



# 1 **Reviews and syntheses: Assessment of Biogeochemical Models in** 2 **the Marine Environment**

3 Kaltham A. Ismail, Maryam R. Al-Shehhi

4 Department of Civil, Infrastructure and Environmental Engineering, Khalifa University, Abu Dhabi, UAE

5 *Correspondence to:* Maryam R. Al-Shehhi ([maryamr.alshehhi@ku.ac.ae](mailto:maryamr.alshehhi@ku.ac.ae))

6 **Abstract.** Marine biogeochemical models are key tools utilized to quantify numerous aspects of  
7 biogeochemistry including primary productivity, cycling of nutrients, redistribution of plankton, and  
8 variability of the carbon cycle in the ocean. These models are typically coupled to physical models with a  
9 horizontal resolution varying from few kilometers to more than 400 kilometers. Many of the existing  
10 biogeochemical models are commonly based on the NPZD model structure however, these models differ  
11 in their complexity determined by the number of state variables and the functional forms. Therefore, this  
12 review illustrates the types of the common biogeochemical models categorized based on the complexity  
13 levels and the governing equations. Then, applications of these models in several ecosystems of the world  
14 ocean are presented through a comprehensive assessment and evaluation of their performance in  
15 reproducing biogeochemical parameters such as chlorophyll-a, nutrients, as well as carbon and oxygen. In  
16 general, models based on functional group approach when coupled to high-resolution physical models show  
17 good estimates of surface nutrients such as nitrogen (N), phosphorous (P), silica (S) in global oceans with  
18 correlation coefficients ( $r$ ) of  $\geq 0.85$ ,  $\geq 0.9$ , and  $\geq 0.78$  respectively. Similarly, NPZD based models coupled  
19 to suitable physical models are found to accurately reproduce N, P, and oxygen (O) with coefficients of  
20 determination ( $R^2$ ) around 0.9 (for N & P) and  $\sim > 0.9$  (for O) particularly in the Indian and Pacific waters.  
21 In addition, highest performance for iron prediction in global oceans is found with  $r$  values between 0.7 and  
22 0.86 particularly by functional group approach models. However, chlorophyll-a prediction has shown  
23 varying performances by all types of models with  $r$  ranging from 0.55 and 0.9. So, applications of  
24 biogeochemical models are dependent on the features of the ecosystem and the purpose of the study.  
25 Therefore, the functional group approach models are mainly applied to investigate biogeochemical cycles  
26 while NPZD models are mainly used for physical-biological investigation.

## 27 **1 Introduction**

28 Modelling the biogeochemistry of the ocean is essential to improve our understanding of the primary productivity,  
29 eutrophication, and nutrients variability. The formal definition of biogeochemistry is to quantify the chemical species  
30 exchanged between earth system reservoirs along with transformations in these reservoirs. Thus, biogeochemistry  
31 focuses on carbon and nutrients cycling between the living and non-living compartments of the ocean (Dutkiewicz et  
32 al., 2020). This is translated into including the inorganic nutrients, detrital matter and the explicit representation of the  
33 living components such as phytoplankton and zooplankton in the biogeochemical modelling. In addition, the  
34 importance of the ocean circulation manifests in the redistribution of organic and inorganic pools hence representation  
35 of currents, temperature, mixing, salinity and density are also an integral part of the biogeochemical models and have  
36 a great impact on the primary productivity and nutrients distribution in the oceans (Heinze and Gehlen, 2013).



37 Therefore, the developed biogeochemical models are mainly based on the classical NPZD approach developed by  
38 Fasham et al. (1990) which stands for Nutrients, Phytoplankton, Zooplankton, and Detritus. These main four  
39 compartments, can be categorized into biotic (e.g. phytoplankton, zooplankton, fishes, whales) and abiotic (e.g.  
40 ammonium, nitrate, dissolved organic/inorganic carbon (DOC/DIC), particulate organic carbon (POC)) (Sarmiento et  
41 al., 1993). As for biota, phytoplankton and zooplankton are the core parts of it where phytoplankton are autotrophic  
42 organisms obtaining their energy from sunlight and can fix the carbon dioxide, and zooplankton are heterotrophic  
43 organisms obtaining their energy source by consuming other organisms. For the abiotic components, in addition to  
44 what was mentioned above, the biogeochemical models also consider the main limiting nutrient in the ocean which is  
45 primarily the Dissolved Inorganic Nitrogen termed as DIN. The other important limiting elements that are also  
46 considered include phosphate, iron and silicate (Lachkar et al., 2020). The representation of these compartments is  
47 governed by one or more state variables which can be used to define the trophic levels of the pelagic ecosystems'  
48 evolution (Heinze and Gehlen, 2013).

