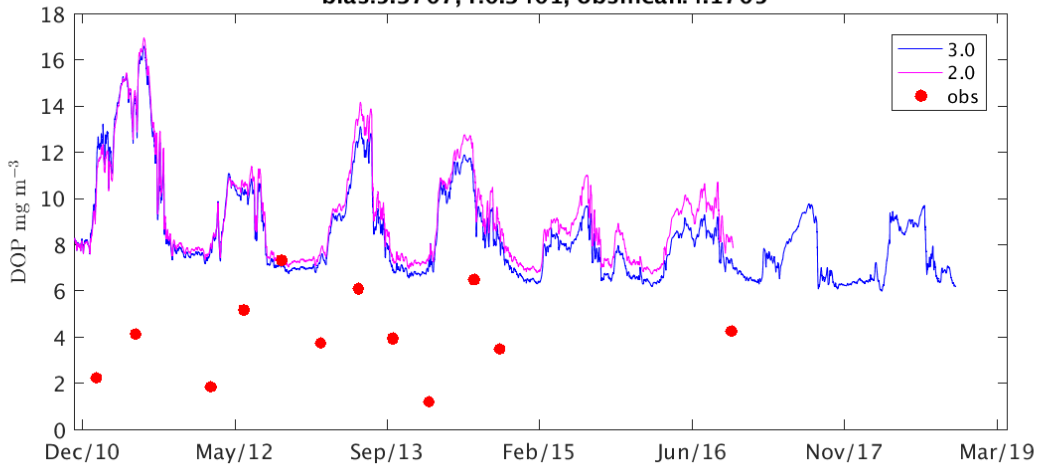
PortD\_0m 3.0 d2:0.23, mape:130.4, rms:5.1598  
bias:4.5438, r:-0.0340, obsmean:4.1186  
PortD\_0m 2.0 d2:0.23, mape:159.4, rms:5.9999  
bias:5.4362, r:0.0120, obsmean:4.0356



Snap\_10m 3.0 d2:0.32, mape:173.3, rms:5.2324  
bias:4.6574, r:0.1434, obsmean:4.1602  
Snap\_10m 2.0 d2:0.29, mape:187.5, rms:5.7602  
bias:5.1843, r:0.1377, obsmean:4.1602



CapeTrib356\_10m 3.0 d2:0.33, mape:171.7, rms:5.5446  
bias:4.9517, r:0.2536, obsmean:4.1705  
CapeTrib356\_10m 2.0 d2:0.33, mape:180.9, rms:5.8735  
bias:5.3707, r:0.3401, obsmean:4.1705



# 17. Simulated EFI assessment against Long Term Monitoring TSS

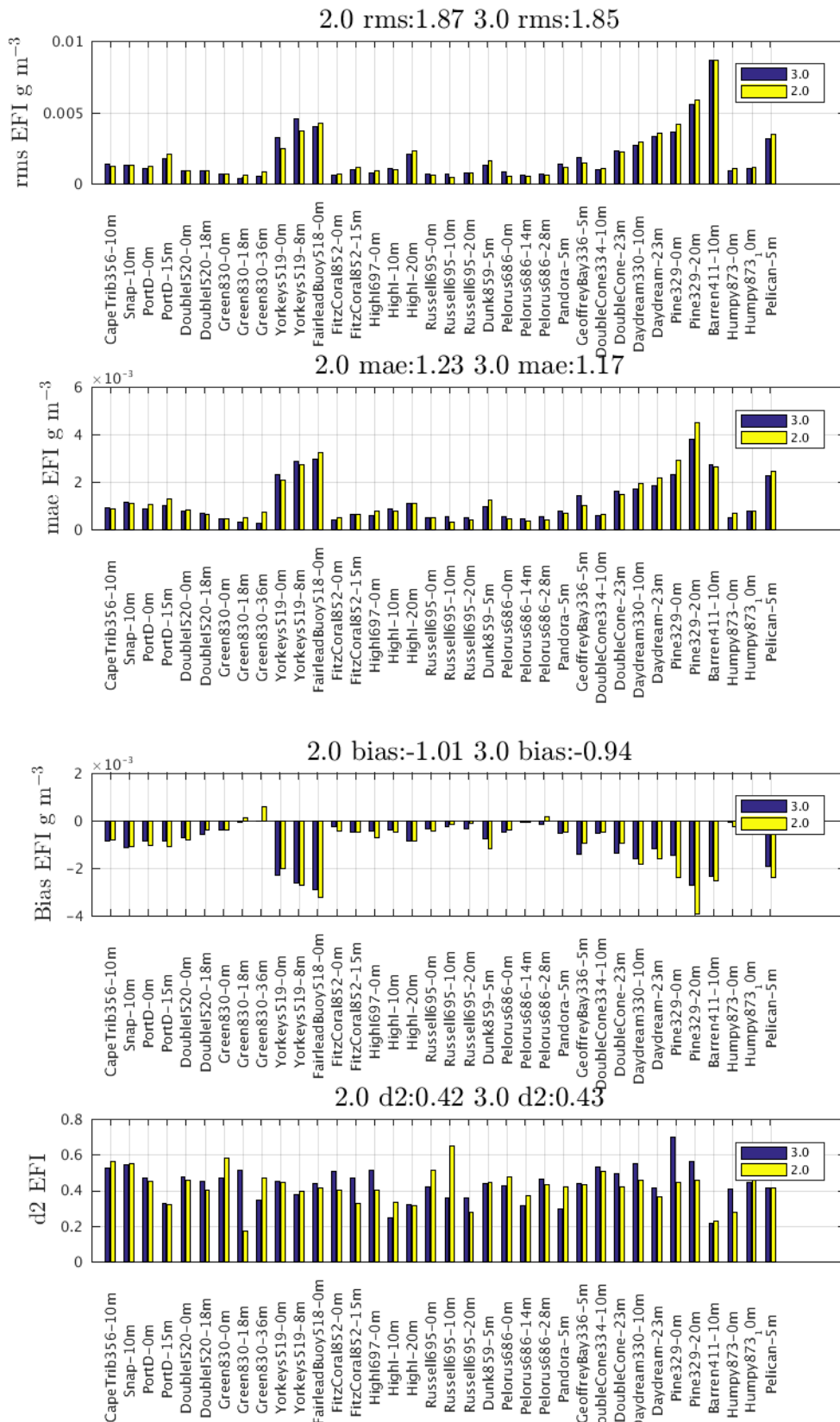
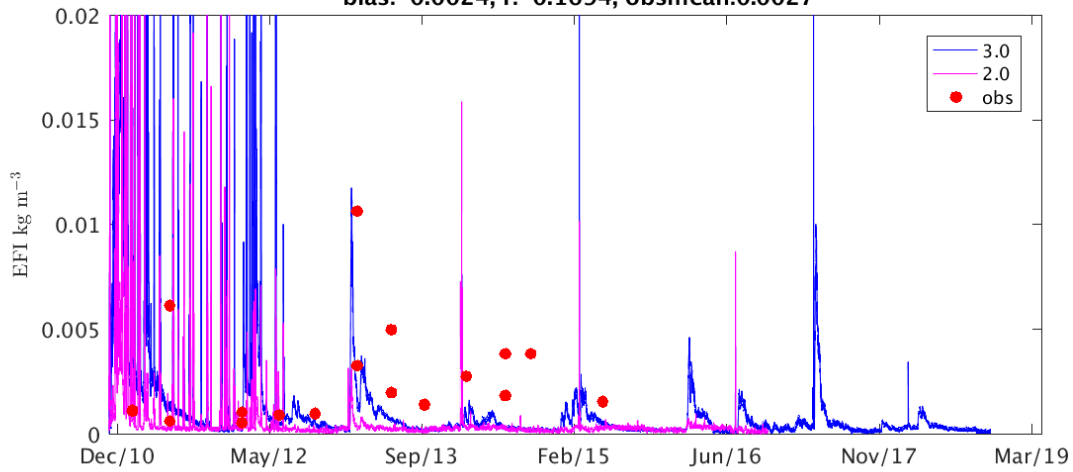
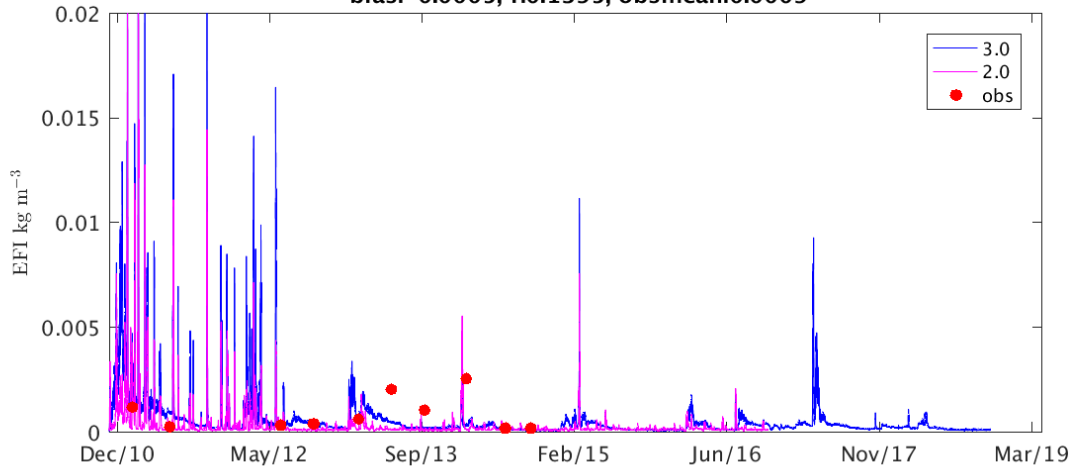


Figure 12 Metrics for Long Term Monitoring sites EFI model assessment against TSS observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

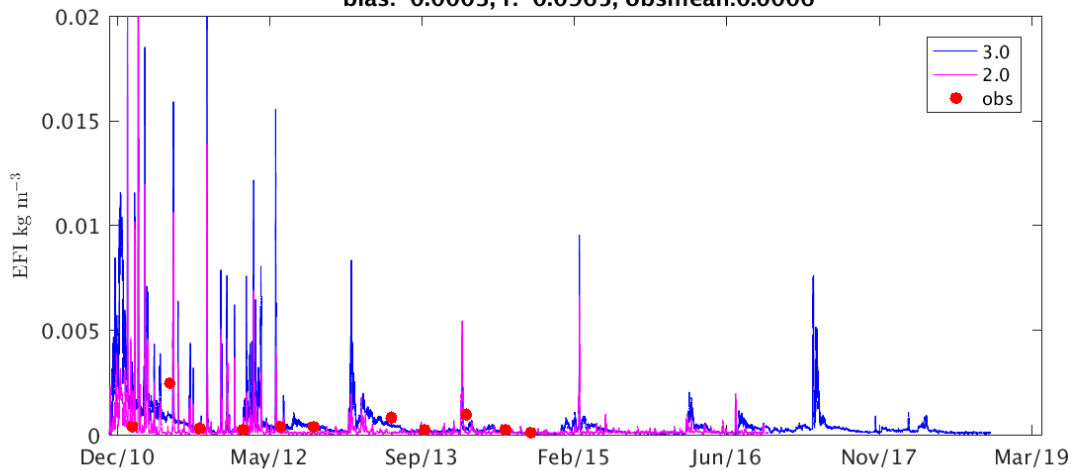
Pelican\_5m 3.0 d2:0.41, mape:79.4, rms:0.0032  
bias:-0.0019, r:0.0770, obsmean:0.0027  
Pelican\_5m 2.0 d2:0.41, mape:81.4, rms:0.0035  
bias:-0.0024, r:-0.1694, obsmean:0.0027



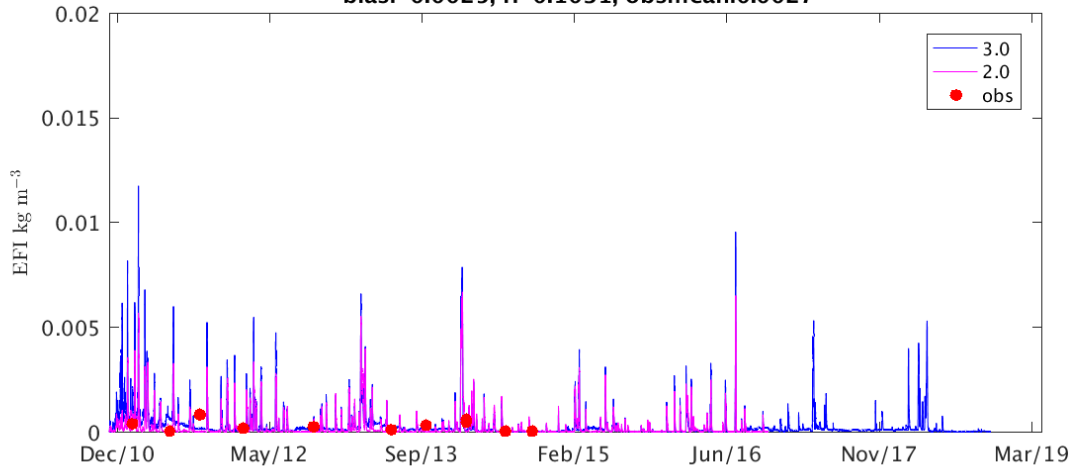
Humpy873\_10m 3.0 d2:0.44, mape:85.4, rms:0.0011  
bias:-0.0002, r:0.1055, obsmean:0.0009  
Humpy873\_10m 2.0 d2:0.50, mape:72.5, rms:0.0011  
bias:-0.0005, r:0.1395, obsmean:0.0009



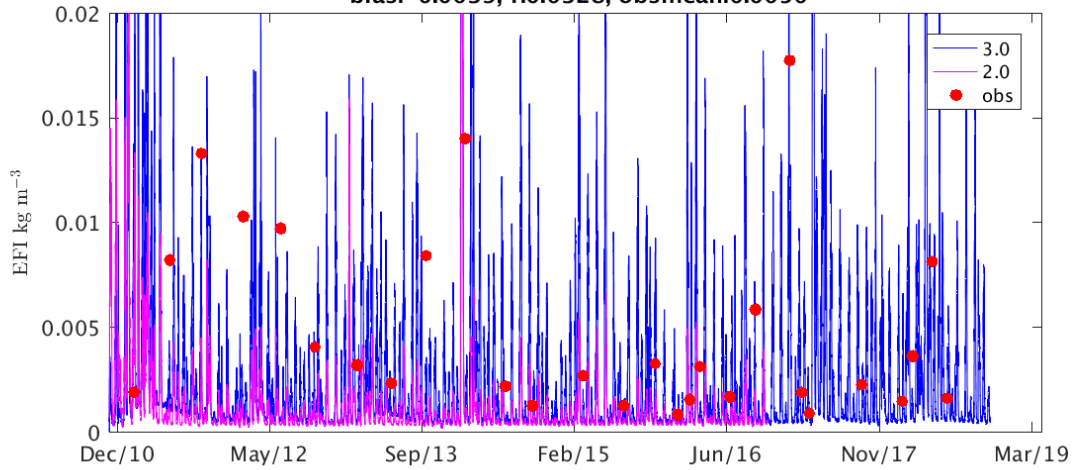
Humpy873\_0m 3.0 d2:0.41, mape:91.6, rms:0.0009  
bias:-0.0001, r:0.1776, obsmean:0.0006  
Humpy873\_0m 2.0 d2:0.28, mape:112.5, rms:0.0010  
bias:-0.0003, r:-0.0965, obsmean:0.0006



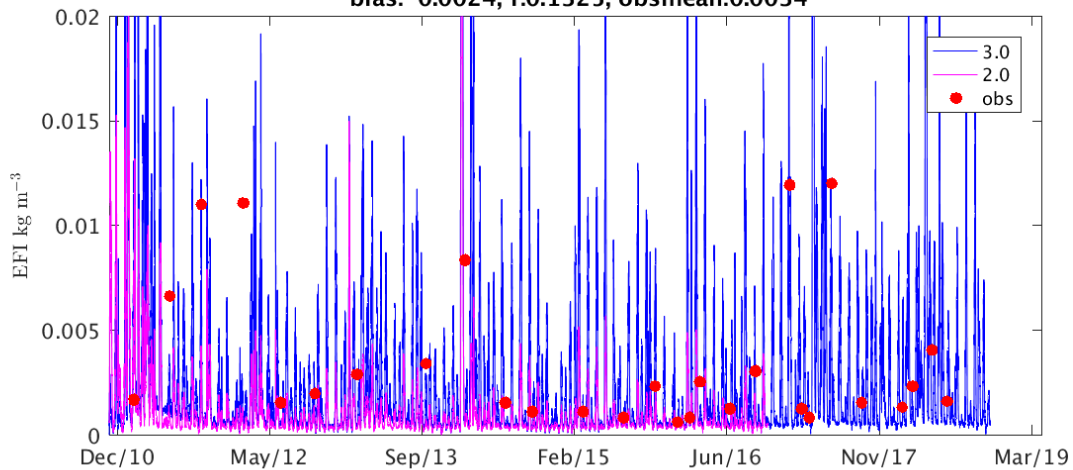
Barren411\_10m 3.0 d2:0.22, mape:165.1, rms:0.0086  
bias:-0.0023, r:-0.1095, obsmean:0.0027  
Barren411\_10m 2.0 d2:0.23, mape:75.0, rms:0.0087  
bias:-0.0025, r:-0.1031, obsmean:0.0027



Pine329\_20m 3.0 d2:0.56, mape:87.1, rms:0.0055  
bias:-0.0027, r:0.2878, obsmean:0.0049  
Pine329\_20m 2.0 d2:0.46, mape:92.4, rms:0.0059  
bias:-0.0039, r:0.0328, obsmean:0.0050

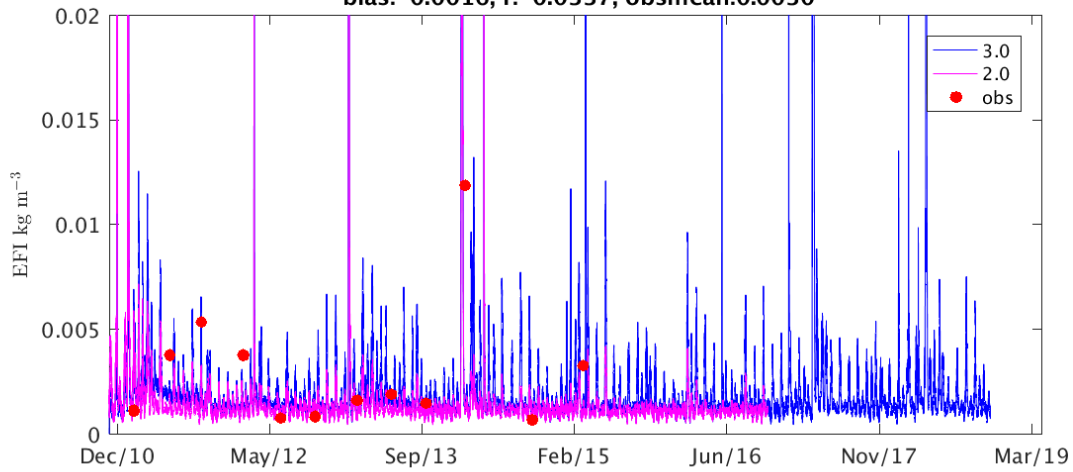


Pine329\_0m 3.0 d2:0.70, mape:70.2, rms:0.0036  
bias:-0.0015, r:0.5206, obsmean:0.0036  
Pine329\_0m 2.0 d2:0.44, mape:81.8, rms:0.0041  
bias:-0.0024, r:0.1325, obsmean:0.0034

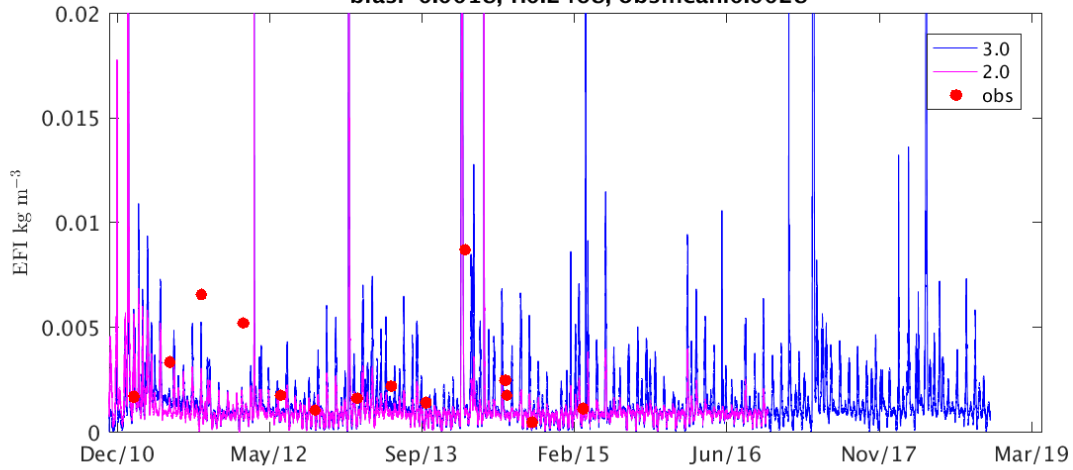




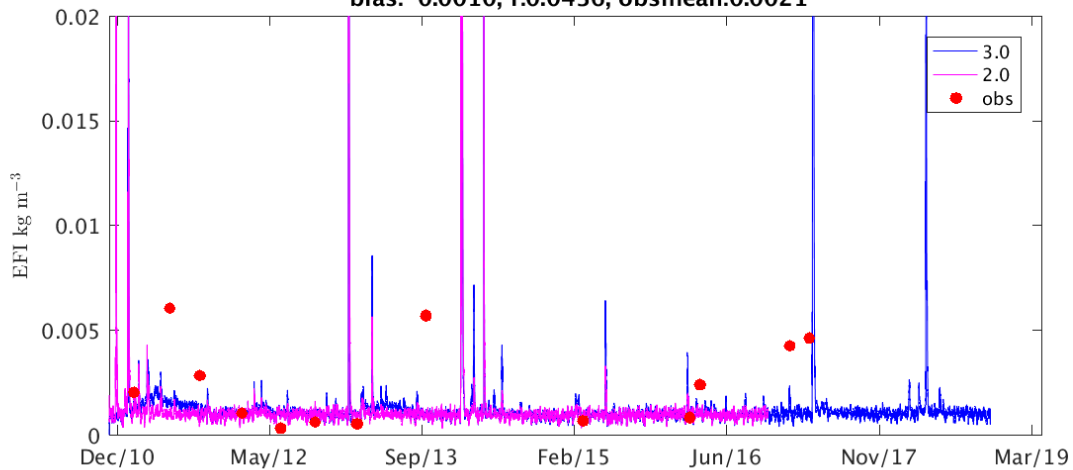
**Daydream\_23m 3.0 d2:0.41, mape:61.2, rms:0.0033**  
**bias:-0.0012, r:0.1259, obsmean:0.0030**  
**Daydream\_23m 2.0 d2:0.36, mape:68.0, rms:0.0035**  
**bias:-0.0016, r:-0.0337, obsmean:0.0030**



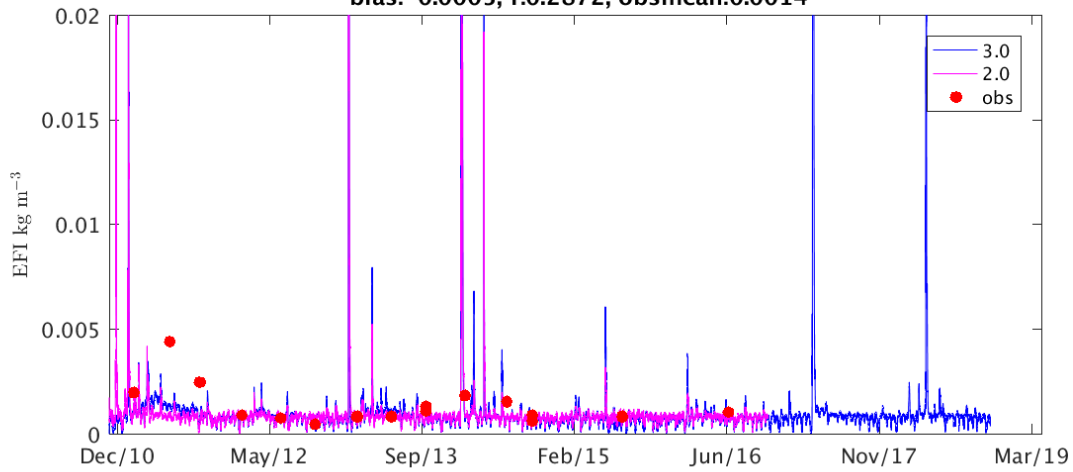
**Daydream330\_10m 3.0 d2:0.55, mape:47.1, rms:0.0026**  
**bias:-0.0016, r:0.4055, obsmean:0.0028**  
**Daydream330\_10m 2.0 d2:0.46, mape:54.5, rms:0.0029**  
**bias:-0.0018, r:0.2468, obsmean:0.0028**



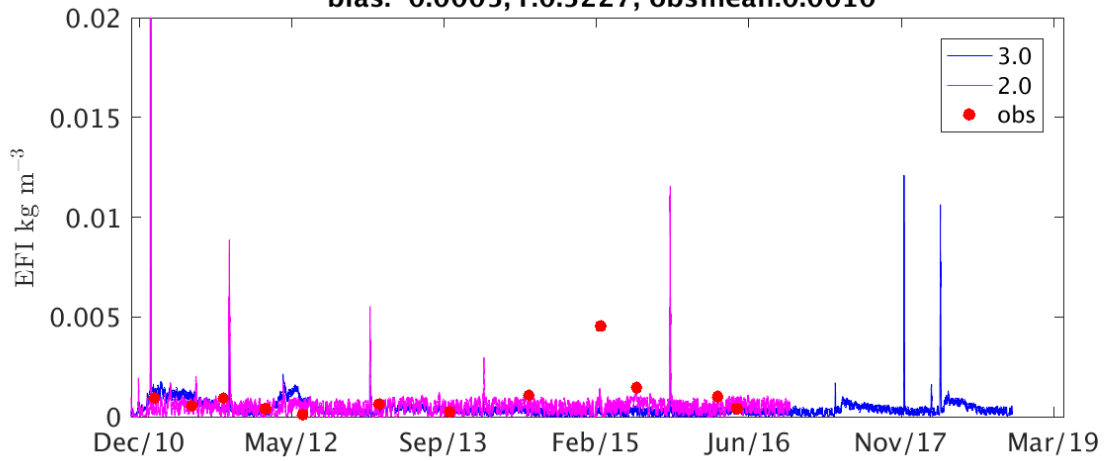
**DoubleCone\_23m 3.0 d2:0.49, mape:61.0, rms:0.0023**  
**bias:-0.0014, r:0.3674, obsmean:0.0025**  
**DoubleCone\_23m 2.0 d2:0.42, mape:68.6, rms:0.0022**  
**bias:-0.0010, r:0.0436, obsmean:0.0021**



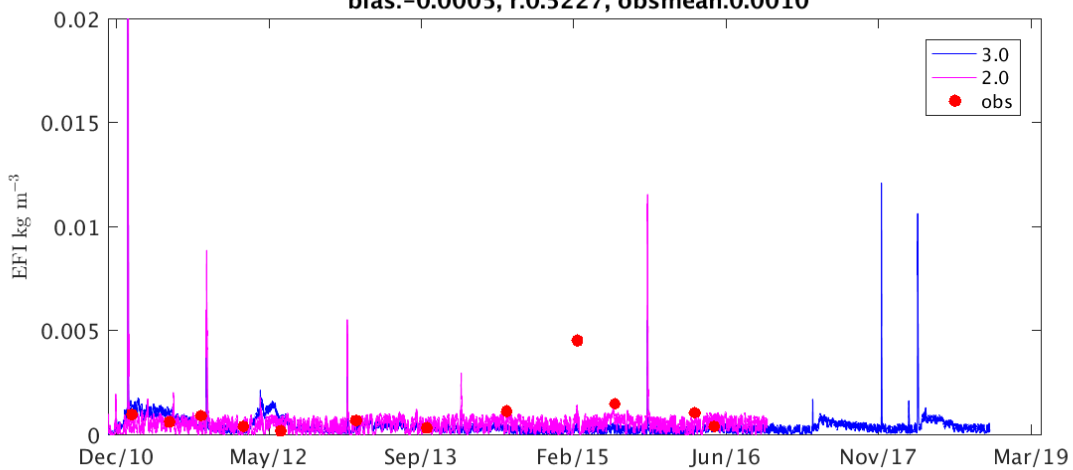
DoubleCone334\_10m 3.0 d2:0.53, mape:32.8, rms:0.0010  
bias:-0.0005, r:0.5558, obsmean:0.0014  
DoubleCone334\_10m 2.0 d2:0.51, mape:30.9, rms:0.0011  
bias:-0.0005, r:0.2872, obsmean:0.0014



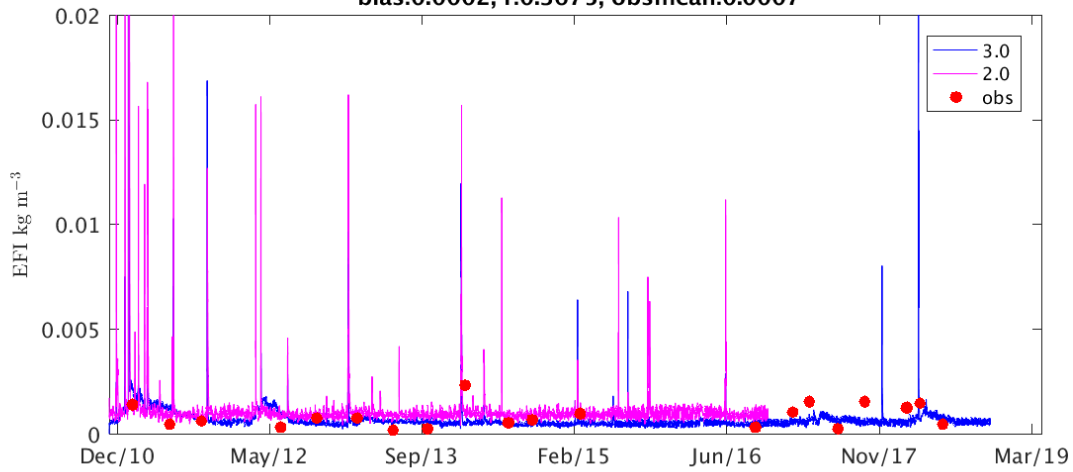
Pandora\_5m 3.0 d2:0.29, mape:91.3, rms:0.0013  
bias:-0.0006, r:-0.0931, obsmean:0.0010  
Pandora\_5m 2.0 d2:0.42, mape:78.4, rms:0.0011  
bias:-0.0005, r:0.5227, obsmean:0.0010



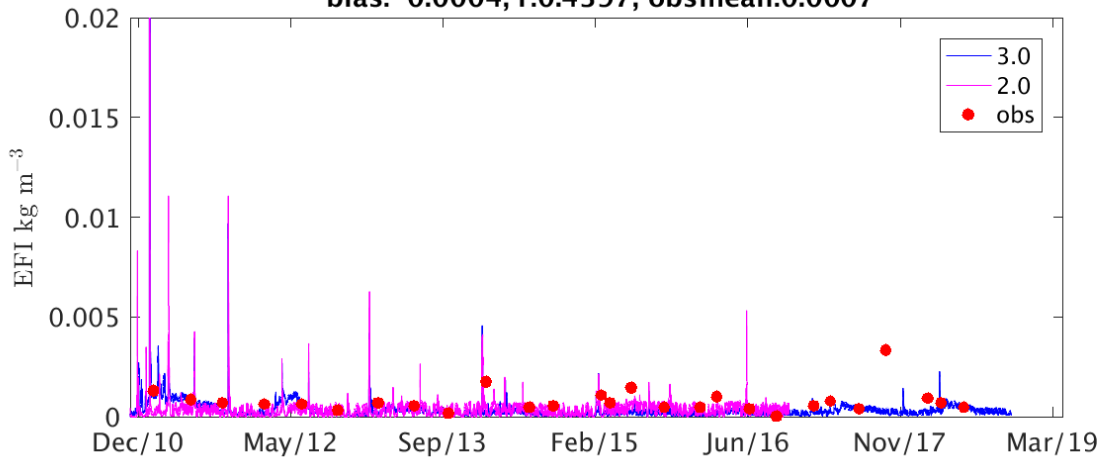
Pandora\_5m 3.0 d2:0.29, mape:91.3, rms:0.0013  
bias:-0.0006, r:-0.0931, obsmean:0.0010  
Pandora\_5m 2.0 d2:0.42, mape:78.4, rms:0.0011  
bias:-0.0005, r:0.5227, obsmean:0.0010



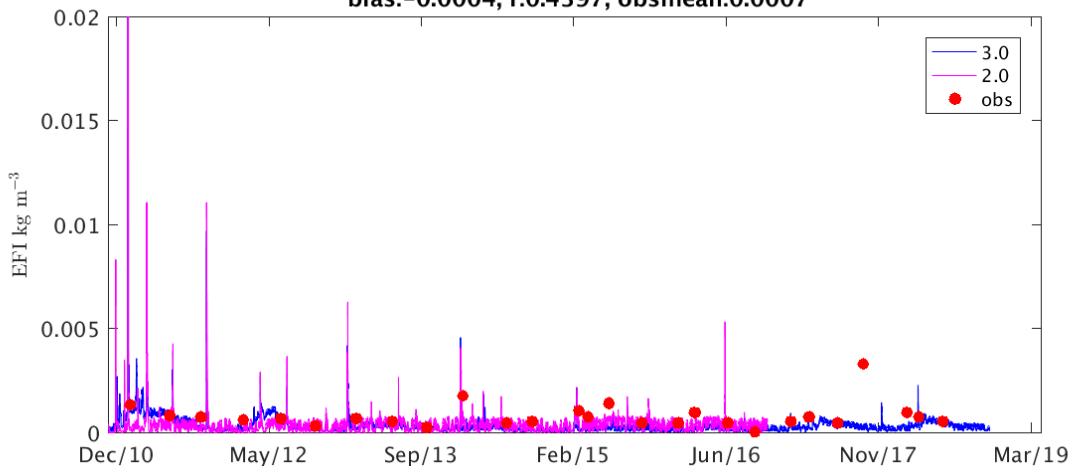
Pelorus686\_28m 3.0 d2:0.46, mape:73.3, rms:0.0007  
bias:-0.0002, r:0.1176, obsmean:0.0009  
Pelorus686\_28m 2.0 d2:0.43, mape:96.6, rms:0.0005  
bias:0.0002, r:0.3675, obsmean:0.0007



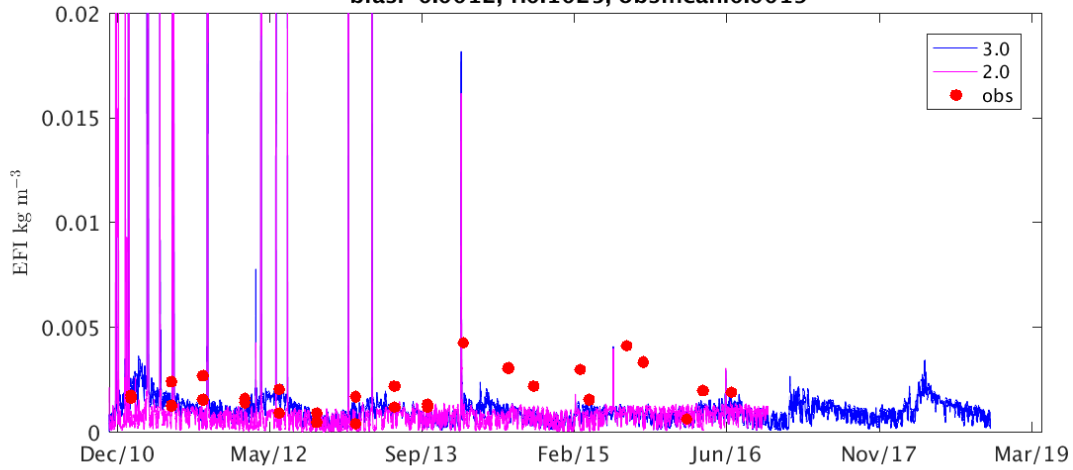
Pelorus686\_0m 3.0 d2:0.42, mape:127.6, rms:0.0008  
bias:-0.0005, r:0.1157, obsmean:0.0008  
Pelorus686\_0m 2.0 d2:0.48, mape:253.4, rms:0.0005  
bias:-0.0004, r:0.4397, obsmean:0.0007



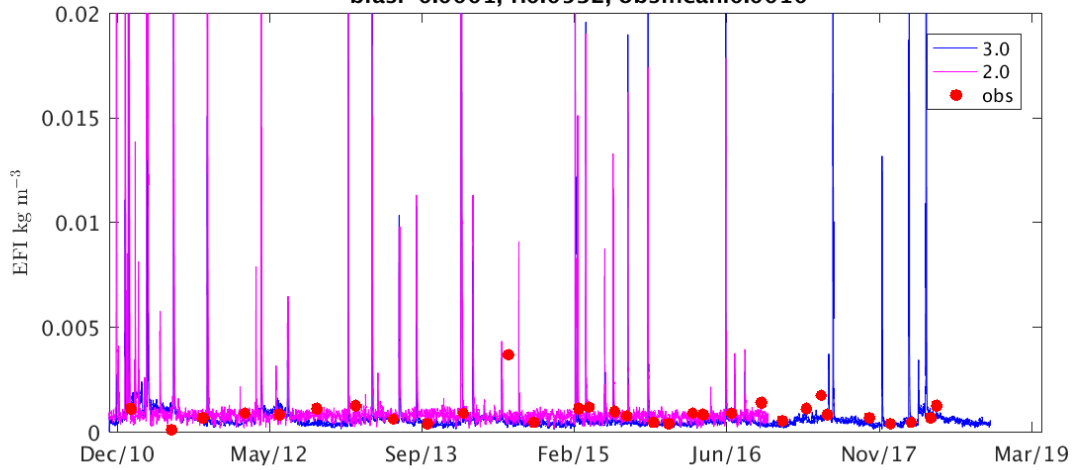
Pelorus686\_0m 3.0 d2:0.42, mape:127.6, rms:0.0008  
bias:-0.0005, r:0.1157, obsmean:0.0008  
Pelorus686\_0m 2.0 d2:0.48, mape:253.4, rms:0.0005  
bias:-0.0004, r:0.4397, obsmean:0.0007



