A mechanistic model of coral bleaching due to temperature-mediated light-driven reactive oxygen build-up in zooxanthellae

Mark E. Baird,^{a,*} Mathieu Mongin^a Farhan Rizwi^a

Line K. Bay^b Neal E. Cantin^b Monika Soja-Woźniak^a

Jennifer Skerratt^a

^a*CSIRO Oceans and Atmosphere, Hobart 7001, Australia*

^b*Australian Institute of Marine Science, Townsville 4810, Australia*

Abstract

Mass coral bleaching has emerged in the 21st century as the greatest threat to the health of the world's reefs. A sophisticated process understanding of bleaching at the polyp scale has now been achieved through laboratory and field studies, but this knowledge is yet to be applied in mechanistic models of shelf-scale reef systems. In this study we develop a mechanistic model of the coral-symbiont relationship that considers temperature-mediated build-up of reactive oxygen species due to excess light, leading to zooxanthellae expulsion. The model explicitly represents the coral host biomass, as well as zooxanthellae biomass, intracellular pigment concentration, nutrient status, and the dynamics of reaction centres and the xanthophyll cycle. Photophysiological processes represented include photoadaptation, xanthophyll cycle dynamics, and reaction centre state transitions. The mechanistic model of the coral-symbiont relationship is incorporated into a ~ 1 km resolution coupled hydrodynamic - biogeochemical model that encompasses the entire ~ 2000 km length of

the Great Barrier Reef. A simulation of the 2016 bleaching event shows the model is able to capture the broadscale features of the observed bleaching, but fails to capture bleaching on offshore reefs due to the model's grid being unable to resolve the bathymetry of shallow platforms surrounded by deep water. To further analyse the model behaviour, a ~ 200 m resolution nested simulation of Davies Reef ($18^{\circ}49'S$, $147^{\circ}38'E$) is undertaken. We use this nested model to demonstrate the depth gradient in zooxanthellae response to thermal stress. Finally, we discuss the uncertainties in the bleaching model, which lie primarily in quantifying the link between reactive oxygen build-up and the expulsion process. Through the mechanistic representation of environmental forcing, this model of coral bleaching applied in realistic environmental conditions has the potential to generate more detailed predictions than the presently-available satellite-based coral bleaching metrics, and can be used to evaluate proposed management strategies.

Key words: *Symbiodinium*; mass bleaching; biogeochemical model; climate change; coral mortality; Great Barrier Reef

1 Introduction

Coral bleaching is the expulsion of the unicellular zooxanthellae symbiont from the coral host, often leading to mortality. The link between a warming surface ocean and mass bleaching events had become obvious after the 1998 global event. It was possible in 1999 to predict from climate model simulations that the thermal tolerances of reef-building corals were likely to be exceeded every year within a few decades, and that events as severe as the 1998 event would likely become commonplace within 20 years (Hoegh-Guldberg, 1999). This 1999 prediction of an unprecedented future has eventuated in the late

* Corresponding author: mark.baird@csiro.au

10 2010s (Hughes et al., 2017). Thus the broadscale patterns of mass bleaching
11 are predictable on decadal scales.

12 New management strategies under consideration for coral reef protection
13 include prioritising those individual reefs that are more resilient to future
14 threats (Hock et al., 2017). Thus it is urgent that we are able to identify reefs
15 with lower thermal stress, or other environmental conditions such as good
16 water clarity, that lead to greater resilience. Furthermore, active intervention
17 strategies are being considered that include the introduction of temperature-
18 tolerant individuals or species (Anthony et al., 2017; van Oppen et al., 2017).
19 To predict the success of these interventions requires models of coral-symbiont
20 bleaching dynamics that explicitly consider the tolerance-enabling trait, such
21 as sensitivity to reactive oxygen concentration. Further these bleaching mod-
22 els must be applied in a realistic, spatially-resolved environmental setting to
23 optimise deployment.

24 Historically, process-based modelling of the coral-symbiont relationship has
25 received relatively little attention compared to other aquatic ecosystem-building
26 functional groups such as seagrass or phytoplankton (e.g. Madden and Kemp
27 (1996); Baird et al. (2003)). This oversight is being addressed with the in-
28 creasing awareness of the impacts of climate change on the coral-symbiont re-
29 lationship. The coral-symbiont relationship was first modelled using a dynamic
30 energy budget approach (Muller et al., 2009; Eynaud et al., 2011). Gustafss-
31 son et al. (2013) also explicitly modelled the coral-symbiont relationship, and
32 included some more mechanistic process description such as diffusive limita-
33 tion of nutrient uptake. Gustafsson et al. (2014) added photo-oxidative stress,
34 and in particular the xanthophyll cycle, reaction centre dynamics and reac-
35 tive oxygen build-up, to their earlier work, showing that heterotrophic feeding

36 provided protection from temperature-enhanced photo-oxidative stress. Most
37 recently, Cuning et al. (2017) have also shown that the balance of autotrophic
38 and heterotrophic nitrogen sources influences the steady-state of the coral-
39 symbiont system, where bleached or unbleached are two final states.

40 The process-based models of the coral-symbiont relationship cited above
41 have been undertaken by considering one polyp in isolation, allowing compar-
42 ison to laboratory experiments, but the output of these one polyp simulations
43 are not easily compared to observations from natural coral reefs. A simpli-
44 fied form of the Gustafsson et al. (2013) model has been implemented in a
45 Great Barrier Reef (GBR) scale model (Baird et al., 2016b; Mongin et al.,
46 2016), but the dynamics of the coral themselves in this complex biogeochem-
47 ical model has only been briefly analysed (Herzfeld et al., 2016). In order to
48 understand the mass bleaching occurring on reefs around the world, and to
49 support a range of management actions, it is necessary to apply process-based
50 coral-symbiont models that consider temperature-mediated light-driven ox-
51 idative stress within biogeochemical / ecosystem models that are capable of
52 predicting the time-varying light, nutrient and prey conditions of natural reef
53 environments.

54 A large, multi-agency collaboration has developed the eReefs coupled hy-
55 drodynamic, sediment and biogeochemical model that simulates at multi-
56 ple scales the environmental conditions of the Great Barrier Reef (Schiller
57 et al., 2014). The project provides ~ 1 and ~ 4 km resolution hindcast and
58 near real time simulations of hydrodynamic and biogeochemical quantities
59 (www.ereefs.info). The models provides skilful predictions of the drivers
60 of coral processes such as temperature, spectrally-resolved bottom light, and
61 water column concentrations of dissolved inorganic nutrients and particulate

62 organic matter across the entire length of the Great Barrier Reef from 2011-
63 present (Skerratt et al., submitted). Furthermore, the eReefs project includes
64 bespoke model generation that allows high-resolution models to be nested
65 within the 1 km regional hindcast (RECOM - RElocatable Coastal Ocean
66 Model).

67 In this paper, we develop a process-based model of the coral-symbiont re-
68 lationship that considers temperature-mediated light-driven oxidative stress
69 resulting in zooxanthellae expulsion. The model explicitly represents the coral
70 host and the zooxanthellae biomass, pigment concentration, nutrient status, as
71 well as the reaction centre and xanthophyll cycle dynamics. The process-based
72 model of the coral-symbiont relationship is incorporated into the eReefs 3D
73 coupled hydrodynamic - biogeochemical model of the Great Barrier Reef, and
74 a simulation run of the 2016 bleaching event in the ~ 1 km configuration and a
75 ~ 200 m Davies Reef configuration. The model behaviour is analysed at both
76 scales, and model uncertainty discussed. Finally, with a model that captures
77 the impact of temperature, solar radiation and water column inorganic and
78 particulate nutrients on coral bleaching, we consider future applications in the
79 management of the Great Barrier Reef.

80 **2 Model description**

81 The ultimate purpose of the mechanistic model of coral bleaching developed
82 in this paper is to be able to predict bleaching in natural environments, and
83 to explore the impact of interventions to reduce bleaching. This requires a
84 model that responds to water column conditions such as nutrients, light and
85 temperature, and produces metrics of stress such as concentration of reactive

86 oxygen species and zooxanthellae expulsion rates.

87 The coral-symbiont model developed here is an extension of the coral polyp
88 model of Gustafsson et al. (2013) and the photosystem bleaching model of
89 Gustafsson et al. (2014). Further we have included the photoadaptation model
90 of Baird et al. (2013) and the multiple nutrient limitation microalgae model
91 of Baird et al. (2016b). This combination of process descriptions is applied
92 in a complex biogeochemical model of the Great Barrier Reef that has been
93 described elsewhere (Mongin et al., 2016), and was developed in the eReefs
94 Project (Schiller et al., 2014).

95 The following description of the coral-symbiont model description is split
96 into three sections: (1) the interactions between the coral host, the symbiont
97 and the environment; (2) photoadaptation through pigment synthesis and the
98 xanthophyll cycle; and (3) photosynthesis, reaction centre dynamics and re-
99 active oxygen production leading to zooxanthellae expulsion.

100 2.1 Coral host, symbiont and the environment

101 The state variables for the coral polyp model (Table A.1) include the biomass
102 of coral tissue, CH (g N m^{-2}), and the structure material of the zooxanthellae
103 cells, CS (mg N m^{-2}). The structure material of the zooxanthellae, CS , in
104 addition to nitrogen, contains carbon and phosphorus at the Redfield ratio.
105 The zooxanthellae cells also contain reserves of nitrogen, R_N (mg N m^{-2}),
106 phosphorus, R_P (mg P m^{-2}), and carbon, R_C (mg C m^{-2}).

107 The zooxanthellae light absorption capability is resolved by considering the
108 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 β -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 A.1).

Fig. 1. Schematic showing the coral-symbiont relationship and its interaction with the overlying water column.

The coral host is able to assimilate organic nitrogen either through translocation from the zooxanthellae cells or through the capture of water column organic detritus and/or plankton (Fig. 1). 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.,

125 1994), based on a structure material at the Redfield ratio, but with variable
 126 internal reserves. The fluxes of C, N and P with the overlying water column
 127 (nutrient uptake and detrital / mucus release) can therefore vary from the
 128 Redfield ratio.

129 An explanation of the individual processes follows, with tables in the Ap-
 130 pendix listing all the model state variables (Table A.1), derived variables (Ta-
 131 ble A.2), equations (Tables A.3, A.4, A.5 and A.6), and parameters values
 132 (Tables A.7 and A.8).

133 2.1.1 *Effective projected area fraction of corals*

134 A key component of the coral-symbiont model is to relate the biomass of the
 135 polyp to coral cover (the fraction of the bottom covered when viewed from
 136 above). This relationship is important as it determines, for a given biomass
 137 of coral host, the area of the bottom the polyp covers. The bottom cover
 138 impacts on the nutrient flux from the water column, and limits the number of
 139 zooxanthellae per unit area. Following the derivation of Baird et al. (2016a), we
 140 use a mathematical form that captures the likelihood that an independently-
 141 placed polyp will lie over the top of another polyp, and is similar to a Poisson
 142 distribution:

$$143 \quad A_{eff} = 1 - \exp(-\Omega_{CH} CH) \quad (1)$$

144 where A_{eff} is the effective projected area fraction of the coral community (m^2
 145 m^{-2}), CH is the biomass of the coral host, and Ω_{CH} is the nitrogen-specific
 146 polyp area coefficient ($\text{m}^2 \text{ g N}^{-1}$).

147 In the coarser configurations, coral communities are restricted to a size that

Fig. 2. Schematic showing the geometric calculation of the sub-grid parameterisation of the effective projected area fraction of corals, A_{CH} . Nominal width of dense coral communities, $x = 200$ m, grid cell dimensions h_1 and h_2 are 1000 m for the 1 km grid, and R is the equivalent circular radius of the grid cell.

is often much less than the model grid size, due to their existence on the rims of reefs (Baird et al., 2004b). To consider this sub-grid scale patchiness, Eq. 1 is slightly modified resulting in the effective projected area for corals calculated by:

$$A_{eff} = A_{CH} (1 - \exp(-\Omega_{CH} CH/A_{CH})) \quad (2)$$

The area coefficient, A_{CH} , represents the fraction of a grid cell that the corals can occupy. In the case of 200 m grids, this will be up to 1, representing dense corals on the whole cell. For coarser grids, A_{CH} is reduced to represent that the cell contains both dense coral communities on the forereef / reef crest and also sparse coral communities on the reef flat / lagoon areas. In the 1 km grid, A_{CH} represents the fraction of the area of dense corals to total reef area, and is of order 0.36. The geometrically-derived equation for A_{CH} is given by (Fig. 2):

$$A_{CH} = 1 - \frac{(R-x)^2}{R^2}, \quad R = \sqrt{h_1 h_2 / \pi}, \quad R > x \quad (3)$$

where x is the width of dense coral communities on the reef, and R is the equivalent circular radius of the grid cell.