49 Several substantial biochemical parameters have been studied in various ecosystems of the global oceans using  
50 different types of biogeochemical models, these parameters include chlorophyll-a, macronutrients (nitrate, phosphate,  
51 silicate), micronutrients (Fe), carbon and oxygen cycles. Chlorophyll-a is typically used as a metric of biomass  
52 concentration instead of carbon biomass in the ocean due to its unique optical properties and it is one of the widely  
53 studied parameter in the biogeochemical modelling. The level of this parameter is affected by several basic factors  
54 including: the solar radiation intensity penetrating the water column, dissolved nutrients gradients with depth,  
55 temperature, and the mixed layer depth (Sverdrup, 1953; Wroblewski et al., 1988). Although the chlorophyll-a to  
56 carbon and nutrient ratio (Chl: C:nutrient) is highly variable due to an acclimatize response to changes in  
57 environmental conditions such as irradiance, temperature, and nutrient availability, this flexibility is neglected by  
58 many large-scale biogeochemical models for the sake of simplicity and lowering complexity (Anugerahanti et al.,  
59 2021). Whereas Macronutrients such as Nitrate ( $\text{NO}_3$ ), Silicate ( $\text{SiO}_3$ ), and Phosphate ( $\text{PO}_4$ ) play a critical role in  
60 phytoplankton growth and ocean dynamics and these nutrients are considered to be key limiting nutrients impacting  
61 oceanic primary productivity; however, iron is recently well established to be also one of the key limiting nutrients  
62 highly impacting phytoplankton dynamics and primary productivity. These limiting nutrients can be supplied to the  
63 ocean through several sources including: dust deposition from atmosphere, riverine inputs, sea ice, sediment  
64 mobilization, as well as hydrothermal vents (Aumont et al., 2015). Unlike other nutrients, iron sources in the ocean



65 mainly come from the atmosphere, transported as aerosols and commonly related to soil dust. Different phytoplankton  
66 groups have different sensitivity to iron limitation, for example diatoms exhibited a large sensitivity to iron limitation  
67 (Gregg et al., 2003) compared to other phytoplankton types. Likewise, carbon is the primary element in the  
68 photosynthesis process carried out by autotrophs mainly phytoplankton in the surface of the ocean. It is also the energy  
69 source for many aerobic heterotrophs and autotrophs living in the ocean. The inorganic form of carbon can be oxidized  
70 through remineralization to form inorganic sources to be utilised by photo synthesizers. While the latter convert the  
71 inorganic form back into organics for the heterotrophs. So, the atmospheric carbon dioxide is regulated by biological  
72 carbon pump which is highly impacted by the role of zooplankton in the ocean (Cavan et al., 2017). Oxygen is a by-  
73 product of photosynthesis and can be dissolved into the ocean from the atmosphere. This parameter is important for  
74 aerobic heterotrophs living in the ocean and its reduction in the ocean can lead to amplify denitrification creating  
75 oxygen minimum zone (OMZ) which is found in some regions of the global oceans (Lachkar et al., 2016, 2019, 2020).  
76 These parameters have been modelled by several bio-geochemical models to better understand the ocean ecosystems  
77 and therefore the aim of this work is to describe the most common biogeochemical models and carry out a complete  
78 assessment of these biogeochemical models in estimating the aforementioned biochemical properties in different  
79 ecosystems. This includes reporting the performance of the models, strengths, uncertainties and limitations. This  
80 review begins with the models' section describing their components, assumptions and structure as well as examples  
81 of well-known models developed based on these approaches. Then, the major modelled parameters studied in the  
82 several ecosystems of the global oceans are discussed.

## 83 **2 Biogeochemical Modelling Approaches** 84

85 The existing biogeochemical models are categorized here into three types in terms of complexity, the number of state  
86 variables, and the governing equations that is formed based on the functional forms, as follow,

### 87 **2.1 Classical NPZD approach** 88

89 This approach basically considers a single variable for each compartment (nutrients - phytoplankton - zooplankton –  
90 detritus sometimes includes bacteria) neglecting the differences between the species (Evans et al., 1985; Fasham et  
91 al., 1990, 1993; Franks P, 2002). In this approach, nitrogen is typically considered a limiting nutrient and detritus  
92 component account for the organic matter pool which are derived from fecal materials and / non-assimilated fraction



93 of grazing by zooplankton and phytoplankton decay. This detritus is recycled through two ways which are utilization  
94 by bacteria and degradation of dissolved organic nitrogen/zooplankton assimilation (Leles et al., 2016).

95 The general form of NPZD is presented in equations 1-4.

$$96 \quad \frac{dN}{dt} = -f(I)g(N)P + R(D)D \quad (1)$$

$$97 \quad \frac{dP}{dt} = f(I)g(N)P - h(P)Z - i(P)P \quad (2)$$

$$98 \quad \frac{dZ}{dt} = \gamma Z h(P) - j(Z)Z \quad (3)$$

$$99 \quad \frac{dD}{dt} = i(P)P + j(Z)Z + (1 - \gamma)h(P)Z - R(D)D \quad (4)$$

100 Five transfer equations are involved in the model including: light limitation (phytoplankton response to  
101 light/irradiance)  $f(I)$ ; nutrient limitation (uptake of nutrients by phytoplankton)  $g(N)$ ; grazing by zooplankton  $h(P)$ ;  
102 loss terms due to excretion, death, and predation by other organisms  $i(P)P, j(Z)Z$ ; degradation of detritus  $R(D)$ .