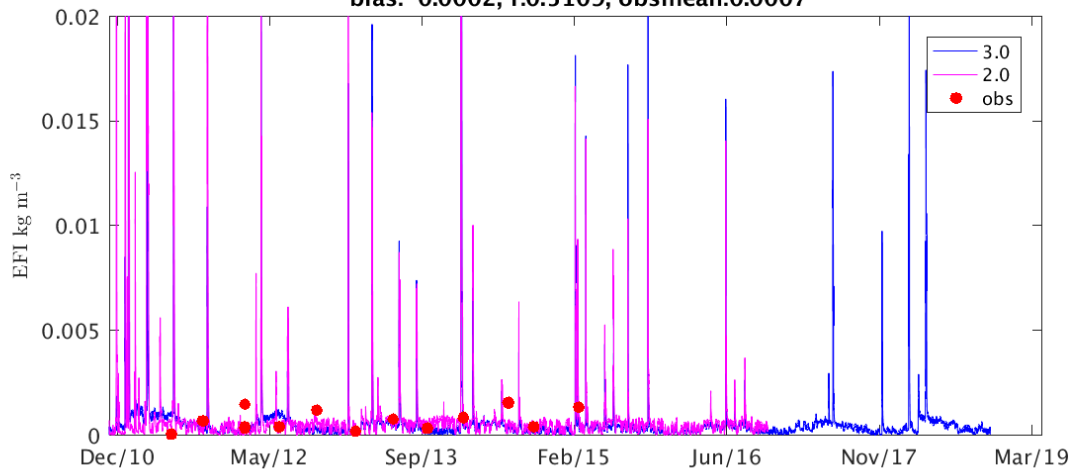
Dunk859\_5m 3.0 d2:0.44, mape:44.5, rms:0.0013  
bias:-0.0008, r:-0.0062, obsmean:0.0019  
Dunk859\_5m 2.0 d2:0.45, mape:57.5, rms:0.0016  
bias:-0.0012, r:0.1025, obsmean:0.0019



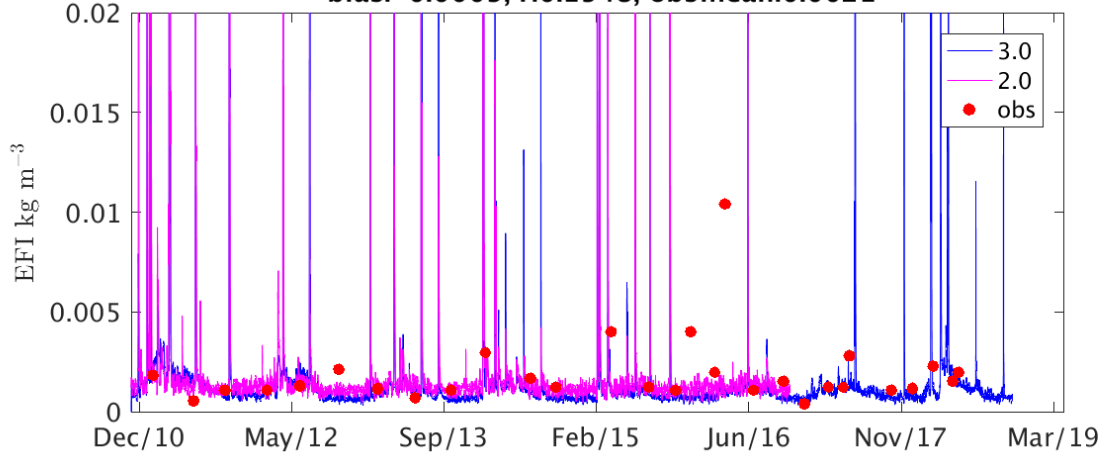
Russell695\_20m 3.0 d2:0.36, mape:71.5, rms:0.0007  
bias:-0.0003, r:0.0144, obsmean:0.0009  
Russell695\_20m 2.0 d2:0.28, mape:58.1, rms:0.0007  
bias:-0.0001, r:0.0532, obsmean:0.0010



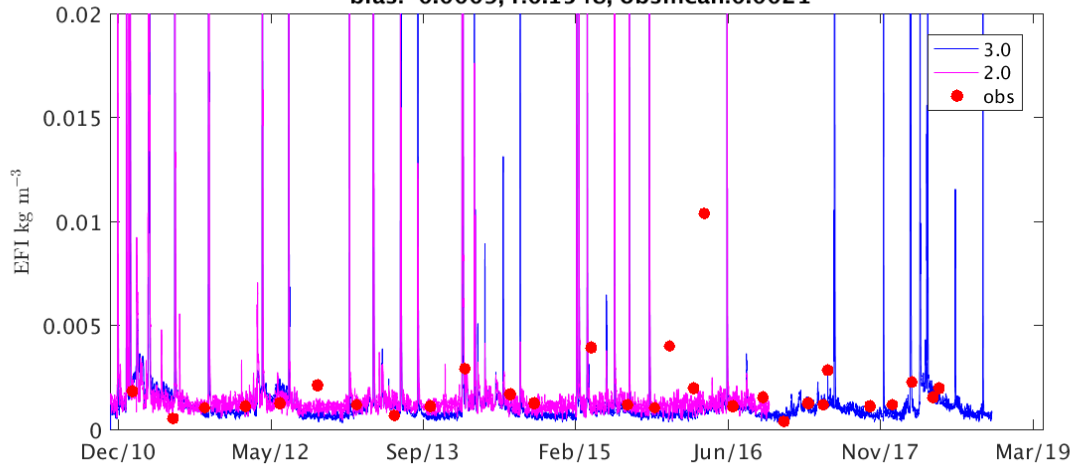
Russell695\_10m 3.0 d2:0.36, mape:277.0, rms:0.0006  
bias:-0.0002, r:-0.1517, obsmean:0.0007  
Russell695\_10m 2.0 d2:0.65, mape:145.8, rms:0.0004  
bias:-0.0002, r:0.5109, obsmean:0.0007



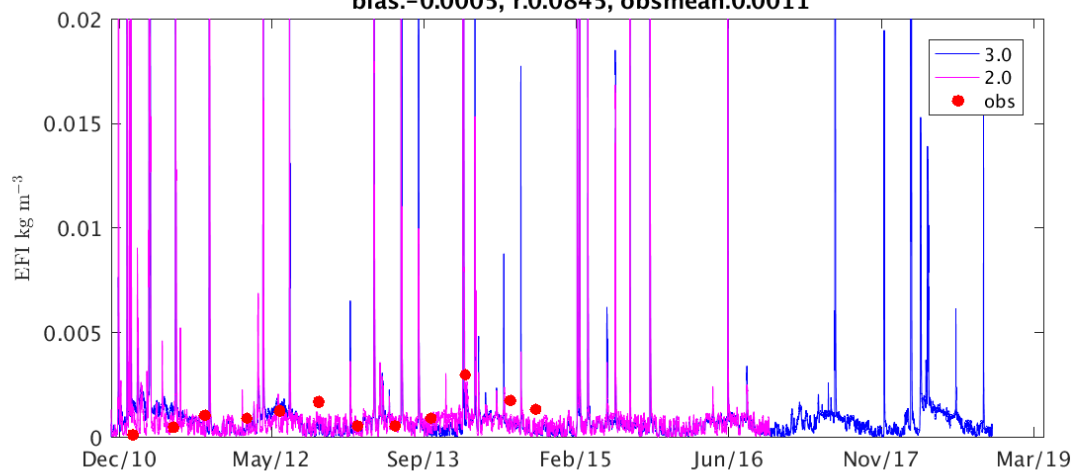
**Highl\_20m 3.0 d2:0.32, mape:48.0, rms:0.0020**  
**bias:-0.0009, r:0.0646, obsmean:0.0019**  
**Highl\_20m 2.0 d2:0.32, mape:38.1, rms:0.0023**  
**bias:-0.0009, r:0.1548, obsmean:0.0021**



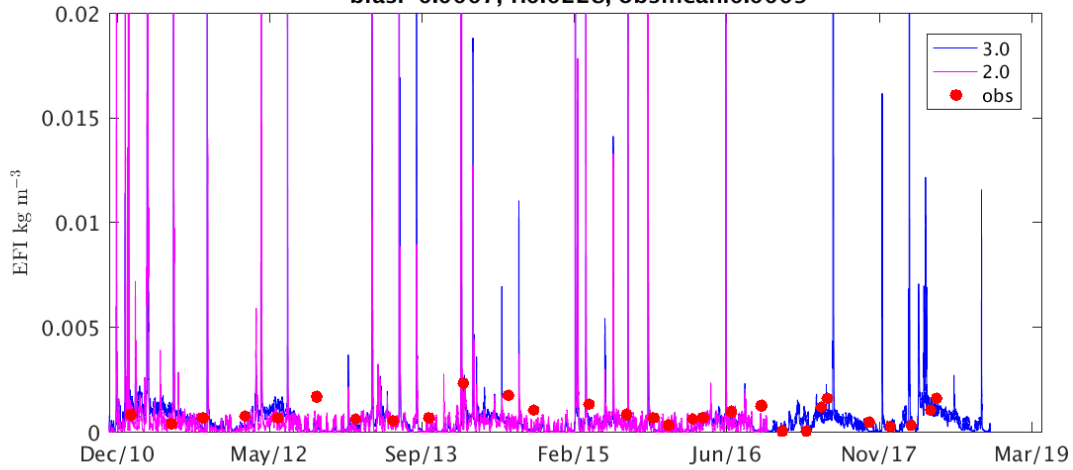
**Highl\_20m 3.0 d2:0.32, mape:48.0, rms:0.0020**  
**bias:-0.0009, r:0.0646, obsmean:0.0019**  
**Highl\_20m 2.0 d2:0.32, mape:38.1, rms:0.0023**  
**bias:-0.0009, r:0.1548, obsmean:0.0021**



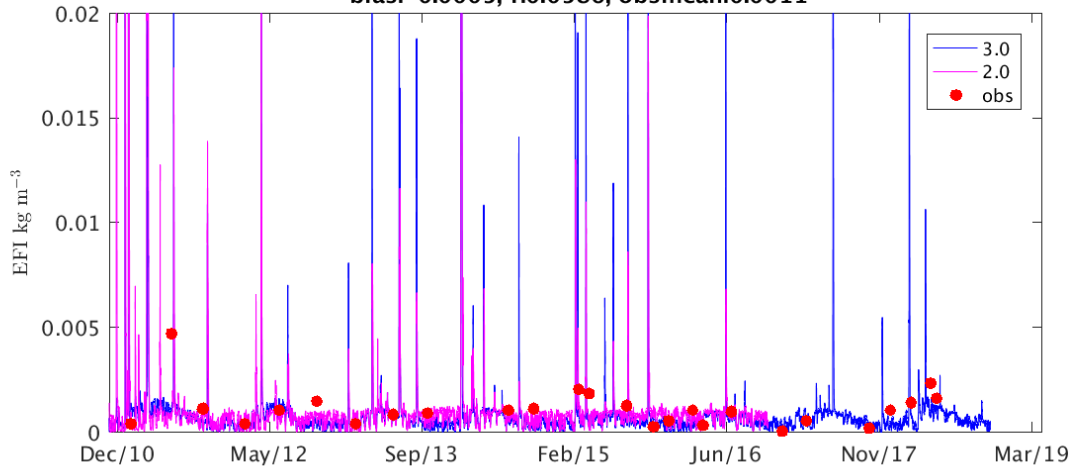
**Highl\_10m 3.0 d2:0.24, mape:167.1, rms:0.0010**  
**bias:-0.0004, r:-0.2611, obsmean:0.0011**  
**Highl\_10m 2.0 d2:0.33, mape:141.6, rms:0.0009**  
**bias:-0.0005, r:0.0845, obsmean:0.0011**



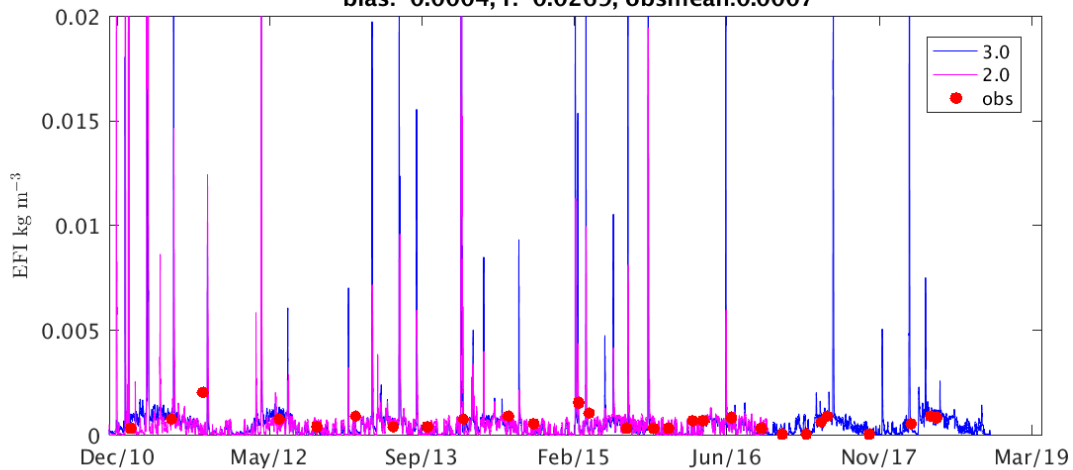
High1697\_0m 3.0 d2:0.51, mape:156.0, rms:0.0007  
bias:-0.0004, r:0.2283, obsmean:0.0009  
High1697\_0m 2.0 d2:0.40, mape:76.1, rms:0.0009  
bias:-0.0007, r:0.0228, obsmean:0.0009



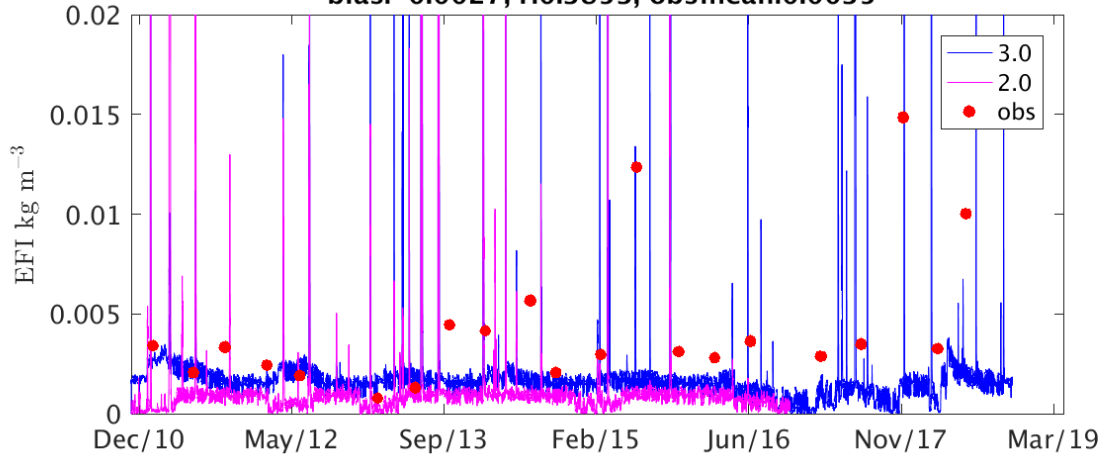
FitzCoral852\_15m 3.0 d2:0.47, mape:160.7, rms:0.0010  
bias:-0.0005, r:0.4042, obsmean:0.0011  
FitzCoral852\_15m 2.0 d2:0.32, mape:60.3, rms:0.0011  
bias:-0.0005, r:0.0586, obsmean:0.0011



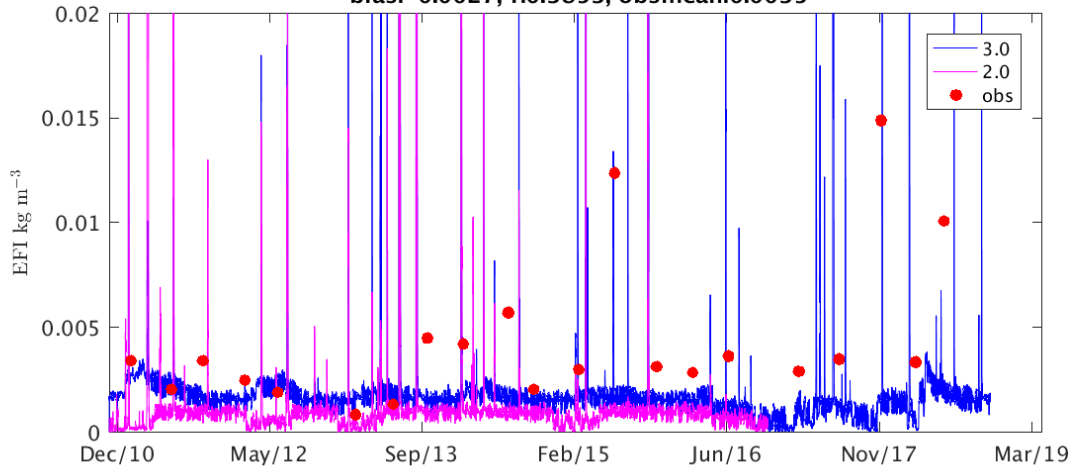
FitzCoral852\_0m 3.0 d2:0.51, mape:87.5, rms:0.0006  
bias:-0.0003, r:0.1662, obsmean:0.0006  
FitzCoral852\_0m 2.0 d2:0.40, mape:65.8, rms:0.0007  
bias:-0.0004, r:-0.0269, obsmean:0.0007



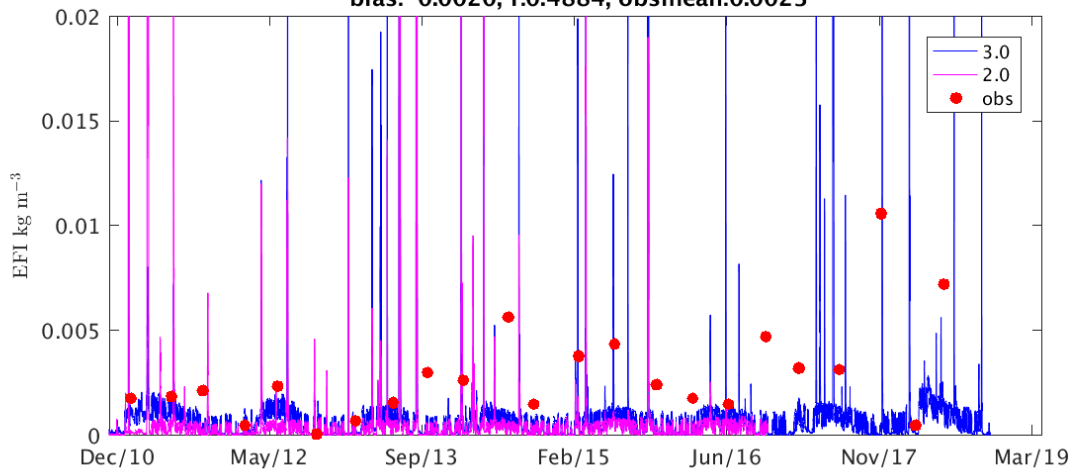
**Yorkeys519\_8m 3.0 d2:0.38, mape:55.0, rms:0.0045**  
**bias:-0.0026, r:-0.1355, obsmean:0.0043**  
**Yorkeys519\_8m 2.0 d2:0.40, mape:68.8, rms:0.0037**  
**bias:-0.0027, r:0.3853, obsmean:0.0035**



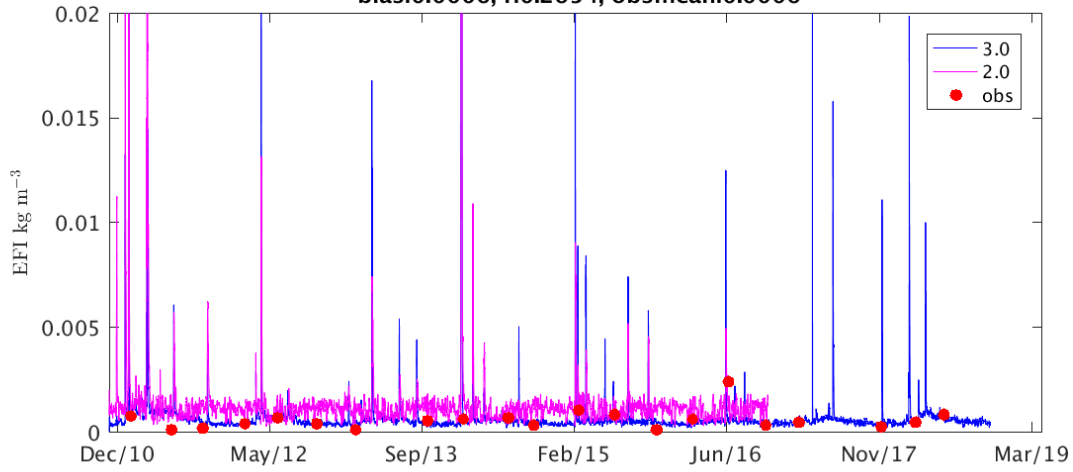
**Yorkeys519\_8m 3.0 d2:0.38, mape:55.0, rms:0.0045**  
**bias:-0.0026, r:-0.1355, obsmean:0.0043**  
**Yorkeys519\_8m 2.0 d2:0.40, mape:68.8, rms:0.0037**  
**bias:-0.0027, r:0.3853, obsmean:0.0035**



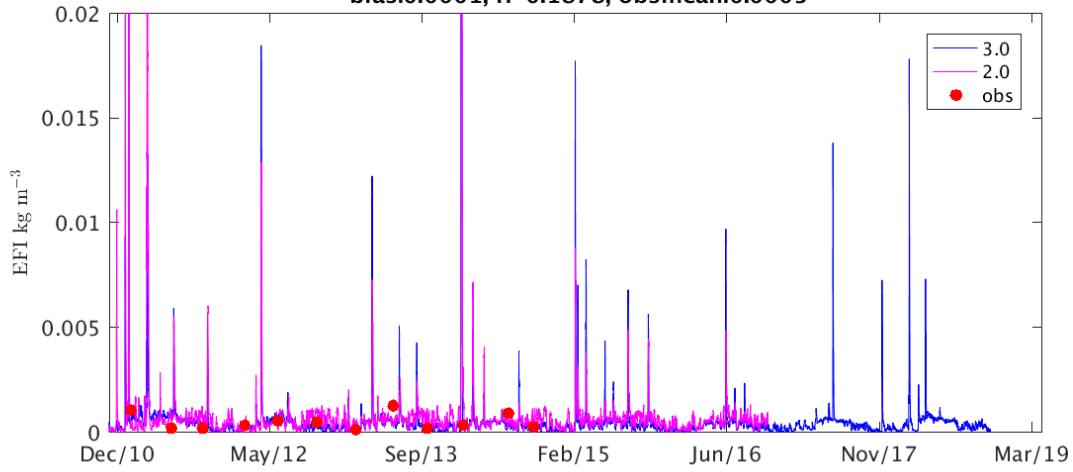
**Yorkeys519\_0m 3.0 d2:0.45, mape:70.4, rms:0.0032**  
**bias:-0.0023, r:0.3135, obsmean:0.0029**  
**Yorkeys519\_0m 2.0 d2:0.44, mape:83.9, rms:0.0025**  
**bias:-0.0020, r:0.4884, obsmean:0.0023**



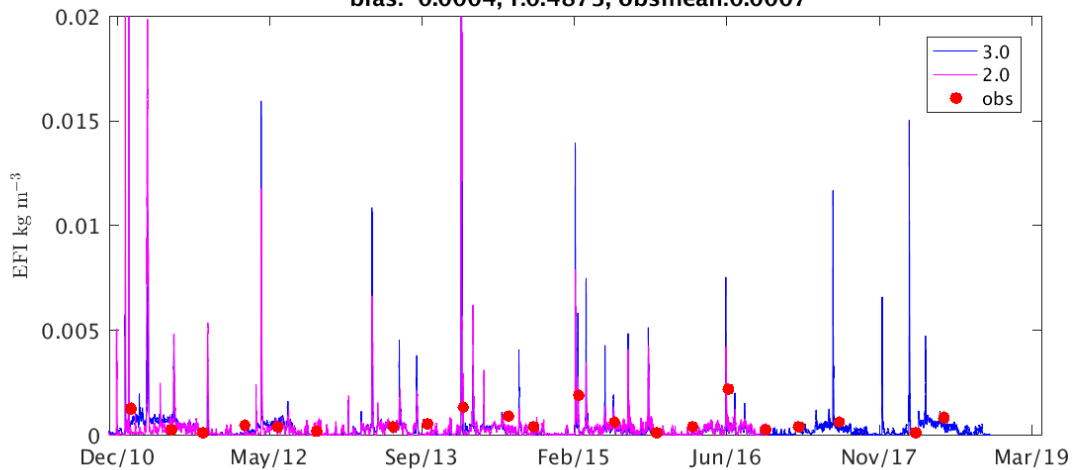
**Green830\_36m 3.0 d2:0.35, mape:78.1, rms:0.0005**  
**bias:-0.0000, r:0.2181, obsmean:0.0006**  
**Green830\_36m 2.0 d2:0.47, mape:246.0, rms:0.0008**  
**bias:0.0006, r:0.2654, obsmean:0.0006**



**Green830\_18m 3.0 d2:0.51, mape:82.5, rms:0.0004**  
**bias:-0.0001, r:0.3274, obsmean:0.0005**  
**Green830\_18m 2.0 d2:0.17, mape:141.1, rms:0.0006**  
**bias:0.0001, r:-0.1878, obsmean:0.0005**

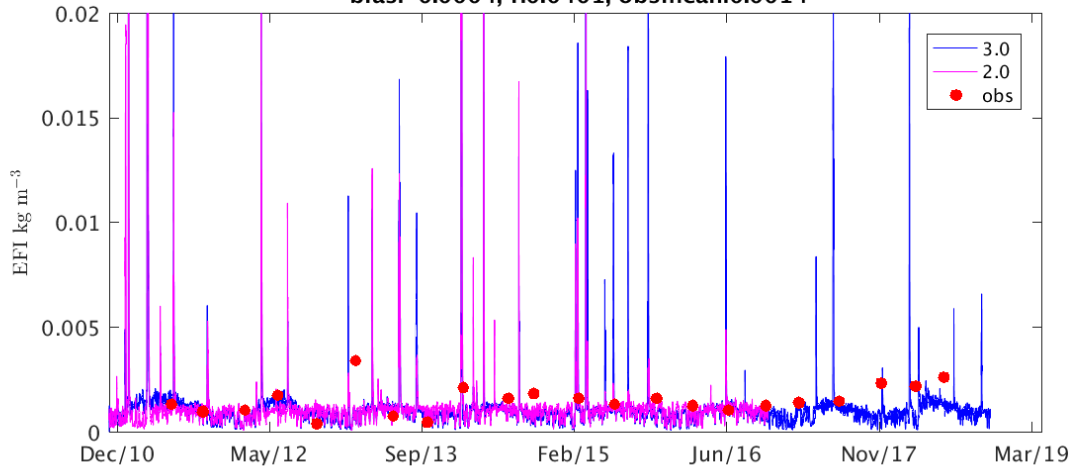


**Green830\_0m 3.0 d2:0.47, mape:67.2, rms:0.0007**  
**bias:-0.0004, r:0.2557, obsmean:0.0006**  
**Green830\_0m 2.0 d2:0.58, mape:68.1, rms:0.0007**  
**bias:-0.0004, r:0.4873, obsmean:0.0007**

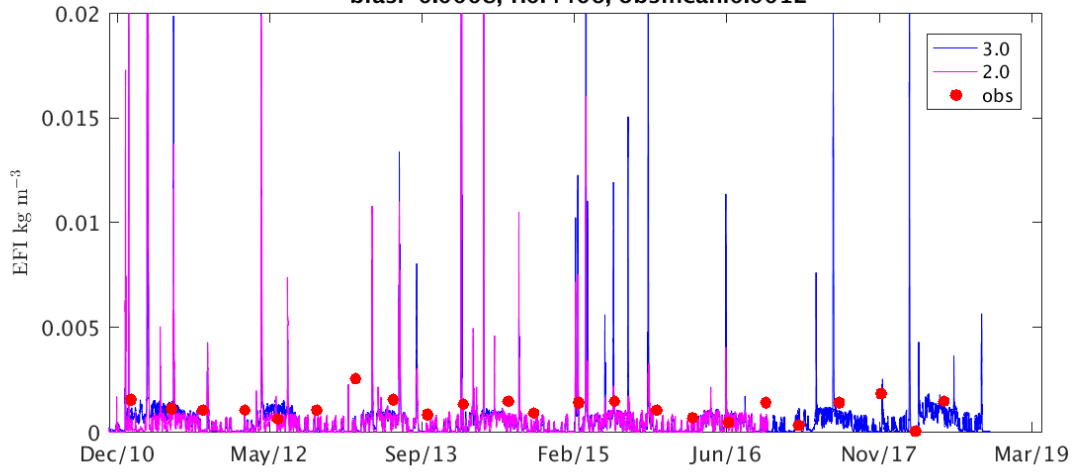




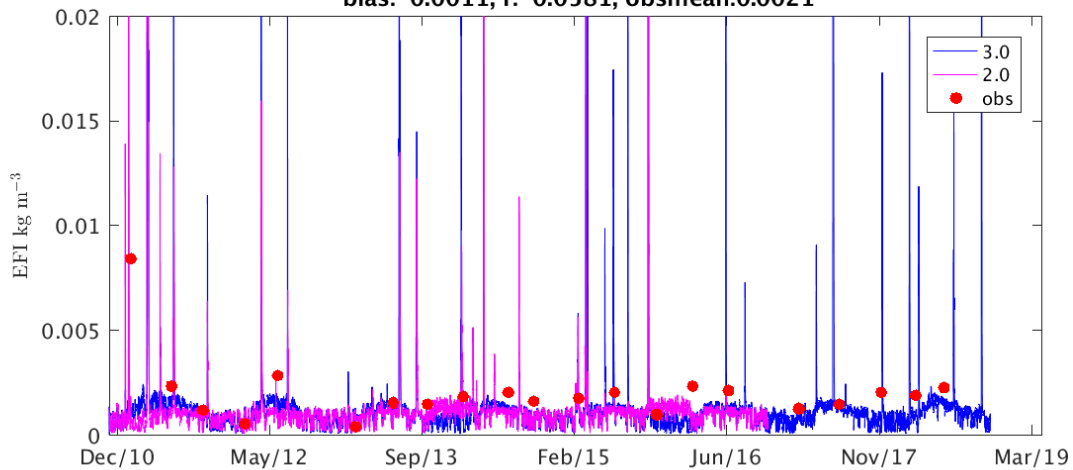
DoubleI520\_18m 3.0 d2:0.45, mape:44.4, rms:0.0009  
bias:-0.0006, r:0.1142, obsmean:0.0015  
DoubleI520\_18m 2.0 d2:0.40, mape:45.5, rms:0.0009  
bias:-0.0004, r:0.0401, obsmean:0.0014



DoubleI520\_0m 3.0 d2:0.47, mape:64.1, rms:0.0009  
bias:-0.0007, r:0.3371, obsmean:0.0012  
DoubleI520\_0m 2.0 d2:0.46, mape:68.5, rms:0.0009  
bias:-0.0008, r:0.4406, obsmean:0.0012



PortD\_15m 3.0 d2:0.32, mape:50.4, rms:0.0018  
bias:-0.0009, r:0.1628, obsmean:0.0020  
PortD\_15m 2.0 d2:0.32, mape:57.7, rms:0.0021  
bias:-0.0011, r:-0.0581, obsmean:0.0021

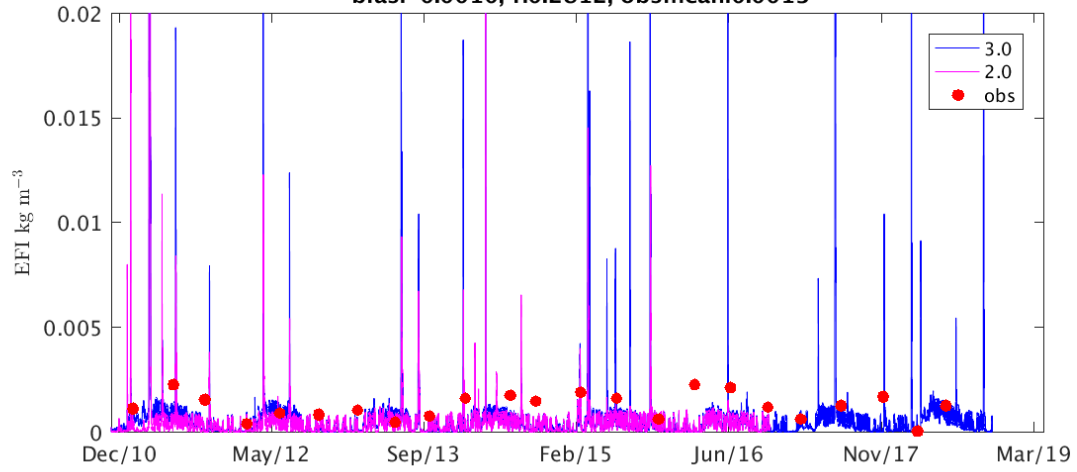


PortD\_0m 3.0 d2:0.47, mape:66.0, rms:0.0011

bias:-0.0009, r:0.2280, obsmean:0.0012

PortD\_0m 2.0 d2:0.45, mape:74.2, rms:0.0012

bias:-0.0010, r:0.2812, obsmean:0.0013

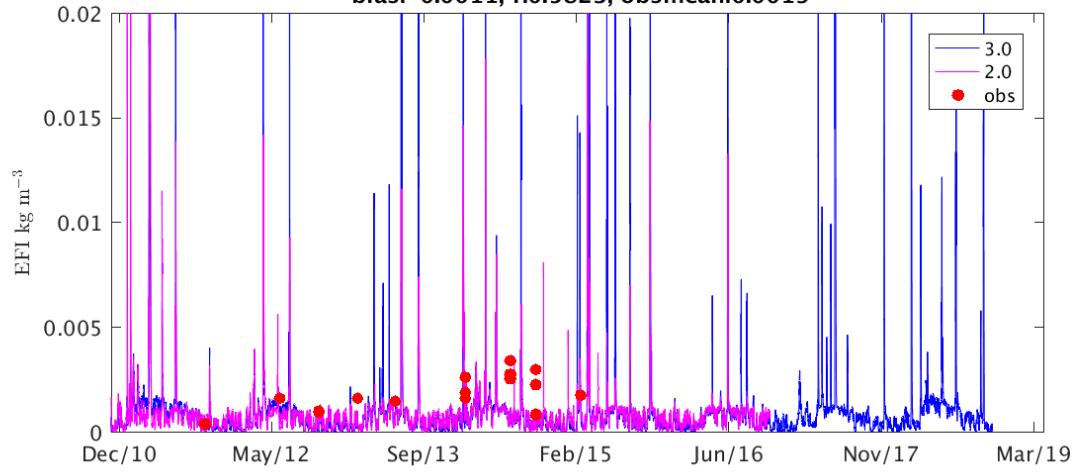


Snap\_10m 3.0 d2:0.54, mape:57.9, rms:0.0013

bias:-0.0011, r:0.5667, obsmean:0.0019

Snap\_10m 2.0 d2:0.55, mape:57.3, rms:0.0013

bias:-0.0011, r:0.5823, obsmean:0.0019



## 18. Simulated Chl *a* assessment against IMOS NRS HPLC Chl *a*

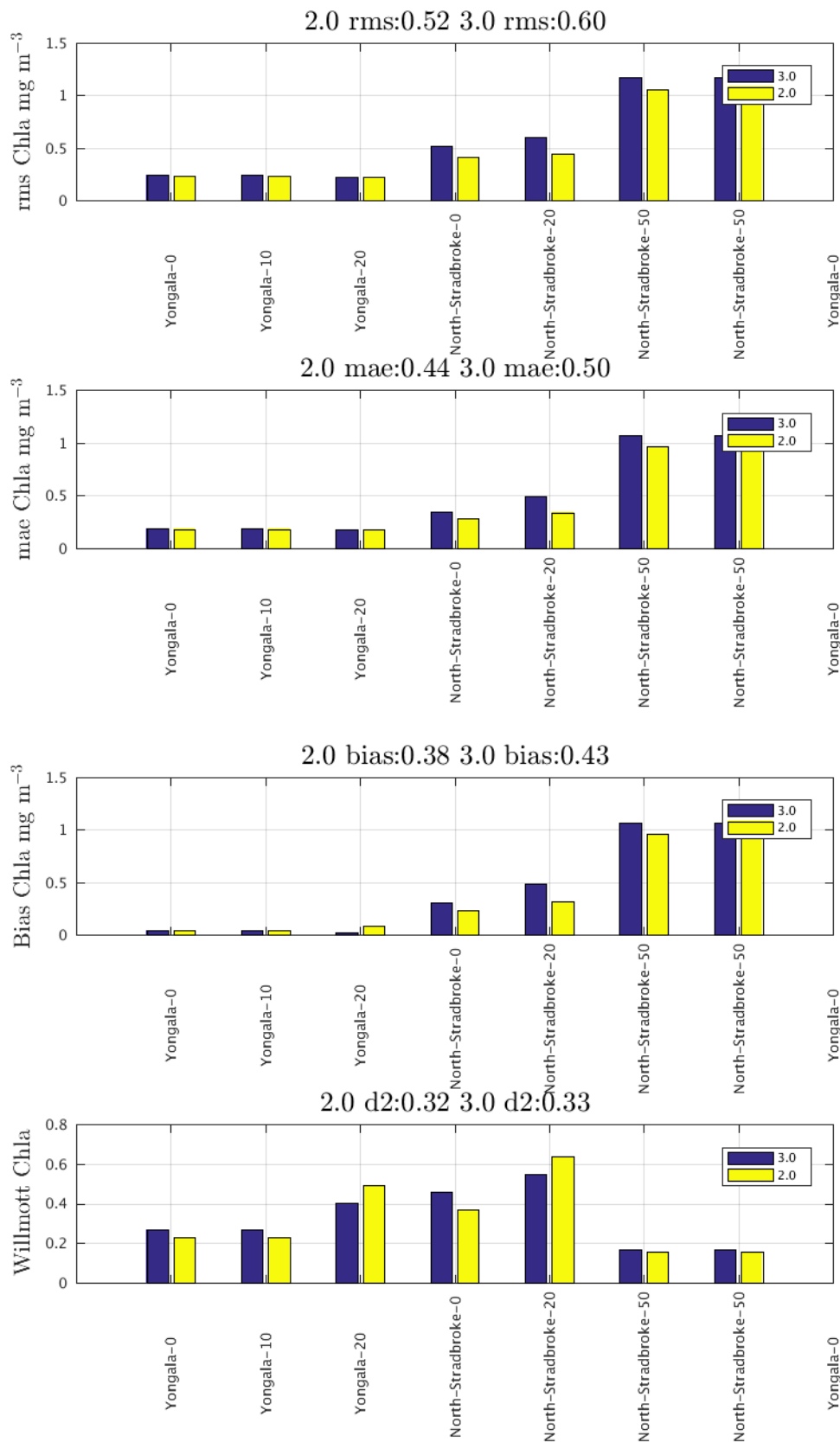


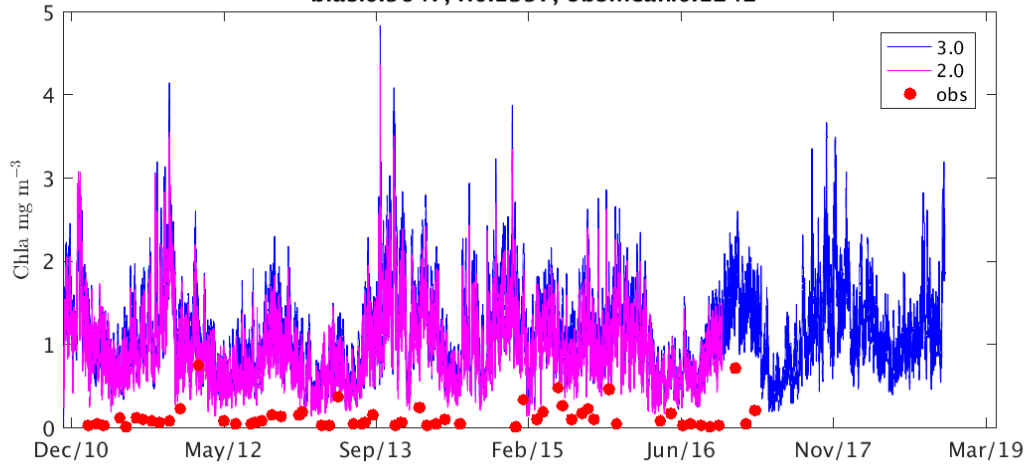
Figure 13 Metrics for IMOS NRS sites Chlorophyll assessment against observations for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27. mae: mean absolute error, rms root mean square