The impact of concentrating corals into one portion of a grid cell, as quan-

165 tified by A_{CH} , only affects the calculations when the concentrated area be-
 166 gins self-shading. Thus, in Eq. 2, when $\Omega_{CH} CH/A_{CH}$ is small, $A_{eff} \sim (1 -$
 167 $\exp(-\Omega_{CH} CH/A_{CH}))$. But if $\Omega_{CH} CH/A_{CH} \rightarrow 1$ and $A_{CH} < 1$ the coral biomass
 168 saturates due to space limitation at a lower biomass than it would for $A_{CH} = 1$.

169 The eReefs model contains macroalgae that grow above the corals at the
 170 seabed. For the case of macroalgae over-growing corals, the effective projected
 171 area occupied by corals is further reduced by the presence of macroalgal leaves:

$$172 \quad A_{eff} = A_{CH} \exp(-\Omega_{MA} MA) (1 - \exp(-\Omega_{CH} CH/A_{CH})) \quad (4)$$

173 where MA is the biomass of macroalgae, and Ω_{MA} is the nitrogen-specific leaf
 174 area coefficient ($\text{m}^2 \text{g N}^{-1}$). We assume that the fraction of the bottom covered
 175 by the macroalgae, $\exp(-\Omega_{MA} MA)$, is evenly spread across the surface. Thus
 176 the portion covered by corals is also reduced by the same factor, resulting in the
 177 multiplication of the $\exp(-\Omega_{MA} MA)$ and $A_{CH} (1 - \exp(-\Omega_{CH} CH/A_{CH}))$ in
 178 Eq. 4. In the eReefs biogeochemical model, the macroalgae is parameterised
 179 more like a filamentous epiphytic macroalgae rather than a leafy seaweed.
 180 Larger seaweeds, including *Halimeda* beds that are extensive in the north-
 181 ern GBR (McNeil et al., 2016), may exclude the corals (or seagrasses) via a
 182 different mechanisms than captured in Eq. 4, but are not represented in the
 183 model.

184 2.1.2 Growth rate of zooxanthellae cells

185 The model considers the diffusion-limited supply of dissolved inorganic nu-
 186 trients (N and P) and the absorption of light, delivering N, P and fixed C to
 187 the internal reserves of the cell (Fig. 1). Nitrogen and phosphorus are taken di-
 188 rectly into the reserves, but carbon is first fixed through photosynthesis (Kirk,

189 1994):

191 More on Eq. 5 is derived in Sec. 2.2.2. The internal reserves of C, N, and P
 192 are consumed to form structural material at the Redfield ratio (Redfield et al.,
 193 1963):

194 Note that while oxygen balances across the two equations, the oxygen re-
 195 leased from NO_3^- in Eq. 6 appears as a product in the photosynthesis equation
 196 (Eq. 5). Ignoring this small mismatch in time of oxygen production simplifies
 197 the model equations while maintaining oxygen conservation.

198 The growth rate of a microalgae cell is given by the maximum growth rate,
 199 μ^{max} , multiplied by the normalised reserves, R^* , of each of N, P and C:

$$200 \quad \mu = \mu^{max} R_N^* R_P^* R_C^* \quad (7)$$

201 Fig. 3 is a simple schematic showing the impact of growth alone on internal
 202 reserves for a population of two cells growing into exactly three cells, although
 203 the equations are continuous in time for a population. The mass of the re-
 204 serves (and therefore the total C:N:P:Chl *a* ratio) of the cell depends on the
 205 interaction of the supply and consumption rates. When consumption exceeds
 206 supply, and the supply rates are non-Redfield, the normalised internal reserves
 207 of the non-limiting nutrients approach 1 while the limiting nutrient becomes

208 depleted. Thus the model behaves like a 'Law of the Minimum' growth model,
 209 except during fast changes in nutrient supply rates.

210 The molar ratio of a cell is given by:

211
$$C : N : P = 106(1 + R_C^*) : 16(1 + R_N^*) : 1 + R_P^* \quad (8)$$

Fig. 3. 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 circle - pigment content. Here a full 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 through 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. (2004a). 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.

212 2.1.3 Uptake of nutrients and particulate matter from the overlying water

213 The maximum flux of nutrients and prey to the surface of the coral is speci-
 214 fied as a mass transfer limit per projected area of coral (Atkinson and Bilger,
 215 1992; Baird et al., 2004b), as given by (Falter et al., 2004; Zhang et al., 2011):

$$216 \quad S_x = 2850 \left(\frac{2\tau}{\rho} \right)^{0.38} Sc_x^{-0.6}, Sc_x = \frac{\nu}{D_x} \quad (9)$$

217 where S_x is the mass transfer rate coefficient of element $x = N, P$, τ is the
 218 shear stress on the bottom, ρ is the density of water and Sc_x is the Schmidt
 219 number. The Schmidt number is the ratio of the diffusivity of momentum, ν ,
 220 and mass, D_x , and varies with temperature, salinity and nutrient species. The
 221 mass transfer rate constant S_x can be thought of the height of water cleared
 222 of nutrient per unit of time by the water-coral exchange.

223 The capture of organic particles (phytoplankton, zooplankton, labile detri-
 224 tus) is also represented as an areal flux. Ribes and Atkinson (2007) considered
 225 whether mass transfer limits apply to particulate matter on reefs, and found
 226 for coral rubble communities only a weak velocity dependence, suggesting filter
 227 feeders overcame any diffusion limitations (see also Monismith et al. (2010)).
 228 Thus, instead of using a velocity-dependent mass transfer rate like was used
 229 for dissolved tracers (Eq. 9), capture of organic particles, G , is represented
 230 by a constant mass transfer rate coefficient, S_{part} , multiplied by the sum of
 231 the concentration of each of organic constituents in the water column. The
 232 calculated capture rate is limited to the maximum growth rate of the coral
 233 tissue, $\mu_{CH}^{max} CH$ (Table A.4).

234 The maximum fluxes of both nutrients and particulates from the overlying
 235 water are multiplied by the effective projected area fraction of the coral (A_{eff})

236 to account for corals covering only a fraction of the bottom.

237 2.1.4 Translocation between zooxanthellae and coral host

238 Translocation here represents the one-way consumption of zooxanthellae or-
239 ganic matter produced through either zooxanthellae growth or mortality.

240 A fraction, f_{tran} , of zooxanthellae growth is translocated to the coral tissue.
241 This fraction is given by the ratio of the projected area of the zooxanthellae
242 cells to twice the surface area of the coral polyp, $2CH\Omega_{CH}$:

$$243 \quad f_{tran} = \frac{\pi r_{CS}^2 CS / m_N}{2CH\Omega_{CH}} \quad (10)$$

244 where r_{CS} is the radius of the zooxanthellae cells. When $f_{tran} < 0.5$, zoox-
245 anthellae growth is primarily used for increasing symbiont population, and
246 for $f_{tran} > 0.5$, it is primarily translocated. The initial number of symbiont
247 cells is set so that $(\pi r_{CS}^2 CS / m_N) / (2CH\Omega_{CH})$ is less than 1. Under this initial
248 condition, as $(\pi r_{CS}^2 CS / m_N) / (2CH\Omega_{CH})$ approaches 1, all symbiont growth
249 is translocated, so f_{tran} never has a value above 1.

250 This translocation formulation represents a geometrically-derived space lim-
251 itation on zooxanthellae, being located within two layers of gastrodermal cells
252 (Gustafsson et al., 2013). The geometric derivation has avoided the need for
253 uncertain and/or poorly-defined mass-specific space limitation coefficients.

254 2.1.5 Coral polyp net production

255 Coral host biomass, CH , grows at a maximum rate, $\mu_{CH}^{max} CH$, conditional
256 on the availability of organic matter either taken up from the water column as
257 particulate organic matter by the host itself (Eq. 9), or through translocation

from zooxanthellae. It is assumed that the realised heterotrophic feeding rate of zooxanthellae, G' , is independent of the physiology of the coral host, and further, that the fraction of the zooxanthellae growth that is translocated depends only on the unavailability of space for the zooxanthellae population to reside in (see above).

$$G' = \min [\min [\mu_{CH}^{max} CH - f_{tran} \mu_{CS} CS - \zeta_{CS} CS, 0], G] \quad (11)$$

Should this rate of translocation, plus the flux of organic matter due to zooxanthellae mortality, exceed the maximum growth rate of coral host biomass, $\mu_{CH}^{max} CH$, then the coral host grows at its maximum rate, and the excess is released into the environment as mucus. Should the translocation rate and the particulate organic matter flux be less than $\mu_{CH}^{max} CH$, then the coral host grows at the sum of the two. Finally, should the sum of the translocation rate and the particulate organic matter flux be greater than $\mu_{CH}^{max} CH$, then the host will use all of the translocated organic matter, and a fraction of captured particulate organic matter, with the fraction being composed of fractions of each particulate components based on the relative concentration of organic matter in each category.

2.1.6 Non-bleaching mortality of coral polyps

There are two mortality terms: the mortality of the entire polyp (ζ_{CH}), affecting both coral and zooxanthellae biomass, and mortality of the zooxanthellae (ζ_{CS}). The polyp mortality term has a quadratic mortality coefficient, ζ_{CH} , that stabilises the biomass of coral tissue to μ_{CH}/ζ_{CH} . For a maximum growth rate of coral, $\mu_{CH}^{max} = 0.05 \text{ d}^{-1}$, ζ_{CH} has been set to $0.01 \text{ (g N m}^{-2}\text{)}^{-1} \text{ d}^{-1}$, so the biomass of coral tissue CH stabilises at $0.05 / 0.01 = 5 \text{ g N m}^{-2}$. As this

282 biomass is per unit area, and includes a correction for corals being only viable
283 on A_{eff} of the area, ζ_{CH} needs to be divided by A_{eff} in the equations.

284 The model does not consider coral host mortality due to thermal stress di-
285 rectly. The impact of zooxanthellae expulsion on the host is a reduced translo-
286 cation of organic matter from the symbiont to the host, reducing growth if
287 heterotrophic feeding is growth limiting.

288 2.2 Photoadaptation through pigment synthesis and the xanthophyll cycle

289 The model considers the photoacclimation or photoadaptation of the zoox-
290 anthellae cells through the processes of pigment synthesis and xanthophyll
291 pigment cycling (Fig. 4, left). The model assumes a constant ratio of xan-
292 thophyll pigments to chlorophyll, $\Theta_{chl2xan}$. This ratio is maintained constant
293 through time by assuming xanthophyll synthesis is $\Theta_{chl2xan}$ multiplied by the
294 chlorophyll synthesis. For simplicity we assume all synthesised xanthophyll is
295 of the photosynthesising form. Similarly, a constant ratio of synthesis of peri-
296 dinin, chlorophyll c_2 and β -carotene accessory pigments to chlorophyll a en-
297 sures these accessory pigments also maintain a constant ratio. The de-coupling
298 of zooxanthellae growth and pigment synthesis results in a variable carbon to
299 chlorophyll ratio through time.

300 The rate of synthesis of pigment is based on the incremental benefit of adding
301 pigment to the rate of photosynthesis. This calculation includes a reduced
302 benefit when carbon reserves are replete, $(1 - R_C^*)$, the reduced benefit due to
303 self-shading, χ , and the fraction of inhibited reaction centres, (Q_{in}/Q_T) . The
304 factor χ is calculated for the derivative of the absorption cross-section per unit
305 projected area, α/PA , with non-dimensional group $\rho = \gamma c_i r$. For a sphere of

Fig. 4. Schematic showing photosynthetic (Chl *a*, peridinin, β -carotene, Chl *c*₂, and the photosynthetic xanthophyll diadinoxanthin, *X_p*) and the photoprotective (xanthophyll diatoxanthin, *X_h*), xanthophyll cycling and reaction centre dynamics. Red arrows depict fluxes of photons / electrons. Black arrows show transformations of state of either reaction centres or xanthophyll cycle pigments. Note that energy (or photons) are conserved in this flow, significantly reducing the need for empirical rate constants.

radius r (Baird et al., 2013):

$$\frac{1}{PA} \frac{\partial \alpha}{\partial \rho} = \frac{1 - e^{-2\rho}(2\rho^2 + 2\rho + 1)}{\rho^3} = \chi \quad (12)$$

where χ represents the area-specific incremental rate of change of absorption with ρ . For the multi-spectral calculation used in this paper, we calculate the quantum-weighted mean of χ , $\bar{\chi}$.

The rate of chlorophyll synthesis is given by:

$$\frac{\partial c_i}{\partial t} = k_{\text{Chl}}^{\max} (1 - R_C^*) (1 - Q_{in}/Q_T) \bar{\chi} \quad \text{if } C : \text{Chl} > \theta_{min} \quad (13)$$

where $k_{\text{Chl}}^{\max}$ is the maximum rate of synthesis and θ_{min} is the minimum C:Chl ratio. Below θ_{min} , pigment synthesis is zero. Both self-shading, and the rate of photosynthesis itself, are based on photon absorption rather than energy ab-

316 sorption as experimentally shown in microalgae (Nielsen and Sakshaug, 1993).