103 The zooplankton assimilation is termed as  $\gamma$  which is commonly modelled by a simple linear function of food ingestion  
104 (Franks P, 2002). The functional forms representation of phytoplankton response to incident light ranges from a simple  
105 linear form to nonlinear functions including saturation and photo-inhibition response (see Table 1). The Michaelis-  
106 Menten/Monod saturation function is the most applied form of nutrient uptake by phytoplankton which can relate the  
107 growth rates to the concentration of a limiting nutrient (Dugdale, 1967). The dependency of the growth on nutrient  
108 concentration is regulated by two kinetic parameters which represent the population traits: the maximum utilization  
109 rate,  $V_{max}$ ; and the affinity constant,  $k$ , which presents an organism ability to capture nutrient ions at low nutrient  
110 concentration  $N$ . The phytoplankton acclimation determines the ability of the cell to adapt its kinetic parameters in  
111 response to changes in environmental conditions. So, if  $V_{max}$  is constant then the acclimation will be discarded in the  
112 Michaelis-Menten formulation because the maximum uptake rate is associated with the total number of uptake sites  
113 of the cell (Bonachela et al., 2015). However, the Michaelis-Menten assumption was argued by (Droop, 1973, 1983)  
114 which has assumed that the growth rate is more likely dependent on the internal content of the nutrients than the  
115 external concentration showing luxury uptake of nutrients (utilization of non-limiting nutrient exceeding the level  
116 required for growth) (Cherif and Loreau, 2010). Hence, the growth of phytoplankton is described by a function of  
117 internal concentration (Quota model), as shown in Table 2. In addition, it is argued that the growth rate is determined



118 by the most limiting process either photosynthesis or nutrient uptake permitting for switching between the two limiting  
119 processes based on the conditions (Franks P, 2002). Whereas zooplankton functional response is typically modelled  
120 with a simple functional form represented by (HOLLING CS, 1959): Holling Type I with linear function, Holling  
121 Type II with hyperbolic curve like Monod function accounting for saturation; and Holling Type III accounting for  
122 saturation and switching when the prey is low in density (sigmoidal). The zooplankton is considered as the closure  
123 term in plankton models and the zooplankton grazing functional forms impact model outputs greatly. For example,  
124 high oscillations of the states over time (destabilization effect) are determined using type II while steady state  
125 (stability) is easily obtained with type III and no impact on model stability was determined with type I. Phytoplankton  
126 and zooplankton mortality functions ranges from linear to non-linear forms (Tables 3 and 4).

127 Modifications have been also made in the NPZD approaches such as by replacing the bacteria compartment with  
128 chlorophyll-a to enhance the estimation of nitrogen flux (Fennel et al., 2006) and introducing a nitrogen based  
129 nutrient-phytoplankton-heterotroph model which is of intermediate complexity with respect to Fasham &  
130 McGillicuddy models (Fasham et al., 1990; McGillicuddy et al., 1995). The number of compartments has also been  
131 increased including more variables (plankton species as well as nutrients) as seen in Chai and Leonard models which  
132 are based on five and nine compartments NPZD models respectively (Chai et al., 1996; Leonard et al., 1999).  
133 Nevertheless, Galbraith et al. (2009) has developed a model based on NPZD but with Light Iron Nutrients and Gasses  
134 called BLING model, This model can isolate the global impact of iron on maximum light-saturated photosynthesis  
135 rates from photosynthetic efficiency. It considers an implicit representation of phytoplankton which is determined  
136 from the growth rate of phytoplankton. The iron representation doesn't rely on Liebig law of the minimum that is  
137 typical in the biogeochemical models, however, the nutrient-light co-limitation is incorporated in accordance with  
138 field and laboratory measurements of phytoplankton. There have been other extensions of the classical NPZD which  
139 have been applied regionally in (Doney et al., 1996; Fennel et al., 2001; Hinckley et al., 2009; Hood et al., 2003;  
140 Kearney et al., 2020; McCreary et al., 1996; McCreary et al., 2001).

## 141 **2.2 Carbon cycle-based approach**

142

143 In this approach, the marine biota model is introduced into a full ocean carbon cycle model to study the impact of  
144 biology on the oceanic carbon cycle. The carbon cycle model typically includes dissolved inorganic carbon and total  
145 alkalinity components. An example of this approach is the Hamburg model of the oceanic carbon cycle (HAMOCC)



146 developed by (Maier-Reimer and Hasselmann, 1987) which is a pure inorganic carbon cycle model and was utilised  
147 to evaluate both the  $^{12}\text{C}$  cycle and the ocean model residence time properties. The model neglects biological sources  
148 and sinks. Therefore, it has been used as a reference for numerical experiments interpretation with extensions  
149 performed by (Bacastow and Maier-Reimer, 1990; Heinze and Maier-Reimer, 1991; Maier-Reimer, 1993) to include  
150 the marine biota and ecosystem processes. Bacastow & Maier-Reimer (1990) has included the first order  
151 representation of the ocean plankton impacts on the ocean global inorganic oceanic carbon cycle model. While the  
152 first ocean carbon cycle model featuring the representation of marine ecosystem explicitly was given by (Six and  
153 Maier-Reimer, 1996). This latter is based on an extended NPZD model which includes five compartments: single  
154 phytoplankton, single zooplankton, detritus, dissolved organic carbon (DOC), and single nutrient (phosphate).  
155 Equations 5-11 represent the rate of change of nutrients as an example of the carbon components including: DOC and  
156 particulate organic carbon (POC) embedded in the plankton model as described by (Six and Maier-Reimer, 1996).