North\_Stradbroke\_50 3.0 d2:0.17, mape:2287.1, rms:1.1762

bias:1.0697, r:0.2079, obsmean:0.1346

North\_Stradbroke\_50 2.0 d2:0.16, mape:2140.4, rms:1.0548

bias:0.9647, r:0.1397, obsmean:0.1242

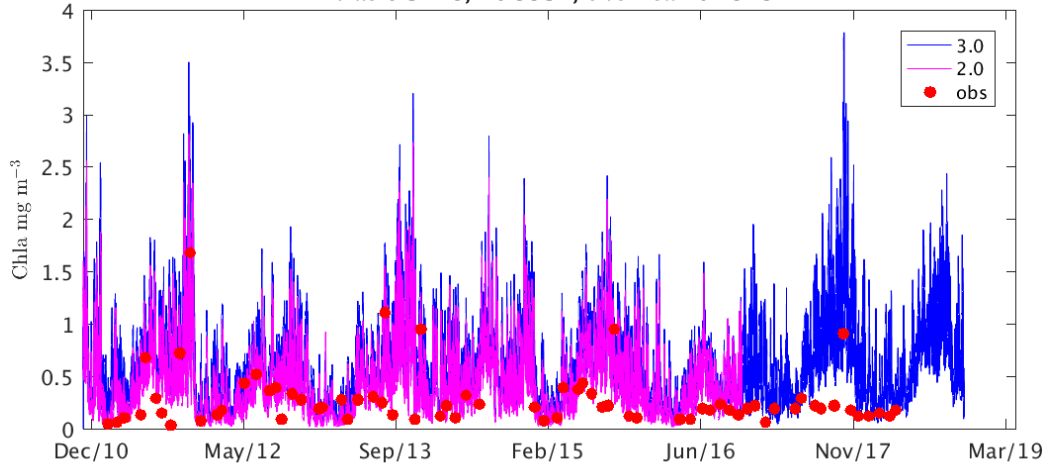


North\_Stradbroke\_20 3.0 d2:0.55, mape:296.5, rms:0.6018

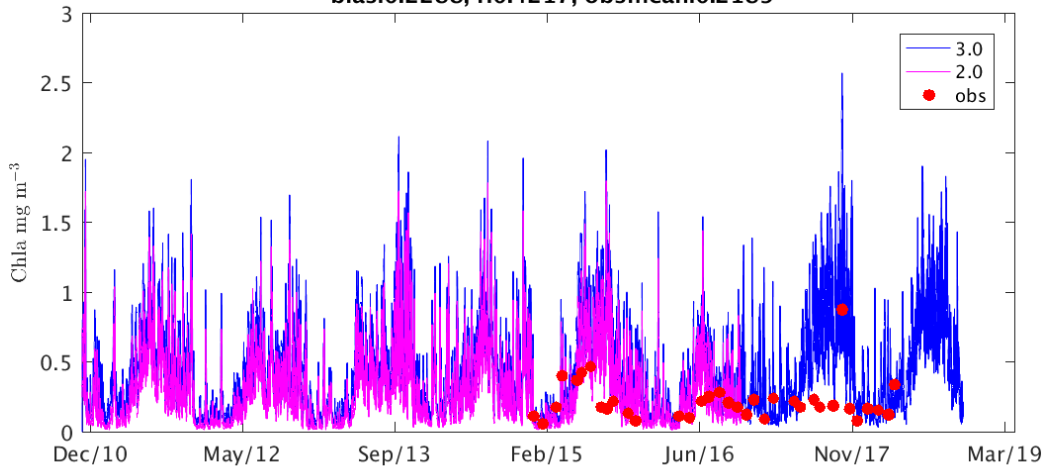
bias:0.4862, r:0.6304, obsmean:0.2812

North\_Stradbroke\_20 2.0 d2:0.64, mape:208.7, rms:0.4469

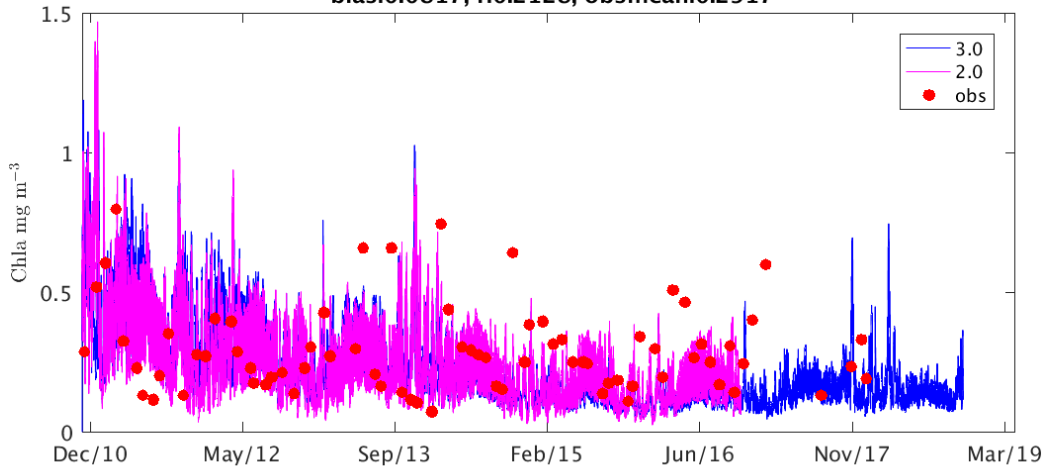
bias:0.3178, r:0.5934, obsmean:0.2975



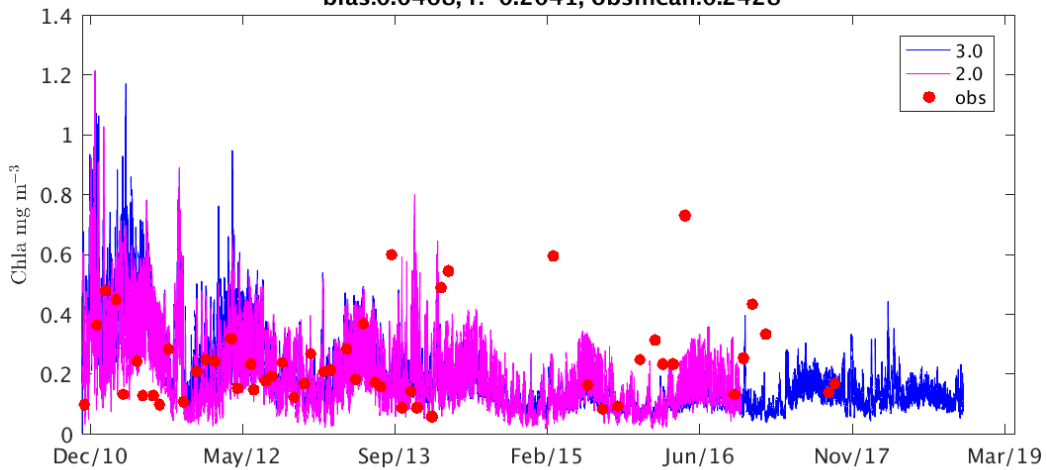
North\_Stradbroke\_0 3.0 d2:0.46, mape:165.5, rms:0.5133  
 bias:0.3062, r:0.6512, obsmean:0.2211  
 North\_Stradbroke\_0 2.0 d2:0.37, mape:137.6, rms:0.4160  
 bias:0.2288, r:0.4217, obsmean:0.2189



Yongala\_20 3.0 d2:0.40, mape:76.7, rms:0.2234  
 bias:0.0175, r:0.0439, obsmean:0.2928  
 Yongala\_20 2.0 d2:0.49, mape:83.6, rms:0.2215  
 bias:0.0817, r:0.2128, obsmean:0.2917



Yongala\_10 3.0 d2:0.27, mape:102.8, rms:0.2473  
 bias:0.0439, r:-0.1568, obsmean:0.2450  
 Yongala\_10 2.0 d2:0.23, mape:108.2, rms:0.2281  
 bias:0.0468, r:-0.2041, obsmean:0.2428



19. Simulated Chl *a* and Fluorescence assessment against AIMS MMP fluorescence (includes scatter plots)

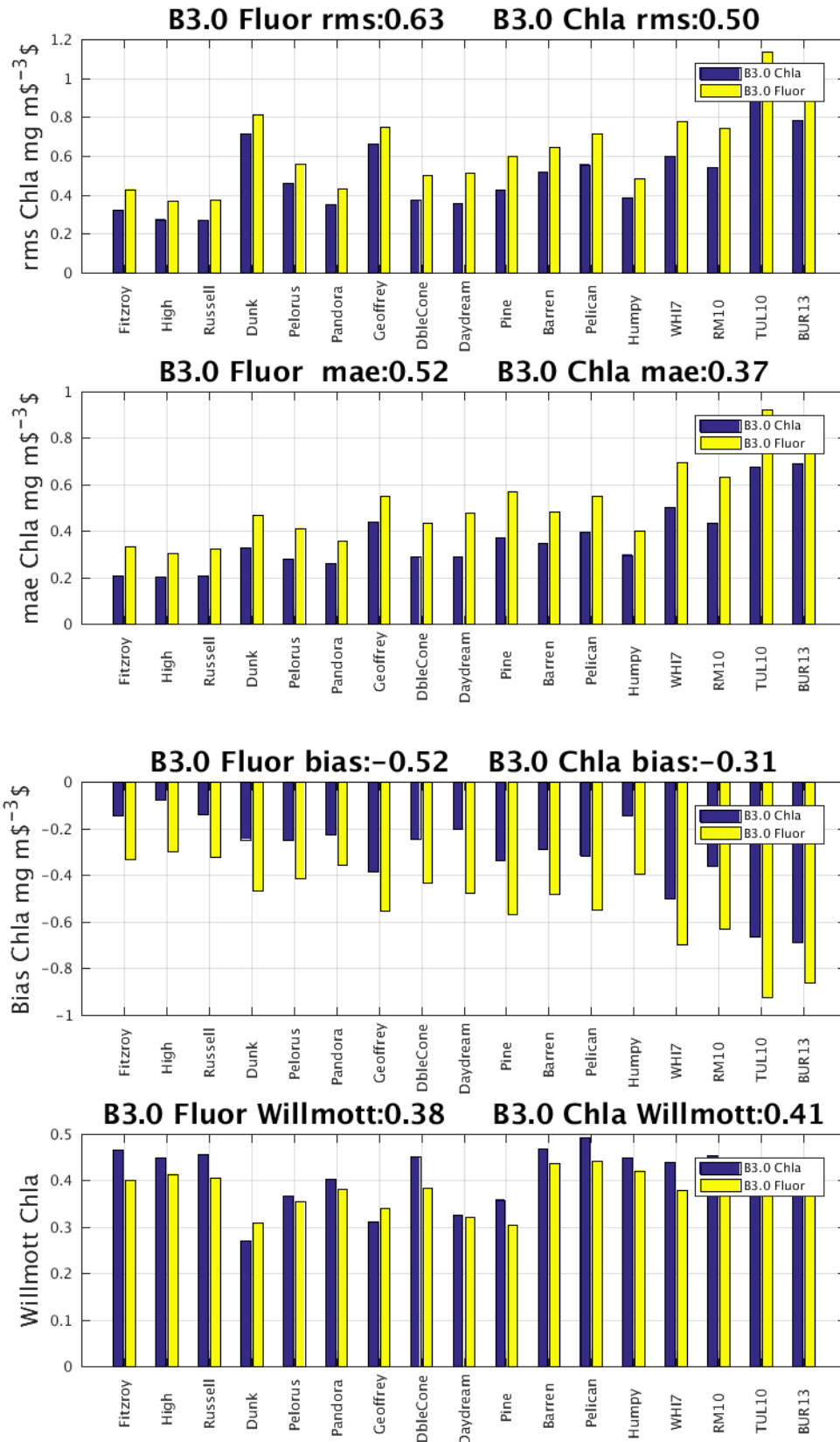
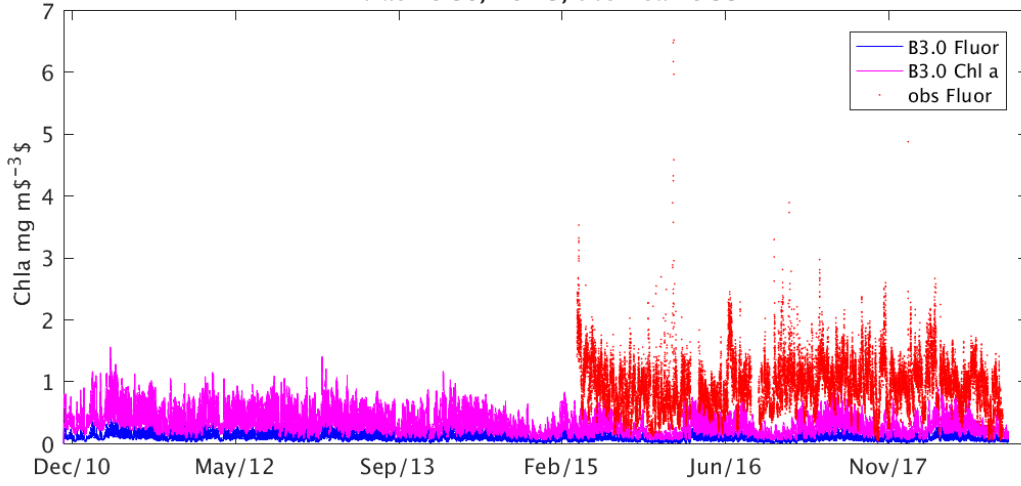
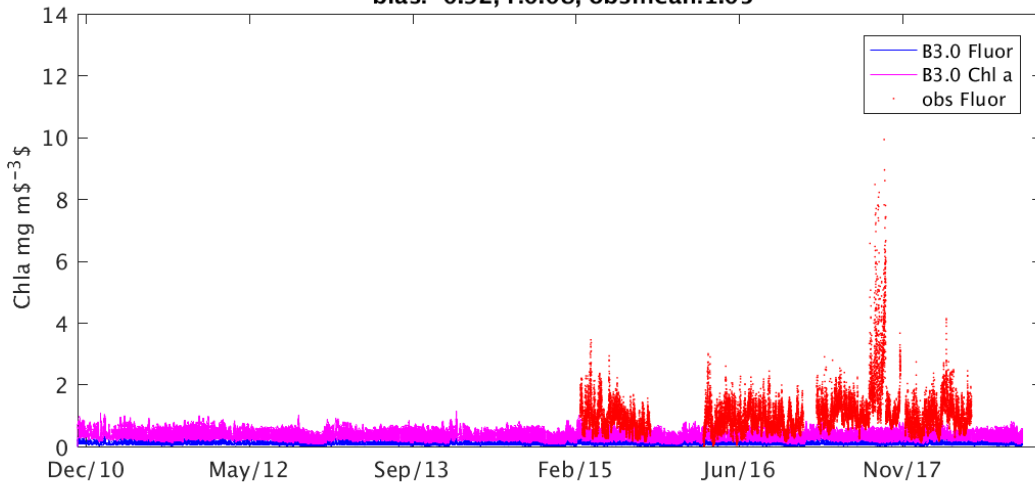


Figure 14 Metrics for AIMS MMP fluorescence against Chl *a* and fluorescence for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

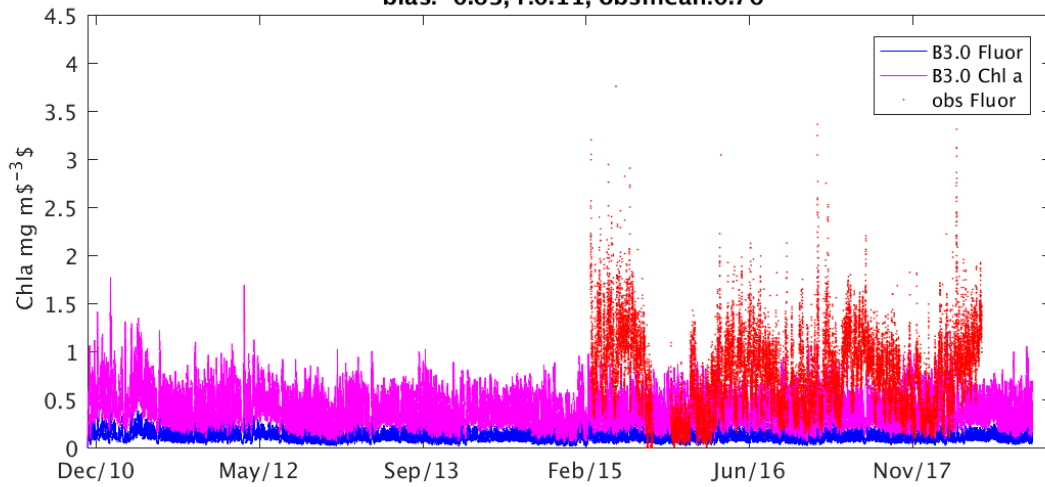
**BUR13 B3.0 Chla Willmott:0.42, mape:70.1, rms:0.79**  
**bias:-0.69, r:0.26, obsmean:0.95**  
**BUR13 B3.0 Fluor Willmott:0.37, mape:89.8, rms:0.94**  
**bias:-0.86, r:0.25, obsmean:0.95**



**TUL10 B3.0 Chla Willmott:0.39, mape:58.1, rms:0.94**  
**bias:-0.66, r:0.09, obsmean:1.05**  
**TUL10 B3.0 Fluor Willmott:0.37, mape:84.6, rms:1.14**  
**bias:-0.92, r:0.08, obsmean:1.05**



**RM10 B3.0 Chla Willmott:0.45, mape:66.6, rms:0.54**  
**bias:-0.36, r:0.14, obsmean:0.76**  
**RM10 B3.0 Fluor Willmott:0.42, mape:79.3, rms:0.74**  
**bias:-0.63, r:0.11, obsmean:0.76**

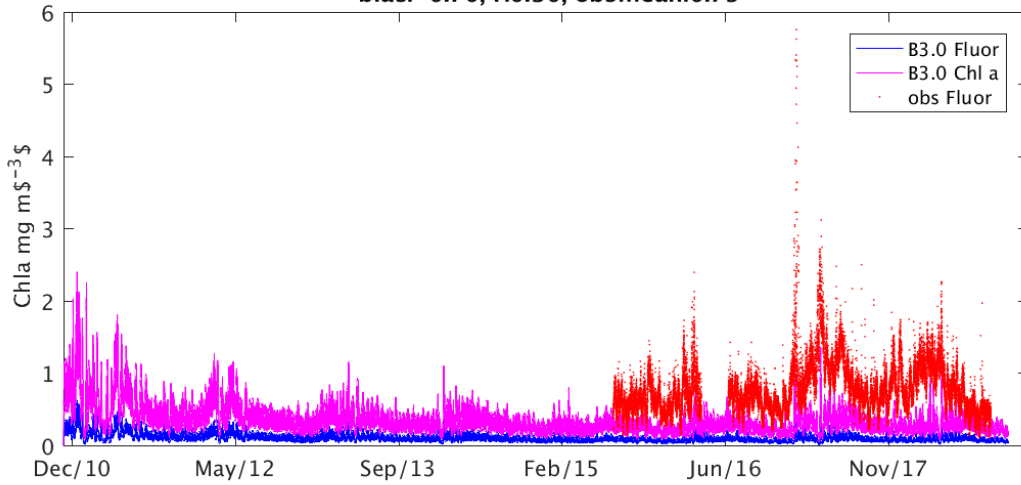


**WHI7 B3.0 Chla Willmott:0.44, mape:59.4, rms:0.60**

**bias:-0.50, r:0.32, obsmean:0.79**

**WHI7 B3.0 Fluor Willmott:0.38, mape:86.8, rms:0.78**

**bias:-0.70, r:0.30, obsmean:0.79**

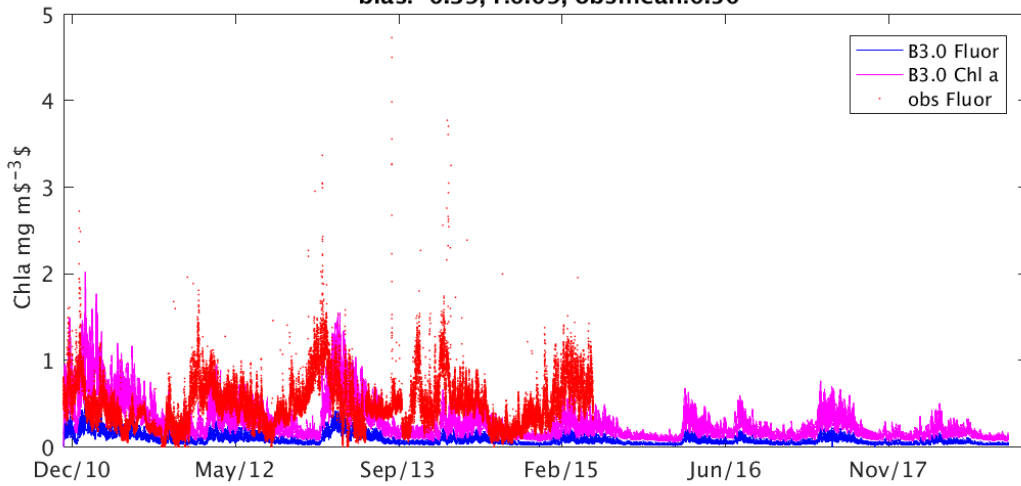


**Humpy\_5m B3.0 Chla Willmott:0.45, mape:74.5, rms:0.39**

**bias:-0.15, r:0.10, obsmean:0.50**

**Humpy\_5m B3.0 Fluor Willmott:0.42, mape:76.1, rms:0.49**

**bias:-0.39, r:0.09, obsmean:0.50**

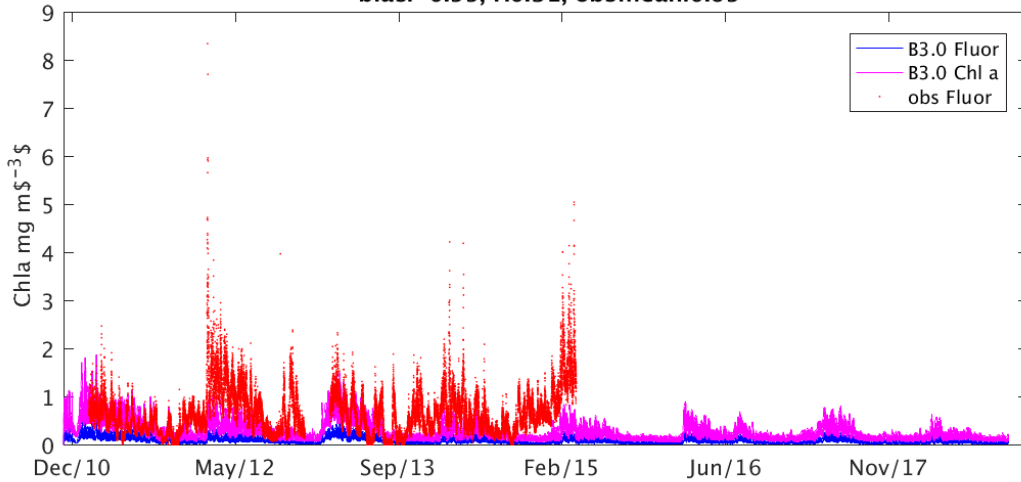


**Pelican\_5m B3.0 Chla Willmott:0.49, mape:82.2, rms:0.56**

**bias:-0.32, r:0.31, obsmean:0.65**

**Pelican\_5m B3.0 Fluor Willmott:0.44, mape:83.0, rms:0.71**

**bias:-0.55, r:0.31, obsmean:0.65**



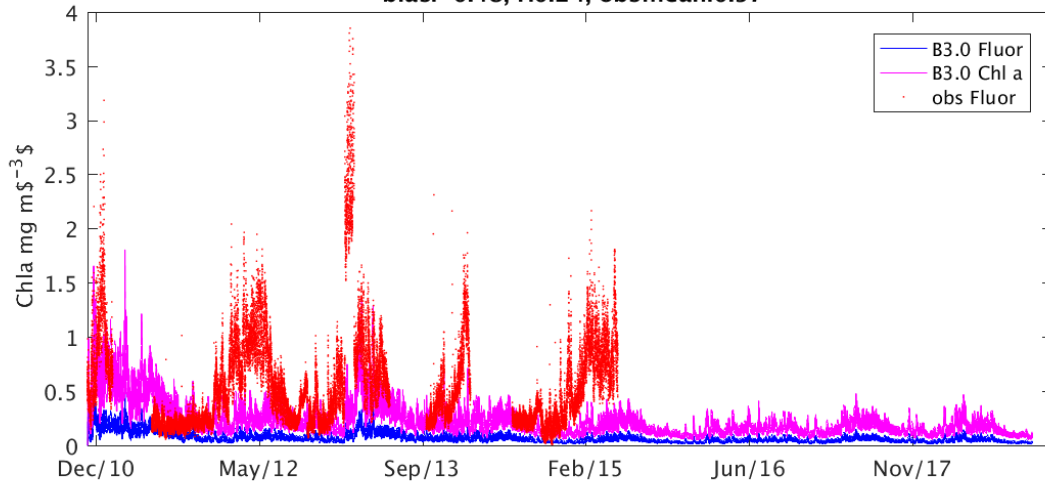


Barren\_5m B3.0 Chla Willmott:0.47, mape:56.6, rms:0.52

bias:-0.29, r:0.25, obsmean:0.57

Barren\_5m B3.0 Fluor Willmott:0.44, mape:77.7, rms:0.65

bias:-0.48, r:0.24, obsmean:0.57

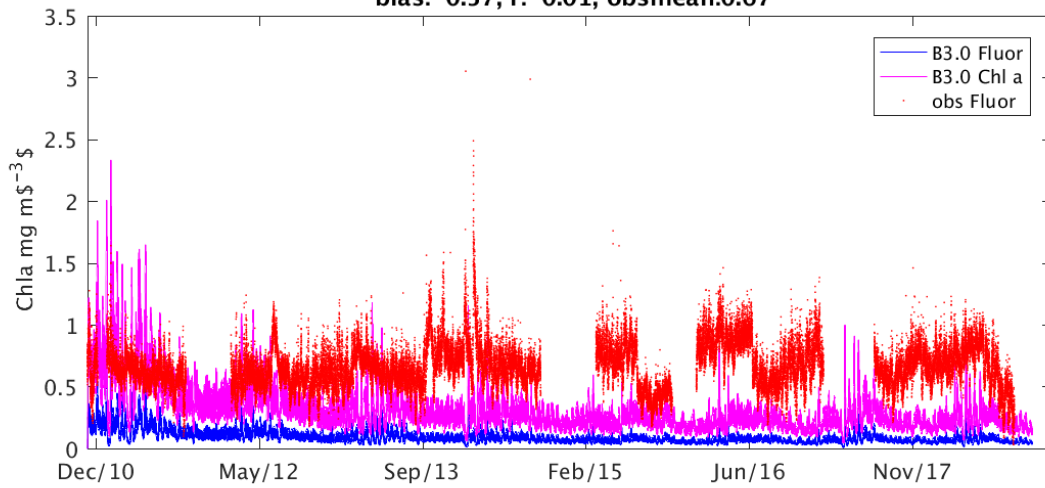


Pine\_5m B3.0 Chla Willmott:0.36, mape:53.1, rms:0.43

bias:-0.34, r:-0.01, obsmean:0.67

Pine\_5m B3.0 Fluor Willmott:0.30, mape:83.6, rms:0.60

bias:-0.57, r:-0.01, obsmean:0.67

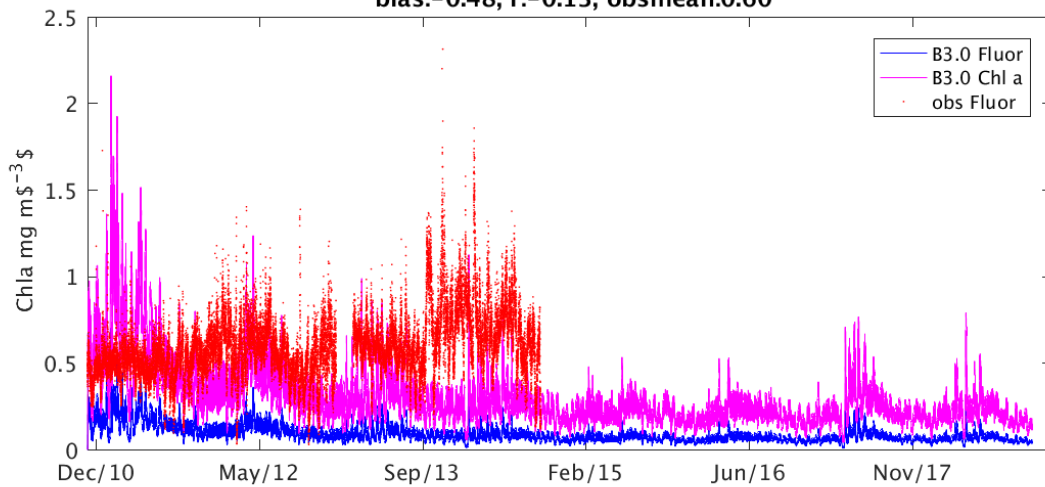


Daydream\_5m B3.0 Chla Willmott:0.33, mape:47.0, rms:0.36

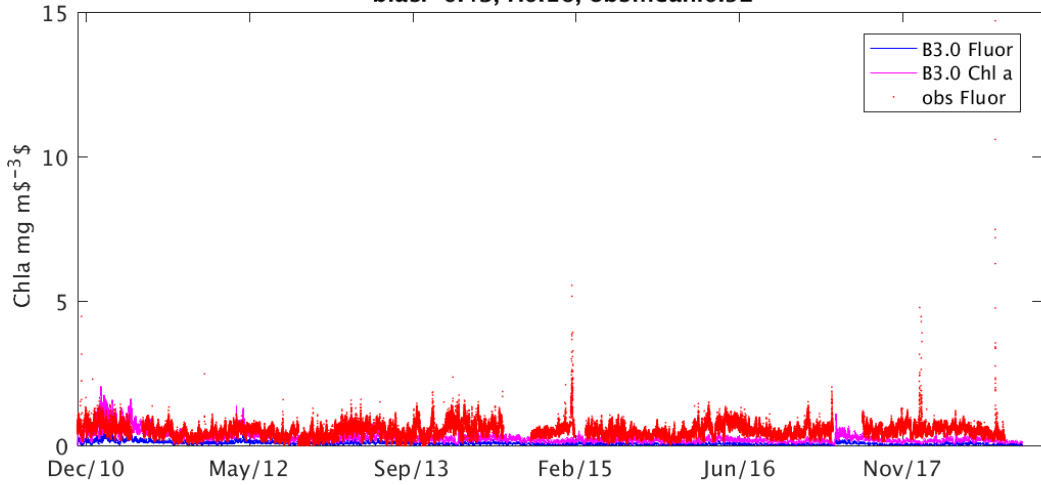
bias:-0.20, r:-0.14, obsmean:0.60

Daydream\_5m B3.0 Fluor Willmott:0.32, mape:77.9, rms:0.52

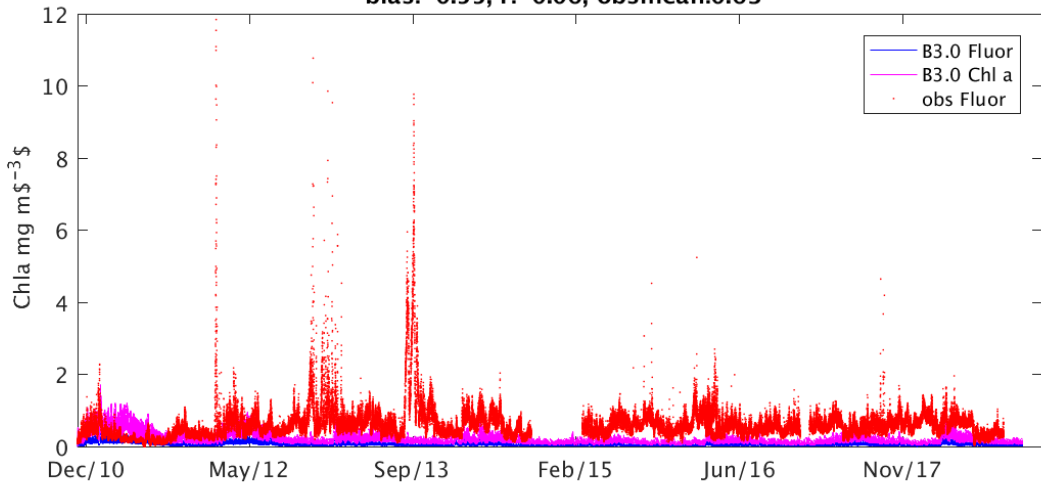
bias:-0.48, r:-0.13, obsmean:0.60



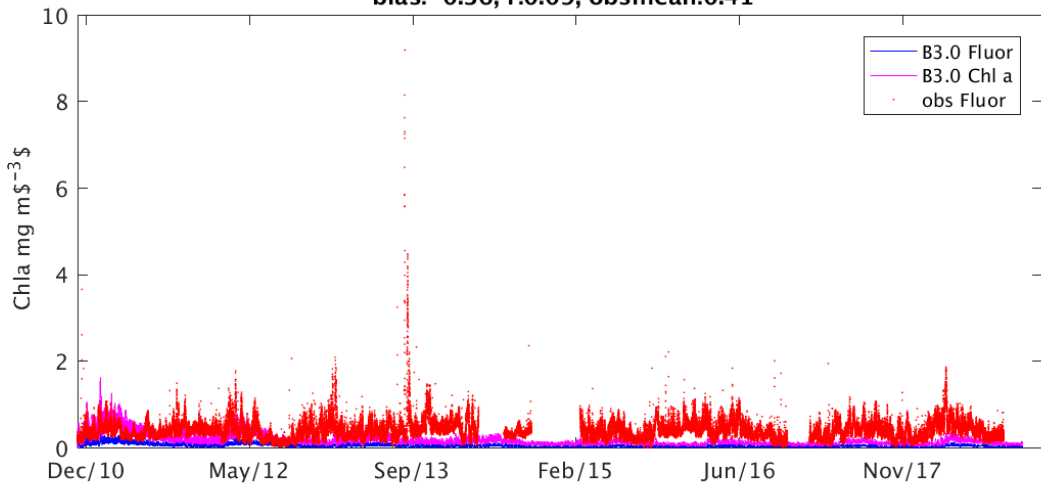
**DoubleCone\_5m B3.0 Chla Willmott:0.45, mape:56.5, rms:0.38**  
**bias:-0.24, r:0.17, obsmean:0.52**  
**DoubleCone\_5m B3.0 Fluor Willmott:0.38, mape:81.4, rms:0.50**  
**bias:-0.43, r:0.16, obsmean:0.52**



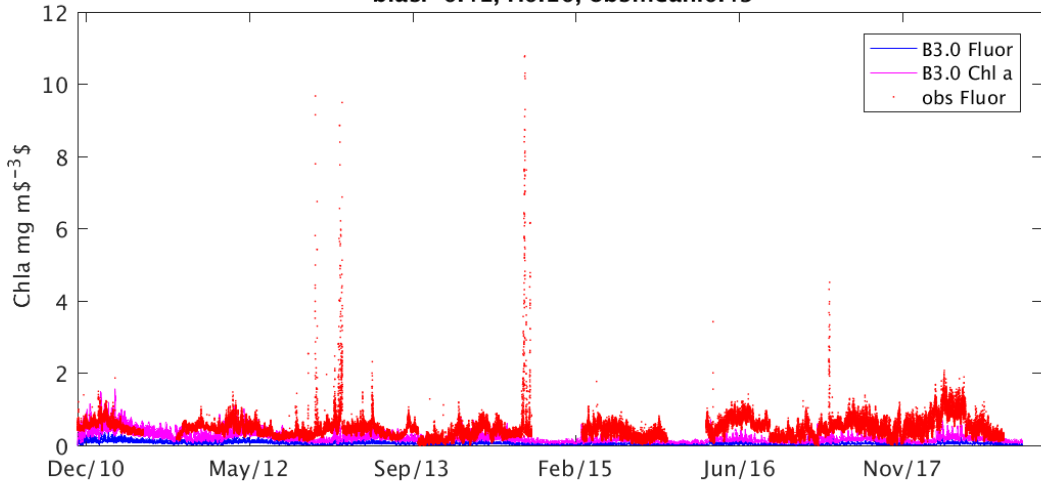
**GeoffreyBay336\_5m B3.0 Chla Willmott:0.31, mape:70.2, rms:0.66**  
**bias:-0.39, r:-0.07, obsmean:0.63**  
**GeoffreyBay336\_5m B3.0 Fluor Willmott:0.34, mape:83.4, rms:0.75**  
**bias:-0.55, r:-0.06, obsmean:0.63**