317 2.2.1 Xanthophyll cycle

Fig. 5. Pigment-specific absorption coefficients for the dominant pigments found in *Symbiodinium* determined using laboratory standards in solvent in a 1 cm vial undertaken. Green lines are photosynthetic pigments, red lines are photoprotective 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. 18), with the weighting calculated from the ratio of each pigment concentration to chlorophyll *a*. Black crosses represent the chl *a*-specific absorption coefficient of all pigments at the wavelengths used in the simulations. 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*, chlorophyll *c*₂ and β -carotene; 1.361 for ethanol used with peridinin, diadinoxanthin and diatoxanthin; 1.330 for water). The integral from 340 to 700 nm of the chl *a*-specific absorption coefficient using the 23 model wavelengths is only 0.72 % greater than using the 563 measured wavelengths. Thus for white light incident on cells with a zero package effect, 23 wavelengths is sufficient to compute the spectrally-resolved absorption. For highly packaged cells, the absorption cross-section is flattened (Kirk, 1994), so the error will be even less than 0.72 %.

318 The symbiont cell contains six pigments, chlorophyll *a*, chlorophyll *c*₂, peri-

319 dinin, β -carotene and diadinoxanthin that absorb light and pass the pho-
 320 tons on through the photosystem; and diatoxanthin, that absorbs light and
 321 dissipates it as heat. Diadinoxanthin and diatoxanthin are almost identical
 322 molecules. Diatoxanthin is the de-epoxidised form of diadinoxanthin. The xan-
 323 thophyll cycle (Falkowski and Raven, 2007) is the reversible switching of di-
 324 adinoxanthin to diatoxanthin under potentially damaging excess light, and
 325 vice-versa under light-limiting conditions. The xanthophyll cycle in the model
 326 is represented by two state variables, the areal concentration of diadinoxan-
 327 thin (X_p) and of diatoxanthin (X_h), and requires one new parameter, τ_{xan} , the
 328 time-scale of switching.

329 The rate at which the xanthophyll pigments switch from diadinoxanthin to
 330 diatoxanthin (or vice versa) is assumed to be relatively fast when compared
 331 to the synthesis of pigments. The reversible processes is given by:

$$332 \quad \frac{\partial X_p}{\partial t} = -8(Q_{in}/Q_T - 0.5)^3 \tau_{xan} \Phi(X_p + X_h) = -\frac{\partial X_h}{\partial t} \quad (14)$$

333 where the time scale, $1/\tau_{xan}$, is order of 10 minutes (Gustafsson et al., 2014).
 334 The direction of switching in Eq. 14 is set by the term $(Q_{in}/Q_T - 0.5)^3$, such
 335 that cells with a large fraction of inhibited reaction centres ($Q_{in}/Q_T > 0.5$)
 336 switch from diadinoxanthin (X_p) to diatoxanthin (X_h), and a small fraction of
 337 oxidised reaction centres vice versa. The term $8(Q_{in}/Q_T - 0.5)^3$ also increases
 338 cubically from zero to 1 (for $Q_{in}/Q_T > 0.5$) or decreases from zero to -1 (for
 339 $Q_{in}/Q_T < 0.5$) as the cell becomes more or less inhibited respectively. Using
 340 a cubic power that takes a small value in the vicinity of 0.5 prevents fast
 341 switching between diadinoxanthin (X_p) and diatoxanthin (X_h) in the region
 342 of 0.5. The constant 8 arises from $8 \times 0.5^3 = 1$, where 3 is the cubic power. A
 343 odd power is necessary to retain the direction of switching.

344 The final bracketed term, $(X_p + X_h)$, recognises that the switching is quanti-
 345 fied for the population of cells, and so is proportional to the total xanthophyll
 346 pigment concentration of the population.

347 Finally, the rate of conversion slows as one pigment pool is reduced to zero, as
 348 determined by a parabolic term Φ (Eq. 15). If $Q_{in}/Q_T < 0.5$ and $X_h > X_p$ (i.e.
 349 uninhibited reaction centres with more heat dissipating than light absorbing
 350 pigment) or $Q_{in}/Q_T > 0.5$ and $X_p > X_h$ (i.e. inhibited reaction centres with
 351 more light absorbing than heat dissipating pigment) then $\Phi = 1$, and the rate
 352 of switching is independent of the present mix of heat and light absorbing
 353 pigment. Otherwise, a parabolic form for Φ is used to reduce the rate of
 354 switching as the processes completes:

$$355 \quad \Phi = 1 - 4 \left(\frac{X_p}{X_p + X_h} - 0.5 \right)^2 \quad (15)$$

356 The parabola is at a maximum at $X_p = X_h$, but decreases by the square
 357 of the difference between the fraction of diadinoxanthin (X_p) and 0.5. The
 358 square ensures that the fractional term does not change the overall sign of the
 359 switching, which, as already mentioned, is set by the reaction centre status
 360 (i.e. $8(Q_{in}/Q_T - 0.5)^3$). The value of the parabolic term is zero at $X_p =$
 361 X_h . At $X_p \gg X_h$, or $X_p \ll X_h$, the parabolic term is equal to 0.25. The
 362 parabolic term is multiplied by 4 so that when switching is complete, $\phi =$
 363 $1 - 1 = 0$, thus preventing X_p or X_h either exceeding $X_p + X_h$, or becoming
 364 negative. In summary the full switching term (Eq. 14) results in the relatively
 365 quick switching of the xanthophyll pigments between light absorbing and heat
 366 dissipating based on the oxidation status of the reaction centres.

367 The processes of light absorption by diadinoxanthin, chlorophyll *a*, chloro-
 368 phyll *c*₂, peridinin and β -carotene is called photochemical quenching (PQ),

369 while light absorbed and dissipated by diatoxanthin (X_h) is called non-photochemical
 370 quenching (NPQ). A common measure of PQ is $(1-F_v/F_m)$ (Raven, 1997),
 371 where F_v is the difference between maximum fluorescence, F_m , and mini-
 372 mum fluorescence (i.e. variable fluorescence). F_v/F_m is a measurable ratio
 373 that represents the maximum potential quantum efficiency of Photosystem II
 374 if all capable reaction centres are open, which is equivalent in this model to
 375 Q_{ox}/Q_T .

376 2.2.2 Carbon fixation / respiration

377 When photons are captured by oxidised reaction centres (photosynthesis)
 378 there an increase in the cellular reserves of carbon, R_C , and an accompanying
 379 uptake of dissolved inorganic carbon, $\frac{106}{1060}12k_I(Q_{ox}/Q_T)a_{Q_{ox}}^*(1-R_C^*)$, and
 380 release of oxygen per cell, $\frac{138}{1060}32k_I(Q_{ox}/Q_T)a_{Q_{ox}}^*(1-R_C^*)$, to the water column
 381 (Table A.3). While the reserves of nutrients have been defined generically
 382 above (a quantity of N, P taken up but not yet combined at the Redfield
 383 ratio), the reserves of carbon are a generic photosynthate - they represent the
 384 point at which a photon has been absorbed AND its energy used to produce
 385 fixed carbon and release oxygen.

386 Basal respiration represents a constant cost of cell maintenance. The loss
 387 of internal reserves, $\mu_{CS}^{\max}m_C\phi R_C^*$, results in a gain of water column dissolved
 388 inorganic carbon per cell, $\frac{106}{1060}\frac{12}{14}\mu_{CS}^{\max}\phi R_C^*$, as well as a loss in water column
 389 dissolved oxygen per cell, $\frac{138}{1060}\frac{32}{14}\mu_{CS}^{\max}\phi R_C^*$ (Table A.3). The loss in water col-
 390 umn dissolved oxygen per cell represents an instantaneous respiration of the
 391 fixed carbon of the reserves. Basal respiration decreases internal reserves, and
 392 therefore growth rate, but does not directly lead to cell mortality at zero car-
 393 bon 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 below.

2.3 *Photosynthesis, reaction centre dynamics and reactive oxygen production*

To model the processes of photoinhibition we include a submodel of reaction centre dynamics that captures the fate of photons absorbed by the cell as a changing oxidation state of the reaction centre of photosystem II (PSII). The model contains state variables for the concentration of oxidised reaction centre, Q_{ox} , reduced reaction centre concentration, Q_{red} , and inhibited reaction centre concentration, Q_{in} , as well as the concentration of reactive oxygen species, [ROS] (Fig. 4). The reaction centre dynamics is based on stoichiometric relationships between reaction centre numbers, photons absorbed and the rate of generation of reactive oxygen species.

To follow the path of a photon as it moves through the reaction centres (Fig. 4), photons are absorbed by either a photosynthetic pigment, or a heat dissipating pigment, in the ratio of the concentration of the two pigment types. If the photon is absorbed by a heat dissipating pigment it is lost. If the photon is absorbed by a photosynthetic pigment, then it will result in a change in either the internal reserves of carbon, the reaction centre state, or the concentration of reactive oxygen species. Like absorption by pigments, the photons interact with the reaction centres as a proportion of the total number of reaction centres. If the photon encounters an oxidised reaction centre, the reserves are depleted and the Rubisco enzyme active, then the only change will be an increase in carbon reserves (i.e. carbon fixation). If the photon encounters an oxidised reaction centre, but fixation is inhibited, then an oxidised reaction

centre becomes reduced. If the photon hits a reduced reaction centre, then a reduced reaction centre becomes inhibited. The final alternative, if the photon interactions with an inhibited reaction centre, then the reaction centre remains inhibited, and a reactive oxygen species is generated, adding to the reactive oxygen pool. The following sections derives rates for these pathways.

2.3.1 Light absorption and photoinhibition

The total rate of photon absorption due to photosynthetic pigments (chlorophyll a , chlorophyll c_2 , peridinin, β -carotene and diadinoxanthin) across all wavelengths, λ , is given by:

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int \alpha_\lambda E_{d,\lambda} \lambda d\lambda \quad (16)$$

where h , c and A_V are fundamental constants (Table A.7). The absorption-cross section (α) of a spherical cell of radius (r), with a wavelength-dependent pigment-specific absorption coefficient of chlorophyll and accessory pigments (γ_{chl+}) and diadinoxanthin (γ_{dia}), and homogeneous intracellular pigment concentration (c_i and x_p respectively), can be calculated using geometric optics (i.e. ray tracing) without considering internal scattering, and is given by (Dy-sens, 1956; Kirk, 1975):

$$\alpha = \pi r^2 \left(1 - \frac{2(1 - (1 + 2(\gamma_{chl+}c_i + \gamma_{dia}x_p)r)e^{-2(\gamma_{chl+}c_i + \gamma_{dia}x_p)r})}{(2(\gamma_{chl+}c_i + \gamma_{dia}x_p)r)^2} \right) \quad (17)$$

where πr^2 is the projected area of the spherical zooxanthellae, and the bracketed term is 0 for no absorption ($(\gamma_{chl+}c_i + \gamma_{dia}x_p)r = 0$) and approaches 1 as the cell becomes fully opaque ($(\gamma_{chl+}c_i + \gamma_{dia}x_p)r \rightarrow \infty$). The pigment-specific absorption coefficient of chlorophyll and accessory pigments (γ_{chl+} , Fig. 5 black

line) is given by:

$$\gamma_{chl+} = \gamma_{chl_a} + \Theta_{chla2chlc} \gamma_{chlc} + \Theta_{chla2per} \gamma_{per} + \Theta_{chla2caro} \gamma_{car} \quad (18)$$

The component of light absorbed by oxidised reaction centres, and therefore available for carbon fixation, is:

$$k_{I,fix} = k_I \left(\frac{Q_{ox}}{Q_T} \right) a_{Q_{ox}}^* (1 - R_C^*) \quad (19)$$

where the oxidised fraction of reaction centres is (Q_{ox}/Q_T) and the fixation rate can be limited by the carbon reserves ($1 - R_C^*$). If the carbon reserves are full (R_C^* approaches 1) then fixation does not consume photons.