$$157 \quad R_{C:P} \frac{dN}{dt} = \begin{aligned} & -\text{phytoplankton growth} \\ & +\text{remineralisation from herbivores} \\ & +\text{remineralisation from carnivores} \\ & +\text{DOC degradation} + \text{POC remineralisation} \end{aligned} \quad (5)$$

158 where  $R_{C:P}$  represents the Redfield ratio of carbon to phosphate. Whereas phytoplankton and zooplankton are  
159 described as follows:

$$160 \quad \frac{dP}{dt} = \begin{aligned} & \text{phytoplankton growth} \\ & -\text{loss due to grazing} - \text{natural decay} \\ & -\text{exudation of DOC} \end{aligned} \quad (6)$$

$$161 \quad \frac{dZ}{dt} = \begin{aligned} & \text{zooplankton growth} \\ & -\text{loss due to grazing by carnivores} - \text{DOC excretion} \end{aligned} \quad (7)$$

162 Then, the carbon components (DOC & POC) are modelled as follows:

$$163 \quad \frac{dDOC}{dt} = \gamma_P(P - P_{min}) + \gamma_Z(Z - Z_{min}) - r_{doc}(N)DOC \quad (8)$$

164 where the first term represents the DOC exudation from phytoplankton; the second term represents the DOC excretion  
165 from zooplankton; and the last term represents DOC degradation.



166 
$$\frac{dPOC}{dt} = F(X) - l(O_2) \quad (9)$$

167 where  $l(O_2)$  represents remineralization of POC (for  $X = (d_p, d_z, \epsilon_{her}, \epsilon_{can}, P, Z, z)$  and  $F(X)$  is the flux of dead organic  
 168 carbon to the ocean interior

169  $F(X) = 0$  ; for  $0 < z < 100\text{m}$

170 Otherwise

171 
$$F(X) = TPP \frac{\partial}{\partial z} \left( \frac{z}{100\text{m}} \right)^{-0.8} \quad (10)$$

172 Where TPP is the total particle production including the particles from natural decay as well as fecal pellet production  
 173 in the euphotic zone:

174

175 
$$TPP = \int_0^{100\text{m}} \left( (1 - z_{inges}) (1 - \epsilon_{her}) \text{ growth of zooplankton} \right. \\ \left. + \text{phytoplankton mortality} \right. \\ \left. + (1 - \epsilon_{can}) \text{ zooplankton mortality} \right) \quad (11)$$

Parameter	Symbol
Mortality rate of phytoplankton	$d_p$
Mortality rate of zooplankton	$d_z$
Ingestion as fecal pellets from herbivores	$\epsilon_{her}$
Ingestion as fecal pellets from carnivores	$\epsilon_{can}$
Assimilation efficiency	$z_{inges}$
Phytoplankton	$P$
Zooplankton	$Z$
Nutrient	$N$
Depth	$z$

176

177 The Hadley Centre Ocean Carbon Cycle (HadOCC) model is another example of Carbon cycle-based approach that  
 178 is initially developed for global ocean carbon cycle modelling studies (Cox et al., 2000). The model simulates the  
 179 important aspects of carbonate chemistry, the export and production of biology. Several tracers are included to model  
 180 the carbon cycle including dissolved inorganic carbon, total alkalinity, single nutrient (nitrogen), oxygen, single  
 181 phytoplankton, single zooplankton, as well as detritus (Palmer and Totterdell, 2001).



182 **2.3 Phytoplankton Functional group approach (PFT)**

183

184 This approach includes different plankton functional types (PFTs) making it the most intricate model with at least 15  
 185 state variables relative to the other model approaches (Gregg, 2000; Gregg et al., 2003; Moore et al., 2004; Le Quére  
 186 et al., 2005). The major plankton functional types include mesozooplankton, protozooplankton, diatoms  
 187 (phytoplankton silicifiers), phaeocystis, nitrogen fixers, coccolithophores, picoheterotrophs and each of these groups  
 188 function differently in terms of their roles in biogeochemical cycles (Hood et al., 2006). These functional traits that  
 189 reflect the functions and biochemical pathways are defined by how the cell uses energy and nutrients. The classical  
 190 NPZD doesn't consider these functional types in which the aggregation of taxonomic and functional organisms in  
 191 ocean ecosystems is only considered. Therefore, in the PFTs based approach, species are grouped based on their  
 192 common ecological and biogeochemical functions (Hood et al., 2006; Le Quére et al., 2005). Equations 12-14 present  
 193 the general form of this approach where several phytoplankton types  $P_j$  are nourished by various nutrients  $N_i$  and  
 194 grazed by many zooplankton types  $Z_{ki}$  as follow,

195 
$$\frac{dN_i}{dt} = -\sum_j [\mu_j P_j M_{ij}] + S_{N_i} \quad (12)$$

196 
$$\frac{dP_j}{dt} = \mu_j P_j - m_j^P P_j - \sum_k [g_{jk} Z_{k,i=1}] - \frac{\partial(w_j^P P_j)}{\partial z} \quad (13)$$