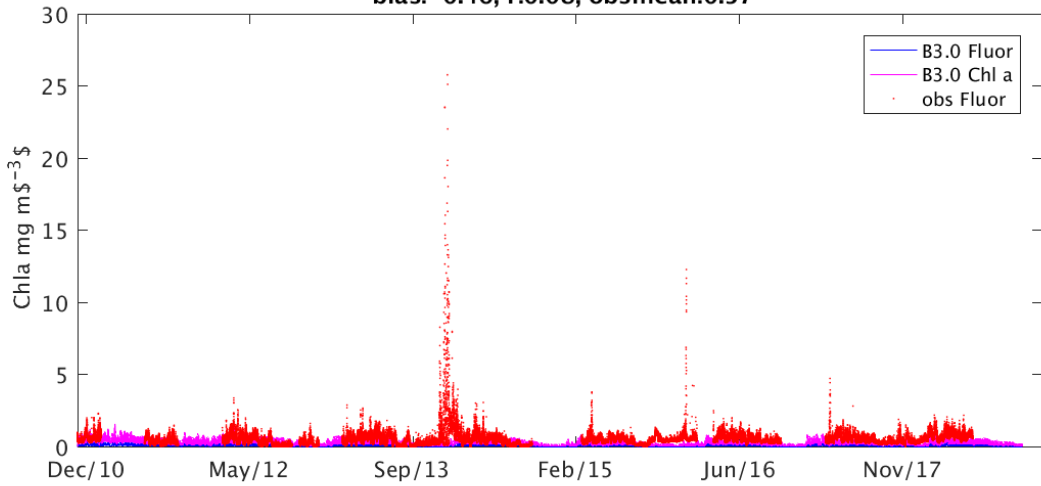
**Pandora\_5m B3.0 Chla Willmott:0.40, mape:59.9, rms:0.35**  
**bias:-0.23, r:0.09, obsmean:0.41**  
**Pandora\_5m B3.0 Fluor Willmott:0.38, mape:82.5, rms:0.43**  
**bias:-0.36, r:0.09, obsmean:0.41**



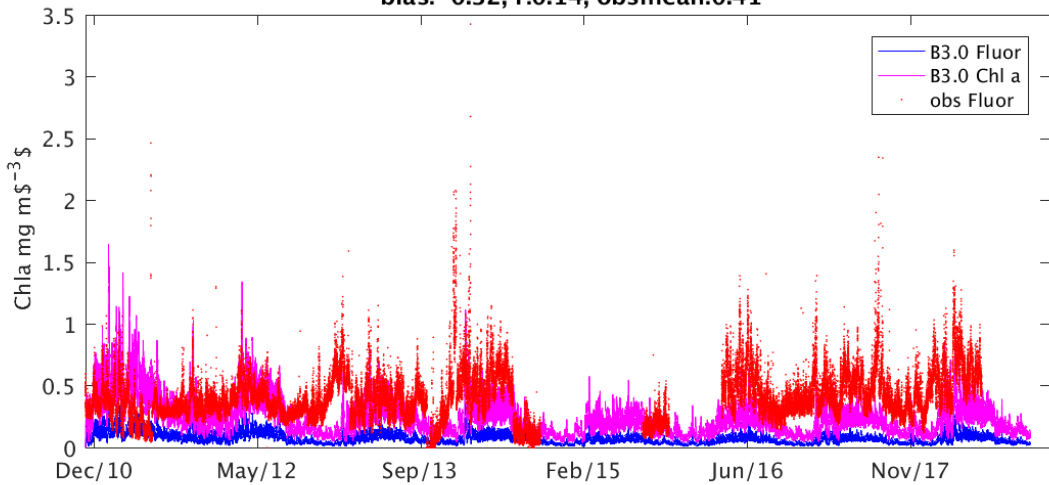
**Pelorus\_5m B3.0 Chl a Willmott:0.37, mape:53.1, rms:0.46**  
**bias:-0.25, r:0.11, obsmean:0.49**  
**Pelorus\_5m B3.0 Fluor Willmott:0.35, mape:80.9, rms:0.56**  
**bias:-0.41, r:0.10, obsmean:0.49**



**Dunk859\_5m B3.0 Chl a Willmott:0.27, mape:93.6, rms:0.72**  
**bias:-0.25, r:0.09, obsmean:0.57**  
**Dunk859\_5m B3.0 Fluor Willmott:0.31, mape:83.3, rms:0.81**  
**bias:-0.46, r:0.08, obsmean:0.57**



**Russell\_5m B3.0 Chl a Willmott:0.46, mape:58.4, rms:0.27**  
**bias:-0.14, r:0.14, obsmean:0.41**  
**Russell\_5m B3.0 Fluor Willmott:0.40, mape:77.0, rms:0.38**  
**bias:-0.32, r:0.14, obsmean:0.41**

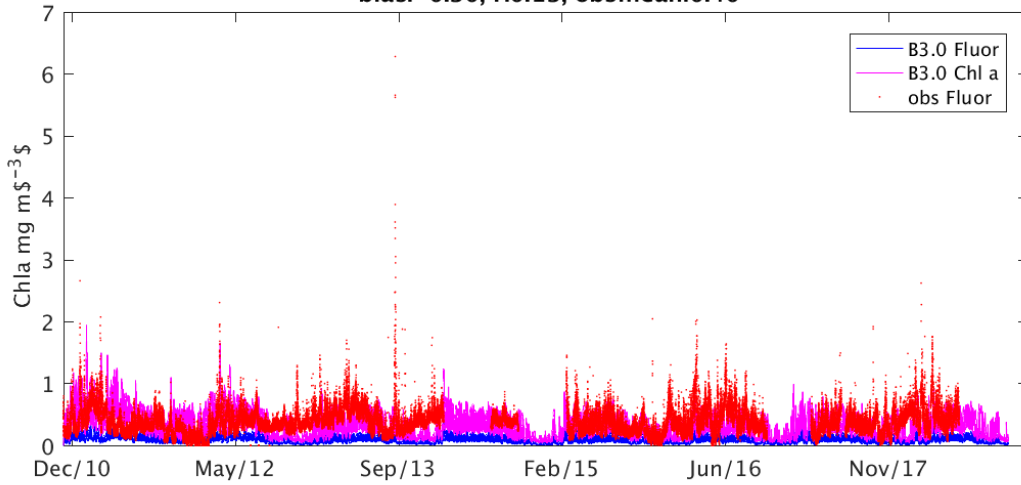


High\_5m B3.0 Chl a Willmott:0.45, mape:72.4, rms:0.27

bias:-0.08, r:0.14, obsmean:0.40

High\_5m B3.0 Fluor Willmott:0.41, mape:74.6, rms:0.37

bias:-0.30, r:0.13, obsmean:0.40

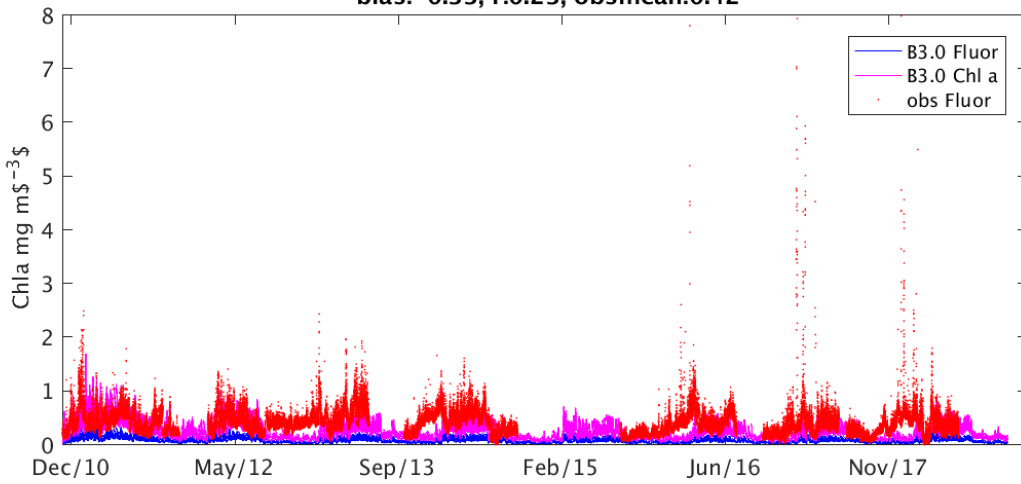


Fitz\_5m B3.0 Chl a Willmott:0.47, mape:50.5, rms:0.32

bias:-0.15, r:0.24, obsmean:0.42

Fitz\_5m B3.0 Fluor Willmott:0.40, mape:76.3, rms:0.43

bias:-0.33, r:0.23, obsmean:0.42



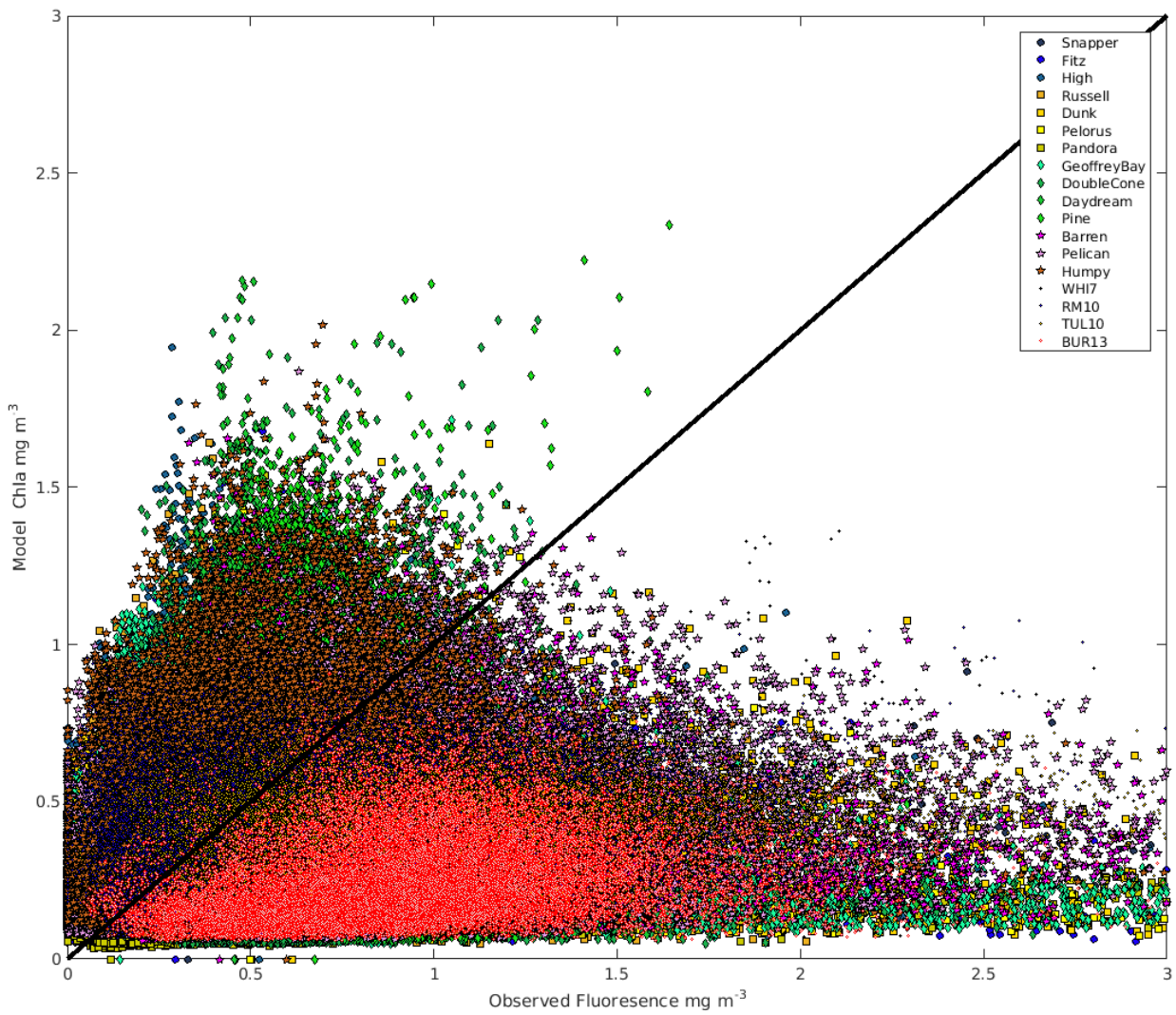
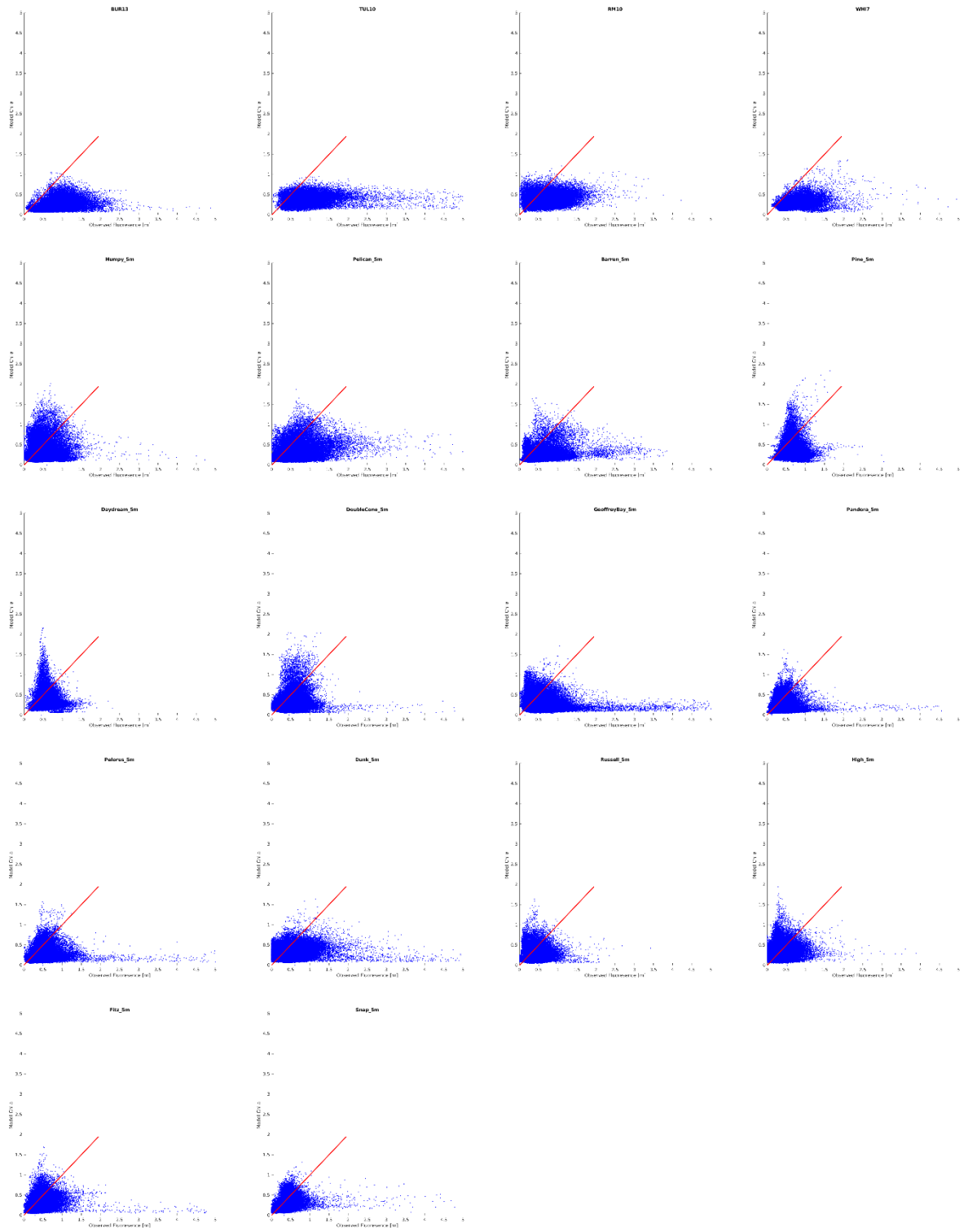


Figure 15 Scatter plot of observed Fluorescence for AIMS MMP assessment against simulated Chl a for model version 3p0



## 20. Simulated Turbidity assessment against AIMS MMP Turbidity

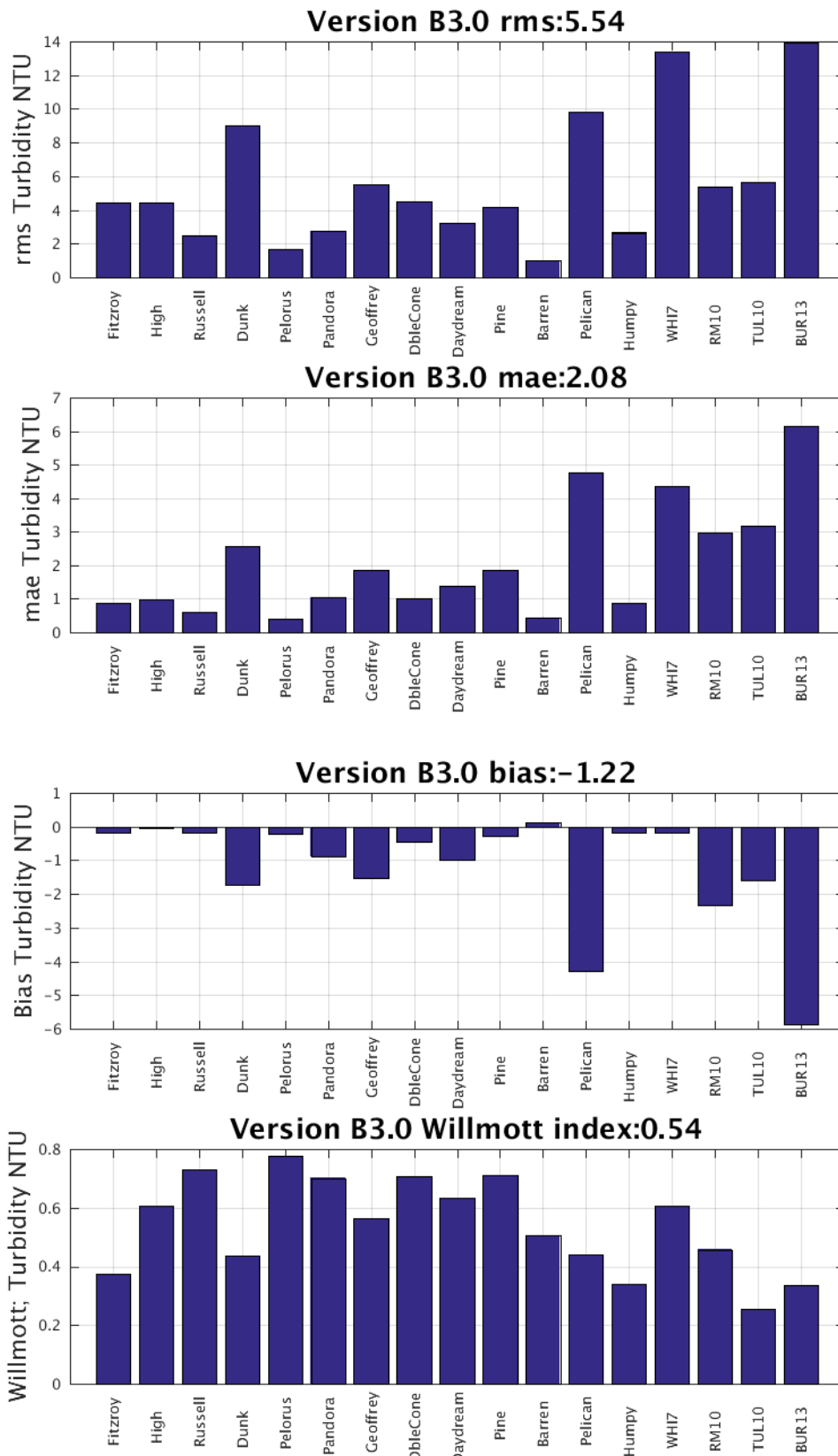
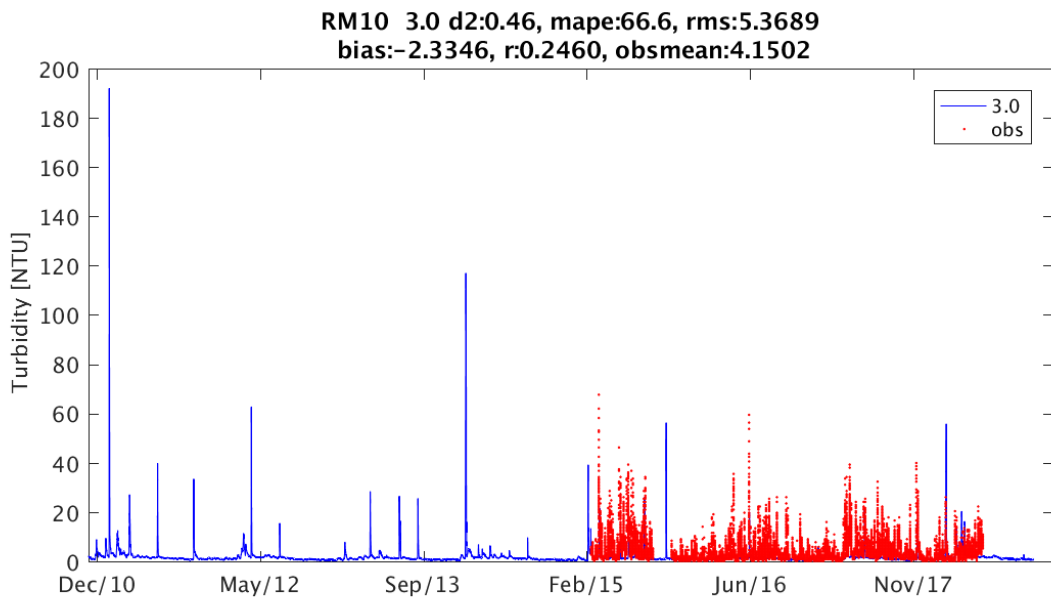
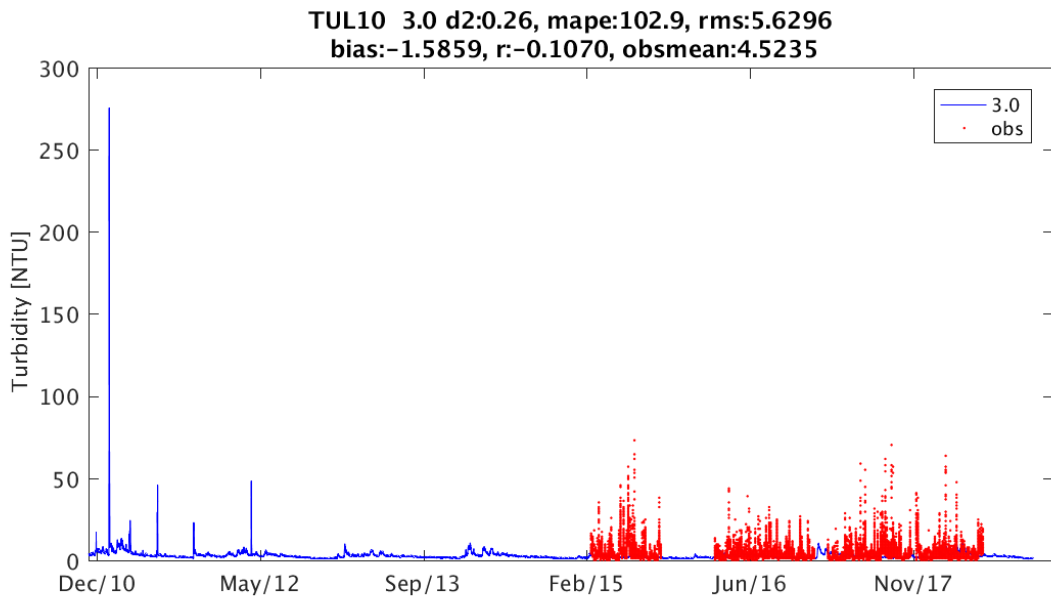
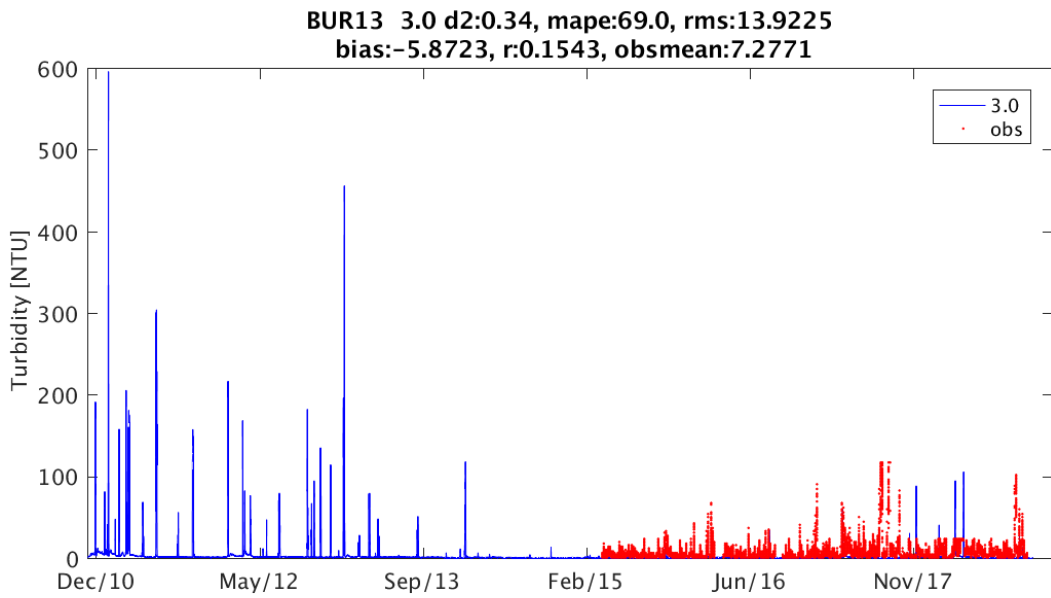


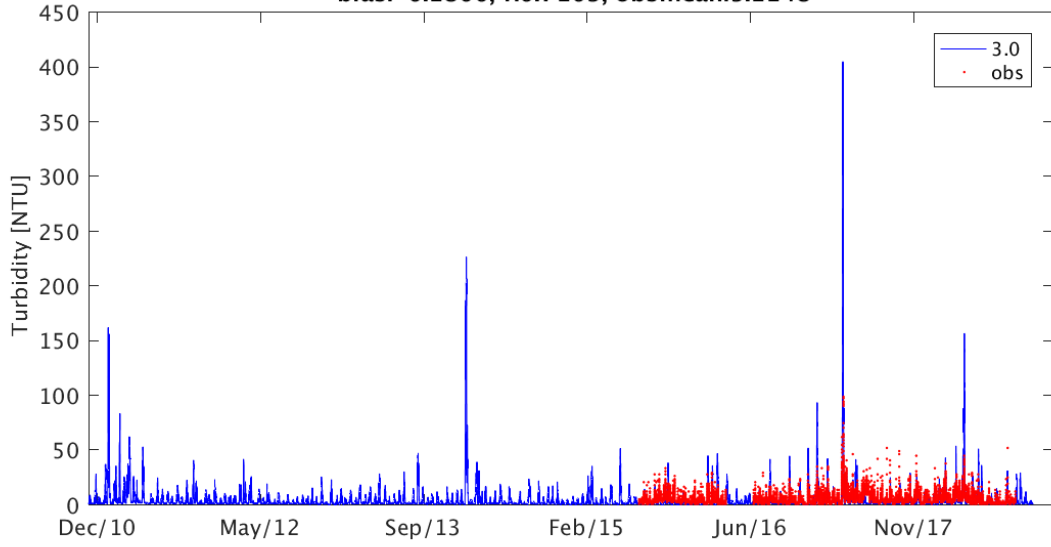
Figure 16 Metrics for AIMS MMP turbidity against simulated turbidity Dec 2010 to November 2018 for model version 3p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

Simulated and observed turbidity at MMP sites (y axis to max extent)

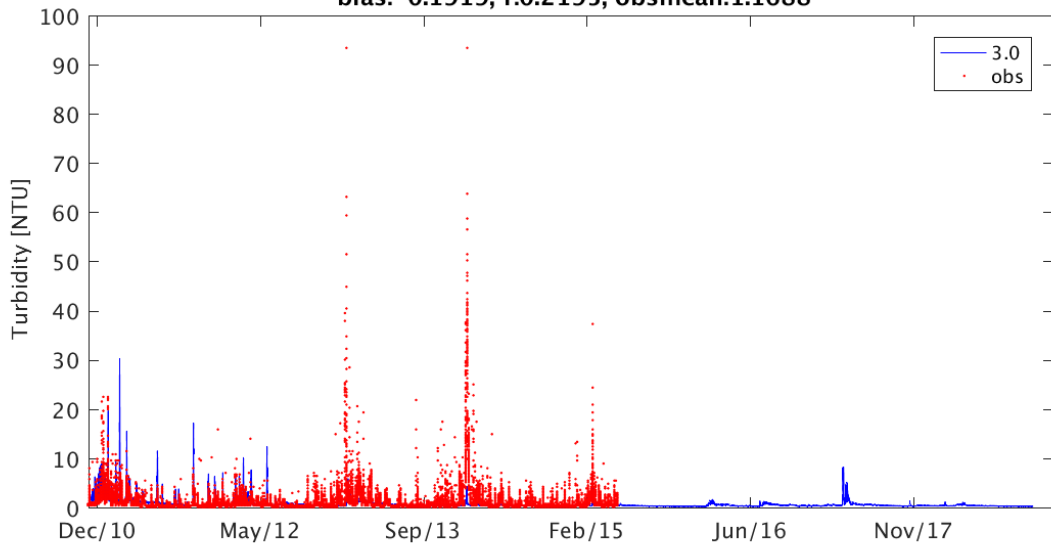




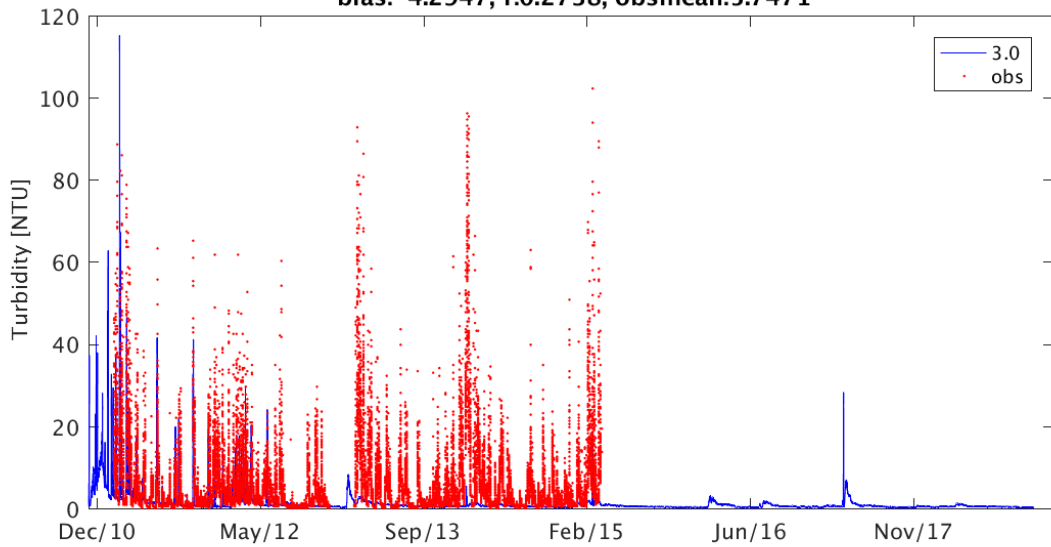
WHI7 3.0 d2:0.61, mape:68.9, rms:13.4203  
bias:-0.1800, r:0.7109, obsmean:5.1148



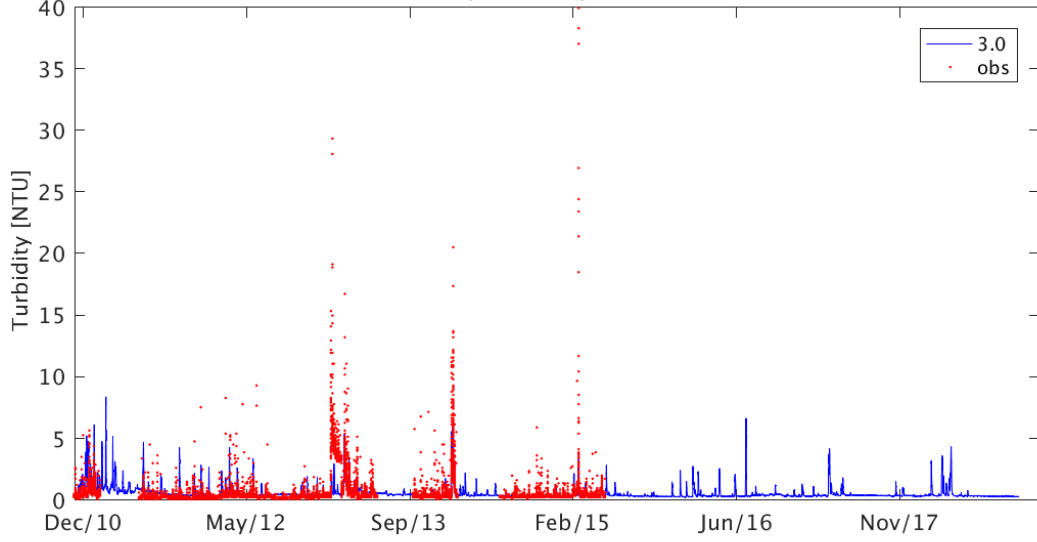
Humpy\_5m 3.0 d2:0.34, mape:75.5, rms:2.7050  
bias:-0.1919, r:0.2195, obsmean:1.1688



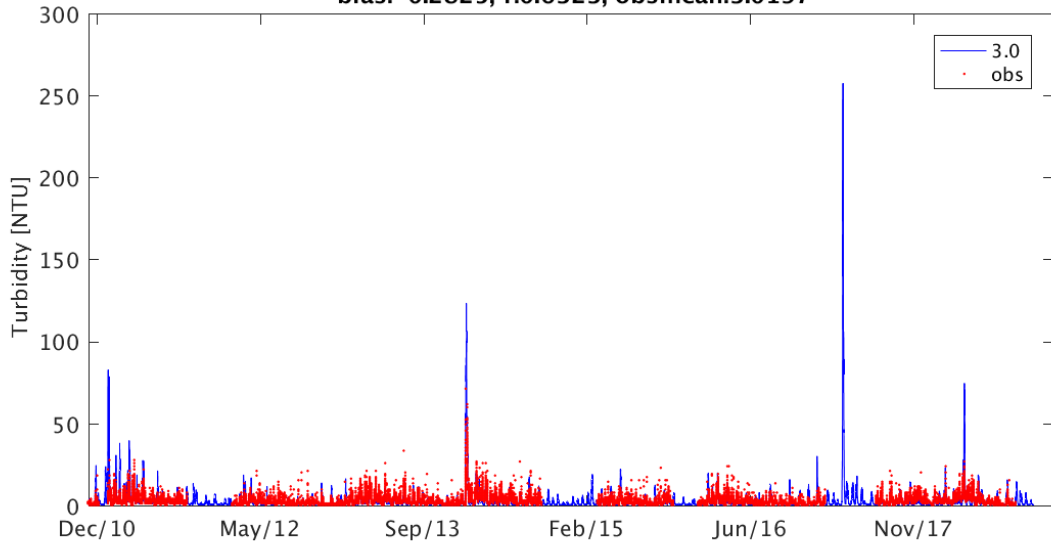
Pelican\_5m 3.0 d2:0.44, mape:75.9, rms:9.8490  
bias:-4.2947, r:0.2738, obsmean:5.7471



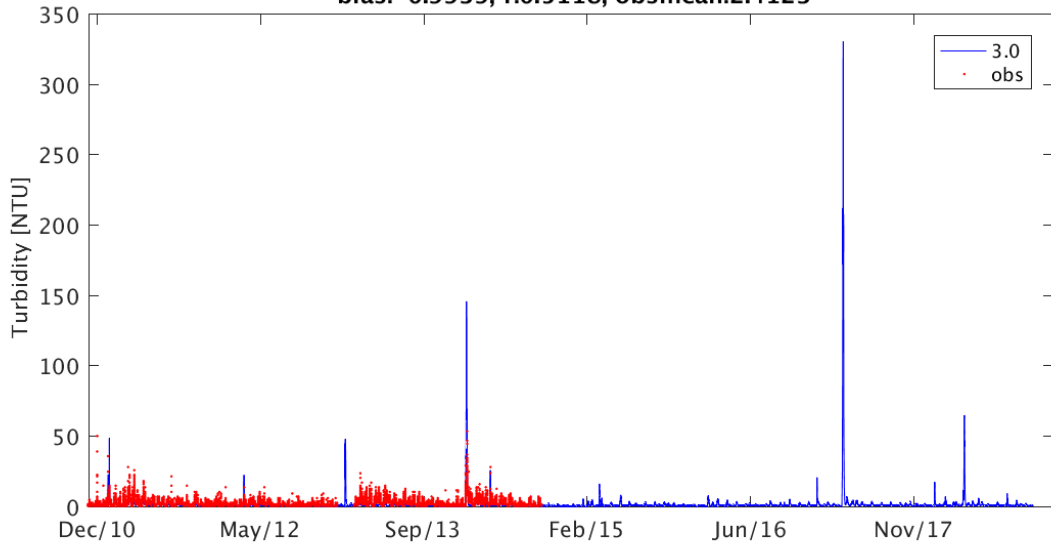
**Barren\_5m 3.0 d2:0.51, mape:168.8, rms:1.0377  
bias:0.1193, r:0.3797, obsmean:0.4807**