Carbon fixation is also reduced by the temperature inhibition of the active component of the reaction centres. This is the key term in coral bleaching. The mechanism through which this occurs is understood to be the inactivation of the Ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO, Lilley et al. (2010)). Field observations show bleaching occurs relative to the climatological value for each reef site (Liu et al., 2014), suggesting a mechanism for corals to adapt to local conditions. For practical purposes, we propose the following equation for the temperature-dependent inhibition of carbon fixation:

$$a_{Q_{ox}}^* = (1 - \exp(-(2 - \Delta T))) / (1 - \exp(-2)) \quad (20)$$

where ΔT is the temperature anomaly and is calculated as the difference between the model bottom temperature and the spatially and temporally-varying climatological temperature at that depth (Ridgway and Dunn, 2003). The form of Eq. 20 was based on a general line of reasoning that bleaching stress begins at a temperature anomaly of 1°C (the NOAA bleaching index uses 1°C above climatology that would reduce $a_{Q_{ox}}^*$ in Eq. 20 to 0.73), and

463 that for a sustained period (2 summer months) 2°C (equivalent to 16 degree
 464 heating weeks) causes maximal stress ($a_{Q_{ox}}^* = 0$). If the climatological tem-
 465 perature is below 26°C , then ΔT is given by the model bottom temperature
 466 minus 26°C . The constant 2°C represents the temperature anomaly above
 467 which activity of oxidised reaction centres is zero. For $\Delta T < 0^\circ\text{C}$, $a_{Q_{ox}}^* = 1$,
 468 and all oxidised reaction centres are active, and $\Delta T > 2^\circ\text{C}$, $a_{Q_{ox}}^* = 0$, and all
 469 oxidised reaction centres are inactive. Both the constant 2°C , and the use of
 470 a seasonally-varying seabed climatological temperature which is based on all
 471 available, but nonetheless limited, number of *in situ* observations and inter-
 472 polated onto a coarse 0.5° grid, are key uncertainties worth consideration in
 473 future work.

474 The component of total absorption that is absorbed by oxidised reaction
 475 centres but not used in fixation and therefore responsible for moving reaction
 476 centres from an oxidised to reduced state is the remaining light absorbed at
 477 the oxidised centres:

$$478 \quad k_{I,unfix} = k_I \left(\frac{Q_{ox}}{Q_T} \right) - k_{I,fix} \quad (21)$$

479 Photons are absorbed by the reaction centres in each of the three oxidation
 480 states in proportion to the fraction in each state, independent of the carbon
 481 reserves. Absorption of a photon by an oxidised state is discussed above. Ab-
 482 sorption by a reduced state moves it to an inhibited state. Absorption by an
 483 inhibited state does not change the state but produces ROS (see below):

$$\frac{\partial Q_{ox}}{\partial t} = -k_{In} m_{RCH} \frac{Q_{ox}}{Q_T} (1 - a_{Q_{ox}}^* (1 - R_C^*)) \quad (22)$$

$$\frac{\partial Q_{red}}{\partial t} = k_{In} m_{RCH} \frac{Q_{ox}}{Q_T} (1 - a_{Q_{ox}}^* (1 - R_C^*)) - k_{In} m_{RCH} \frac{Q_{red}}{Q_T} \quad (23)$$

$$\frac{\partial Q_{\text{in}}}{\partial t} = k_I n m_{\text{RCII}} \frac{Q_{\text{red}}}{Q_{\text{T}}} \quad (24)$$

where k_I is the rate of photon absorption (Eq. 16), n is the number of zooxanthellae cells and m_{RCII} is a stoichiometric coefficient, and is one over the number of photons needed to reduce a whole reaction centre (Table A.8).

The reaction centre turn-over time is shorter than the chlorophyll synthesis or carbon fixation terms. To illustrate this point, Suggett et al. (2008) gives the cross-sectional area of an individual reaction centre as $385 \times 10^{-20} \text{ m}^2$. Thus for a photon flux of $250 \text{ mol photon m}^{-2} \text{ d}^{-1}$, a relatively low light level for midday, the time-interval between individual photon interceptions is $385 \times 10^{-20} / (250 / A_V) \times (1/86400) \approx 0.1 \text{ s}$. As this turnover is much quicker than other processes represented in the photosystem model, it has the potential to slow the model integration. A solution is to divide the terms in Eqs. 23 - 25 by 10^6 . This results in reaction centre dynamics varying on an hourly, rather than second, time-scale. The slower response of the reaction centres has only small feedbacks to other terms in the photosystem model, and maintains conservation of reaction centre numbers in the calculation.

2.3.2 Production of reactive oxygen

Photons absorbed by inhibited reaction centres generate reactive oxygen species, [ROS]:

$$\frac{\partial [\text{ROS}]}{\partial t} = 32 \frac{138}{106} \frac{1}{10} k_I n m_{\text{RCII}} \left(\frac{Q_{\text{in}}}{Q_{\text{T}}} \right) \quad (25)$$

where the stoichiometric conversions are $32 \text{ g O mol O}_2^{-1}$, $\frac{138}{106} \text{ mol O mol C}^{-1}$ $\frac{1}{10} \text{ mol C mol photon}^{-1}$. Reactive oxygen species are not considered part of

the oxygen mass balance, as it is assumed to be sourced and returned to the mass of water (H₂O).

2.3.3 Repair rate of inhibited reaction centres

The repair rate of inhibited reactions centres is difficult to quantify, and may be a function of temperature (Hill et al., 2011). We took the assumption that the reaction centres would need to be able to repair damaged caused by 10 mol photon m⁻² d⁻¹. This relatively low daily averaged light intensity represents a threshold below which surface-adapted coral species show an impact due to low light, and might therefore be a reasonable minimum repair rate. As discussed later, this is one of the most uncertain components of the model.

To repair damaged caused by 10 mol photon m⁻² d⁻¹,

$$\frac{\partial Q_{\text{in}}}{\partial t} = -268 m_{RCH} Q_{\text{in}} = -\frac{\partial Q_{\text{ox}}}{\partial t} \quad (26)$$

where m_{RCH} is a stoichiometric coefficient [mol photon (mol reaction centre)⁻¹], and the constant 268 arises from the 10 mol photon m⁻² d⁻¹ limit.

2.3.4 Rate of detoxification of reactive oxygen species

Reactive oxygen species are reduced through a temperature-dependent processes (Hill et al., 2011):

$$\frac{\partial [\text{ROS}]}{\partial t} = -f(T) R_N^* R_P^* R_C^* [\text{ROS}] \quad (27)$$

where $f(T)$ is a function of temperature, and here is set at the maximum growth rate of the zooxanthellae cells. This particularly uncertain assumption results in the cells detoxifying at the same rate as they grow. The logic for

526 this term is as simple as a healthier symbiont is one that grows faster, and
 527 coincidentally, would have more resources for detoxification.

528 2.4 *Zooxanthellae expulsion*

529 The rate of expulsion of zooxanthellae cells is function of the reactive oxygen
 530 concentration, [ROS]:

$$531 \quad \frac{\partial CS}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{threshold}]}{m_O} \right] CS \quad (28)$$

532 where γ is the maximum expulsion rate, $m_O = (138/16)(32/14)m_N$ is the
 533 stoichiometric coefficient for the oxygen content of the structural component
 534 a cell, and $[\text{ROS}_{threshold}]$ is the limit below which no bleaching occurs. A similar
 535 rate of loss is applied to Q_{ox} , Q_{red} , Q_{in} , C , X_p , X_h , R_C , R_N , R_P and [ROS].
 536 Expulsion leads to an increase in detritus at the Redfield ratio, D_{Red} , in the
 537 bottom water column layer from the zooxanthellae structural material, and
 538 an increased in dissolved nutrients (carbon, DIC , nitrogen in the form of
 539 ammonia $[NH_4]$, and phosphorus, P) due to the loss of reserves (Table A.6).

540 2.5 *Description of the eReefs coupled hydrodynamic - biogeochemical model*

541 The eReefs model (Fig. 6) configuration used simulates the circulation, op-
 542 tics, biogeochemistry and sediment dynamics from December 1, 2014 - present.
 543 More details on the model grid and hydrodynamic configuration are given in
 544 Herzfeld and Gillibrand (2015) and Herzfeld (2015). The sediment (Margve-
 545 lashvili et al., 2016), optical (Baird et al., 2016b) and biogeochemical (Mongin
 546 et al., 2016) models are similarly described in detail, with a further 600+ pages

documenting model configuration and skill assessment (Herzfeld et al., 2016;
Skerratt et al., submitted).

Fig. 6. Schematic showing the eReefs coupled hydrodynamic, sediment, optical, biogeochemical model. Orange labels represent components that either scatter or absorb light, thus influencing seabed light levels.

GBR-wide configuration. The eReefs coupled hydrodynamic, optical, sediment and biogeochemical model has been configured at ~ 1 km resolution for the northeast Australian continental shelf, from $28^{\circ}40'S$ to the Papua New Guinea coastline. The model's curvilinear grid has 2389 cells in the alongshore direction, 510 in the offshore direction, and 44 depth levels. The hydrodynamic model is run with a 1.2 s barotropic time step, and the current fields used to calculate mass conserving fluxes of sediment and biogeochemical constituents (Gillibrand and Herzfeld, 2016). The sediment and biological processes are integrated using a 1 hour timestep.

A 5th-order Dormand-Prince ordinary differential equation integrator (Dormand and Prince, 1980) with adaptive step control is used to integrate the

560 local rates of changes due to ecological processes. This requires 7 function
561 evaluations for the first step and 6 for each step after. A tolerance of 1×10^{-5}
562 mg N m^{-3} is required for the integration step to be accepted. The mass of
563 carbon, nitrogen, phosphorus and oxygen are checked at each model timestep
564 to ensure conservation.

565 The model is forced using atmospheric conditions from the Bureau of Me-
566 teorology ACCESS-R and OceanMaps atmospheric and ocean products, and
567 concentrations of dissolved and particulate constituents from 21 rivers along
568 the Queensland coast (north to south: Normanby, Daintree, Barron, combined
569 Mulgrave+Russell, Johnstone, Tully, Herbert, Haughton, Burdekin, Don, O’Connell,
570 Pioneer, Fitzroy, Burnett, Mary, Calliope, Boyne, Caboolture, Pine, combined
571 Brisbane+Bremer, and combined Logan+Albert) and the Fly River in Papua
572 New Guinea. River concentrations of sediment and nutrient were based on
573 mean values from observations over a 10 year period (Furnas, 2003). Sepa-
574 rate means were obtained for wet- (the Fly, and the northern most 6 rivers in
575 Queensland) and dry- (remainder) catchment rivers, and multiplied by gauged
576 flows to obtain river loads. The model uses a novel river boundary condition
577 (Herzfeld, 2015) that discharges the river freshwater load in a brackish surface
578 plume whose salinity and thickness is calculated to account for upstream flow
579 in the salt wedge and in-estuary mixing between density layers. The coral dis-
580 tribution in the model is a combination of the eAtlas features map, or, where
581 available, a satellite-derived coral zonation (Roelfsema et al., 2018).

582 *Davies Reef configuration.* The ~ 200 m model of Davies Reef off Townsville
583 (centred on $18^{\circ}49'S$, $147^{\circ}38'E$, Andrews and Gentien (1982)) was built using
584 the eReefs Project RECOM automatic nesting capability (<https://research.csiro.au/ereefs/mo>)
585 The model bathymetry was interpolated from the GBR100 bathymetry (Bea-

man, 2010) version 4 with improved resolution of reef tops. Atmospheric forcing was the same as the 1 km model above. The initial conditions of water column state variables are interpolated from a previous run of the 1 km model (GBR1_H2p0_B1p9_Chhd_Dhnd), while some benthic variables (seagrass and coral distributions) have distributions re-interpolated from the high resolution benthic maps, and assigned values from the nearest neighbour in the initialising model.

The ~ 200 m nested model uses boundary conditions provided by a standard eReefs 1 km model simulation (GBR1_H2p0_B1p9_Chhd_Dhnd) that did not include coral bleaching. Thus the model that generated the boundary conditions for the nested model is slightly different to the 1 km configuration described above, but the water column properties that are advected into the nested model, which depend primarily on nutrient / plankton processes in the water column, will be very similar. The boundary condition for all water column tracers was formulated using the advection scheme (Van Leer, 1977) used within the model domain itself. This consistency of boundary and advection schemes ensures diffusion and dispersion errors are minimised.

3 Results

The coral bleaching model presented in this paper details new formulations for the processes of zooxanthellae growth as a function of the interaction of nutrient and light uptake; photoadaptation through the pigment synthesis and xanthophyll cycling; photoinhibition through reaction centre dynamics; and zooxanthellae expulsion through a build-up of reactive oxygen species. Here we describe the model behaviour in a ~ 1 km configuration along the entire

610 Great Barrier Reef during a mass bleaching event in early 2016; in a ~ 200 m
611 nested model of Davies Reef; and finally, at the scale of one polyp through
612 analysing a time-series at two depths in the Davies Reef model.

613 3.1 *GBR-scale behaviour of the zooxanthellae model*

614 The 2016 bleaching event was the most severe experienced by the Great
615 Barrier Reef, with the greatest bleaching occurring in the far north (Hughes
616 et al., 2017). This extreme event provides a good test of the model. On January
617 1, the simulated water temperature at the coral surface was only just above
618 the summer monthly maximum, as shown by the simulated RuBisCO activity
619 being close to 1 (i.e. not inhibited by thermal stress) (Fig. 7, left). By February
620 1 the temperature relative to climatology had increased significantly, and did
621 not reduce until after April 1.