197 
$$\frac{dZ_{ki}}{dt} = Z_{ki} \sum_j [\zeta_{jk} g_{jk} M_{ij}] - m_k^Z Z_{ki} \quad (14)$$

Parameter	Symbol
Growth rate of phytoplankton j	$\mu_j$
Matrix of the ratio of element i to currency (which can be phosphorous, nitrogen, etc.)	$M_{ij}$
Sources of tracer $N_i$	$S_{N_i}$
Rate of mortality/excretion of phytoplankton j	$m_j^P$
Grazing of zooplankton k on phytoplankton j	$g_{jk}$
Sinking rate for phytoplankton j	$w_j^P$
Grazing efficiency of zooplankton k on phytoplankton j	$\zeta_{jk}$
Rate of mortality/excretion of zooplankton k	$m_k^Z$

198





199 The common PFTs' models include the European Regional Seas Ecosystem Model versions (1 & 2) : ERSEM I,  
200 ERSEM II (Baretta-Bekker et al., 1997; Baretta et al., 1995; Blackford et al., 2004) which are based on a generic lower  
201 trophic approach developed to study the cycling of carbon as well as nutrients. In ERSEM, the ecosystem is divided  
202 into three functional types in which the biotic groups are classified by their functional role not by species. For instance,  
203 phytoplankton as producers; bacteria as decomposers; zooplankton as consumers which are further subdivided based  
204 on trait-size and uptake of silica to represent a food web. The functional group dynamics are represented by including  
205 population processes such as growth, migration, and mortality as well as physiological processes such as ingestion,  
206 respiration, excretion, and egestion. The phytoplankton groups involve pico-phytoplankton, nano-phytoplankton,  
207 diatoms, and non-siliceous macro-phytoplankton, while zooplankton groups include micro-zooplankton, heterotrophic  
208 nano-flagellates, and meso-zooplankton. The ERSEM model was initially applied to the North Sea to study the  
209 seasonal cycling of nutrients (N, P, S, C). A further modification has been made to the ERSEM to produce another  
210 version called Biogeochemical Flux Model (BFM). This latter accounts for the Chemical Functional Families (CFFs)  
211 in the state variables. The CFFs is split into living, non-living, and inorganic states (Vichi et al., 2007).

212 The Pelagic Interactions Scheme for Carbon and Ecosystem Studies (PISCES) model is another example of PFTs  
213 based model that is a modified version of HAMOCC considering 24 state variables including  $\text{NO}_3$ ,  $\text{NH}_4$ ,  $\text{PO}_4$ ,  $\text{SiO}_2$ ,  
214 Fe; small phytoplankton, large phytoplankton, small zooplankton, large zooplankton, DOM, small detritus, and large  
215 detritus (O. Aumont et al., 2003). PISCES model has been extensively used to study several ecosystems and widely  
216 applied in more than hundred studies that are based on this approach either directly or indirectly (Aumont et al., 2015).  
217 Likewise, the NASA Ocean Biogeochemical Model (NOBM) is another type of PFTs based model originally coupled  
218 to the Ocean-Atmosphere Spectral Irradiance Model (OASIM) (Gregg, 2001; Gregg et al., 2009). NOBM comprises  
219 of four phytoplankton groups, four nutrient groups (nitrate, regenerated ammonium, silica, and iron), a single  
220 zooplankton group, and three detrital pools (organic material storage, sinking, and remineralization) (Gregg, 2000;  
221 Das et al., 2019; Gregg et al., 2003; Gregg and Casey, 2007; Trull et al., 2018) (Gregg, 2001) (Gregg et al., 2003).  
222 Additionally, the PlankTOM biogeochemical model is a dynamic ocean model describing lower trophic level of  
223 marine ecosystems. This model has several extensions through varying in the number of PFTs resolved. For example,  
224 six PFTs: diatoms, coccolithophores, mixed phytoplankton, bacteria, protozooplankton and meso-zooplankton are  
225 included in PlankTOM6 (Le Quéré et al., 2005). However, additional PFTs such as nitrogen fixers, Phaeocystis,  
226 picophytoplankton and macro-zooplankton are added into PlankTOM10 (Buitenhuis et al., 2013) to evaluate the



227 interactions between climate and ocean biogeochemistry with the wide use of data synthesis for parametrizations of  
228 the PFTs growth rates (Kwiatkowski et al., 2014). PlankTOM resolves the cycle of carbon (C), nitrogen (N), oxygen  
229 (O), phosphorous (P), Silicon (Si), iron (Fe) cycle, three types of organic detritus, air sea fluxes of CO<sub>2</sub>, O<sub>2</sub>, Dimethyl  
230 sulphide (DMS) and N<sub>2</sub>O.