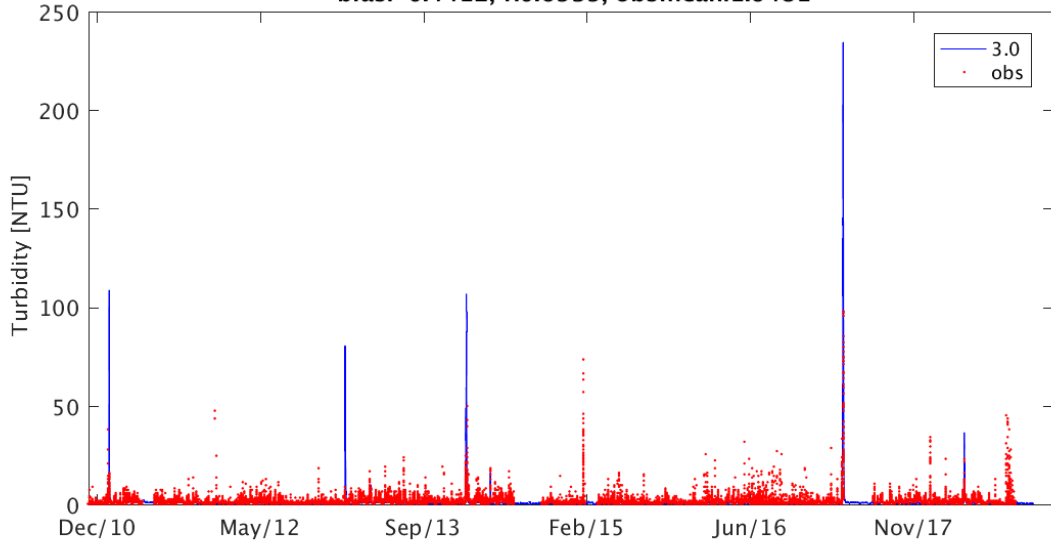
**Pine\_5m 3.0 d2:0.71, mape:53.2, rms:4.2012  
bias:-0.2825, r:0.6323, obsmean:3.0197**



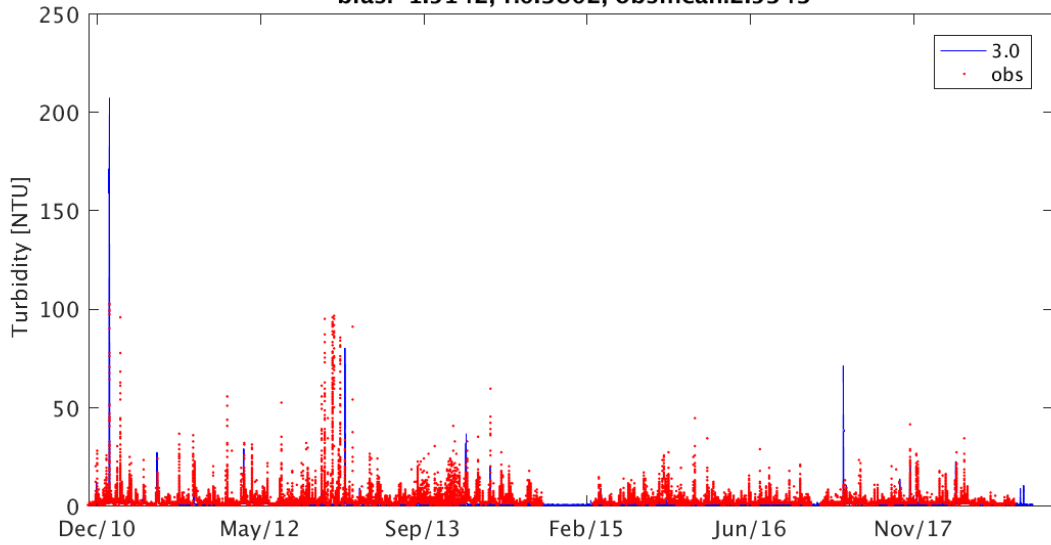
**Daydream\_5m 3.0 d2:0.63, mape:46.0, rms:3.2591  
bias:-0.9939, r:0.5118, obsmean:2.4123**



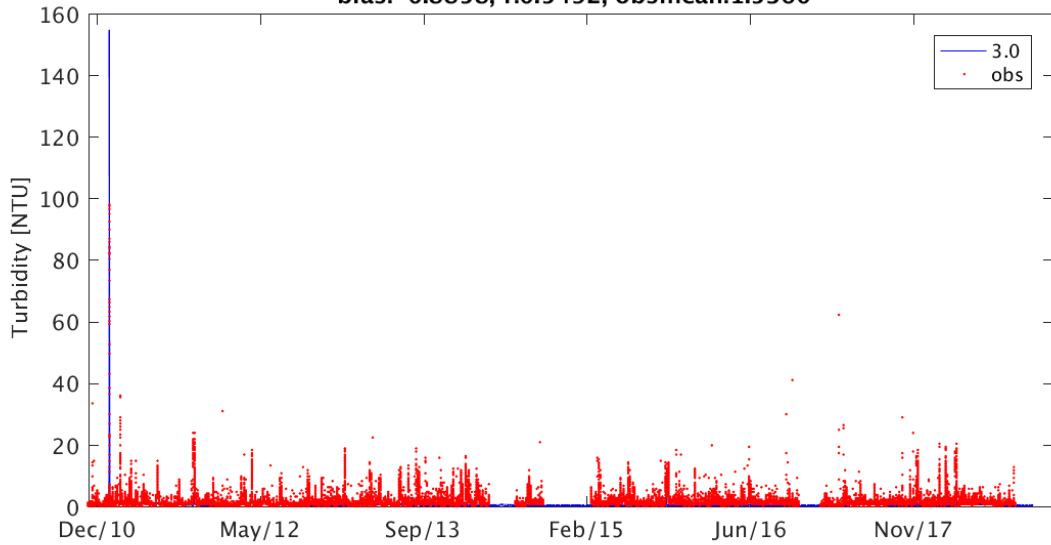
**DoubleCone\_5m 3.0 d2:0.71, mape:44.4, rms:4.4994  
bias:-0.4412, r:0.6939, obsmean:1.6481**



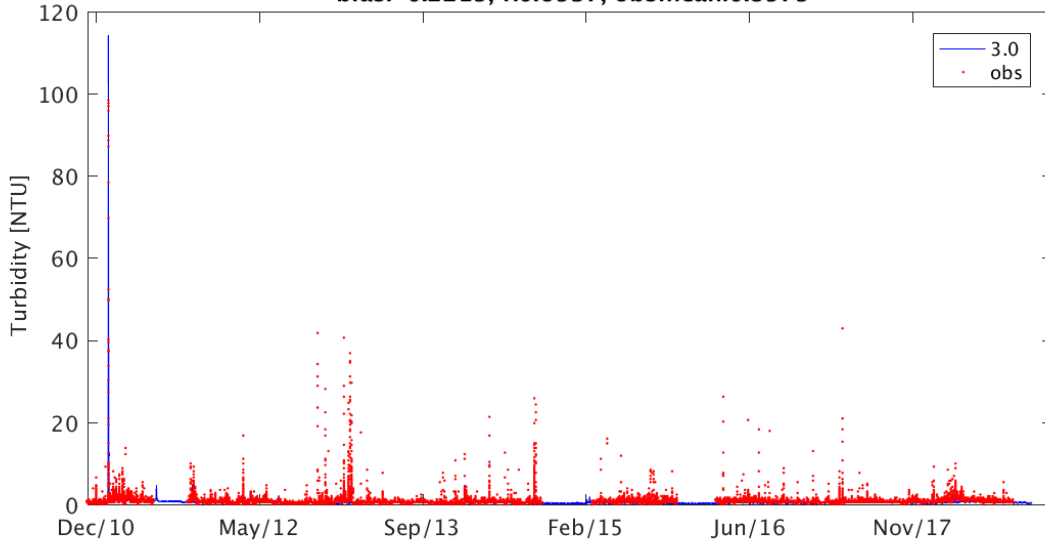
**GeoffreyBay336\_5m 3.0 d2:0.57, mape:58.0, rms:5.5019  
bias:-1.5142, r:0.3802, obsmean:2.5343**



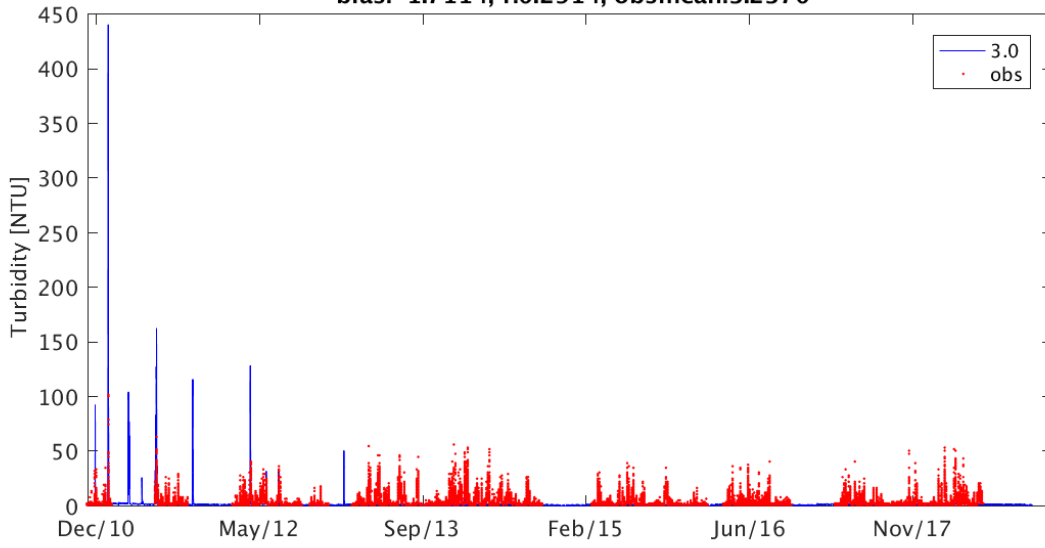
**Pandora\_5m 3.0 d2:0.70, mape:57.3, rms:2.7270  
bias:-0.8858, r:0.5492, obsmean:1.5360**



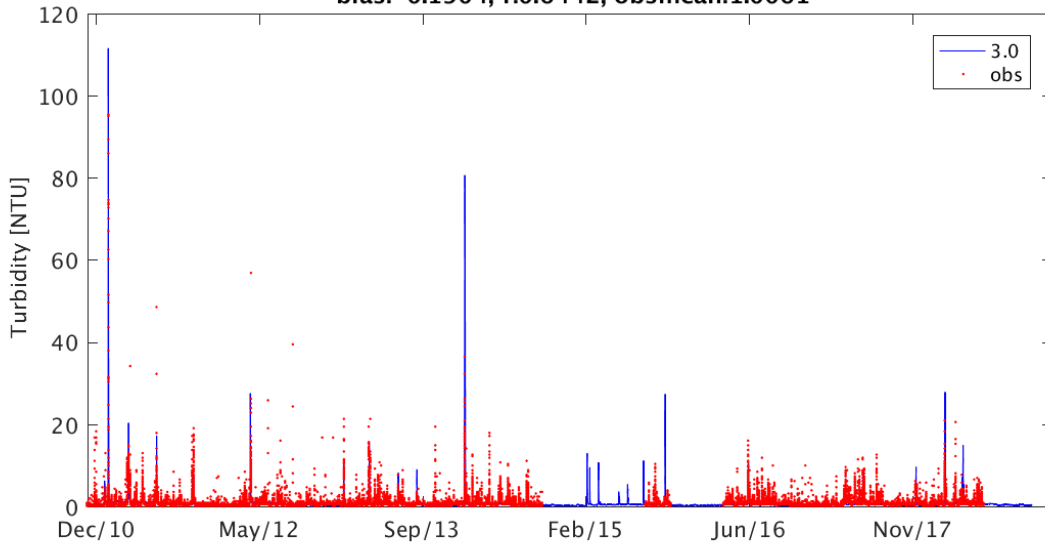
**Pelorus\_5m 3.0 d2:0.78, mape:40.3, rms:1.6540  
bias:-0.2219, r:0.6537, obsmean:0.8579**



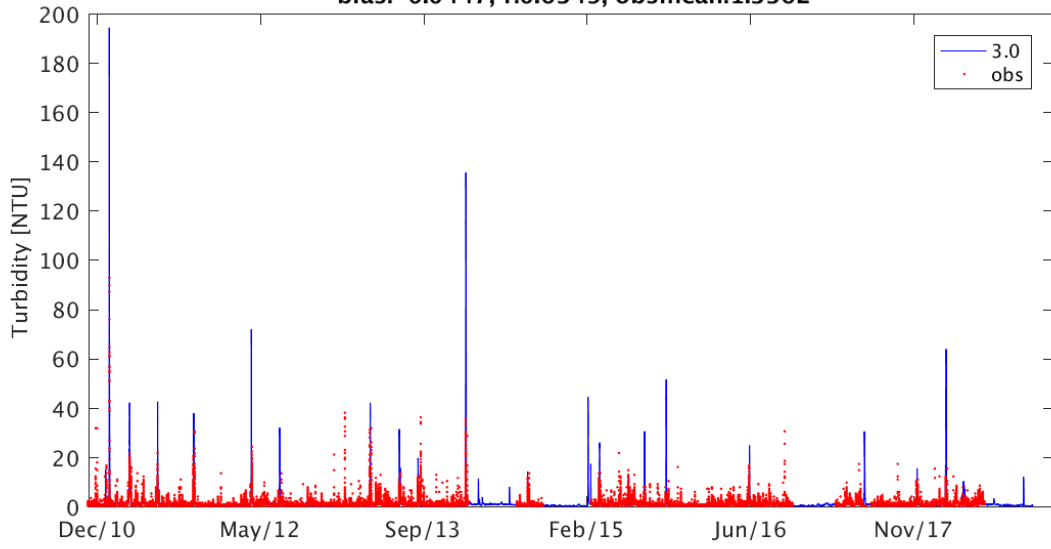
**Dunk859\_5m 3.0 d2:0.44, mape:55.3, rms:9.0171  
bias:-1.7114, r:0.2914, obsmean:3.2370**



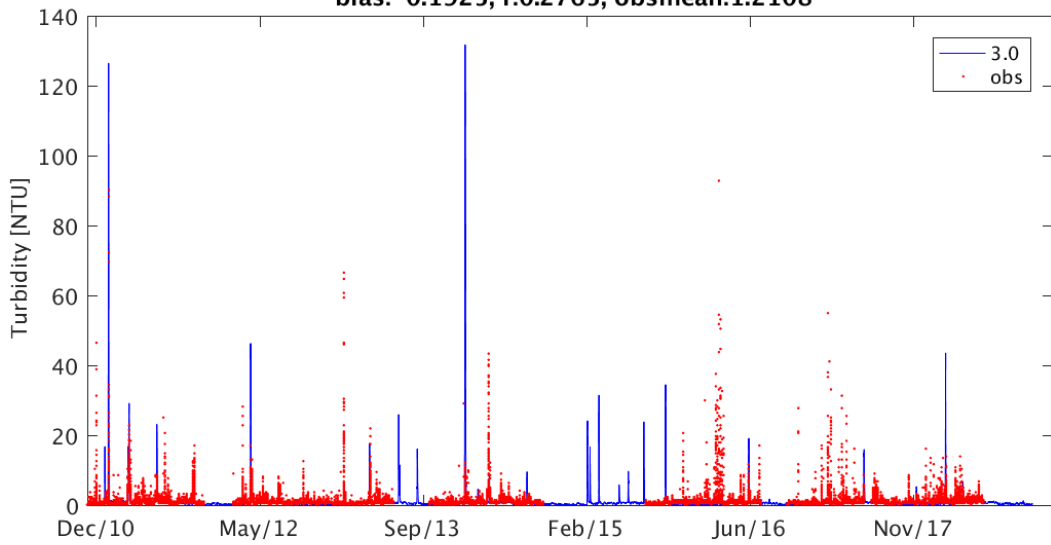
**Russell\_5m 3.0 d2:0.73, mape:50.8, rms:2.4572  
bias:-0.1904, r:0.6442, obsmean:1.0061**



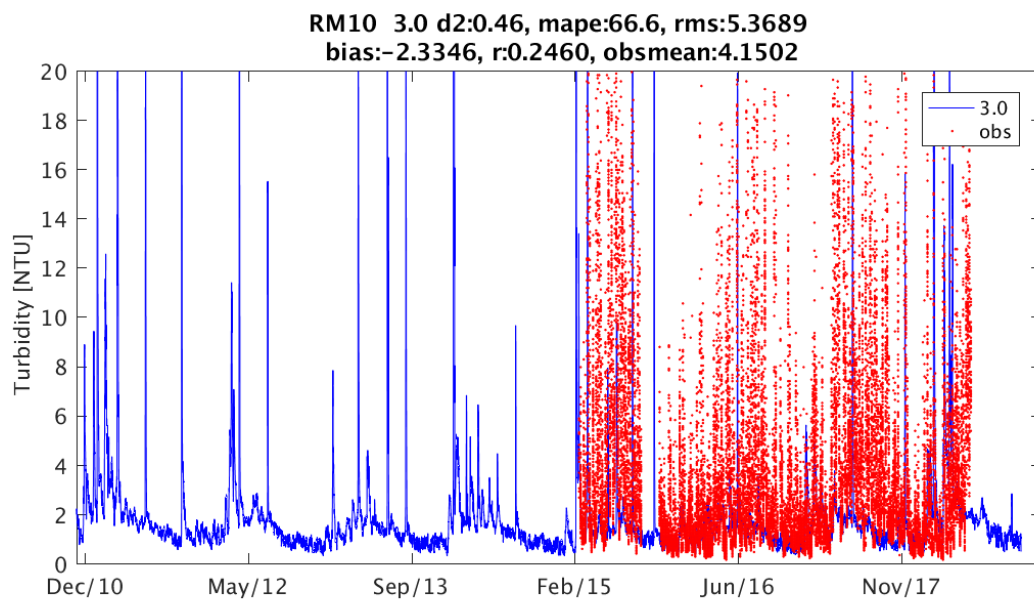
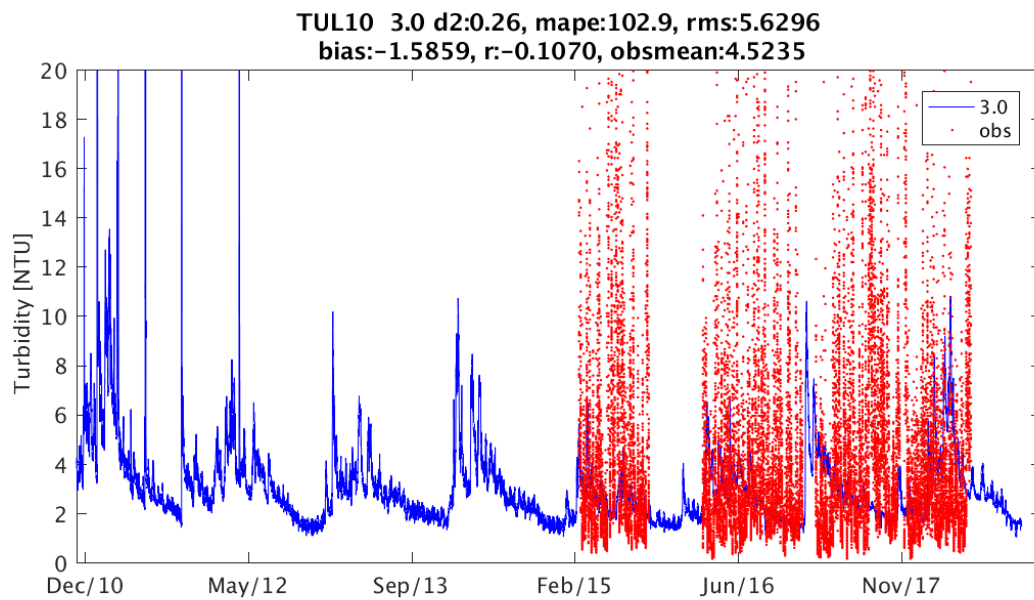
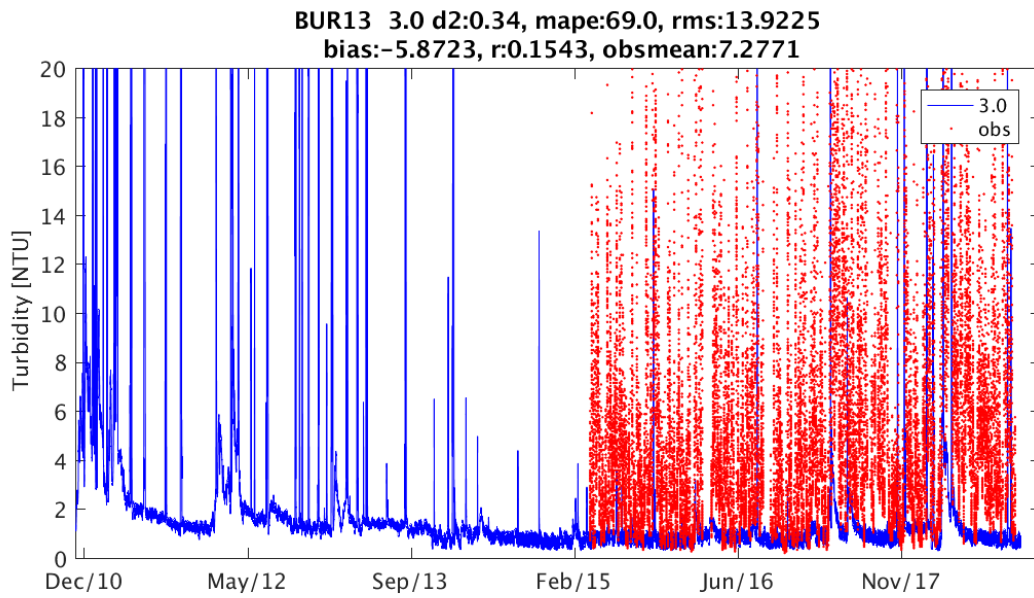
High\_5m 3.0 d2:0.61, mape:52.8, rms:4.4620  
bias:-0.0447, r:0.6349, obsmean:1.3362



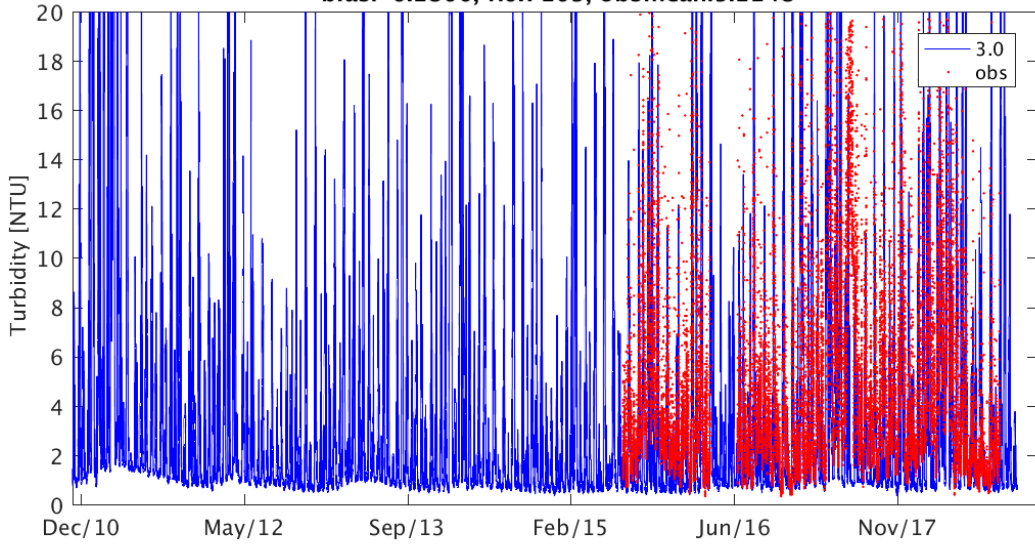
Fitz\_5m 3.0 d2:0.37, mape:57.3, rms:4.4454  
bias:-0.1925, r:0.2765, obsmean:1.2108



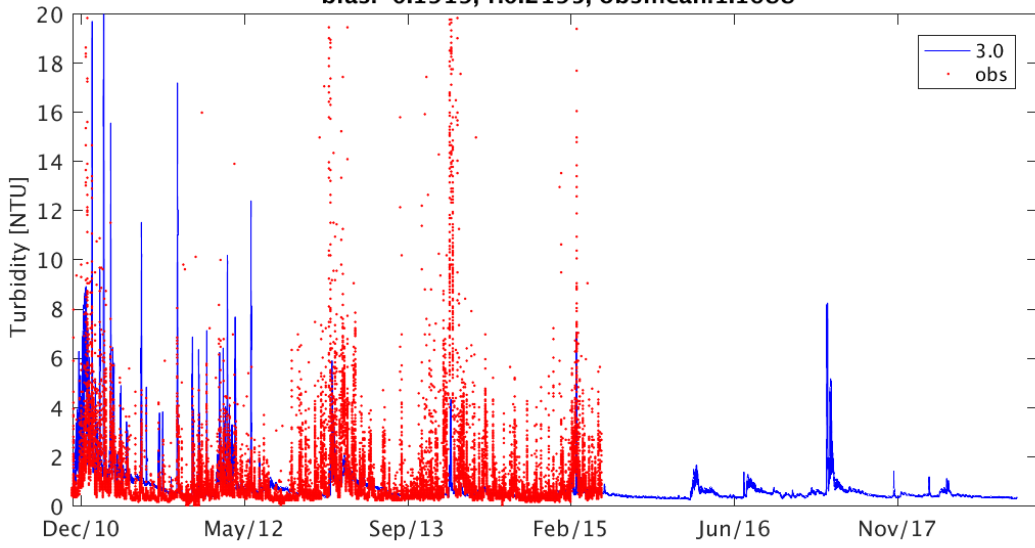
Simulated and observed turbidity at MMP sites (y axis fixed at 20 NTU)



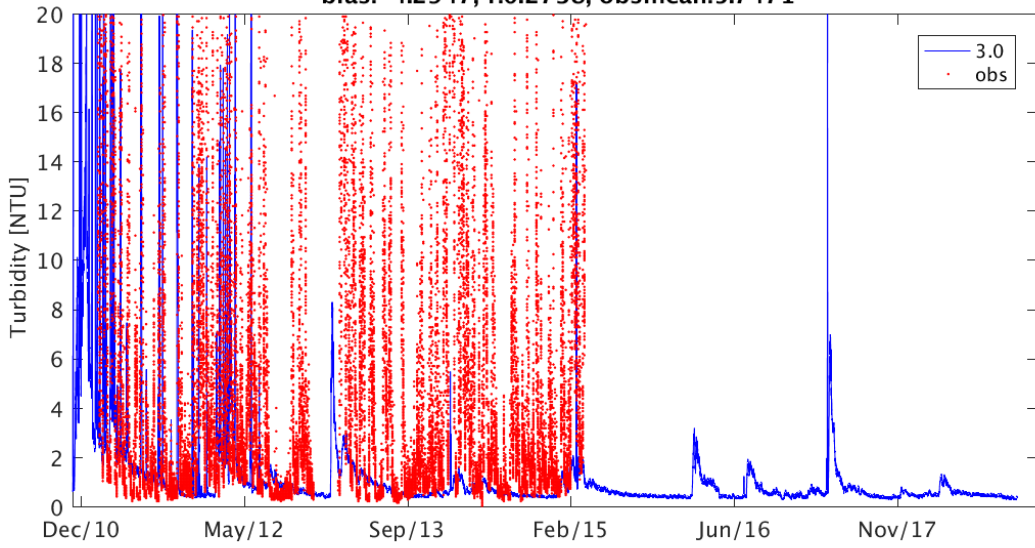
**WHI7 3.0 d2:0.61, mape:68.9, rms:13.4203**  
**bias:-0.1800, r:0.7109, obsmean:5.1148**



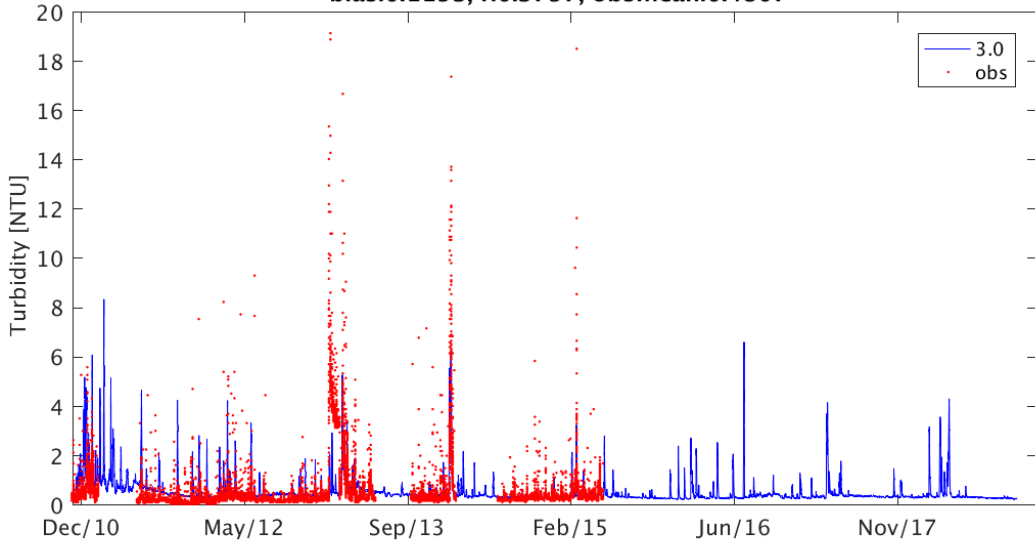
**Humpy\_5m 3.0 d2:0.34, mape:75.5, rms:2.7050**  
**bias:-0.1919, r:0.2195, obsmean:1.1688**



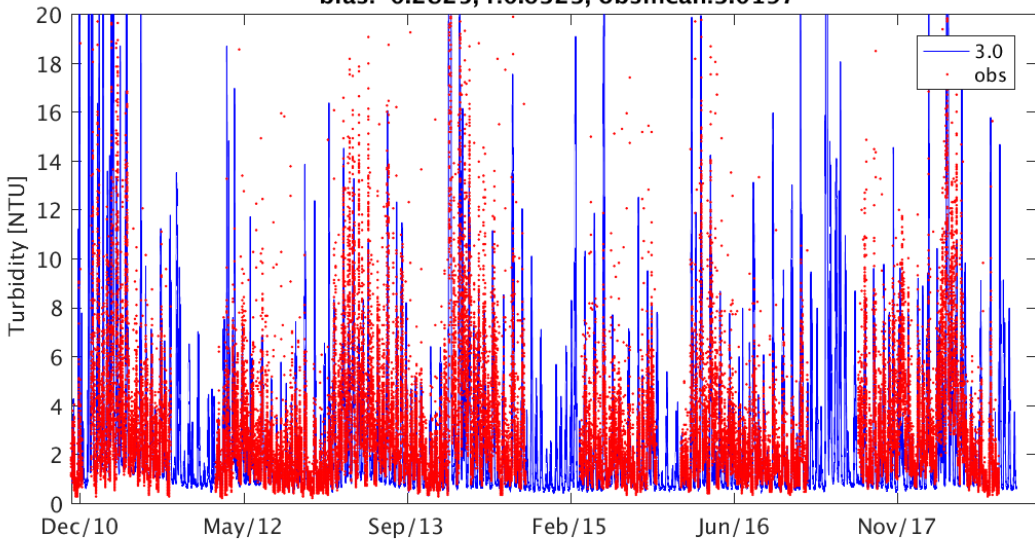
**Pelican\_5m 3.0 d2:0.44, mape:75.9, rms:9.8490**  
**bias:-4.2947, r:0.2738, obsmean:5.7471**



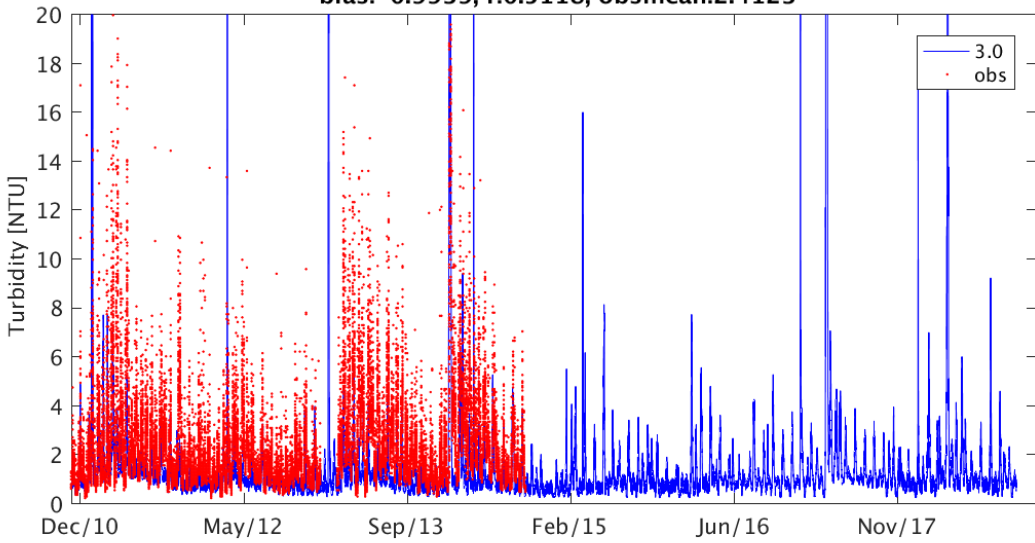
**Barren\_5m 3.0 d2:0.51, mape:168.8, rms:1.0377  
bias:0.1193, r:0.3797, obsmean:0.4807**



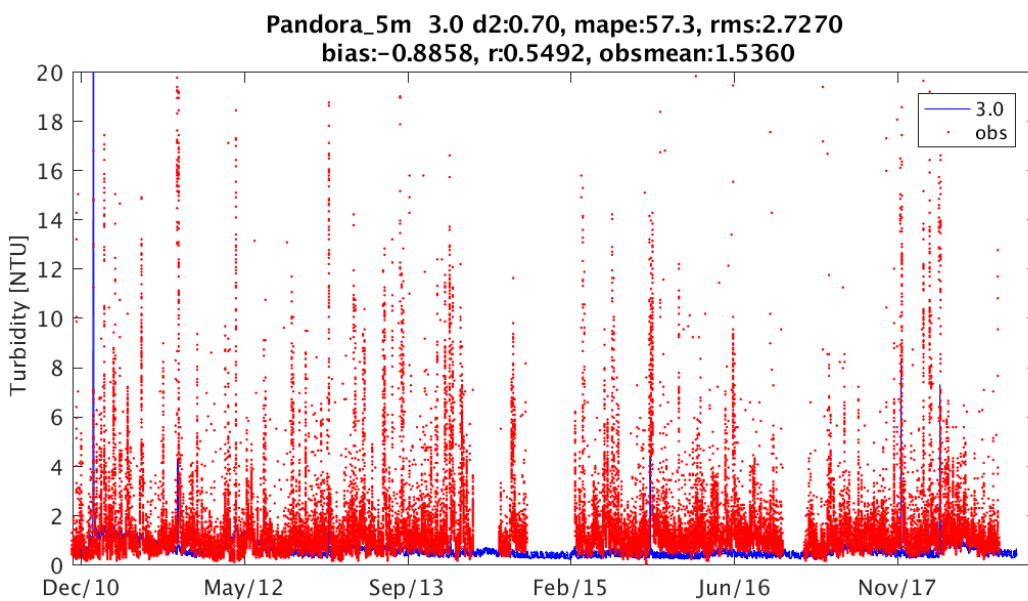
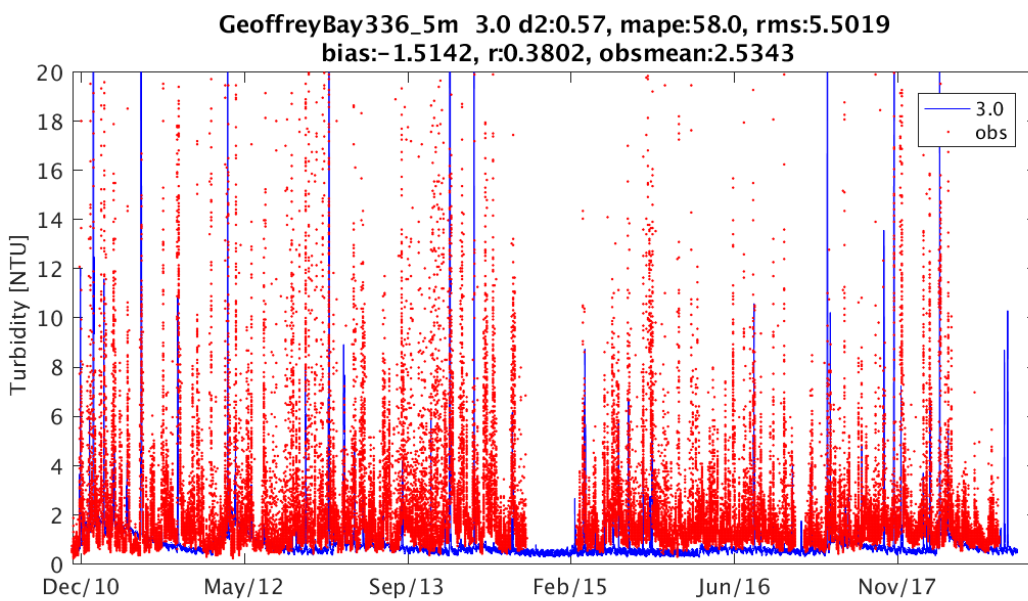
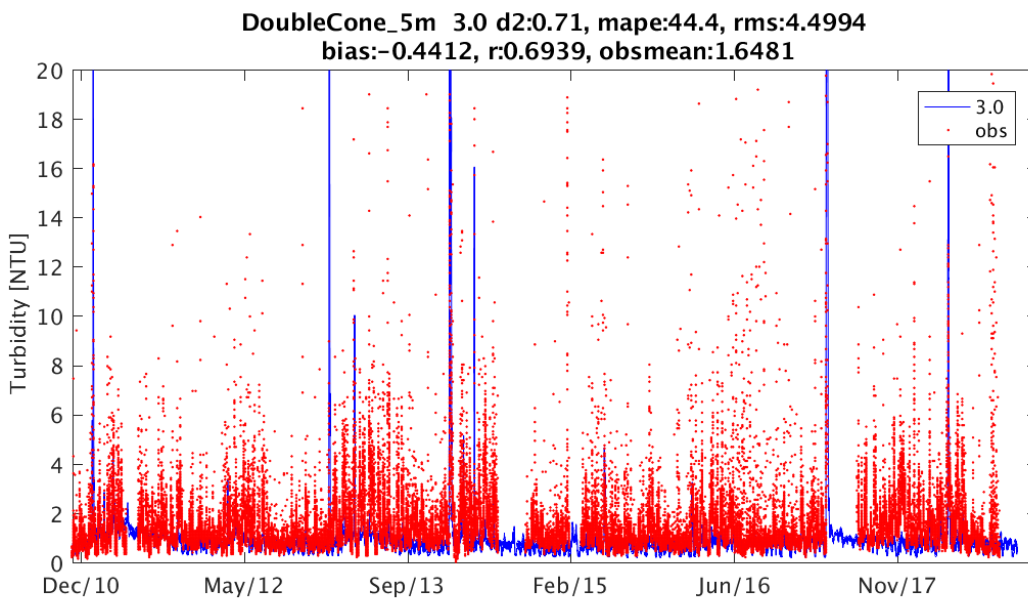
**Pine\_5m 3.0 d2:0.71, mape:53.2, rms:4.2012  
bias:-0.2825, r:0.6323, obsmean:3.0197**