622 The response in concentration of reactive oxygen on January 1 (Fig. 8) shows
623 zooxanthellae on some shallow reefs had relatively high levels of oxidative
624 stress. By February 1, most of the reefs north of Hinchinbook Island shows
625 high levels of reactive oxygen, although interestingly this reduced somewhat
626 by March 1. The model predicted reactive oxygen stress has a similar spatial
627 distribution as the observed bleaching from aerial surveys (Fig. 8, bottom
628 left) with the exception that the model bathymetry is too deep at most of the
629 offshore reefs to accumulate oxidative stress. While these results are promising,
630 they illustrate that for the purposes of predicting coral bleaching, the ~ 1 km
631 model suffers from poor resolution of many of the outer-reef reef tops.

Fig. 7. Activity of the RuBisCO enzyme, $a_{Q_{ox}}^*$ (Eq. 20), from left to right, at midday on the 1st of January, February, March and April of 2016 based on simulated seabed temperature. A value of $a_{Q_{ox}}^* = 1$ allows full use of photons absorbed by oxidised reaction centres to fix carbon, thereby quenching photons and filling carbon reserves (Fig. 4). For a value of zero, a result of being greater than 2°C above the climatology, all photons move oxidised and / or reduced reaction centres towards the inhibited state.

632 3.2 Individual (Davies) reef scale behaviour

633 Davies Reef is a 4 km x 2 km kidney-shaped reef located off Townsville
 634 (Fig. 9). In the ~ 1 km model described above Davies consists of approxi-
 635 mately 8 grid cells with a minimum depth of 15 m below mean sea level. In
 636 the ~ 200 m nested model, which can resolve reef tops far better, the mini-
 637 mum depth is 3.8 m. This allows for a much greater spatial variation in light
 638 at the seabed (Fig. 9, photosynthetically available radiation, PAR). Other en-
 639 vironmental variables such as temperature, DIN, DIP, and particulate organic
 640 matter (POM) also show variation across the reef as the fast-moving overlying

Fig. 8. Snapshots of reactive oxygen accumulation per zooxanthellae cell in the 1 km eReefs model, from left to right, on the 1st of January, February, March and April of 2016, and compared to the aerial bleaching surveys conducted in March-April 2016 (left, Hughes et al. (2017)). The background water colour is the model output simulated true colour (Baird et al., 2016b), and can be used as an indicator of water clarity between reefs on the day. Reefs ($\sim 1 \text{ km}^2$ in the model) are coloured white if deeper than 20 m, to indicate they are too deep to bleach in the model; grey if they are sufficiently shallow to potentially bleach, but have reactive oxygen concentrations below $[\text{ROS}_{\text{threshold}}]$, and yellow through to red to indicate increasing reactive oxygen stress. The ARC Centre of Excellence National Bleaching Taskforce bleach index scales from 0 ($< 1\%$ of colonies bleached), 1 (1-10%), 2 (10-30%), 3 (30-60%) and 4 (60-100%). Two thin black lines show the extent of the Bleaching Survey on the model domain. The reactive oxygen concentration per zooxanthella and bleaching index can be qualitatively compared, but a quantitative comparison would rely on uncertain components of the model.

641 waters are altered by fluxes with the benthos.

642 Focusing on the diurnal change, at 6 am, all xanthophyll pigments are photoabsorbing, and the reaction centres are primarily oxidised (Fig. 9). The
 643
 644 nitrogen assimilation by corals is dominated by organic nitrogen uptake (i.e.
 645 heterotrophic feeding), which in the model is only allowed in dark conditions.
 646 By 3 pm, most xanthophyll pigments have switched to heat dissipating, with
 647 the exception of those below 20 m that remain photoabsorbing. The reaction

648 centres in shallow waters have become strongly inhibited, although again at
649 depth remain primarily oxidised. Interestingly, the reserves of C, N, and P, as
650 well as the reactive oxygen concentration, remain relatively constant through
651 the day. This is because the growth of zooxanthellae is relatively slow, so the
652 reserves are not being depleted quickly.

653 As the reactive oxygen concentration is relatively constant, the bleaching
654 rate is only moderately stronger during the day. Bleaching is occurring only
655 in waters less than 10 m. The temperature-mediated inactivity of RuBisCO,
656 $a_{Q_{ox}}$, is more evenly spread across the reef - thus the reduced bleaching below
657 10 m is due to lower light levels rather than less thermal stress.

Fig. 9. Coral-related state variables at Davies Reef. Variables that are shown only on the reef are seabed values (i.e. PAR is downwelling light just above the coral surface), while DIN, Age, DIP, and POM are near surface fields with off reef values shown. The * refers to a normalised value, such that reserves of C, N, and P are values between 0 (deplete) and 1 (replete), while the sum of normalised xanthophyll pigments ($X_h^* + X_p^*$) and normalised reaction centres ($Q_{ox}^* + Q_{red}^* + Q_{in}^*$) is 1. The white circle and black cross in the depth panel identify the location of the shallow (3.8 m) and deep (18.0 m) time-series sites in Fig. 11.

Fig. 10. Coral-related state variables at 3 pm on 22 March 2016 in the ~ 200 m nested model at Davies Reef. For more information see Fig. 9.

658 3.3 Polyp-scale behaviour of the zooxanthellae model

659 Analysis of time-series at two depths in the Davies Reef nested configuration
660 can be used to further investigate the behaviour of the coral bleaching model.
661 We have chosen two adjacent sites, one shallow and one deep (Fig. 9, depth
662 panel). Here we are looking at the physiological response of the zooxanthellae
663 photosystem to different light levels under thermal stress (Fig. 11).

664 3.3.1 Zooxanthellae growth limitation

665 Zooxanthellae growth is a function of the maximum growth rate, and the
666 reserves of nitrogen, phosphorus and carbon. Each normalised reserve, R^* ,
667 is a value between zero and one. The normalised reserved increases when the
668 supply of the nutrient exceeds the consumption for growth, and decreases when
669 consumption for growth exceeds the nutrient supply (Baird et al., 2003). In
670 coral reef environments, nutrients are generally strongly limiting in the surface
671 waters, and less so at depth. One exception to this generality is if RuBisCO
672 becomes inactive at high temperatures, and then absorption does not add to
673 carbon reserves and growth can become limited by fixed carbon.

674 At the shallow site (Fig. 11A) carbon reserves are high (~ 0.7), phosphorus
675 reserves intermediate (~ 0.6), and nitrogen reserves low (< 0.1). Thus growth
676 is strongly N limited. High carbon reserves can be maintained in part because
677 RuBisCO is moderately active ($a_{Q_{ox}}^* \sim 0.5$, Fig. 11B), although on the 3rd
678 March the carbon reserves can be seen to drop when RuBisCO became inactive
679 for 24 hours (Fig. 11B). At the deep site (Fig. 11D), we see that the carbon
680 reserves are also high and the zooxanthellae are still nitrogen limited. This is
681 possible because of the clear water (bottom light is only halved from the 3.8

682 m site), and because of photoacclimation described in next section.

683 3.3.2 *Zooxanthellae photoacclimation*

684 Photoacclimation occurs through changing rates of pigment synthesis and
685 xanthophyll pigment switching.

686 *Pigment synthesis.* At the shallow site, the cells adjust to high light by reduc-
687 ing pigment synthesis resulting in a high C:Chl ratio of ~ 100 g/g (Fig. 11B).
688 A high C:Chl ratio is a low cellular chlorophyll concentration. At the deep
689 site, the C:Chl is reduced to ~ 40 g/g as chlorophyll synthesis is greater to
690 capture a higher percentage of the photons that are hitting the cells.

691 *Xanthophyll cycle.* At the shallow site the reaction centres are inactive during
692 the day, with recovery over night (Fig. 11C). As a result, the xanthophyll cycle
693 is primarily in the heat dissipating state during the day, and light absorbing in
694 the early morning. In contrast at the deeper site (Fig. 11F), a greater fraction
695 of the reaction centres are oxidised, and therefore the xanthophyll pigments
696 are all in the photosynthesising state. The photoacclimation processes are able
697 to keep the carbon reserves to a relatively similar level at the two sites despite
698 light levels varying from 8 to 80 mol photon $\text{m}^{-2} \text{d}^{-1}$. This is in part due to
699 impact of nitrogen limitation on the other reserves.

700 3.3.3 *Reactive oxygen accumulation and bleaching.*

701 The rate of ROS build up depends on both the fraction of inhibited reaction
702 centres, and the flux of photons to the reaction centres. Thus at the deep
703 site the reactive oxygen concentration is low, and the bleaching rate is zero
704 (Fig. 11F). In contrast, at the shallow site there was a substantial fraction

705 of inactive reaction centres (Fig. 11C), and a large photon flux, so reactive
706 oxygen concentration builds up. At the shallow site in early March, when Ru-
707 BisCO became totally inactive, more photons hit inactive reaction centres, and
708 there was an even greater accumulation of ROS, leading to more zooxanthellae
709 expulsion (Fig. 11C).

710 4 Discussion

711 In this paper we have introduced new formulations of coral host-symbiont
712 interactions, photoadaptation, xanthophyll cycling and reactive oxygen dy-
713 namics. Outputs of a simulation at the GBR-wide scale show promise for
714 predicting mass bleaching events, and the behaviour at the scale of the Davies
715 Reef appear reasonable. At this point in the model development, components
716 of the model derivation are uncertain, and the laboratory and field data sets
717 to assess the model outputs are still emerging. Nonetheless, this represents
718 the first application of a sophisticated coral bleaching model applied across a
719 entire shelf system.

720 4.1 Model formulation

721 The coral-symbiont model presented here is derived from process representa-
722 tions that take advantage, where possible, of geometric or physical constraints.
723 The geometric descriptions used include: (1) a relationship between polyp
724 biomass and coral cover derived from a random-placement geometric model
725 (Eq. 2); (2) the limiting term for zooxanthellae self-shading based on the
726 derivative of the absorption cross-section against absorption of the pigments

(Eq. 12); (3) the uptake of dissolved nutrients through a diffusive boundary layer (Eq. 9); and (4) the space-limitation of zooxanthellae using zooxanthellae projected areas in a two layer gastrodermal cell anatomy (Eq. 10). One advantage of this geometric approach is that it often requires fewer and better constrained parameters than more empirical process descriptions. This approach has proven successful in other marine biogeochemical applications (Baird et al., 2004a; Wild-Allen et al., 2013), and is fundamental to the formulation of the eReefs biogeochemical model (Baird et al., 2016b).

The mathematical formulations also take advantage of stoichiometric relationships between reaction centre numbers, photons absorbed and the concentration of reactive oxygen species created. It is a unique characteristic of the eReefs biogeochemical water column optical model (Baird et al., 2016b) that the processes of absorption by photoautotrophs are photon conserving, such that the photosynthetic growth processes in phytoplankton and benthic plants are a function of stoichiometric combination of photons and nitrogen and phosphorus (Baird et al., 2001). This approach is also applied in zooxanthellae, with the absorption coefficient of the multiple pigments determining the number of photons absorbed, and then this quantity reduces reaction centres, or accumulates carbon or reactive oxygen, in stoichiometrically determined ratios. By using these constraints the model is able to resolve reaction centre state (Fig. 4), and include the processes of photoinhibition and reactive oxygen generation, with the inclusion of just a few new model parameters, such as the stoichiometric ratio of RCII units to photons, m_{RCII} , and a few temperature-dependent reaction rates.

We openly recognise that we do not have the knowledge to follow all processes mechanistically. Thus, the inactivation of the RuBisCO-mediated carbon fix-

753 ation (Eq. 20), the repair rate of inhibited reaction centres (Eq. 26), and
754 the detoxification rate of reactive oxygen species (Eq. 27) are temperature-
755 dependent empirical formulations, for which the underlying biochemical reac-
756 tions are not resolved. Additionally, the reactive oxygen concentration that
757 initiates bleaching, $ROS_{threshold}$, and the mathematical form of the expul-
758 sion above this threshold (Eq. 28), are based on simple reasoning. Emerging
759 laboratory techniques (Murphy et al., 2017) may provide the quantitative un-
760 derstanding necessary to formulate more mechanistic process descriptions.

761 The descriptions of ROS dynamics that are empirically formulated are the
762 characteristics that would be considered unique for temperature tolerant corals
763 (Bay et al., 2016), and thus those that may determine the resilience of reefs in
764 the future (Matz et al., 2018). As these uncertainties are fundamental to some
765 management strategies being considered (Anthony et al., 2017), it is urgent
766 that modellers use the emerging understanding of the processes driving ROS
767 toxicity as it becomes available.

768 There is also considerable uncertainty of the role of all pigments in the elec-
769 tron chain. Fujiki and Taguchi (2001) propose that the photosynthetic xan-
770 thophyll pigment diadinoxanthin does not pass photons onto chlorophyll *a*,
771 while other works suggest photosynthetic xanthophylls do drive carbon fixa-
772 tion (Falkowski and Raven, 2007). In this paper we provide a path from di-
773 adinoxanthin absorption to carbon fixation (Fig. 4). Other detailed structural
774 studies show that the morphology of the pigment bed changes with physiolog-
775 ical status (Liu et al., 2004), thus potentially changing the roles of pigments.
776 The challenge of including knowledge from detailed biochemical studies like
777 these is formidable, and is not attempted here.