231 Moreover, the Model of Ecosystem Dynamics, nutrient Utilization, Sequestration and Acidification (MEDUSA) is  
232 developed by (Yool et al., 2011, 2013) is a model of intermediate complexity, constructed beyond the standard NPZD  
233 formulations. The biogeochemical cycles of iron, silicon, and nitrogen as well as small and large plankton size classes  
234 are included in this model. In this specific model, an explicit representation of internal chlorophyll quotas is included  
235 to allow for light acclimation. The key focus of MEDUSA is the biological sequestration of carbon in the deep ocean.  
236 The model is developed to study the biogeochemical response particularly of the so-called biological pump to human-  
237 induced driven change in the global ocean. Nevertheless, the tracers of phytoplankton with allometric zooplankton  
238 (TOPAZ) model is based on the interactions between the biogeochemical and the carbon cycles including two  
239 dissolved organic matter forms, dissolved inorganic species for coupled carbon (C), nitrogen (N), Phosphorous (P),  
240 Silica (S), Iron (Fe), calcium carbonate (CaCO<sub>3</sub>), dissolved oxygen (O<sub>2</sub>) heterotroph, lithogenic cycling. Additionally,  
241 processes such as gas exchange, scavenging, atmospheric deposition, denitrification and nitrogen fixation, sediment  
242 processes, and river inputs were included (Dunne et al., 2010). This model has been implemented in several studies  
243 such as (Bronse laer et al., 2020; Jung, et al., 2019; Sharada et al., 2020). The extended version of TOPAZ is the  
244 Carbon, Ocean Biogeochemistry and Lower Trophics (COBALT) which was developed to improve the planktonic  
245 food web dynamics resolution to examine the influence of climate on the flow of energy from phytoplankton to fish  
246 (Stock et al., 2014). The planktonic food web representation in TOPAZ is highly idealized including an implicit  
247 representation of zooplankton and bacteria hence, an implicit modelling of the impacts of these groups on  
248 phytoplankton and biogeochemical processes were applied. Therefore, these limitations were addressed in COBALT  
249 by including three explicit zooplankton groups, bacteria with a mechanistic parametrizations of the impacts of these  
250 groups on biogeochemistry (Stock et al., 2014b). COBALT has resolved the global scale cycles of nitrogen, carbon,  
251 phosphate, silicate, iron, calcium carbonate, oxygen and lithogenic material where small and large phytoplankton are  
252 involved. Nevertheless, DARWIN biogeochemical model is a more complex PFTs based model consisting of 78  
253 phytoplankton types, heterotrophs, organic and inorganic forms of nitrogen, phosphorous, iron, and silica. This model  
254 was developed first to study the phytoplankton distribution especially for the cyanobacterium *Prochlorococcus* species



255 by (Follows et al., 2007). The model was coupled with the general circulation model in (Wunsch and Heimbach,  
256 2007) and was initially applied for the global distributions of phytoplankton and physiological traits. It has been  
257 applied in a followed study which has considered more biogeochemical components and enhancement of optical  
258 properties (Dutkiewicz et al., 2015; Lo et al., 2019). Nonetheless, Regulated ecosystem model (REcoM) based on  
259 functional group approach (two phytoplankton group: diatoms and nanophytoplankton; one class of zooplankton) is  
260 based on the Quota model in which the internal phytoplankton cells stoichiometry is affected by the conditions of  
261 temperature, light, and nutrients (Schourup-Kristensen et al., 2014). REcoM has also been commonly used in the  
262 Southern Ocean studies (Hauck and Völker, 2015; Losch et al., 2014; Taylor et al., 2013).

263 The complexity of the aforementioned PFTs models depends on number of the independent elements along with the  
264 number of PFTs considered. As regards the PFTs, simple models include one PFT which is of single phytoplankton  
265 and single zooplankton such as in HadOCC (Palmer and Totterdell, 2001). Simple models can also include two to  
266 three PFTs such as MEDUSA (Yool et al., 2013) and PISCES (Aumont et al., 2015). However, as the number of PFTs  
267 increases, the complexity of the model increases as well. As for the average elemental composition of particulate  
268 matter, it is constrained in the sea despite of the variations in the carbon to chlorophyll (C/Chl) ratios (Anugerahanti  
269 et al., 2021). The commonly used average proportion of the main elements in phytoplankton is: 106 C (carbon): 16 N  
270 (nitrogen): 1 P (phosphorous) (by atoms) and these proportionalities are termed as Redfield ratios (Redfield, 1933).  
271 Generally, adding complexity to the model doesn't necessarily improve the model skill, as has been proven in several  
272 studies which compare models with different complexities (Friedrichs et al., 2007; Kriest et al., 2010; Kwiatkowski  
273 et al., 2014; Ward et al., 2013; Xiao and Friedrichs, 2014).

### 274 **3 Determination of the biochemical parameters**

275

276 The aforementioned models have been applied to resolve the biochemical properties including Chlorophyll-a,  
277 Macronutrients (N,P,S), Micronutrients (Fe), Carbon and Oxygen in different ecosystems. Detailed assessments of  
278 the capabilities of these models are provided here and summarized in Table 5,

#### 279 **3.1 Chlorophyll-a**

280

281 Chlorophyll-a concentrations have been determined using the models described above, however, the PFTs based  
282 models are found to offer more accurate estimates of Chlorophyll-a concentrations by distinguishing the