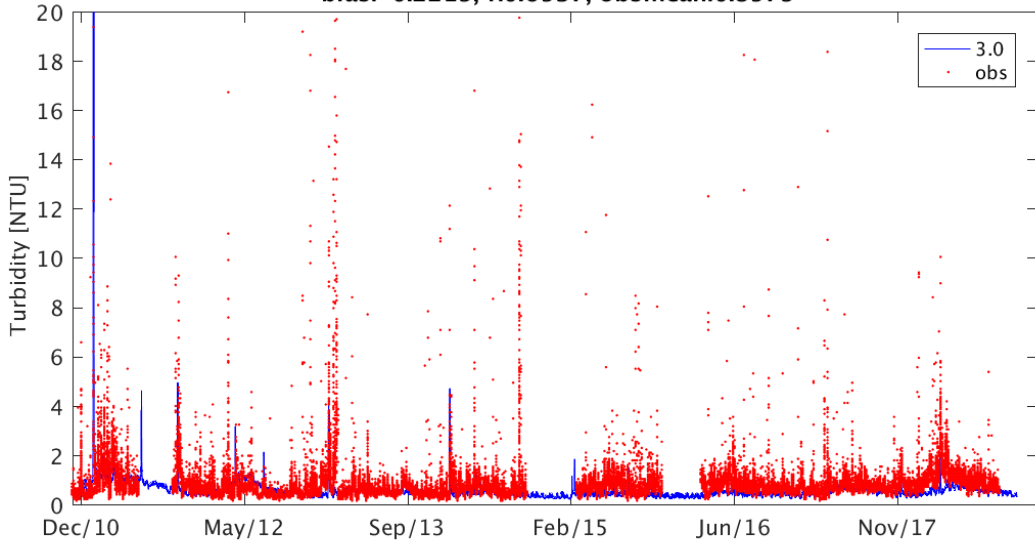
**Daydream\_5m 3.0 d2:0.63, mape:46.0, rms:3.2591  
bias:-0.9939, r:0.5118, obsmean:2.4123**



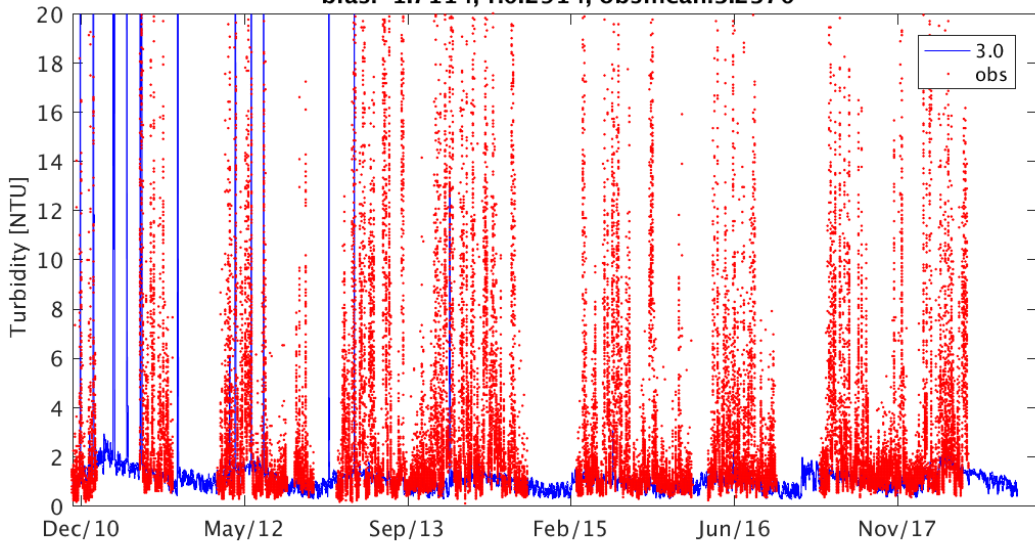




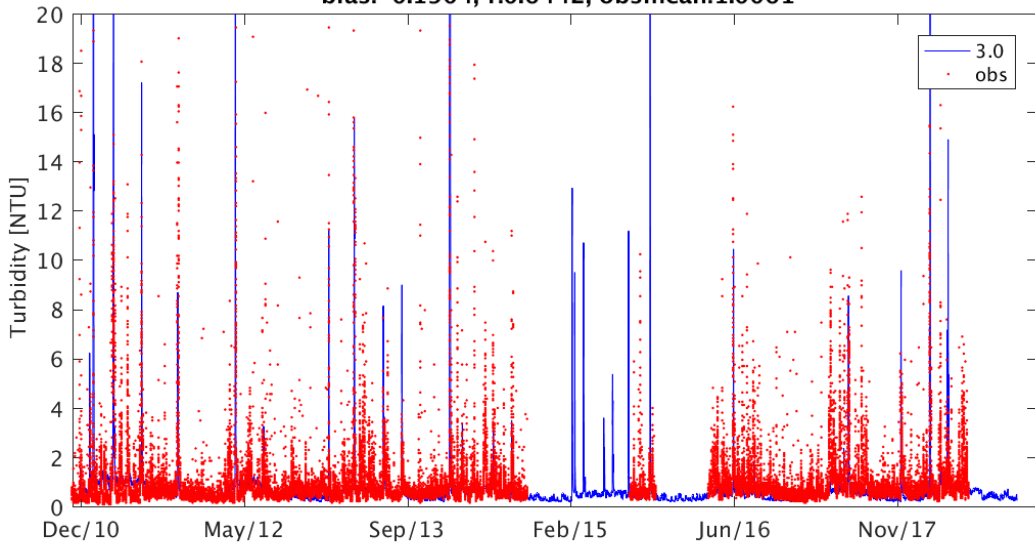
**Pelorus\_5m 3.0 d2:0.78, mape:40.3, rms:1.6540  
bias:-0.2219, r:0.6537, obsmean:0.8579**



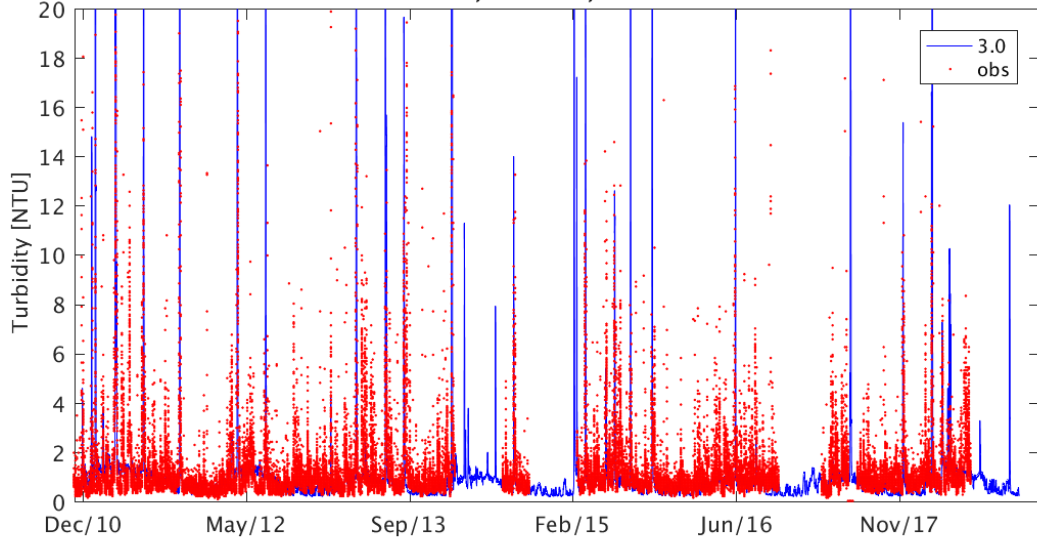
**Dunk859\_5m 3.0 d2:0.44, mape:55.3, rms:9.0171  
bias:-1.7114, r:0.2914, obsmean:3.2370**



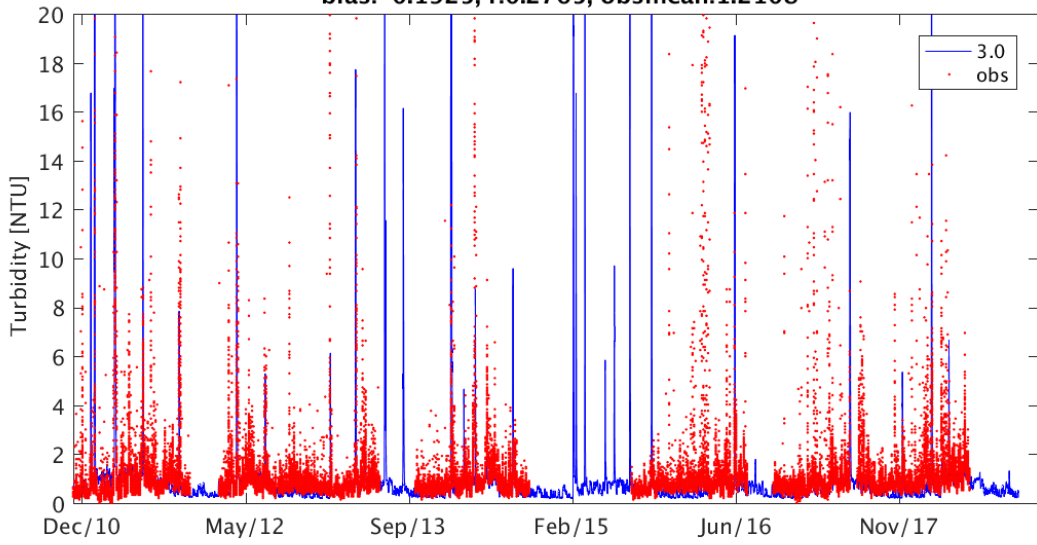
**Russell\_5m 3.0 d2:0.73, mape:50.8, rms:2.4572  
bias:-0.1904, r:0.6442, obsmean:1.0061**



High\_5m 3.0 d2:0.61, mape:52.8, rms:4.4620  
bias:-0.0447, r:0.6349, obsmean:1.3362



Fitz\_5m 3.0 d2:0.37, mape:57.3, rms:4.4454  
bias:-0.1925, r:0.2765, obsmean:1.2108



## 21. Simulated Chl *a* assessment against IMOS/NRS fluorescence

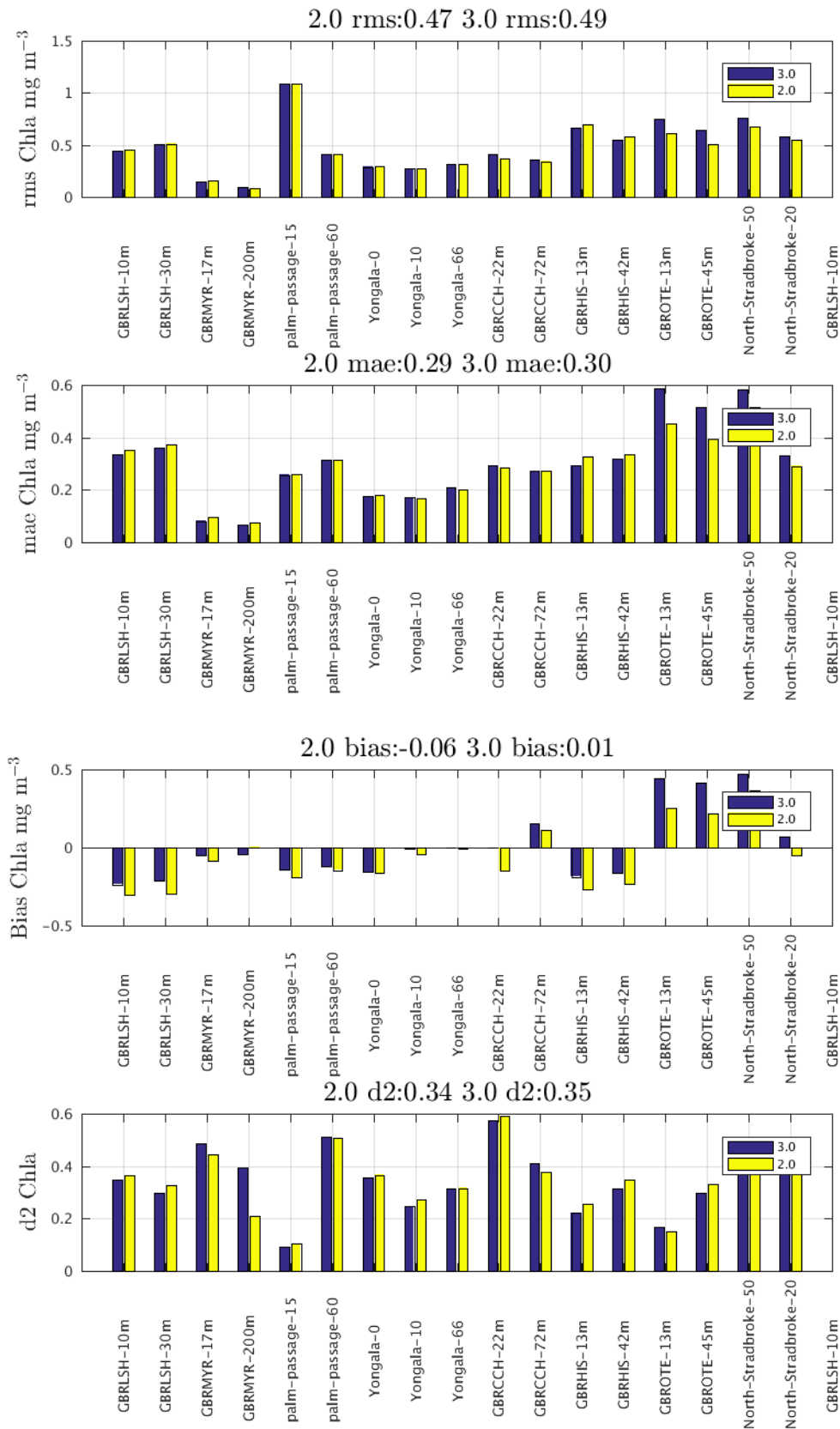


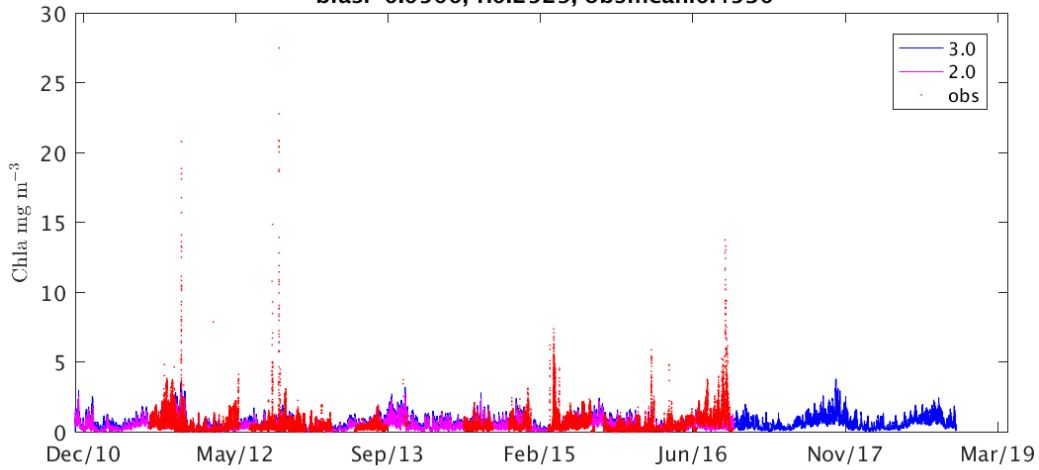
Figure 17 Metrics for IMOS and NRS fluorescence against Chl *a* for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

North\_Stradbroke\_20 3.0 d2:0.45, mape:129.4, rms:0.5768

bias:0.0702, r:0.2402, obsmean:0.4530

North\_Stradbroke\_20 2.0 d2:0.44, mape:98.8, rms:0.5501

bias:-0.0500, r:0.2529, obsmean:0.4530

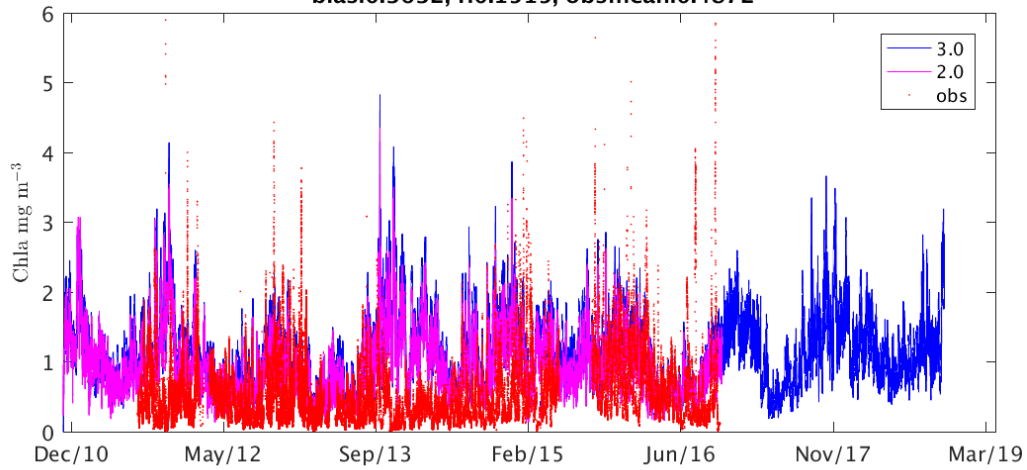


North\_Stradbroke\_50 3.0 d2:0.42, mape:301.7, rms:0.7567

bias:0.4732, r:0.1829, obsmean:0.4872

North\_Stradbroke\_50 2.0 d2:0.42, mape:266.1, rms:0.6750

bias:0.3632, r:0.1515, obsmean:0.4872

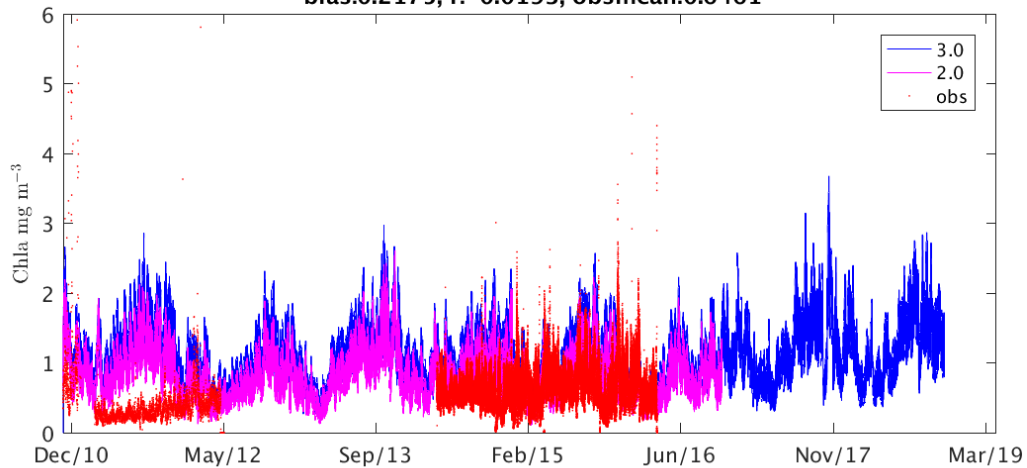


GBROTE\_45m 3.0 d2:0.30, mape:125.5, rms:0.6452

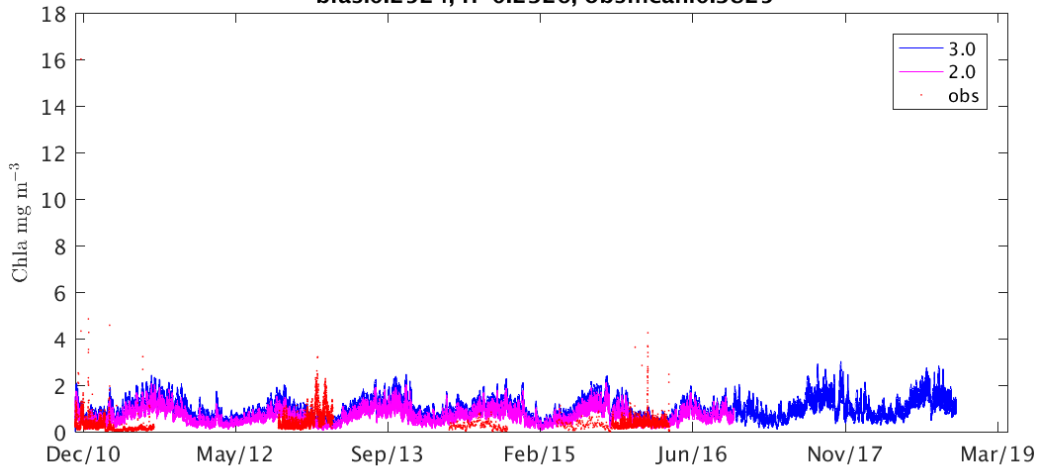
bias:0.4133, r:-0.0315, obsmean:0.6461

GBROTE\_45m 2.0 d2:0.33, mape:94.0, rms:0.5041

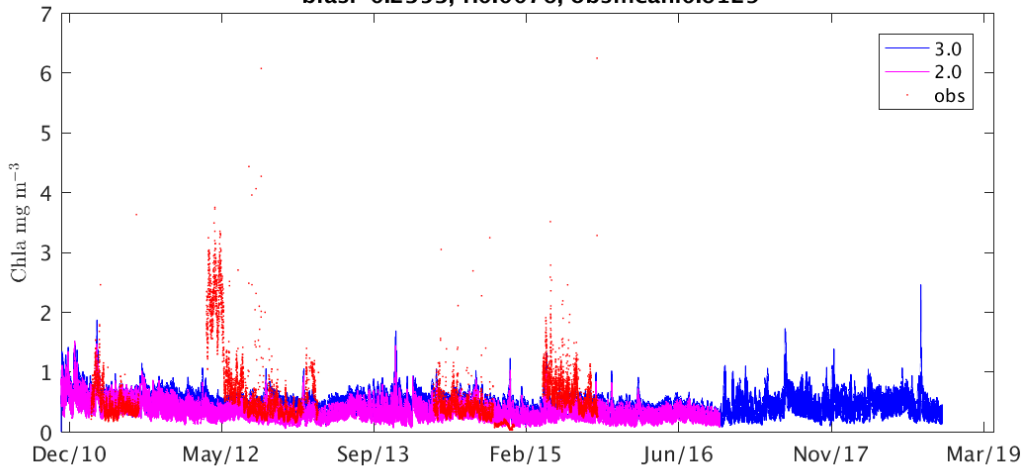
bias:0.2175, r:-0.0193, obsmean:0.6461



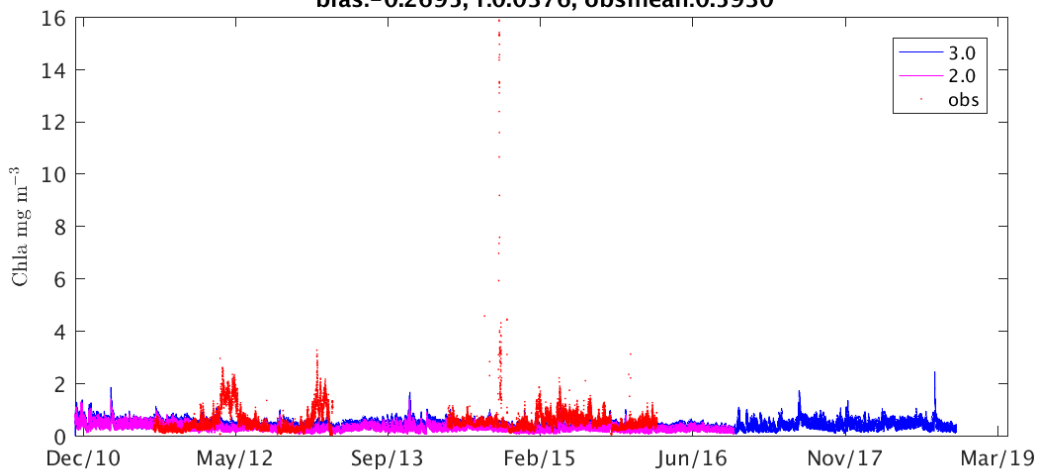
**GBROTE\_13m 3.0 d2:0.17, mape:303.9, rms:0.7526**  
**bias:0.4410, r:-0.2350, obsmean:0.3825**  
**GBROTE\_13m 2.0 d2:0.15, mape:224.1, rms:0.6145**  
**bias:0.2524, r:-0.2326, obsmean:0.3825**



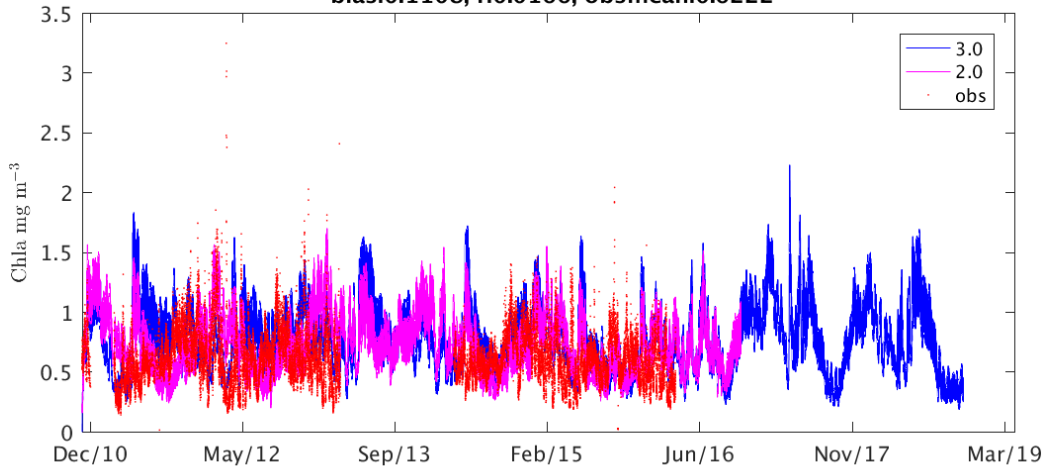
**GBRHIS\_42m 3.0 d2:0.32, mape:59.9, rms:0.5507**  
**bias:-0.1605, r:0.0432, obsmean:0.6129**  
**GBRHIS\_42m 2.0 d2:0.35, mape:54.9, rms:0.5798**  
**bias:-0.2353, r:0.0076, obsmean:0.6129**



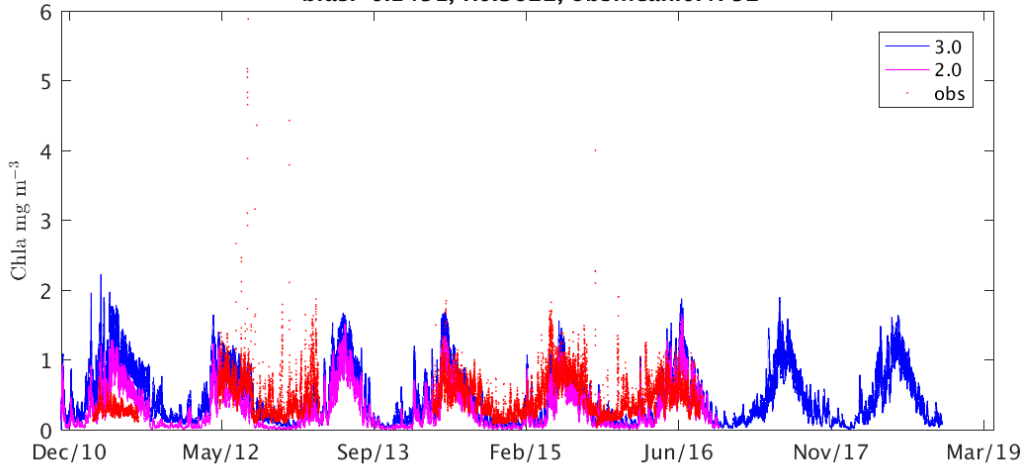
**GBRHIS\_13m 3.0 d2:0.22, mape:47.9, rms:0.6678**  
**bias:-0.1870, r:0.0568, obsmean:0.5930**  
**GBRHIS\_13m 2.0 d2:0.26, mape:48.4, rms:0.6954**  
**bias:-0.2695, r:0.0376, obsmean:0.5930**



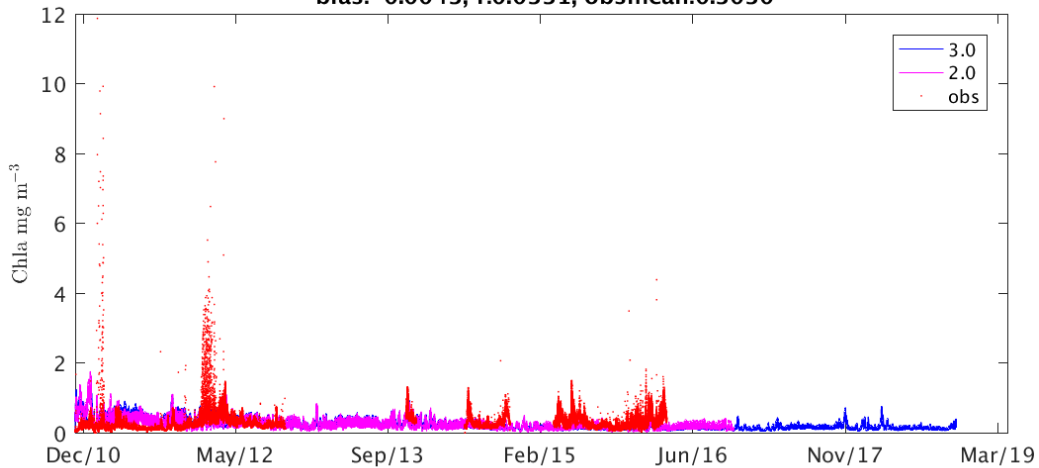
**GBRCCH\_72m 3.0 d2:0.41, mape:54.3, rms:0.3552**  
**bias:0.1563, r:0.0914, obsmean:0.6222**  
**GBRCCH\_72m 2.0 d2:0.38, mape:55.6, rms:0.3431**  
**bias:0.1108, r:0.0166, obsmean:0.6222**



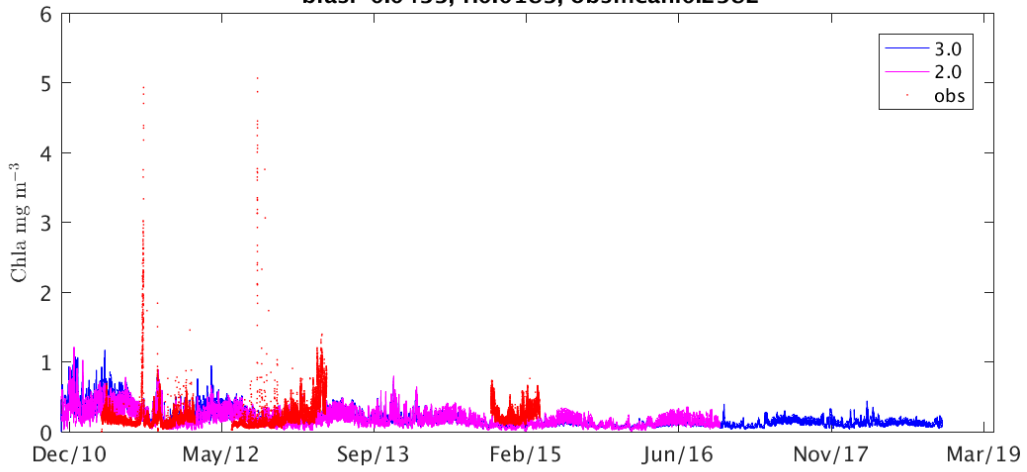
**GBRCCH\_22m 3.0 d2:0.57, mape:73.1, rms:0.4084**  
**bias:-0.0009, r:0.3270, obsmean:0.4752**  
**GBRCCH\_22m 2.0 d2:0.59, mape:67.4, rms:0.3693**  
**bias:-0.1451, r:0.3622, obsmean:0.4752**



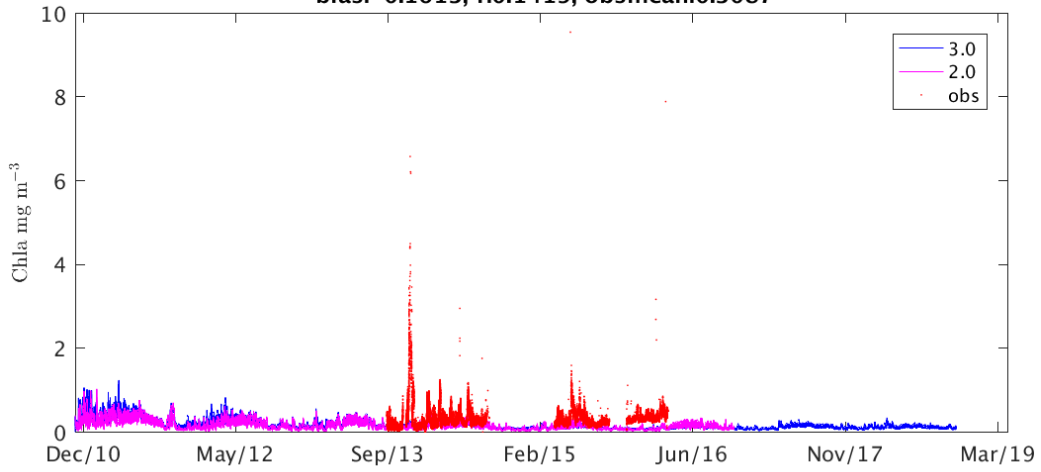
**Yongala\_26 3.0 d2:0.31, mape:93.7, rms:0.3211**  
**bias:-0.0001, r:0.0065, obsmean:0.3030**  
**Yongala\_26 2.0 d2:0.32, mape:88.0, rms:0.3181**  
**bias:-0.0043, r:0.0331, obsmean:0.3030**



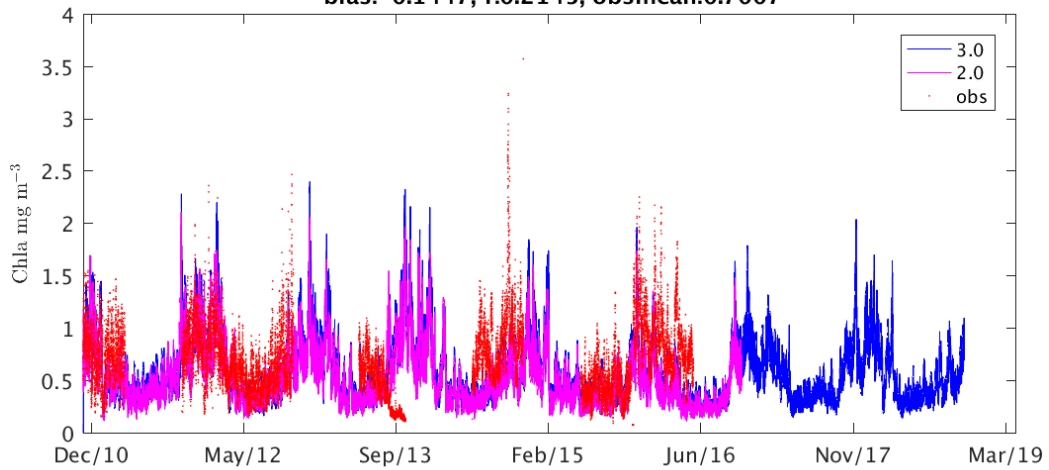
**Yongala\_10 3.0 d2:0.25, mape:84.2, rms:0.2741**  
**bias:-0.0103, r:0.0050, obsmean:0.2382**  
**Yongala\_10 2.0 d2:0.27, mape:79.2, rms:0.2704**  
**bias:-0.0433, r:0.0183, obsmean:0.2382**



**Yongala\_0 3.0 d2:0.35, mape:51.2, rms:0.2904**  
**bias:-0.1563, r:0.1742, obsmean:0.3087**  
**Yongala\_0 2.0 d2:0.37, mape:52.2, rms:0.2970**  
**bias:-0.1613, r:0.1419, obsmean:0.3087**

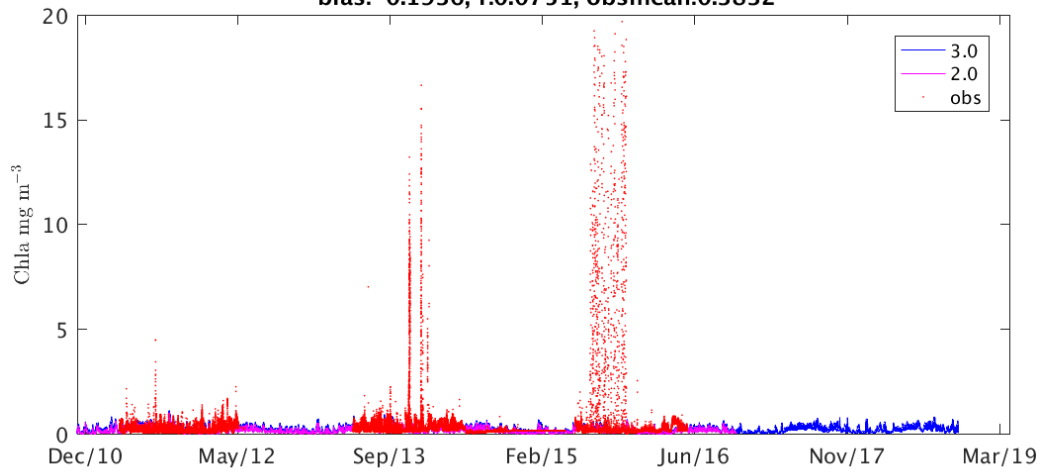


**palm\_passage\_60 3.0 d2:0.51, mape:60.7, rms:0.4143**  
**bias:-0.1187, r:0.2124, obsmean:0.7007**  
**palm\_passage\_60 2.0 d2:0.51, mape:58.3, rms:0.4087**  
**bias:-0.1447, r:0.2145, obsmean:0.7007**