778 Even in the cases where physical constraints are used in the model for-

779 mulation, there is uncertainty regarding their form. For example, the model
780 presented here uses sphere packing geometry in a two layer gastrodermal
781 cell anatomy to determine the translocation fraction of zooxanthellae growth
782 (Eq.10). Another study (van Woesik et al., 2010), for example, considers lay-
783 ers of cells stacked vertically, with the light intensity of lower layers limiting
784 zooxanthellae density. While it may be possible to choose the most appropri-
785 ate mechanistic formulation for a particular coral species, the task of choosing
786 a generic form, as we have attempted here, inevitably has shortcomings.

787 The model developed here does not consider all phenomena relevant to
788 bleaching. For example, the model considers only one mechanism for ther-
789 mal stress induced bleaching, while the existence of bleaching under low light
790 conditions demonstrates that other mechanisms exist (Tolleter et al., 2013).
791 Further only one generic coral type, and one *Symbiodinium* clade, is consid-
792 ered. Thus the simulation here is not able to resolve the differences between
793 temperature tolerances of different corals assemblages (Bay et al., 2016).

794 Finally, the eReefs biogeochemical model (Baird et al., 2016b) that incor-
795 porates the new zooxanthellae photophysiological processes derived in this
796 paper represents only a fraction of the processes affecting coral health. For
797 example, the model represents only one coral type, and one macroalgae type,
798 and considers the only interaction between the two is a competition for nutri-
799 ents and light. A more sophisticated, ecosystem or habitat style model would
800 consider multiple coral and seagrass types inhabiting particular niches on the
801 seabed, and interacting with a range of herbivorous fish (Bozec et al., 2018).
802 Such an improved representation of coral mortality, which could include other
803 processes such as cyclone damage and starfish grazing (Babcock et al., 2016),
804 would remove the need for the ad-hoc quadratic mortality term for coral hosts.

805 Despite all the simplifications and omissions, the model developed here does
806 represent a comprehensive set of processes spanning scales from the polyp
807 processes to the shelf-scale, and from nutrient and photochemical interactions
808 to coral symbiosis.

809 4.2 *Future applications*

810 The use of satellite-derived temperature exposure alone as a measure of coral
811 bleaching severity has been broadly successful (Liu et al., 2014), and is used
812 operationally at a global scale. Nonetheless, it has not captured all bleach-
813 ing events accurately, and work is under way to include solar radiation in
814 bleaching algorithms (Skirving et al., 2018). Even with additional considera-
815 tions such as solar radiation, satellite algorithms will always be limited to the
816 estimation of near-surface properties, and their inability to consider factors
817 affecting bleaching such as dissolved nutrients (D’Angelo and Wiedenmann,
818 2014) that cannot be remotely-sensed. Furthermore satellite observations will
819 never be predictive. Thus, the near real time prediction and forecasting of coral
820 bleaching by a biogeochemical model such as developed here that can consider
821 the history of temperature, light and other environmental conditions at the
822 surface of the corals provides a means to overcome some of these limitations.

823 Finally, a process-based model is capable of explicitly representing man-
824 agement strategies such as local shading (Coelho et al., 2017), marine cloud
825 brightening, or increased stress tolerance of individuals and/or populations of
826 coral or zooxanthellae (Anthony et al., 2017). The eReefs modelling framework
827 has already been used to optimise catchment management for the purposes
828 of improving water quality on the Great Barrier Reef (Brodie et al., 2017).

829 The bleaching model derived here will next be used to quantify the impact
830 of interventions designed to minimise the impacts of a warming ocean on the
831 corals of the Great Barrier Reef.

Fig. 11. Model behaviour at Davies Reef at a shallow (3.8 m, top 3 rows) and a deep (18.0 m, bottom three rows) site in March 2016. Panels A and D show the light at the coral surface (PAR, mol photon m⁻² d⁻¹, scaled on the y -axis to the maximum PAR given in the title), and the normalised reserves of nitrogen, phosphorus and carbon. Panels B and E show the state of the xanthophyll cycle as the fraction of heat absorbing (X_h) and heat dissipating (X_p) pigments, the RuBisCO activity ($a_{Q_{ox}}^*$, varying between inactive at 0 and fully active at 1), and the carbon to chlorophyll ratio (scaled on the y -axis so the minimum C:Chl ratio of 20 g/g is 0, and 1 is 180 g/g). Panels C and F show the state of the reaction centres, and the rate of bleaching ($\times 10$ d⁻¹).

832 5 Acknowledgements

833 The coral bleaching model presented here was developed with funding from
834 CSIRO and the National Environmental Science Programme (NESP) Tropi-
835 cal Water Quality Hub (Project No. 3.3.1). The model simulations were de-
836 veloped as part of the eReefs project, a public-private collaboration between
837 Australia’s leading operational and scientific research agencies, government,
838 and corporate Australia. The authors wish to thank the many scientists in-
839 volved in the project, in particular Mike Herzfeld, John Andrewatha, Nugzar
840 Margvelashvili, Karen Wild-Allen, Barbara Robson, Andy Steven and Cedric
841 Robillot. Observations used in the eReefs project include those from the Inte-
842 grated Marine Observing System (IMOS) and the Marine Monitoring Program
843 (MMP). ARC Centre of Excellence National Bleaching Taskforce survey data
844 was download from <http://dx.doi.org/10.1002/ecy.2092> (Hughes et al., 2017).
845 The authors appreciate fruitful discussions with Peter Ralph as the model was
846 developed from the one-polyp model of Gustafsson et al. (2014) to the model
847 described here. Lesley Clementson kindly provided the pigment-specific ab-
848 sorption coefficients from unpublished experiments conducted at the CSIRO
849 Hobart Laboratories. This absorption data, and the entire model code used in
850 this study, is available on request to the authors.

851 References

- 852 Andrews, J. C., Gentien, P., 1982. Upwelling as a source of nutrients for the
853 Great Barrier Reef Ecosystems: A solution to Darwin’s Question. *Mar. Ecol.*
854 *Prog. Ser.* 8, 257–269.
- 855 Anthony, K., Bay, L. K., Costanza, R., Firn, J., Gunn, J., Harrison, P., Hey-

ward, A., Lundgren, P., Mead, D., Moore, T., Mumby, P. J., van Oppen, M.
J. J., Robertson, J., Runge, M. C., Suggett, D. J., Schaffelke, B., Wachen-
feld, D., Walshe, T., 2017. New interventions are needed to save coral reefs.
Nature Ecol. Evol. 1, 1420–1422.

Atkinson, M. J., Bilger, B. W., 1992. Effects of water velocity on phosphate
uptake in coral reef-flat communities. *Limnol. Oceanogr.* 37, 273–279.

Babcock, R. C., Dambacher, J. M., Morello, E. B., Plagnyi, E. E., KR, K.
R. H., Sweatman, H. P. A., 2016. Assessing different causes of Crown-of-
Thorns starfish outbreaks and appropriate responses for management on
the Great Barrier Reef. *PLoS ONE* 11, e0169048.

Baird, M. E., Adams, M. P., Babcock, R. C., Oubelkheir, K., Mongin, M.,
Wild-Allen, K. A., Skerratt, J., Robson, B. J., Petrou, K., Ralph, P. J.,
O’Brien, K. R., Carter, A. B., Jarvis, J. C., Rasheed, M. A., 2016a. A
biophysical representation of seagrass growth for application in a complex
shallow-water biogeochemical model. *Ecol. Model.* 325, 13–27.

Baird, M. E., Cherukuru, N., Jones, E., Margvelashvili, N., Mongin, M.,
Oubelkheir, K., Ralph, P. J., Rizwi, F., Robson, B. J., Schroeder, T., Sker-
ratt, J., Steven, A. D. L., Wild-Allen, K. A., 2016b. Remote-sensing re-
flectance and true colour produced by a coupled hydrodynamic, optical,
sediment, biogeochemical model of the Great Barrier Reef, Australia: com-
parison with satellite data. *Env. Model. Softw.* 78, 79–96.

Baird, M. E., Emsley, S. M., McGlade, J. M., 2001. Modelling the interacting
effects of nutrient uptake, light capture and temperature on phytoplankton
growth. *J. Plankton Res.* 23, 829–840.

Baird, M. E., Oke, P. R., Suthers, I. M., Middleton, J. H., 2004a. A plankton
population model with bio-mechanical descriptions of biological processes
in an idealised 2-D ocean basin. *J. Mar. Sys.* 50, 199–222.

883 Baird, M. E., Ralph, P. J., Rizwi, F., Wild-Allen, K. A., Steven, A. D. L.,
884 2013. A dynamic model of the cellular carbon to chlorophyll ratio applied
885 to a batch culture and a continental shelf ecosystem. *Limnol. Oceanogr.* 58,
886 1215–1226.

887 Baird, M. E., Roughan, M., Brander, R. W., Middleton, J. H., Nippard, G. J.,
888 2004b. Mass transfer limited nitrate uptake on a coral reef flat, Warraber
889 Island, Torres Strait, Australia. *Coral Reefs* 23, 386–396.

890 Baird, M. E., Walker, S. J., Wallace, B. B., Webster, I. T., Parslow, J. S.,
891 2003. The use of mechanistic descriptions of algal growth and zooplankton
892 grazing in an estuarine eutrophication model. *Est., Coastal and Shelf Sci.*
893 56, 685–695.

894 Bay, L. K., Doyle, J., Logan, M., Berkelmans, R., 2016. Recovery from bleach-
895 ing is mediated by threshold densities of background thermo-tolerant sym-
896 biont types in a reef-building coral. *Royal Society Open Science* 3, 160322.

897 Beaman, R. J., 2010. Project 3DGBR: A high-resolution depth model for the
898 Great Barrier Reef and Coral Sea, pp. 13 plus Appendix 1. Tech. rep.,
899 Marine and Tropical Sciences Research Facility (MTSRF) Project 2.5i.1a
900 Final Report, MTSRF, Cairns, Australia.

901 Beckmann, A., Hense, I., 2004. Torn between extremes: the ups and downs of
902 phytoplankton. *Ocean Dynamics* 54, 581–592.

903 Bozec, Y.-M., Doropoulos, C., Roff, G., Mumby, P. J., Jun 2018. Tran-
904 sient grazing and the dynamics of an unanticipated coral–algal phase shift.
905 *Ecosystems*.

906 Brodie, J., Baird, M., Mongin, M., Skerratt, J., Robillot, C., Waterhouse, J.,
907 2017. Pollutant target setting for the Great Barrier Reef: Using the eReefs
908 framework. In: Syme, G., Hatton MacDonald, D., Fulton, B. and Pianta-
909 dosi, J. (eds), MODSIM2017, 22nd International Congress on Modelling

910 and Simulation. Modelling and Simulation Society of Australia and New
 911 Zealand, December 2017. pp. 1913–1919.

912 Coelho, V. R., Fenner, D., Caruso, C., Bayles, B. R., Huang, Y., Birkeland,
 913 C., 2017. Shading as a mitigation tool for coral bleaching in three common
 914 Indo-Pacific species. *J. Exp. Mar. Biol. Ecol.* 497, 152–163.

915 Cunning, R., Muller, E. B., Gates, R. D., Nisbet, R. M., 2017. A dynamic
 916 bioenergetic model for coral-*Symbiodinium* symbioses and coral bleaching
 917 as an alternate stable state. *J. Theor. Biol.* 431, 49 – 62.

918 D’Angelo, C., Wiedenmann, J., 2014. Impacts of nutrient enrichment on coral
 919 reefs: new perspectives and implications for coastal management and reef
 920 survival. *Current Opinion in Environmental Sustainability* 7, 82 – 93.

921 Dormand., J. R., Prince, P. J., 1980. A family of embedded Runge-Kutta
 922 formulae. *J. Comp. App. Math.* 6, 19–26.

923 Duysens, L. N. M., 1956. The flattening of the absorption spectra of suspen-
 924 sions as compared to that of solutions. *Biochim. Biophys. Acta* 19, 1–12.

925 Eynaud, Y., Nisbet, R. M., Muller, E. B., 2011. Impact of excess and harmful
 926 radiation on energy budgets in scleractinian corals. *Ecological Modelling*
 927 222 (7), 1315 – 1322.

928 Falkowski, P. G., Raven, J. A., 2007. *Aquatic Photosynthesis*, 2nd Edition.
 929 Blackwell Science.

930 Falter, J. L., Atkinson, M. J., Merrifield, M. A., 2004. Mass-transfer limita-
 931 tion of nutrient uptake by a wave-dominated reef flat community. *Limnol.*
 932 *Oceanogr.* 49, 1820–1831.