283 phytoplankton types. The PFT based model PlankTOM, for instance, was used to evaluate the role of grazing versus  
284 iron limitation in the low chlorophyll content (HNLC) areas of the Southern Ocean (Le Quéré et al., 2016). The  
285 PlankTOM was able to produce reasonable surface chlorophyll-a estimates with correlation coefficient ( $r$ ) around 0.8  
286 especially in the summer season when the macro-zooplankton grazing was explicitly involved. PlankTOM5.3 has  
287 shown large improvements of the interannual variation of surface chlorophyll-a relative to PlankTOM5.2 in the global  
288 oceans (with residual sum of squares RSS = -13%) (Buitenhuis et al., 2013) by including a new photosynthesis  
289 formulation with a representation of iron-light colimitation (Geider et al., 1998) in their fixed stoichiometry model.  
290 PlankTOM10 was also compared to PlankTOM6 and applied in the Southern Ocean (Le Quéré et al., 2016). This new  
291 version has similar formulations to the previous versions of the model except that it included more phytoplankton  
292 groups. Both models exhibit similar results for the surface chlorophyll-a concentrations ( $r \sim 0.8$ ), primary and export  
293 production except that PlankTOM6 was unable to reproduce the observed low chlorophyll-a contents in summer  
294 season in the Southern Ocean due to slightly deeper mixed-layer depth in the summertime. Overall, PlankTOM10 has  
295 shown slightly better performance than PlankTOM6 in terms of surface chlorophyll-a distribution (bias% = 1.2%),  
296 whereas the distribution of surface nutrients has been slightly lower by 5% and 2.5% for nitrogen and silica (except  
297 for phosphate which shows similar performance  $r \sim 0.9$ ). Other PFTs based models including ERSEM, DARWIN,  
298 TOPAZ, PISCES, BLING and NOBM have been applied to study chlorophyll-a distribution in the surface and deep  
299 oceans. ERSEM has been applied to study chlorophyll-a dynamics in the Mediterranean and has shown good  $r$  value  
300 of 0.64 for the spatial distribution of the simulated and observed chlorophyll-a. However, a relatively larger bias with  
301 root mean square difference (RMSD) of 0.78 was obtained for the annual mean spatial variability due to the absence  
302 of cyclonic gyres of the Rhodes and South Adriatic causing intermittent blooms. In addition, the PFTs based model  
303 DARWIN coupled with MITgcm in (Dutkiewicz et al., 2015) apprehended large spatial variability in chlorophyll-a  
304 for the global oceans with low  $r$  around 0.55 and have shown overestimation in particularly the Southern Ocean and  
305 higher latitudes. DARWIN was customized to study phytoplankton distribution in the Southern Ocean (Lo et al.,  
306 2019) which has included the abundance of coccolithophores which was improved through increasing the affinity for  
307 nutrients as well as coccolithophores grazing control. Two distinct size classes of diatoms (small & large) were added,  
308 and two different life stages were considered for Phaeocystis (single cell vs colonial). The improvements have  
309 increased the agreement between the simulated coccolithophores and diatoms with the in-situ data. However, the  
310 model inaccurately has simulated diatoms and haptophytes in the Ross Sea and has overestimated the small non-



311 silicified phytoplankton with general mean absolute error for diatoms and haptophytes are  $0.74 \text{ mg m}^{-3}$  and  $0.22 \text{ mg}$   
312  $\text{m}^{-3}$  respectively. This inconsistency can be attributed to inaccuracy in representing PFT phenology and distribution.  
313 Representation of co-existence within coccolithophores and Phaeocystis remains a challenge and any small changes  
314 in DARWIN physiological parameters led to either Phaeocystis or coccolithophores loss. In addition, the sea-ice algae  
315 representation has not been explicitly represented which may not work well in region where ice exists.

316 Concentrated Chlorophyll-a condition (i.e., Phytoplankton blooms) was also captured in the middle latitudes of the  
317 Northern and Southern Hemispheres as well as in the tropical Pacific by both models (NEMO-TOPAZ and NEMO-  
318 PISCES) indicating El Niño-Southern Oscillation (ENSO) condition. Both models showed an overall  $r$  between 0.6-  
319 0.9 across all oceans. While the zonal averaged Chlorophyll-a was overpredicted (by  $\sim 67\%$ ) from  $30^\circ\text{N}$  to  $45^\circ\text{N}$  in  
320 both models especially in the Pacific Ocean east of Japan which is due to mainly an error in the Kuroshio Current path  
321 seen in low resolution models (Jung et al., 2019a). The physical model NEMO has simulated a relatively thicker mixed  
322 layer which in turn simulated bigger spring blooms in this area creating a positive bias in Chlorophyll-a values in the  
323 mid-latitudes of the Northern Hemispheres in biogeochemical models.

324 In contrast, underestimation of surface Chlorophyll-a in the equatorial Atlantic Ocean (bias  $\sim -0.2 \mu\text{g kg}^{-1}$ ) and the  
325 Arabian Sea (bias  $\sim -0.4 \mu\text{g kg}^{-1}$ ) was also found in both models and these two areas encountering mesoscale and sub-  
326 mesoscale processes impacting the biogeochemistry. NEMO-PISCES with the use of higher resolution grid than the  
327 one used in (Jung et al., 2019a) presented better Chlorophyll-a distribution in the Arabian Sea with an average value  
328 of  $\sim 1.3 \text{ mg Chl m}^{-3} \text{ d}$  (Koné et al., 2009). Although both models overpredicted the surface chlorophyll-a in the  
329 Southern and tropical Pacific (STD  $\sim 0.26 \mu\text{g kg}^{-1}$ ), the NEMO-TOPAZ showed a larger bias over the equator (STD  $\sim$   
330  $0.22 \mu\text{g kg}^{-1}$ ) for the surface Chlorophyll-a than PISCES-NEMO which is proved to be caused by the high atmospheric  
331 iron deposition in TOPAZ, which is then replaced with PISCES data resulting in lowering the bias for surface  
332 Chlorophyll-a. Hence, sensitivity experiments on atmospheric iron deposition can be a good task to improve the  
333 surface chlorophyll-a distributions in simulations.