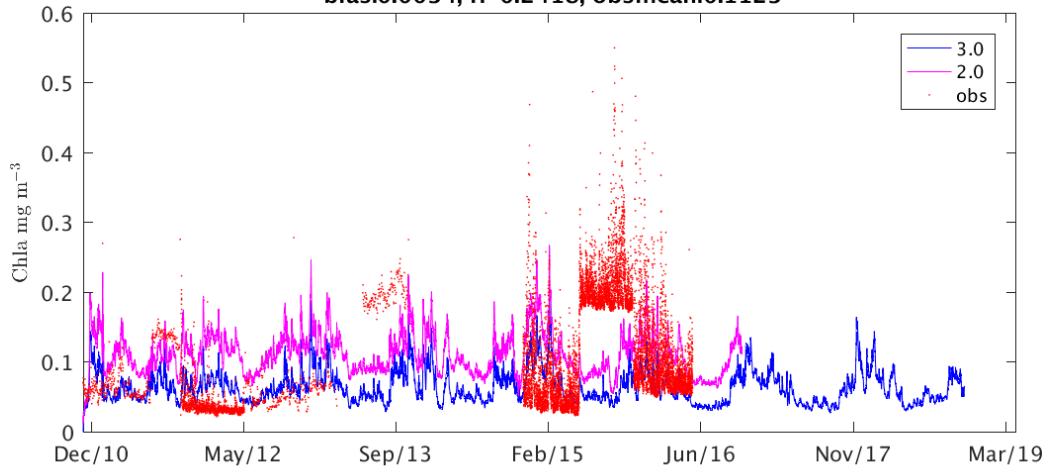




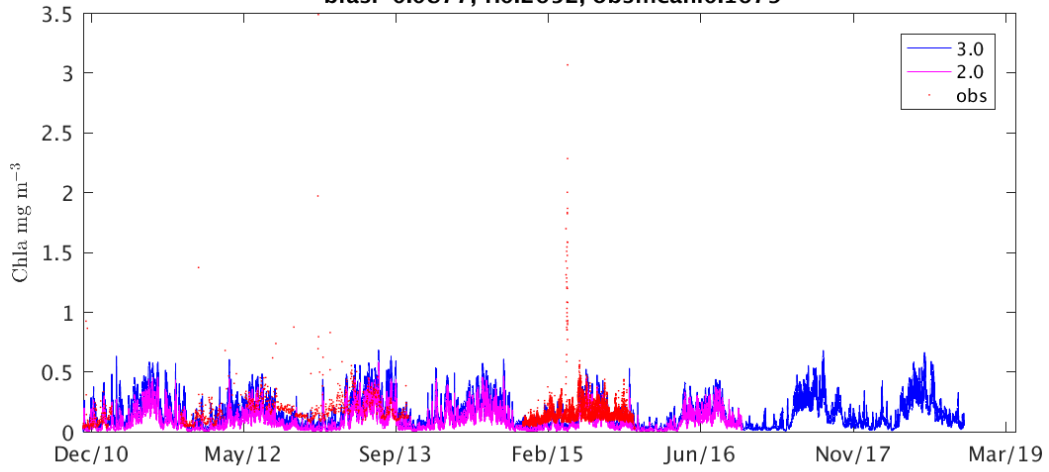
**palm\_passage\_15 3.0 d2:0.09, mape:66.8, rms:1.0897**  
**bias:-0.1422, r:0.0324, obsmean:0.3832**  
**palm\_passage\_15 2.0 d2:0.11, mape:59.8, rms:1.0911**  
**bias:-0.1936, r:0.0751, obsmean:0.3832**



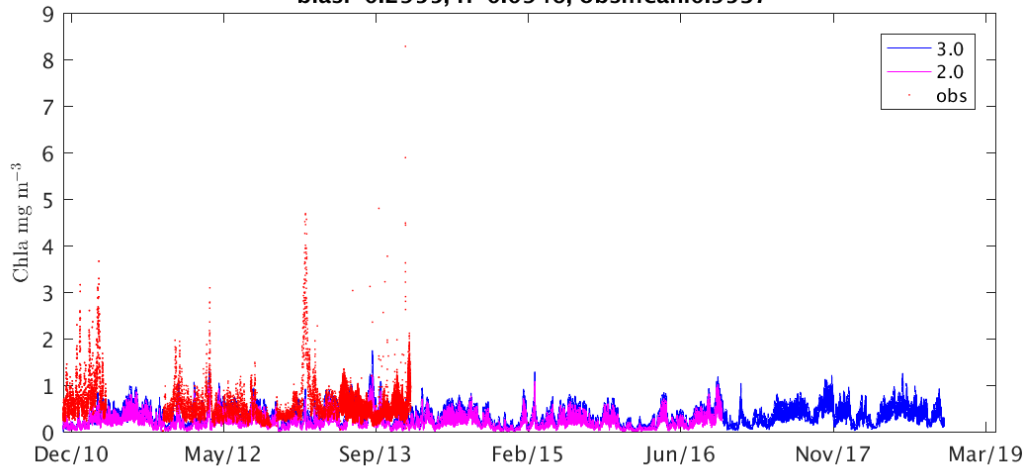
**GBRMYR\_200m 3.0 d2:0.40, mape:59.4, rms:0.0931**  
**bias:-0.0440, r:-0.1409, obsmean:0.1123**  
**GBRMYR\_200m 2.0 d2:0.21, mape:102.3, rms:0.0888**  
**bias:0.0034, r:-0.2418, obsmean:0.1123**



**GBRMYR\_17m 3.0 d2:0.49, mape:47.3, rms:0.1464**  
**bias:-0.0480, r:0.2613, obsmean:0.1679**  
**GBRMYR\_17m 2.0 d2:0.45, mape:58.0, rms:0.1573**  
**bias:-0.0877, r:0.2652, obsmean:0.1679**



**GBRSLH\_30m 3.0 d2:0.30, mape:66.0, rms:0.5020**  
**bias:-0.2140, r:-0.1121, obsmean:0.5537**  
**GBRSLH\_30m 2.0 d2:0.33, mape:64.9, rms:0.5123**  
**bias:-0.2955, r:-0.0946, obsmean:0.5537**



## 22. Simulated NOx assessment against NRS: Yongala and NSI

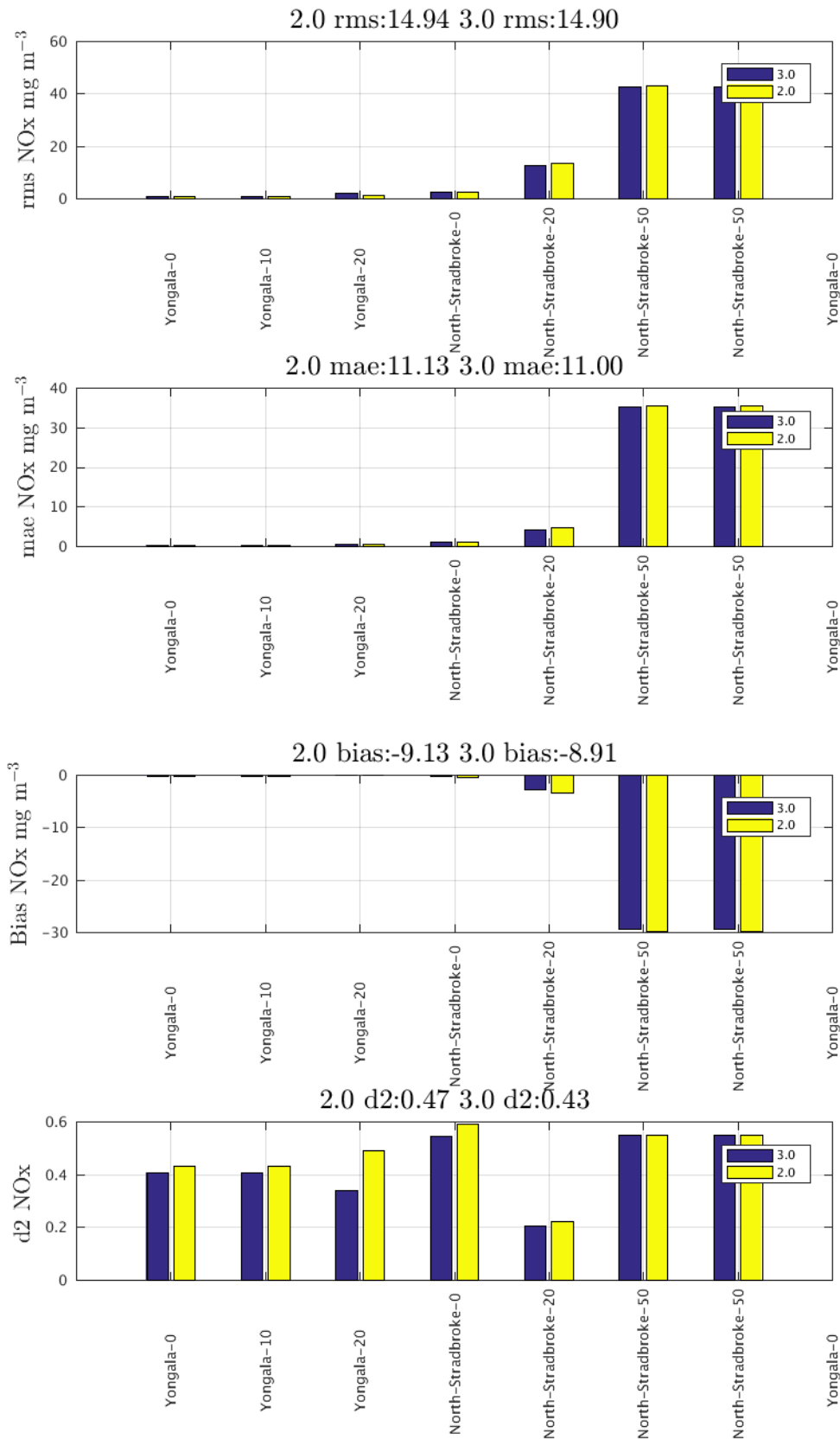


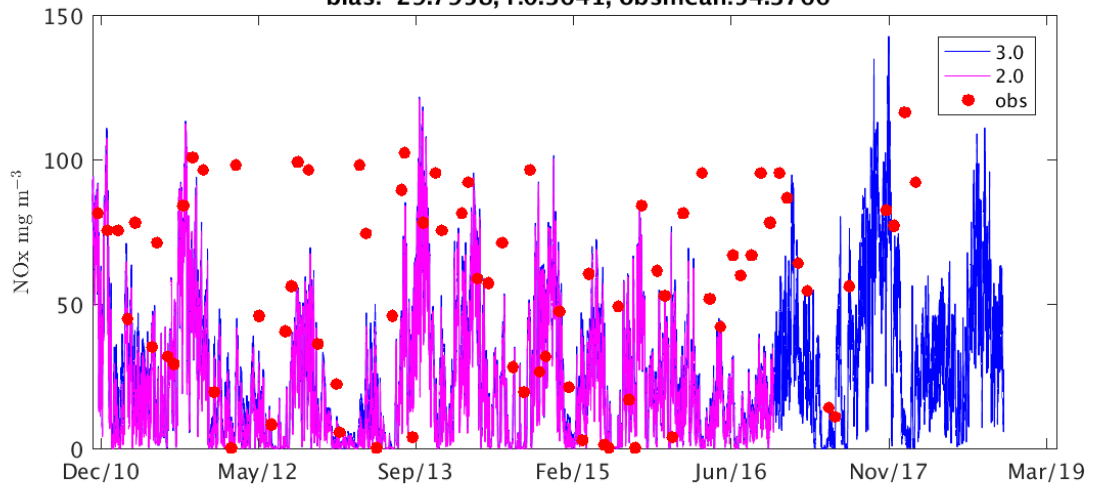
Figure 18 Metrics for NRS NOx against model version 3p0 and 2p0 until 2014 for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

North\_Stradbroke\_50 3.0 d2:0.55, mape:116.2, rms:42.8284

bias:-29.3199, r:0.3570, obsmean:56.3039

North\_Stradbroke\_50 2.0 d2:0.55, mape:120.1, rms:42.9826

bias:-29.7958, r:0.3641, obsmean:54.3766

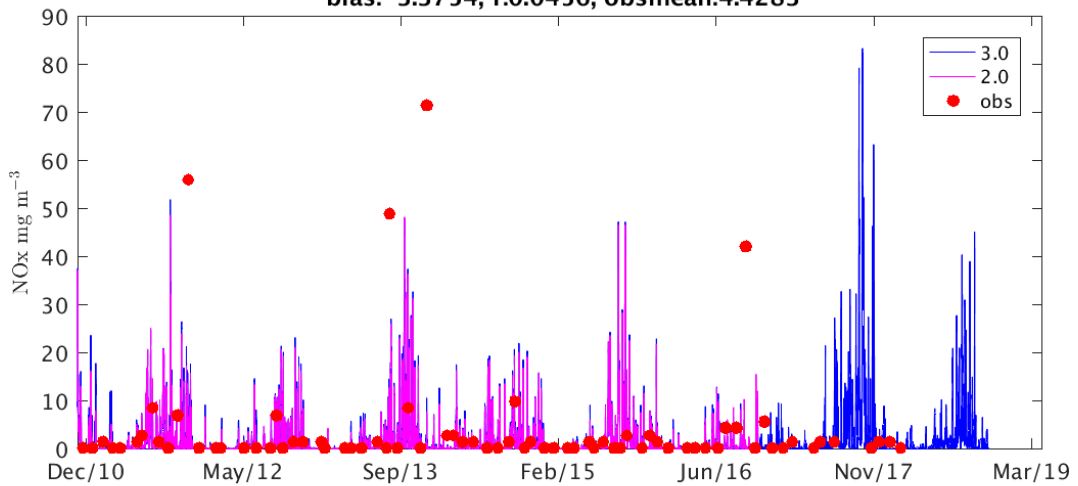


North\_Stradbroke\_20 3.0 d2:0.21, mape:96.0, rms:12.5846

bias:-2.8284, r:0.0675, obsmean:3.9712

North\_Stradbroke\_20 2.0 d2:0.22, mape:100.4, rms:13.6062

bias:-3.3754, r:0.0456, obsmean:4.4283

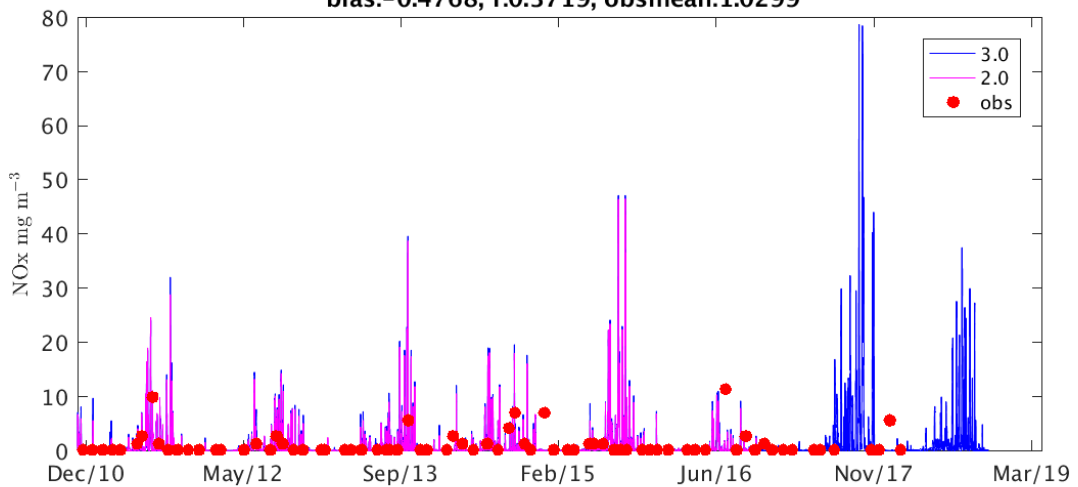


North\_Stradbroke\_0 3.0 d2:0.54, mape:96.3, rms:2.5793

bias:-0.3079, r:0.3055, obsmean:0.9751

North\_Stradbroke\_0 2.0 d2:0.59, mape:84.9, rms:2.4294

bias:-0.4768, r:0.3719, obsmean:1.0299

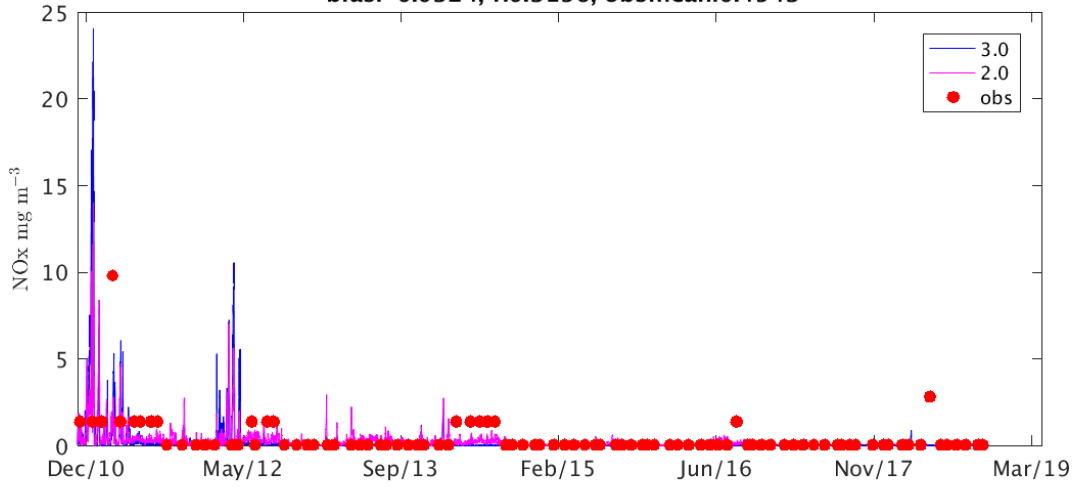


Yongala\_20 3.0 d2:0.34, mape:148.2, rms:1.9444

bias:-0.0721, r:0.2131, obsmean:0.3716

Yongala\_20 2.0 d2:0.49, mape:92.6, rms:1.2867

bias:-0.0324, r:0.3196, obsmean:0.4543

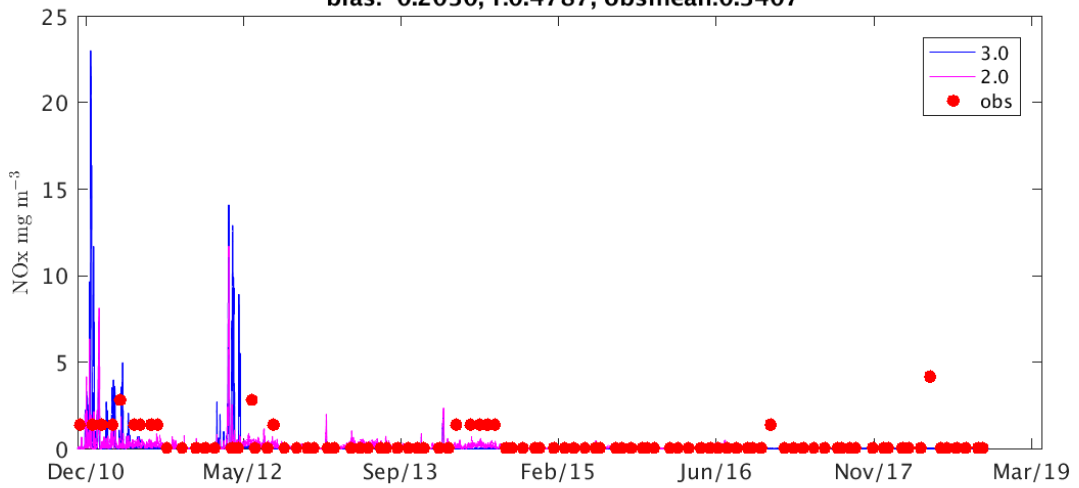


Yongala\_10 3.0 d2:0.41, mape:90.3, rms:0.7520

bias:-0.2569, r:0.2792, obsmean:0.3144

Yongala\_10 2.0 d2:0.43, mape:80.9, rms:0.6571

bias:-0.2030, r:0.4787, obsmean:0.3407



## 23. Simulated NH4 assessment against NRS: Yongala and NSI

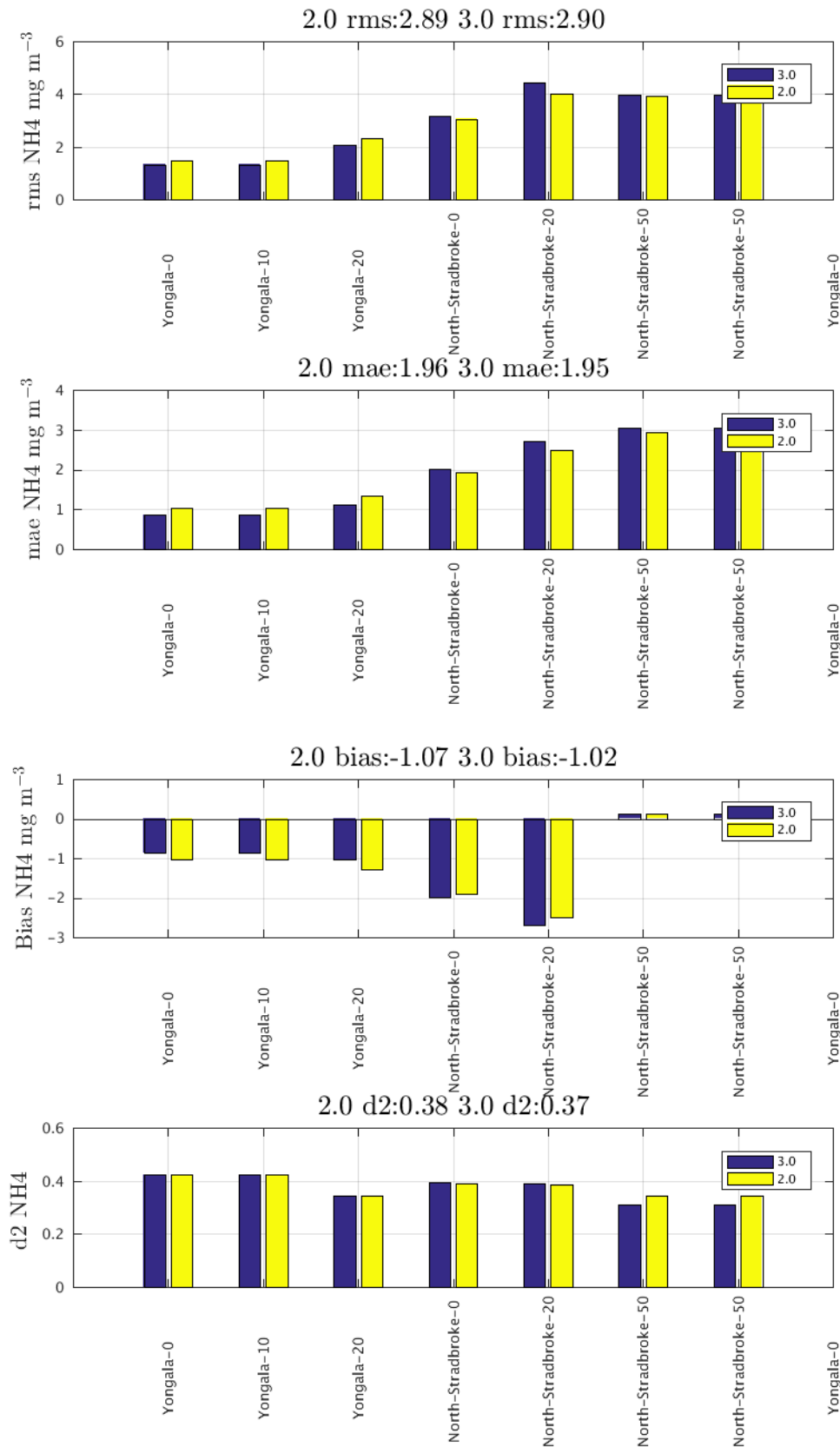


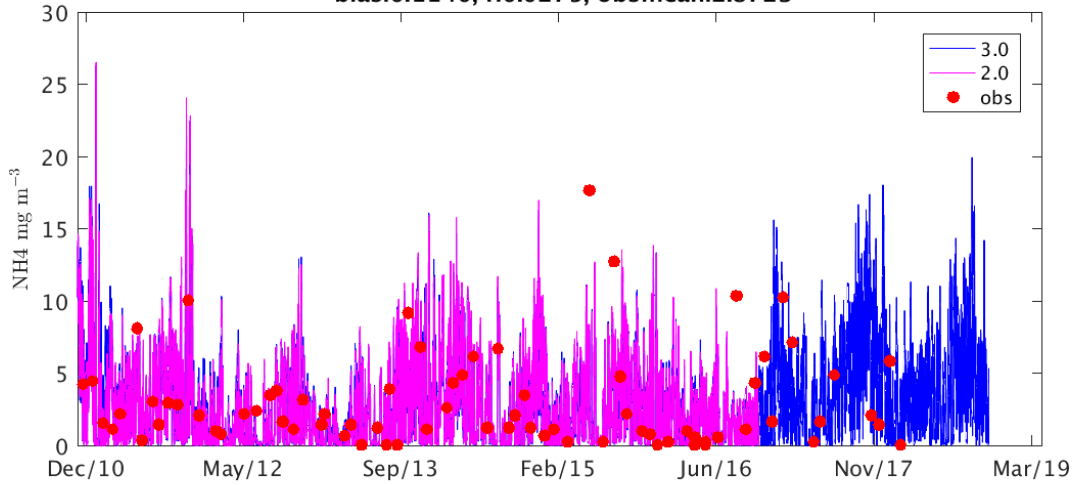
Figure 19 Metrics for NRS NH4 for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

North\_Stradbroke\_50 3.0 d2:0.31, mape:168.9, rms:3.9650

bias:0.1315, r:-0.0367, obsmean:3.0019

North\_Stradbroke\_50 2.0 d2:0.34, mape:164.3, rms:3.9159

bias:0.1140, r:0.0275, obsmean:2.8723

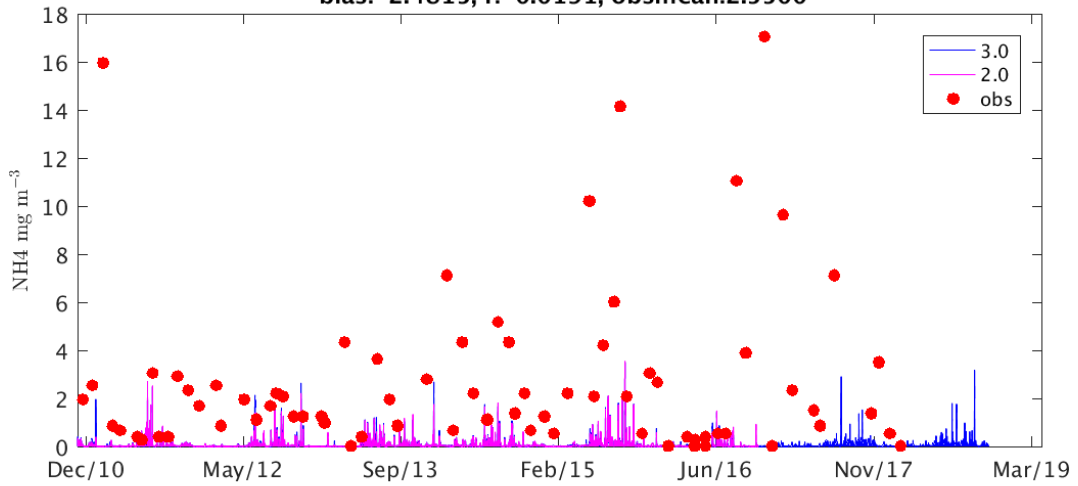


North\_Stradbroke\_20 3.0 d2:0.39, mape:94.1, rms:4.4470

bias:-2.7033, r:-0.0254, obsmean:2.7669

North\_Stradbroke\_20 2.0 d2:0.38, mape:93.5, rms:3.9994

bias:-2.4815, r:-0.0191, obsmean:2.5500

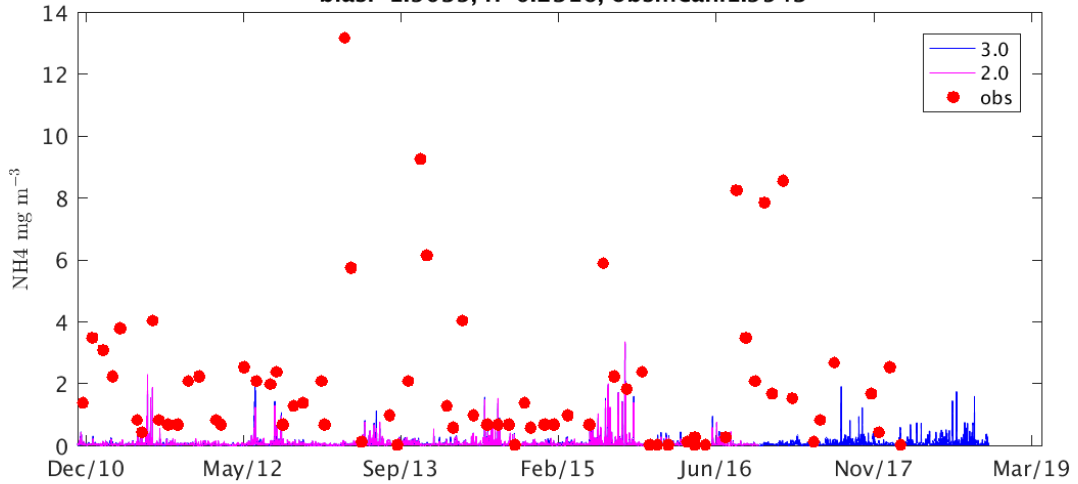


North\_Stradbroke\_0 3.0 d2:0.39, mape:93.1, rms:3.1746

bias:-1.9830, r:-0.2707, obsmean:2.0403

North\_Stradbroke\_0 2.0 d2:0.39, mape:94.4, rms:3.0627

bias:-1.9039, r:-0.2316, obsmean:1.9543

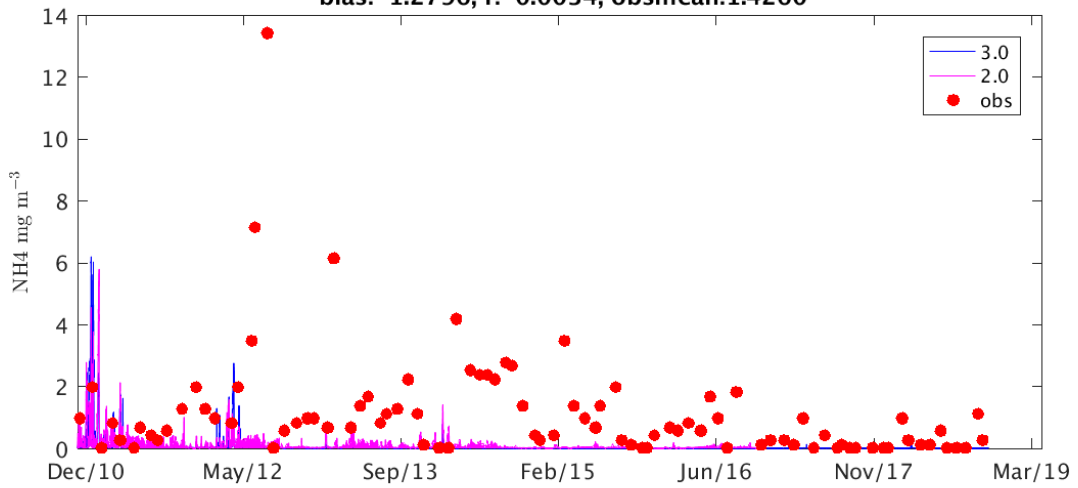


Yongala\_20 3.0 d2:0.34, mape:98.7, rms:2.0681

bias:-1.0401, r:0.0360, obsmean:1.1307

Yongala\_20 2.0 d2:0.34, mape:90.8, rms:2.3246

bias:-1.2796, r:-0.0034, obsmean:1.4260

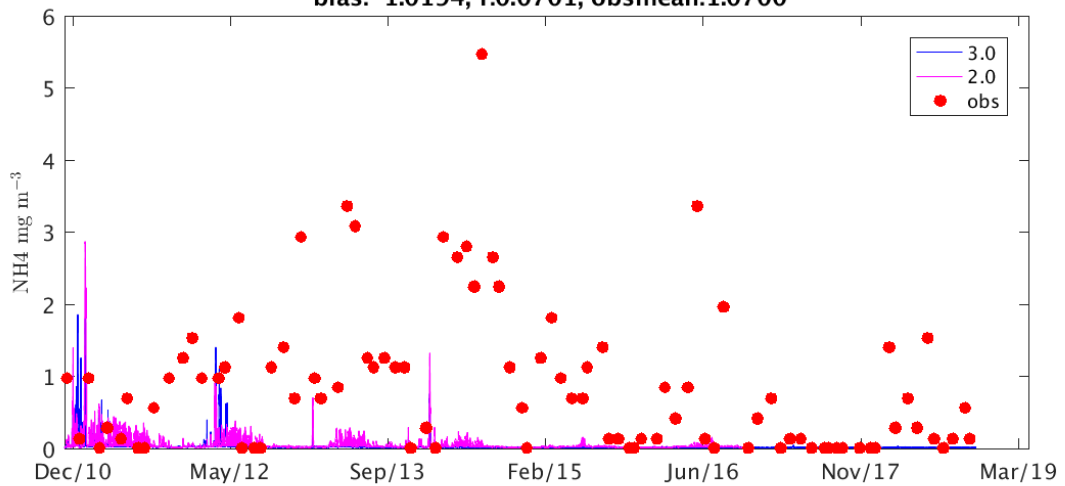


Yongala\_10 3.0 d2:0.42, mape:94.8, rms:1.3301

bias:-0.8479, r:0.0321, obsmean:0.8710

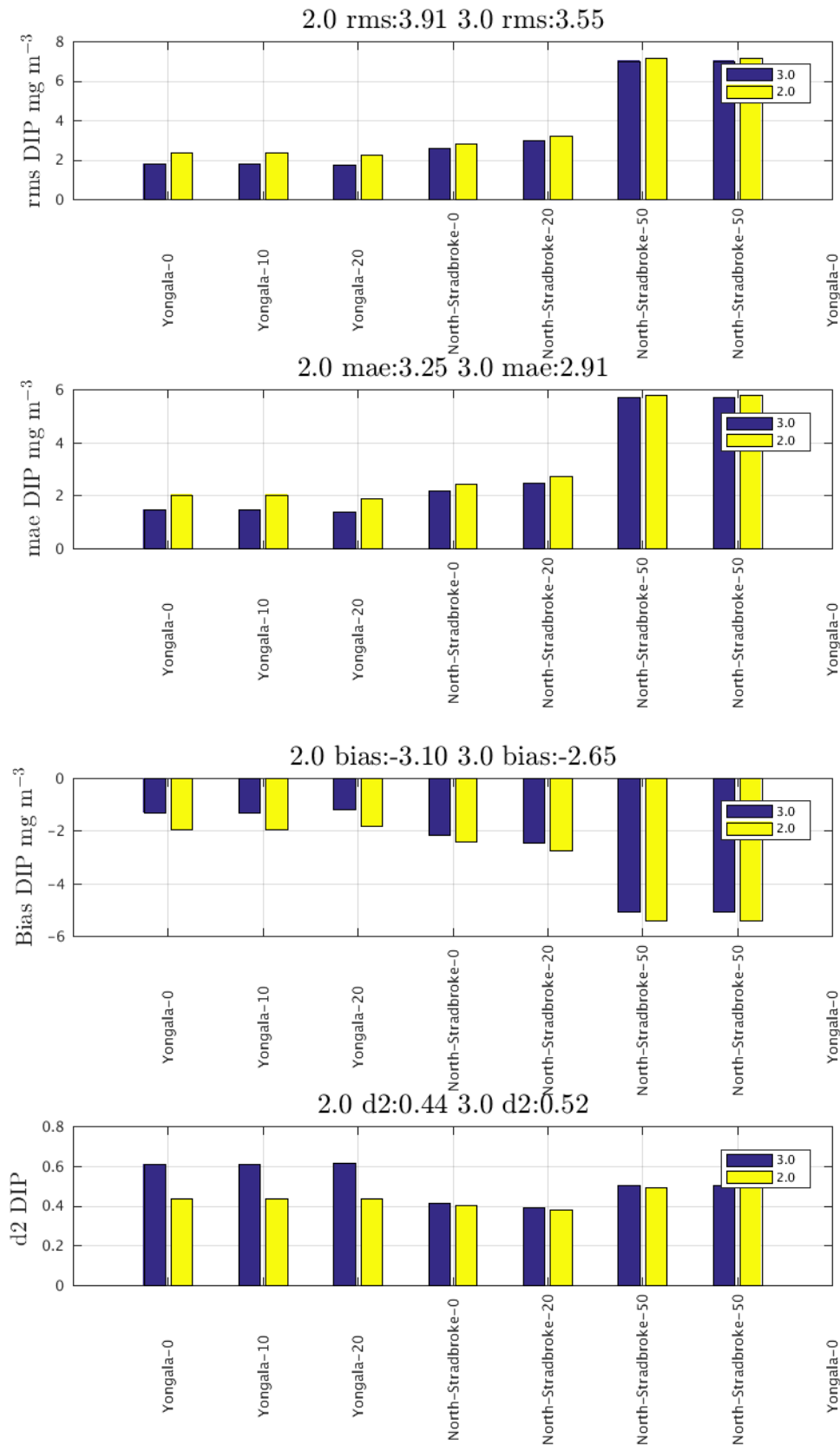
Yongala\_10 2.0 d2:0.43, mape:92.8, rms:1.4893

bias:-1.0194, r:0.0701, obsmean:1.0700





## 24. Simulated DIP assessment against NRS: Yongala and NSI



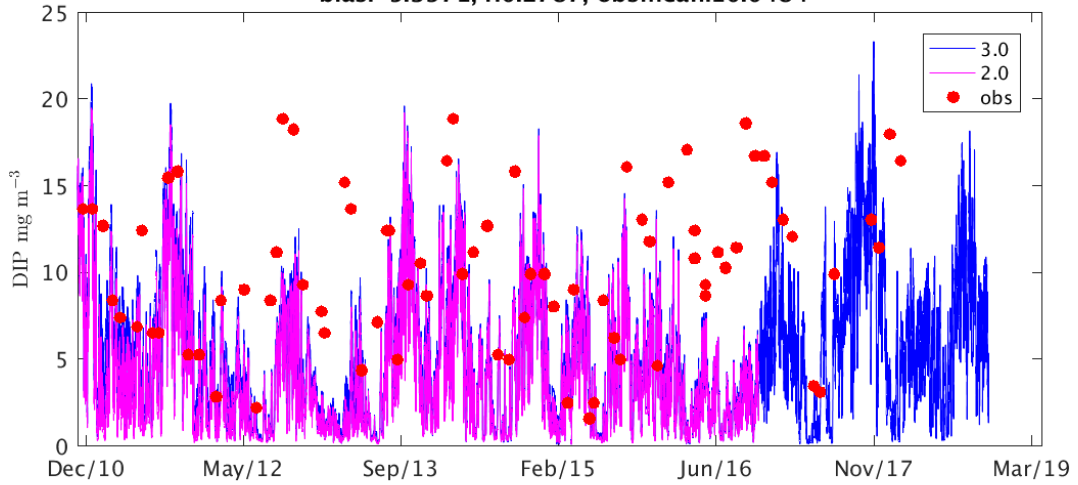
Metrics for IMOS NRS DIP for model version 3p0 and 2p0 d2 = Willmott index see Statistical metric page 27.mae:mean absolute error, rms root mean square