933 Finkel, Z. V., 2001. Light absorption and size scaling of light-limited
 934 metabolism in marine diatoms. *Limnol. Oceanogr.* 46, 86–94.

935 Fujiki, T., Taguchi, S., 2001. Relationship between light absorption and the
 936 xanthophyll-cycle pigments in marine diatoms. *Plankton Biol. Ecol.* 48, 96–

937 103.

938 Furnas, M., 2003. Catchments and corals: terrestrial runoff to the Great Bar-
 939 rier Reefs. Tech. rep., Australian Institute of Marine Science, Queensland,
 940 334 p.

941 Gillibrand, P. A., Herzfeld, M., 2016. A mass-conserving advection scheme for
 942 offline simulation of tracer transport in coastal ocean models. *Env. Model.*
 943 *Soft.* 101, 1–16.

944 Gustafsson, M. S. M., Baird, M. E., Ralph, P. J., 2013. The interchangeabil-
 945 ity of autotrophic and heterotrophic nitrogen sources in scleractinian coral
 946 symbiotic relationships: a numerical study. *Ecol. Model.* 250, 183–194.

947 Gustafsson, M. S. M., Baird, M. E., Ralph, P. J., 2014. Modelling photoinhibi-
 948 tion and bleaching in Scleractinian coral as a function of light, temperature
 949 and heterotrophy. *Limnol. Oceanogr.* 59, 603–622.

950 Herzfeld, M., 2015. Methods for freshwater riverine input into regional ocean
 951 models. *Ocean Model.* 90, 1 – 15.

952 Herzfeld, M., Andrewartha, J., Baird, M., Brinkman, R., Furnas,
 953 M., Gillibrand, P., Hemer, M., Joehnk, K., Jones, E., McKin-
 954 non, D., Margvelashvili, N., Mongin, M., Oke, P., Rizwi, F., Rob-
 955 son, B., Seaton, S., Skerratt, J., Tonin, H., Wild-Allen, K., 2016.
 956 eReefs Marine Modelling: Final Report, CSIRO, Hobart 497 pp.
 957 http://www.marine.csiro.au/cem/gbr4/eReefs_Marine_Modelling.pdf
 958 rm. Tech. rep.

959 Herzfeld, M., Gillibrand, P., 2015. Active open boundary forcing using dual
 960 relaxation time-scales in downscaled ocean models. *Ocean Model.* 89, 71–83.

961 Hill, R., Brown, C. M., DeZeeuw, K., Campbell, D. A., Ralph, P. J., 2011.
 962 Increased rate of D1 repair in coral symbionts during bleaching is insufficient
 963 to counter accelerated photo-inactivation. *Limnol. Oceanogr.* 56, 139–146.

964 Hochberg, E. J., Apprill, A. M., Atkinson, M. J., Bidigare, R. R., 2006. Bio-
 965 optical modeling of photosynthetic pigments in corals. *Coral Reefs* 25, 99–
 966 109.

967 Hock, K., Wolff, N. H., Ortiz, J. C., Condie, S. A., Anthony, K. R. N., Black-
 968 well, P. G., Mumby, P. J., 2017. Connectivity and systemic resilience of the
 969 Great Barrier Reef. *PLoS Biol.* 11, e2003355.

970 Hoegh-Guldberg, O., 1999. Climate change, coral bleaching and the future of
 971 the world’s coral reefs. *Mar. Fresh. Res.* 50, 839–866.

972 Hughes, T. P., Kerry, J. T., Simpson, T., 2017. Large-scale bleaching of corals
 973 on the Great Barrier Reef. *Ecology*.
 974 URL <http://dx.doi.org/10.1002/ecy.2092>

975 Kirk, J. T. O., 1975. A theoretical analysis of the contribution of algal cells
 976 to the attenuation of light within natural waters. I. General treatment of
 977 suspensions of pigmented cells. *New Phytol.* 75, 11–20.

978 Kirk, J. T. O., 1994. *Light and Photosynthesis in Aquatic Ecosystems*, 2nd
 979 Edition. Cambridge University Press, Cambridge.

980 Lilley, R. M., Ralph, P. J., Larkum, A. W. D., 2010. The determination of ac-
 981 tivity of the enzyme rubisco in cell extracts of the dinoflagellate alga symbio-
 982 dinium sp. by manganese chemiluminescence and its response to short-term
 983 thermal stress of the alga. *Plant, Cell & Environment* 33 (6), 995–1004.

984 Liu, G., Heron, S. F., Eakin, C. M., Muller-Karger, F. E., Vega-Rodriguez,
 985 M., Guild, L., Cour, J. L. D. L., Geiger, E. F., Skirving, W. J., Burgess,
 986 T. F. R., 2014. Reef-scale Thermal Stress Monitoring of Coral Ecosystems:
 987 New 5-km Global Products from NOAA Coral Reef Watch. *Remote Sens.*
 988 6, 11579–11606.

989 Liu, Z., Yan, H., Wang, K., Kuang, T., Zhang, J., Gui, L., An, X., Chang, W.,
 990 2004. Crystal structure of spinach major light-harvesting complex at 2.72Å

991 resolution. *Nature* 428, 287–292.

992 Madden, C. J., Kemp, W. M., 1996. Ecosystem model of an estuarine sub-
 993 mersed plant community: calibration and simulation of eutrophication re-
 994 sponses. *Estuaries* 19, 457–474.

995 Margvelashvili, N., Herzfeld, M., Rizwi, F., Mongin, M., Baird, M., Jones,
 996 E., Schaffelke, B., King, E., Schroeder, T., 2016. Emulator-assisted data
 997 assimilation in complex models. *Ocean Dyn.* 66, 1109–1124.

998 Matz, M., Treml, E. A., Aglyamova, G. V., Bay, L. K., 2018. Potential and
 999 limits for rapid genetic adaptation to warming in a Great Barrier Reef coral.
 1000 *PLOS Genetics* 14, e1007220.

1001 McNeil, M. A., Webster, J. M., Beaman, R. J., Graham, T. L., 2016. New
 1002 constraints on the spatial distribution and morphology of the *Halimeda*
 1003 bioherms of the Great Barrier Reef, Australia. *Coral Reefs* 35, 1343–1355.

1004 Mongin, M., Baird, M. E., Tilbrook, B., Matear, R. J., Lenton, A., Herzfeld,
 1005 M., Wild-Allen, K. A., Skerratt, J., Margvelashvili, N., Robson, B. J.,
 1006 Duarte, C. M., Gustafsson, M. S. M., Ralph, P. J., Steven, A. D. L., 2016.
 1007 The exposure of the Great Barrier Reef to ocean acidification. *Nature Com-*
 1008 *munications* 7, 10732.

1009 Monismith, S. G., Davis, K. A., Shellenbarger, G. G., Hench, J. L., Nidzieko,
 1010 N. J., Santoro, A. E., Reidenbach, M. A., Rosman, J. H., Holtzman, R.,
 1011 Martens, C. S., Lindquist, N. L., Southwell, M. W., Genin, A., 2010. Flow
 1012 effects on benthic grazing on phytoplankton by a Caribbean reef. *Limnol.*
 1013 *Oceanogr.* 55, 1881–1892.

1014 Muller, E. B., Sebastiaan, A. L., Kooijman, M., Edmunds, P. J., Doyle, F. J.,
 1015 Nisbet, R. M., 2009. Dynamic energy budgets in syntrophic symbiotic rela-
 1016 tionships between heterotrophic hosts and photoautotrophic symbionts. *J.*
 1017 *Theor. Biol.* 259, 44–57.

1018 Muller-Parker, G., Cook, C. B., D'Elia, C. F., 1994. Elemental composition of
1019 the coral *Pocillopora damicornis* exposed to elevated seawater ammonium.
1020 Pac. Sci. 48, 234–246.

1021 Murphy, C. D., Ni, G., Li, G., Barnett, A., Xu, K., Grant-Burt, J., Liefer, J. D.,
1022 Suggett, D. J., Campbell, D. A., 2017. Quantitating active photosystem
1023 II reaction center content from fluorescence induction transients. Limnol.
1024 Oceanogr. Meth. 15, 54–69.

1025 Nielsen, M. V., Sakshaug, E., 1993. Photobiological studies of *Skeletonema*
1026 *costatum* adapted to spectrally different light regimes. Limnol. Oceanogr.
1027 38, 1576–1581.

1028 Raven, J. A., 1997. Phagotrophy in phototrophs. Limnol. Oceanogr. 42, 198–
1029 205.

1030 Redfield, A. C., Ketchum, B. H., Richards, F. A., 1963. The influence of or-
1031 ganisms on the composition of sea-water. In: Hill, N. (Ed.), The sea, 2nd
1032 Edition. Wiley, pp. 26–77.

1033 Ribes, M., Atkinson, M. J., 2007. Effects of water velocity on picoplankton
1034 uptake by coral reef communities. Coral Reefs 26, 413–421.

1035 Ridgway, K. R., Dunn, J. R., 2003. Mesoscale structure of the mean East
1036 Australian Current System and its relationship with topography. Prog.
1037 Oceanogr. 56, 189–222.

1038 Roelfsema, C., Kovacs, E., Ortiz, J. C., Wolff, N. H., Callaghan, D., Wettle,
1039 M., Ronan, M., Hamylton, S. M., Mumby, P. J., Phinn, S., 2018. Coral
1040 reef habitat mapping: A combination of object-based image analysis and
1041 ecological modelling. Remote Sensing of Environment 208, 27–41.

1042 Schiller, A., Herzfeld, M., Brinkman, R., Stuart, G., Jan. 2014. Monitoring,
1043 predicting and managing one of the seven natural wonders of the world.
1044 Bull. Am. Meteor. Soc., 23–30.

1045 Skerratt, J., Mongin, M., Wild-Allen, K. A., Baird, M. E., Robson, B. J., Schaf-
 1046 felke, B., Soja-Woźniak, M., Margvelashvili, N., Davies, C. H., Richardson,
 1047 A. J., Steven, A. D. L., submitted. Plankton and nutrient dynamics on the
 1048 Great Barrier Reef: Skill assessment and analysis of the eReefs biogeochem-
 1049 ical model. *J. Mar. Sys.* , .
 1050 Skirving, W., Enrquez, S., Hedley, J. D., Dove, S., Eakin, C. M., Mason,
 1051 R. A. B., Cour, J. L. D. L., Liu, G., Hoegh-Guldberg, O., Strong, A. E.,
 1052 Mumby, P. J., Iglesias-Prieto, R., 2018. Remote sensing of coral bleaching
 1053 using temperature and light: progress towards an operational algorithm.
 1054 *Remote Sens.* 10, 18.
 1055 Suggett, D. J., MacIntyre, H. L., Kana, T. M., Geider, R. J., 2009. Com-
 1056 paring electron transport with gas exchange: parameterising exchange rates
 1057 between alternative photosynthetic currencies for eukaryotic phytoplankton.
 1058 *Aquat. Microb. Ecol.* 56, 147–162.
 1059 Suggett, D. J., Warner, M. E., Smith, D. J., Davey, P., Hennige, S., Baker,
 1060 N. R., 2008. Photosynthesis and production of hydrogen peroxide by *Sym-*
 1061 *biodinium* (Pyrrophyta) phylotypes with different thermal tolerances. *J.*
 1062 *Phycol.* 44, 948–956.
 1063 Tolleter, D., Seneca, F. O., DeNofrio, J. C., Krediet, C. J., Palumbi, S. R.,
 1064 Pringle, J. R., Grossman, A. R., 2013. Coral bleaching independent of pho-
 1065 tosynthetic activity. *Current Biol.* 23, 1782 – 1786.
 1066 Van Leer, B., 1977. Towards the ultimate conservative difference scheme. IV.
 1067 A new approach to numerical convection. *J. Comp. Phys.* 23, 276 – 299.
 1068 van Oppen, M. J. H., Gates, R. D., Blackall, L. L., Cantin, N., Chakravarti,
 1069 L. J., Chan, W. Y., Cormick, C., Crean, A., Damjanovic, K., Epstein, H.,
 1070 Harrison, P. L., Jones, T. A., Miller, M., Pears, R. J., Peplow, L. M., Raftos,
 1071 D. A., Schaffelke, B., Stewart, K., Torda, G., Wachenfeld, D., Weeks, A. R.,

1072 Putnam, H. M., 2017. Shifting paradigms in restoration of the world's coral
 1073 reefs. *Global Change Biology* 23 (9), 3437–3448.
 1074 URL <http://dx.doi.org/10.1111/gcb.13647>

1075 van Woesik, R., Shiroma, K., Koksas, S., 2010. Phenotypic variance predicts
 1076 symbiont population densities in corals: A modelling approach. *PLOS One*
 1077 5, e9185.

1078 Wild-Allen, K., Skerratt, J., Whitehead, J., Rizwi, F., Parslow, J., 2013. Mech-
 1079 anisms driving estuarine water quality: a 3D biogeochemical model for in-
 1080 formed management. *Est. Coast. Shelf Sci.* 135, 33–45.

1081 Wyatt, A. S. J., Lowe, R. J., Humphries, S., Waite, A. M., 2010. Particulate
 1082 nutrient fluxes over a fringing coral reef: relevant scales of phytoplankton
 1083 production and mechanisms of supply. *Mar. Ecol. Prog. Ser.* 405, 113–130.

1084 Zhang, Z., Lowe, R., Falter, J., Ivey, G., 2011. A numerical model of wave-
 1085 and current-driven nutrient uptake by coral reef communities. *Ecol. Mod.*
 1086 222, 1456–1470.

A Model state variables, equations and parameter values

Table A.1. Model state variables. Note that water column variables are 3 dimensional, benthic variables are 2 dimensional, and unnormalised reserves are per cell.

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

Table A.2. Derived variables for the coral polyp model.

Variable	Symbol	Units
Downwelling irradiance	E_d	W m^{-2}
Maximum reserves of nitrogen	$R_N^{\max}$	mg N cell^{-1}
Maximum reserves of phosphorus	$R_P^{\max}$	mg P cell^{-1}
Maximum reserves of carbon	$R_C^{\max}$	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	mg m^{-3}
Intracellular diadinoxanthin concentration	x_p	mg m^{-3}
Intracellular diatoxanthin concentration	x_h	mg m^{-3}
Total reaction centre concentration	Q_T	mg m^{-2}
Total active reaction centre concentration	Q_a	mg m^{-2}
Concentration of zooxanthellae cells	n	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}	cell m^{-2}
Absorption cross-section	α	$\text{m}^2 \text{ cell}^{-1}$
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	ρ	kg m^{-3}
Bottom stress	τ	N m^{-2}
Schmidt number	Sc	-
Mass transfer rate coefficient for particles	S_{part}	m d^{-1}
Heterotrophic feeding rate	G	$\text{g N m}^{-2} \text{ d}^{-1}$
Wavelength	λ	nm
Translocation fraction	f_{tran}	-
Active fraction of oxidised reaction centres	$a_{Q_{ox}}^*$	-

Table A.3. Equations for the interactions of coral host, symbiont and environment excluding bleaching loss terms that appear in Table A.6. The term CS/m_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 O₂⁻¹.

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

$$\frac{\partial P}{\partial t} = -S_P P(1 - R_P^*) A_{eff} \quad (A.2)$$

$$\frac{\partial DIC}{\partial t} = - \left(\frac{106}{1060} 12 k_I \frac{Q_{ox}}{Q_T} a_{Q_{ox}}^* (1 - R_C^*) - \frac{106}{16} \frac{12}{14} \mu_{CS}^{\max} \phi R_C^* \right) (CS/m_N) \quad (A.3)$$

$$\frac{\partial [O_2]}{\partial t} = \left(\frac{138}{1060} 32 k_I \frac{Q_{ox}}{Q_T} a_{Q_{ox}}^* (1 - R_C^*) - \frac{138}{16} \frac{32}{14} \mu_{CS}^{\max} \phi R_C^* \right) (CS/m_N) \quad (A.4)$$

$$\frac{\partial R_N}{\partial t} = S_N N(1 - R_N^*) / (CS/m_N) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_N + R_N) \quad (A.5)$$

$$\frac{\partial R_P}{\partial t} = S_P P(1 - R_P^*) / (CS/m_N) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_P + R_P) \quad (A.6)$$

$$\begin{aligned} \frac{\partial R_C}{\partial t} = & k_I \left(\frac{Q_{ox}}{Q_T} \right) a_{Q_{ox}}^* (1 - R_C^*) - \mu_{CS}^{\max} R_P^* R_N^* R_C^* (m_C + R_C) \\ & - \mu_{CS}^{\max} \phi m_C R_C^* \end{aligned} \quad (A.7)$$

$$\frac{\partial CS}{\partial t} = \mu_{CS}^{\max} R_P^* R_N^* R_C^* CS - \zeta_{CS} CS \quad (A.8)$$

$$\frac{\partial c_i}{\partial t} = (k_{chl}^{\max} (1 - R_C^*) (1 - Q_{in}/Q_T) \bar{\chi} - \mu_P^{\max} R_P^* R_N^* R_C^* c_i) (CS/m_N) \quad (A.9)$$

$$\frac{\partial X_p}{\partial t} = \Theta_{xan2chl} (k_{chl}^{\max} (1 - R_C^*) (1 - Q_{in}/Q_T) \bar{\chi}) \quad (A.10)$$

$$- 8 (Q_{in}/Q_T - 0.5)^3 \tau_{xan} \Phi (X_p + X_h) \quad (A.11)$$

$$\frac{\partial X_h}{\partial t} = 8 (Q_{in}/Q_T - 0.5)^3 \tau_{xan} \Phi (X_p + X_h) \quad (A.12)$$

$$\frac{\partial CS}{\partial t} = (1 - f_{tran}) \mu_{CS} CS - \zeta_{CS} CS + f_{remin} \frac{\zeta_{CH}}{A_{eff}} CH^2 \quad (A.13)$$

$$k_I = \frac{(10^9 hc)^{-1}}{A_V} \int \alpha_\lambda E_{d,\lambda} \lambda d\lambda \quad (A.14)$$

$$S_x = 2850 \left(\frac{2\tau}{\rho} \right)^{0.38} S_{c_x}^{-0.6}, S_{c_x} = \frac{\nu}{D_x} \quad (A.15)$$

$$\Phi = 1 - 4 \left(\frac{X_p}{X_p + X_h} - 0.5 \right)^2 \text{ or } \Phi = 1 \quad (A.16)$$

Table A.4. Equations for the coral polyp model. The term CS/m_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 O₂⁻¹. Other constants and parameters are defined in Table A.8.

$$\begin{aligned} \frac{\partial CH}{\partial t} &= G' - \frac{\zeta_{CH}}{A_{eff}} CH^2 & (A.17) \\ \frac{\partial B}{\partial t} &= -S_{part} A_{eff} B \frac{G'}{G} / h_{wc} & (A.18) \\ \frac{\partial Z}{\partial t} &= -S_{part} A_{eff} Z \frac{G'}{G} / h_{wc} & (A.19) \\ \frac{\partial D_{Red}}{\partial t} &= \left(-S_{part} A_{eff} D_{Red} \frac{G'}{G} + (1 - f_{remin}) \frac{\zeta_{CH}}{A_{eff}} CH^2 \right) / h_{wc} & (A.20) \\ f_{tran} &= \frac{\pi r_{CS}^2 n_{CS}}{2CH\Omega_{CH}} & (A.21) \\ G &= S_{part} A_{eff} (B + Z + D_{Red}) & (A.22) \\ G' &= \min [\min [\mu_{CH}^{max} CH - f_{tran} \mu_{CS} CS - \zeta_{CS} CS, 0], G] & (A.23) \\ A_{eff} &= 1 - \exp(-\Omega_{CH} CH) & (A.24) \end{aligned}$$

Table A.5. Reaction centre dynamics. Bleaching loss terms appear in Table A.6.

$$\begin{aligned} \frac{\partial Q_{ox}}{\partial t} &= -k_{In} m_{RCH} \left(\frac{Q_{ox}}{Q_T} \right) \left(1 - a_{Q_{ox}}^* (1 - R_C^*) \right) + f_2(T) R_N^* R_P^* R_C^* Q_{in} & (A.25) \\ \frac{\partial Q_{red}}{\partial t} &= k_{In} m_{RCH} \left(\frac{Q_{ox}}{Q_T} \right) \left(1 - a_{Q_{ox}}^* (1 - R_C^*) \right) - k_{In} m_{RCH} \frac{Q_{red}}{Q_T} & (A.26) \\ \frac{\partial Q_{in}}{\partial t} &= -268 m_{RCH} Q_{in} + k_{In} m_{RCH} \frac{Q_{red}}{Q_T} & (A.27) \\ \frac{\partial [ROS]}{\partial t} &= -f(T) R_N^* R_P^* R_C^* [ROS] + 32 \frac{138}{106} \frac{1}{10} k_{In} m_{RCH} \left(\frac{Q_{in}}{Q_T} \right) & (A.28) \end{aligned}$$

Table A.6. Equations describing the expulsion of zooxanthellae, and the resulting release of inorganic and organic molecules into the bottom water column layer.

$\frac{\partial[\text{NH}_4]}{\partial t} = \max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] CSR_N^*/h_{wc}$	(A.29)
$\frac{\partial P}{\partial t} = \frac{1}{16} \frac{31}{14} \max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] CSR_P^*/h_{wc}$	(A.30)
$\frac{\partial DIC}{\partial t} = \frac{106}{16} \frac{12}{14} \max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] CSR_C^*/h_{wc}$	(A.31)
$\frac{\partial[\text{O}_2]}{\partial t} = -\frac{\partial DIC}{\partial t} \frac{138}{106} \frac{32}{12} \frac{[\text{O}_2]^2}{K_{OA}^2 + [\text{O}_2]^2}$	(A.32)
$\frac{\partial[\text{COD}]}{\partial t} = \frac{\partial DIC}{\partial t} \frac{138}{106} \frac{32}{12} \left(1 - \frac{[\text{O}_2]^2}{K_{OA}^2 + [\text{O}_2]^2} \right)$	(A.33)
$\frac{\partial CS}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] CS$	(A.34)
$\frac{\partial R_N}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] R_N$	(A.35)
$\frac{\partial R_P}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] R_P$	(A.36)
$\frac{\partial R_C}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] R_C$	(A.37)
$\frac{\partial Chl}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] Chl$	(A.38)
$\frac{\partial X_p}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] X_p$	(A.39)
$\frac{\partial X_h}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] X_h$	(A.40)
$\frac{\partial Q_{\text{ox}}}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] Q_{\text{ox}}$	(A.41)
$\frac{\partial Q_{\text{red}}}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] Q_{\text{red}}$	(A.42)
$\frac{\partial Q_{\text{in}}}{\partial t} = -\max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] Q_{\text{in}}$	(A.43)
$\frac{\partial D_{\text{Red}}}{\partial t} = \max \left[\gamma, \frac{[\text{ROS}] - [\text{ROS}_{\text{threshold}}]}{m_O} \right] CS/h_{wc}$	(A.44)

Table A.7. Constants and parameter values used to model coral polyps. V is zooxanthellae cell volume in μm^3 . ^aFig. 5, ^cRedfield et al. (1963) and Kirk (1994), ^dFinkel (2001), ^eRibes and Atkinson (2007); Wyatt et al. (2010), ^{f,g}Gustafsson et al. (2013, 2014).

	Symbol	Value
<i>Constants</i>		
Molecular diffusivity of NO_3	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	$6.626 \times 10^{-34} \text{ J s}^{-1}$
Avagadro constant	A_V	$6.02 \times 10^{23} \text{ mol}^{-1}$
^a Pigment-specific absorption coefficients	γ_λ	$f(\text{pig}, \lambda) \text{ m}^{-1} (\text{mg m}^{-3})^{-1}$
Kinematic viscosity of water	ν	$f(T, S_A) \sim 1.05 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$
<i>Parameters</i>		
^b Nitrogen content of zooxanthellae cells	m_N	$5.77 \times 10^{-12} \text{ mol N cell}^{-1}$
^c Carbon content of zooxanthellae cells	m_C	$(106/16) m_N \text{ mol C cell}^{-1}$
^d Maximum intracellular Chl concentration	$c_i^{\max}$	$3.15 \times 10^6 \text{ mg Chl m}^{-3}$
Radius of zooxanthellae cells	r_{CS}	$5 \mu\text{m}$
Maximum growth rate of coral	$\mu_{CH}^{\max}$	0.05 d^{-1}
^e Rate coefficient of particle capture	S_{part}	3.0 m d^{-1}
Maximum growth rate of zooxanthellae	$\mu_{CS}^{\max}$	0.4 d^{-1}
Quadratic mortality coefficient of polyps	ζ_{CH}	$0.01 \text{ d}^{-1} (\text{g N m}^{-2})^{-1}$
Linear mortality of zooxanthellae	ζ_{CS}	0.04 d^{-1}
^g Remineralised fraction of coral mortality	f_{remin}	0.5
Nitrogen-specific host area coefficient of polyps	Ω_{CH}	$2.0 \text{ m}^2 \text{ g N}^{-1}$
Fractional (of $\mu_{CS}^{\max}$) respiration rate	ϕ	0.1

Table A.8. Constants and parameter values used in the coral bleaching model. ^aIn Suggett et al. (2009). ^b ratio of constant terms in multivariate analysis in Hochberg et al. (2006). ^cFitted parameter based on the existence of non-bleaching threshold (Suggett et al., 2009), and a comparison of observed bleaching and model output in the ~ 1 km model.

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