North\_Stradbroke\_50 3.0 d2:0.50, mape:55.7, rms:7.0137

bias:-5.0577, r:0.2643, obsmean:10.3234

North\_Stradbroke\_50 2.0 d2:0.49, mape:58.1, rms:7.1660

bias:-5.3971, r:0.2787, obsmean:10.0484

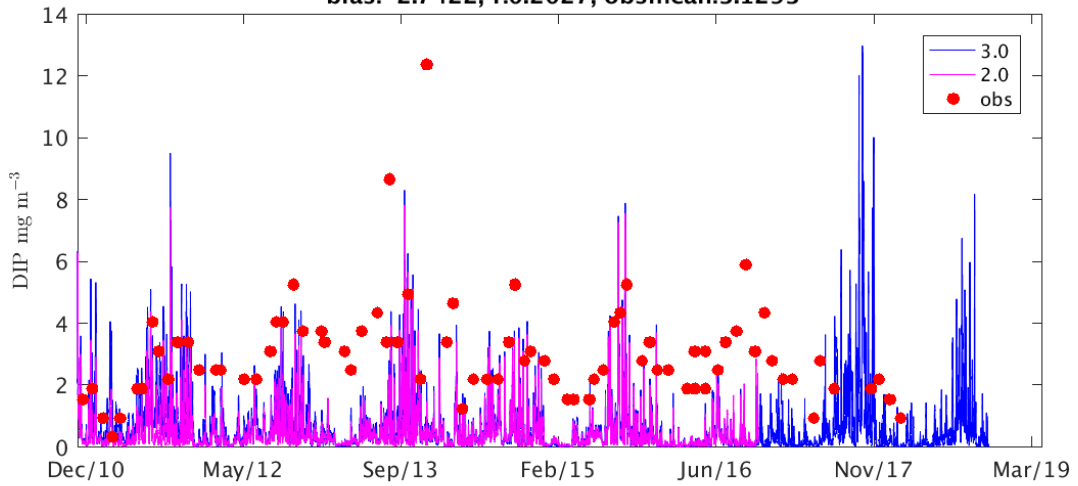


North\_Stradbroke\_20 3.0 d2:0.39, mape:80.4, rms:2.9800

bias:-2.4585, r:0.1857, obsmean:2.9916

North\_Stradbroke\_20 2.0 d2:0.38, mape:86.5, rms:3.2297

bias:-2.7422, r:0.2027, obsmean:3.1293

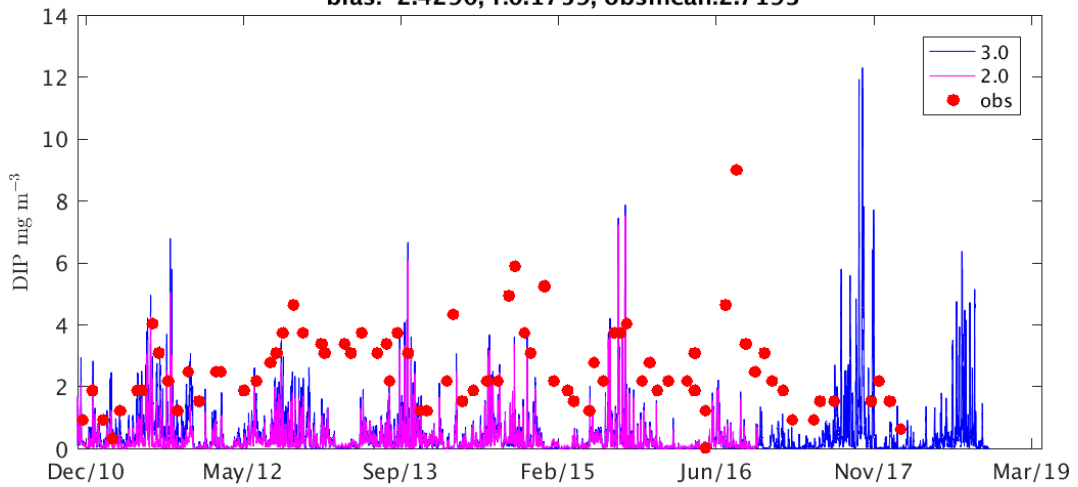


North\_Stradbroke\_0 3.0 d2:0.41, mape:82.3, rms:2.5701

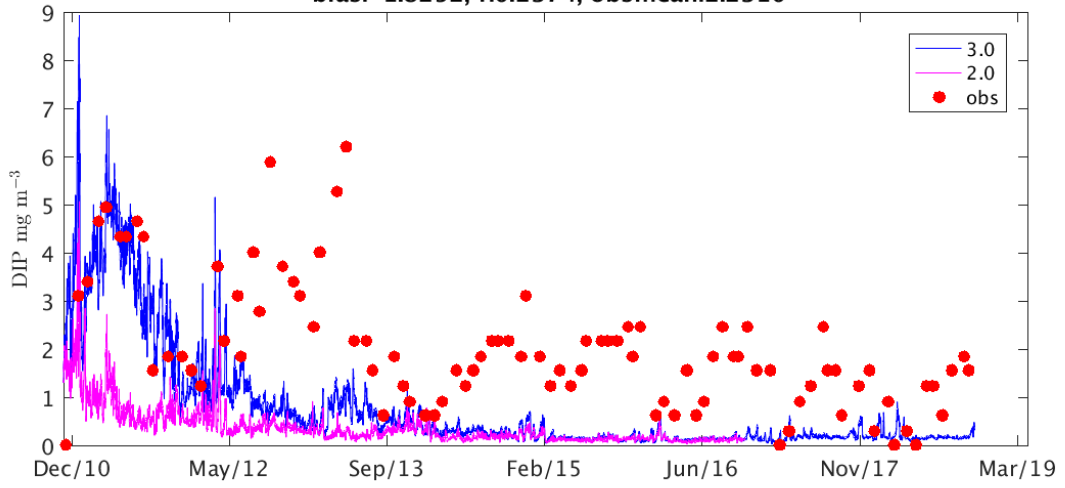
bias:-2.1489, r:0.1245, obsmean:2.5681

North\_Stradbroke\_0 2.0 d2:0.40, mape:87.5, rms:2.7917

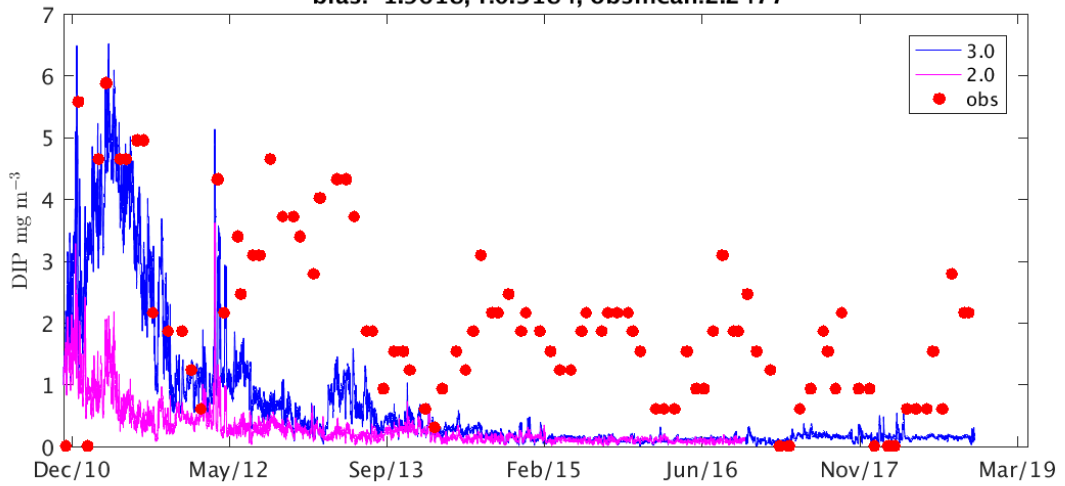
bias:-2.4290, r:0.1759, obsmean:2.7193



Yongala\_20 3.0 d2:0.61, mape:71.1, rms:1.7303  
bias:-1.1670, r:0.4977, obsmean:1.9564  
Yongala\_20 2.0 d2:0.44, mape:80.8, rms:2.2524  
bias:-1.8252, r:0.2374, obsmean:2.2310



Yongala\_10 3.0 d2:0.61, mape:76.3, rms:1.7752  
bias:-1.3186, r:0.5422, obsmean:1.9659  
Yongala\_10 2.0 d2:0.44, mape:87.0, rms:2.3687  
bias:-1.9618, r:0.3184, obsmean:2.2477



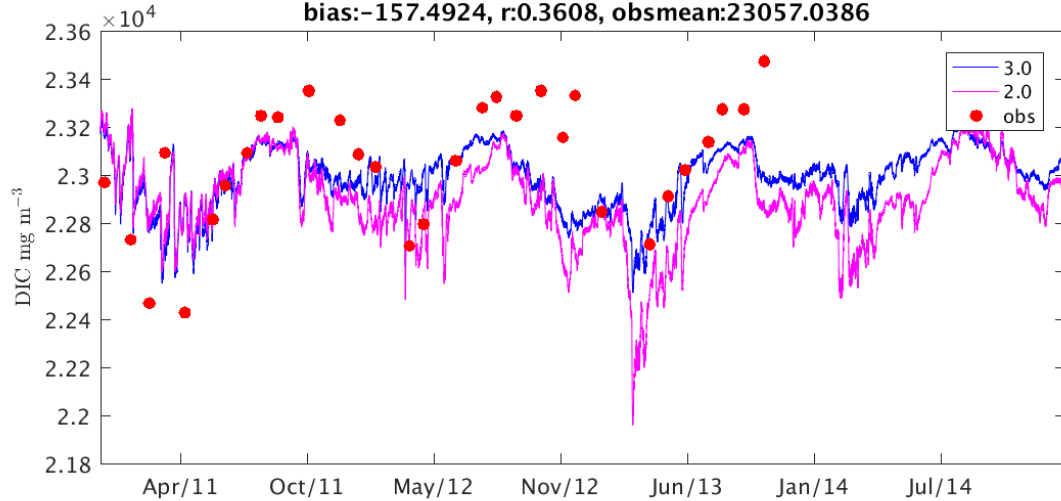
## 25. Simulated DIC assessment against NRS Yongala

**Yongala\_26 3.0 d2:0.58, mape:0.9, rms:251.8943**

**bias:-75.8681, r:0.4184, obsmean:23057.0386**

**Yongala\_26 2.0 d2:0.56, mape:1.1, rms:299.8606**

**bias:-157.4924, r:0.3608, obsmean:23057.0386**

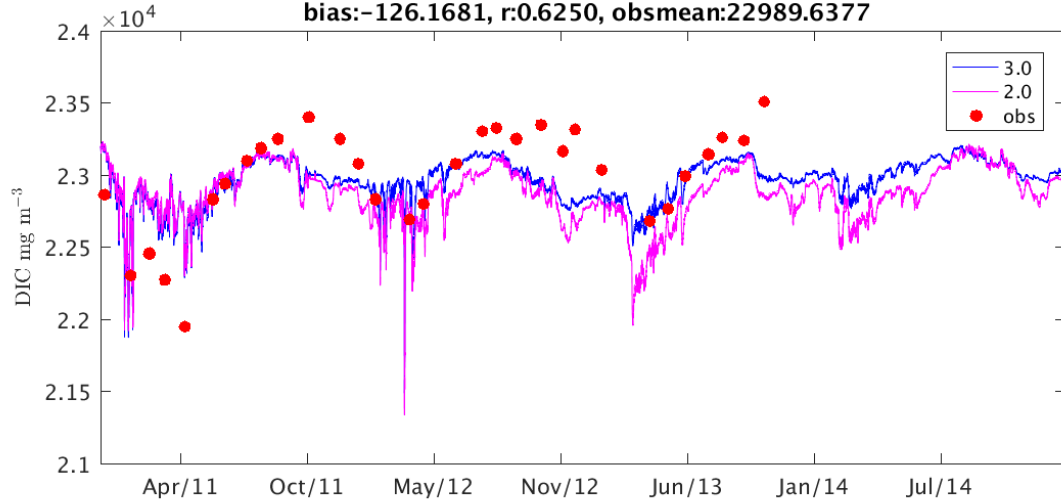


**Yongala\_10 3.0 d2:0.76, mape:0.9, rms:258.2364**

**bias:-44.3495, r:0.7547, obsmean:22989.6377**

**Yongala\_10 2.0 d2:0.69, mape:1.1, rms:310.3398**

**bias:-126.1681, r:0.6250, obsmean:22989.6377**

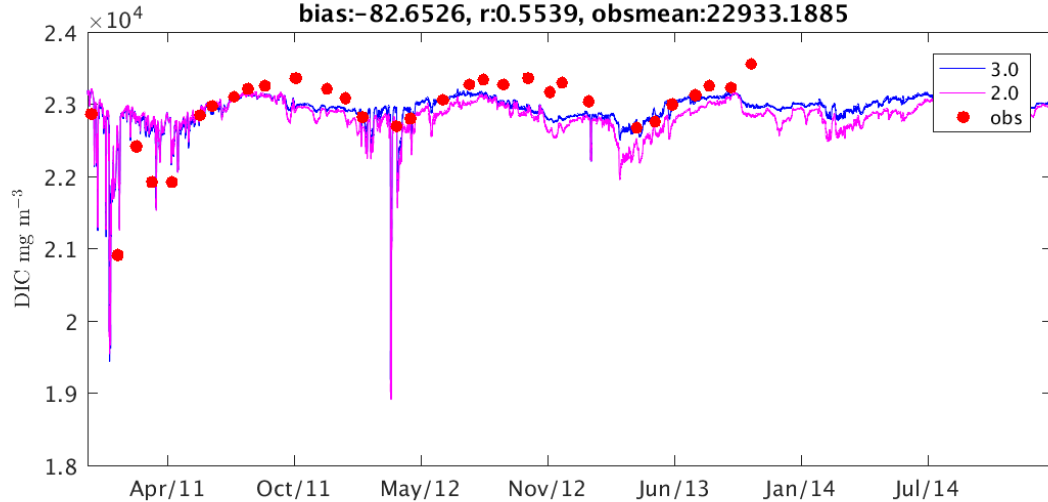


**Yongala\_0 3.0 d2:0.64, mape:1.2, rms:409.6874**

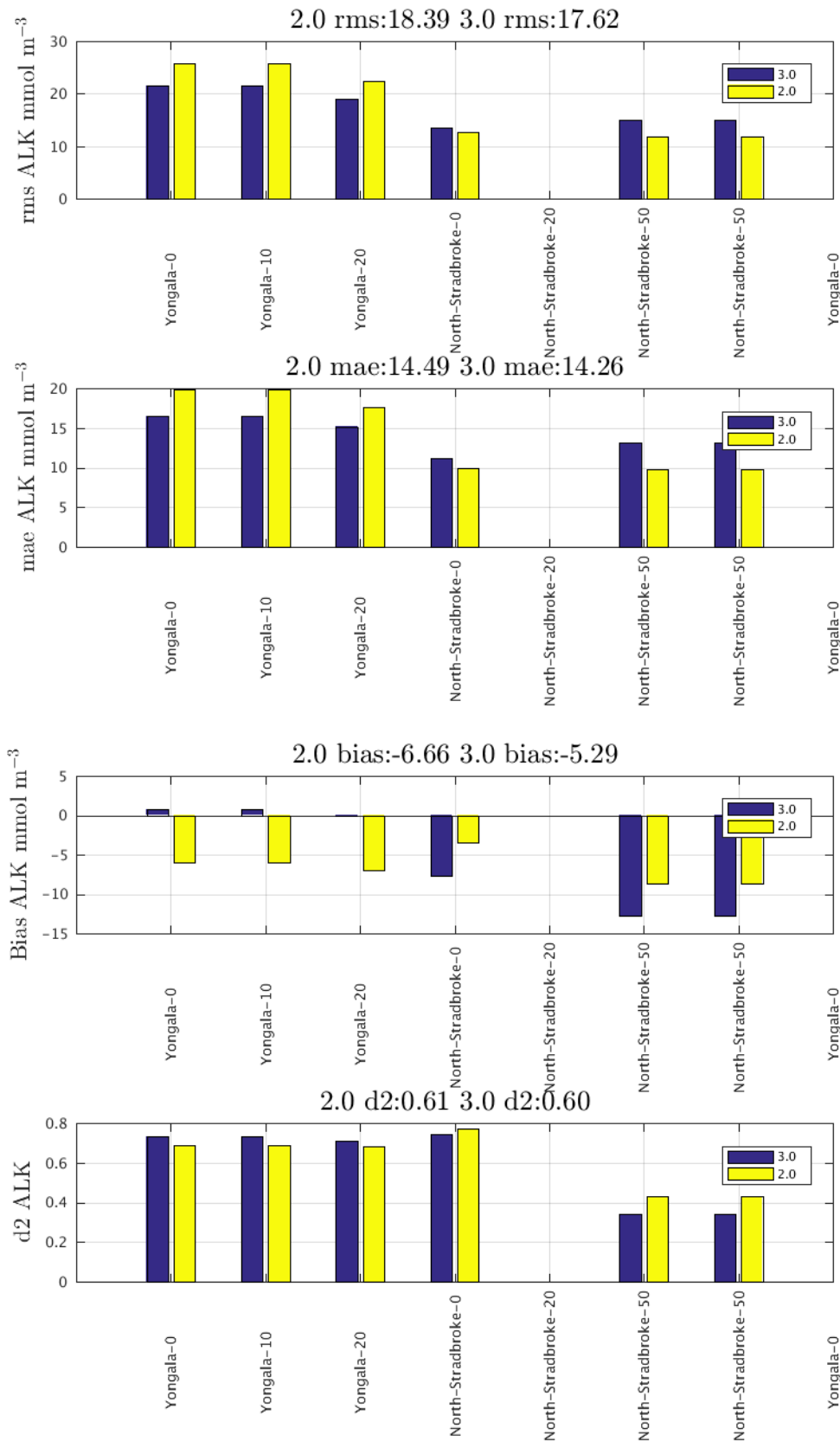
**bias:-2.2563, r:0.7140, obsmean:22933.1885**

**Yongala\_0 2.0 d2:0.57, mape:1.4, rms:452.0324**

**bias:-82.6526, r:0.5539, obsmean:22933.1885**



## 26. Simulated alkalinity assessment against NRS Yongala North Stradbroke

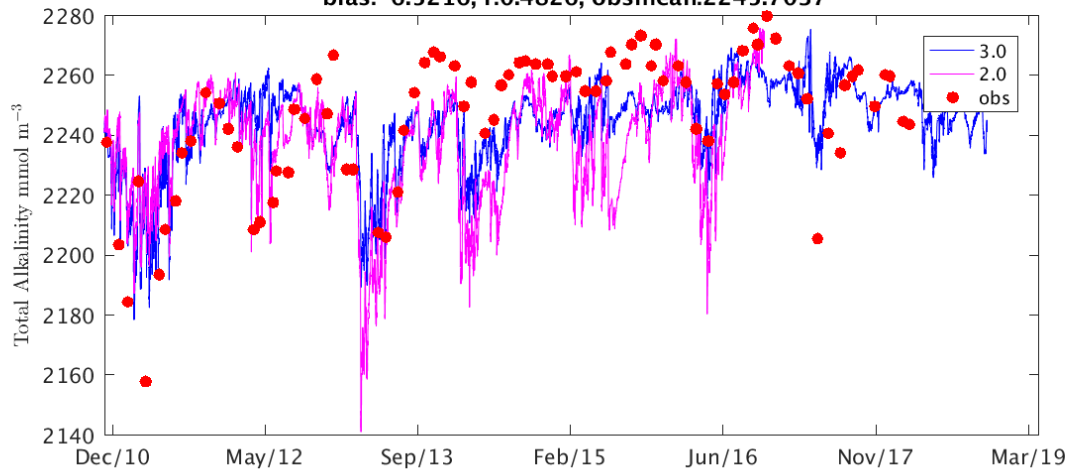


Yongala\_26 3.0 d2:0.69, mape:0.7, rms:18.3375

bias:0.0641, r:0.5781, obsmean:2246.9869

Yongala\_26 2.0 d2:0.65, mape:0.8, rms:21.7963

bias:-6.5216, r:0.4826, obsmean:2245.7037

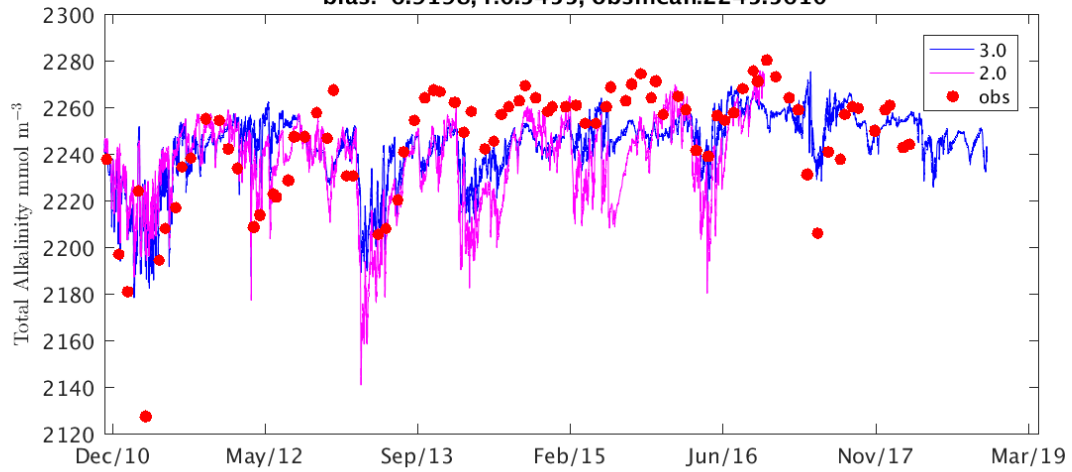


Yongala\_20 3.0 d2:0.71, mape:0.7, rms:19.0163

bias:-0.0493, r:0.6262, obsmean:2246.6614

Yongala\_20 2.0 d2:0.68, mape:0.8, rms:22.3538

bias:-6.9198, r:0.5455, obsmean:2245.5610

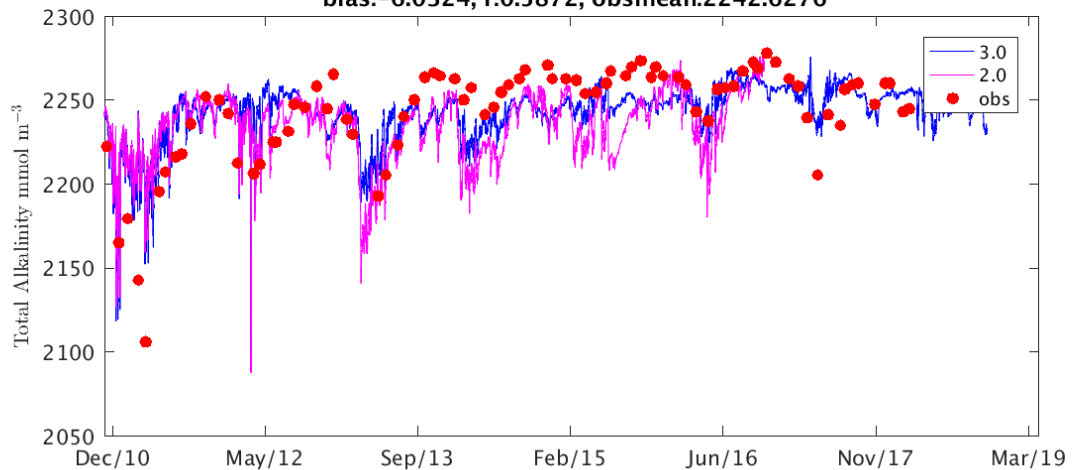


Yongala\_10 3.0 d2:0.73, mape:0.7, rms:21.5717

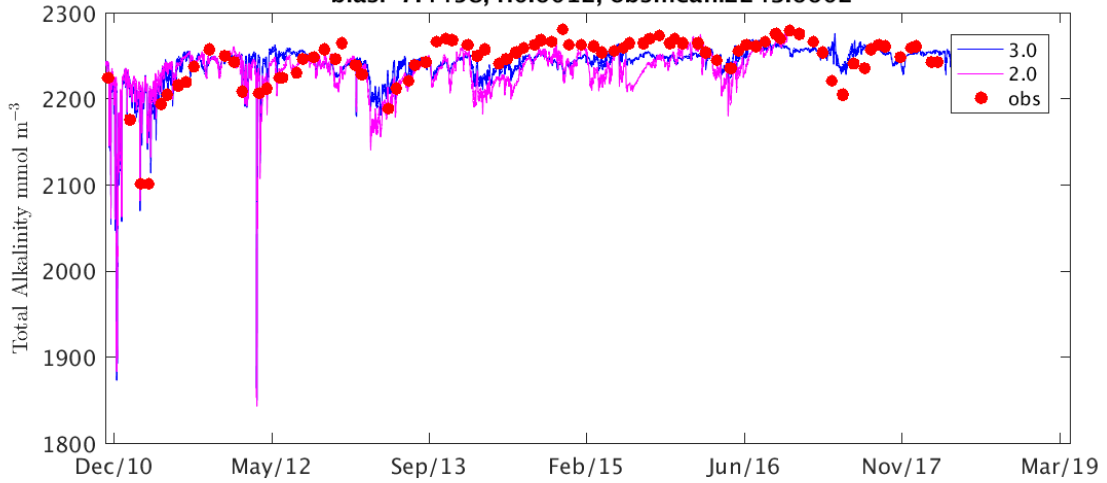
bias:0.8170, r:0.7043, obsmean:2244.2514

Yongala\_10 2.0 d2:0.69, mape:0.9, rms:25.7781

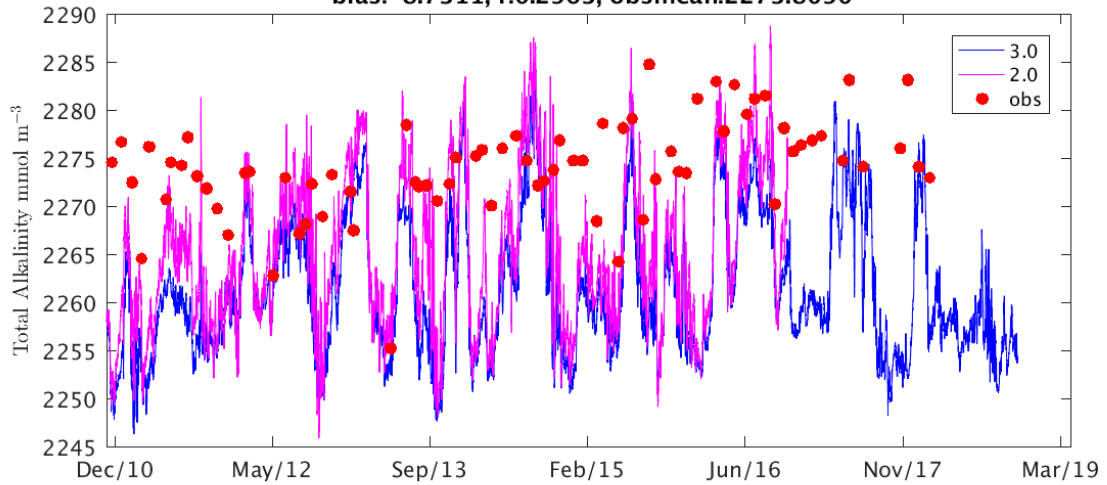
bias:-6.0324, r:0.5872, obsmean:2242.6276



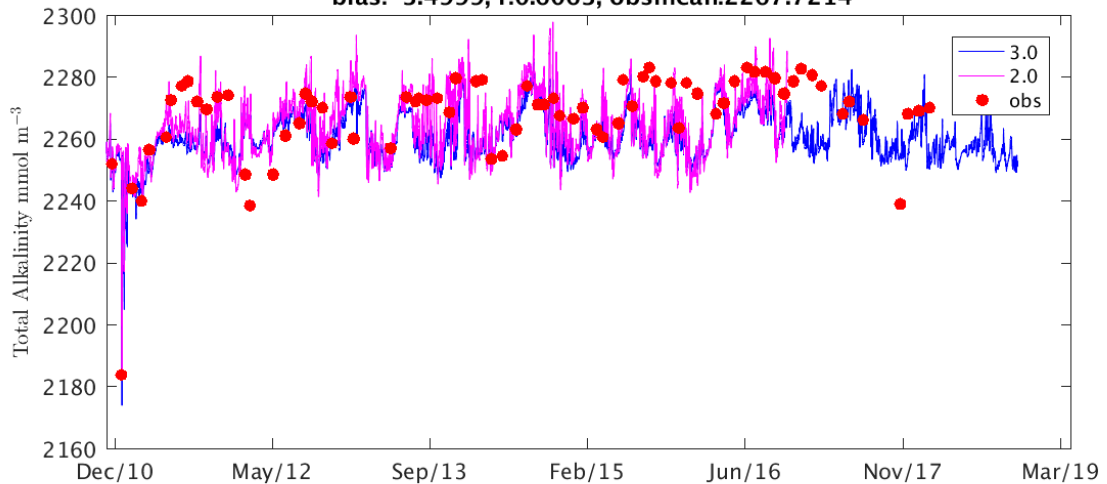
Yongala\_0 3.0 d2:0.73, mape:0.8, rms:22.8977  
bias:-0.4962, r:0.7074, obsmean:2244.9720  
Yongala\_0 2.0 d2:0.69, mape:0.9, rms:27.2858  
bias:-7.4458, r:0.6012, obsmean:2243.6602



North\_Stradbroke\_50 3.0 d2:0.34, mape:0.6, rms:15.0199  
bias:-12.8018, r:0.2477, obsmean:2274.2339  
North\_Stradbroke\_50 2.0 d2:0.43, mape:0.4, rms:11.8997  
bias:-8.7311, r:0.2963, obsmean:2273.8090



North\_Stradbroke\_0 3.0 d2:0.74, mape:0.5, rms:13.5100  
bias:-7.7162, r:0.6444, obsmean:2268.0755  
North\_Stradbroke\_0 2.0 d2:0.77, mape:0.4, rms:12.6298  
bias:-3.4999, r:0.6063, obsmean:2267.7214



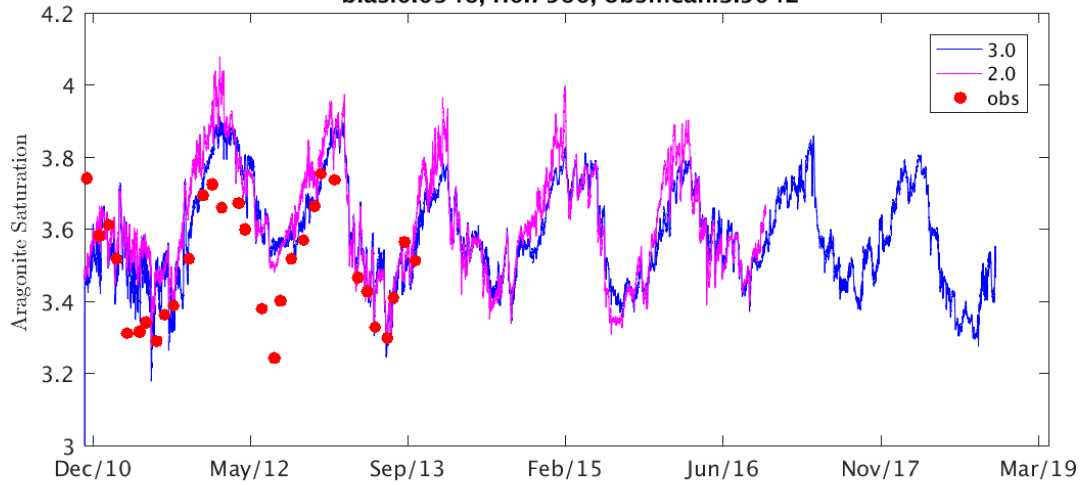
## 27. Simulated aragonite assessment against Yongala

**Yongala\_20 3.0 d2:0.80, mape:3.1, rms:0.1338**

**bias:0.0666, r:0.7046, obsmean:3.5042**

**Yongala\_20 2.0 d2:0.79, mape:3.5, rms:0.1433**

**bias:0.0946, r:0.7560, obsmean:3.5042**

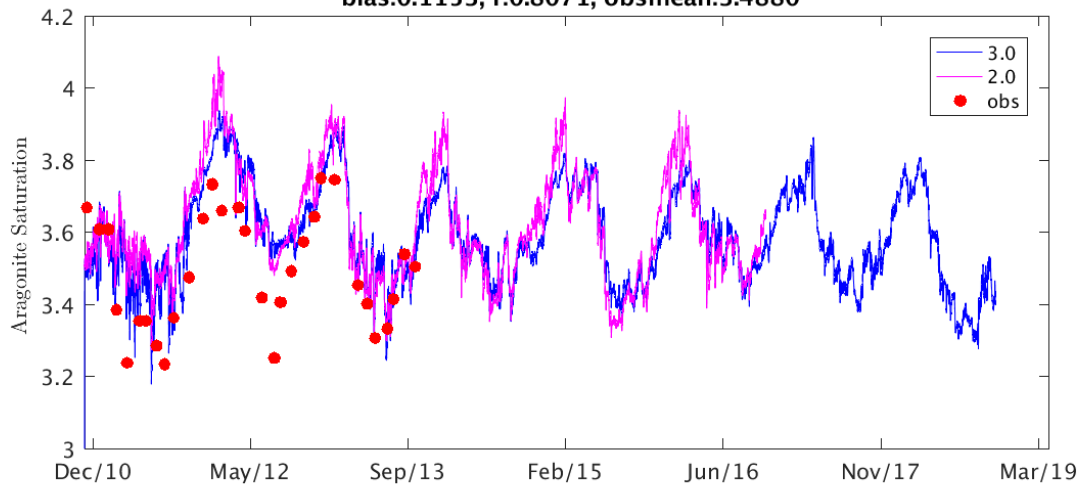


**Yongala\_10 3.0 d2:0.80, mape:3.3, rms:0.1377**

**bias:0.0909, r:0.7704, obsmean:3.4880**

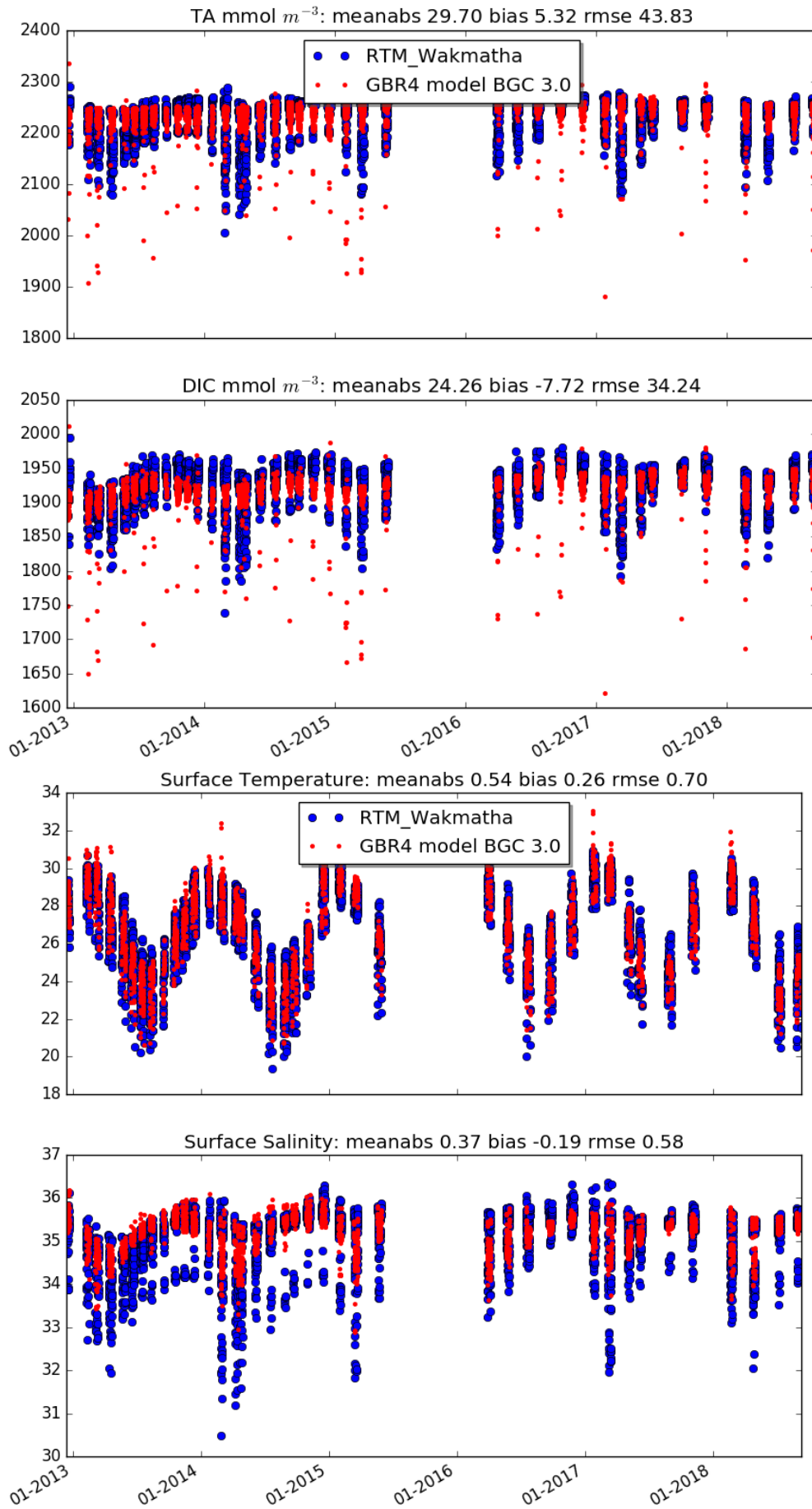
**Yongala\_10 2.0 d2:0.79, mape:3.8, rms:0.1515**

**bias:0.1153, r:0.8071, obsmean:3.4880**





## 28. Wakmatha transect line for Carbon chemistry assessment



29. Satellite images of MMP NRS and LTM sites