334 Similarly, the PFTs based model NOBM was able to predict surface Chlorophyll-a level ( $r > 0.7$ ) in global oceans  
335 (Gregg et al., 2003). However, the correct species abundance was not well identified by the model due to disparities  
336 between the model and observations in particular the Indian Ocean where the observations were mainly concentrated  
337 in the Arabian Sea (the model is modestly dominated by diatoms whereas observations are dominated by



338 cyanobacteria). This might have caused by the strong upwelling in the model thus increasing nutrients concentrations  
339 which trigger faster growing organisms such as diatoms.

340 Nevertheless, BLING-NEMO coupled model was used to study the high Chlorophyll-a levels (i.e. blooms)  
341 (Castro de la Guardia et al., 2019) in which the spring bloom in the Barents Sea (BS) was underestimated by 1.7 mg  
342 chl m<sup>-3</sup> while the autumn bloom underpredicted by 0.7 mg chl m<sup>-3</sup>. This deviation might be attributed to the lack of  
343 nutrients from riverine input by the BLING-NEMO coupled model. Whereas the concentration representing the spring  
344 and autumn bloom in the Labrador Sea (LS) has shown an agreement with the observed seasonality, which is  
345 comparable to that of the satellite data. However, the Chlorophyll-a content is slightly overestimated by 0.2 mg chl  
346 m<sup>-3</sup> during February-April due to an earlier start of the spring bloom in the simulation. Furthermore, the BLING-  
347 NEMO model has mistakenly predicted the spring blooms in March instead of April in the Hudson Bay (HB) and  
348 Baffin Bay (BB). In these two bays, the spring bloom was slightly overpredicted by 0.5 mg chl m<sup>-3</sup> and ~ 0.3 mg chl  
349 m<sup>-3</sup> in the BB and HB respectively. This discrepancy might be attributed to the underprediction of sea ice  
350 concentration.

351 Chlorophyll-a has been also derived by the carbon cycle and simple NPZD models. For example, the carbon cycle  
352 based model: HAMOCC5 was able to reproduce Chlorophyll-a with a value of 0.05 mg Ch m<sup>-3</sup> in the oligotrophic  
353 subtropical gyres (Aumont et al., 2003) with a bias of 0.24 mg chl m<sup>-3</sup>. Unlike the earlier version of the model  
354 (HAMOCC3.1) which has shown a higher concentrations of Chlorophyll-a compared to observation in these regions  
355 (Six and Maier-Reimer, 1996). This version of HAMOCC5 is an extension of HAMOCC3.1 (Six and Maier-Reimer,  
356 1996) with the inclusion of iron and silicate limitation along with the phosphate. HAMOCC5 with its coarse resolution  
357 cannot resolve the coastal upwellings in productive regions such as Peru upwelling. The improvement of the  
358 HAMOCC was mainly in making the Chl: C ratio variable which is decreasing in the centre of the subtropical gyres  
359 to values about 1:150 while in HAMOCC3.1 this ratio remained constant at 1:60. Therefore, this model with this  
360 improvement as well as iron and silicate limiting nutrients inclusion improved the representation of chlorophyll-a  
361 content in subtropical gyres (around 0.2-0.25 mg m<sup>-3</sup>).

362 As for the simple NPZD models, they have shown a better representation of chlorophyll-a when coupled to a high-  
363 resolution physical model as well as including correct physics representations. For example, the involvement of tides  
364 in ROMS in (Fennel et al., 2008) has improved the chlorophyll-a representations over Georges Bank which was not



365 presented in the previous model (Fennel et al., 2006). The same model of (Fennel et al., 2008) was improved by adding  
366 dissolved organic matter (DOM) module along with the other model components (Druon et al., 2010) to study the  
367 DOM dynamics in the Northeastern U.S. continental shelves which showed a well agreement of high chlorophyll-a  
368 concentrations with the satellite data particularly in the inner shelf and on Georges Bank as a result of the tidal mixing  
369 and continuous nutrient supply (Bias: chlorophyll-a (with DOM) = 4 mg chl m<sup>-3</sup>, chlorophyll-a (without DOM) = 6  
370 mg chl m<sup>-3</sup>).

### 371 **3.2 Macronutrients (N, P, S)**

372

373 Nutrients such as nitrate, phosphorous, and silica have been well represented by several biogeochemical models  
374 (Aumont et al., 2015; Das et al., 2019; Dutkiewicz et al., 2015; Jung et al., 2019b; Lachkar et al., 2019; Pant et al.,  
375 2018; Le Quéré et al., 2016; Sankar et al., 2018). The PFTs based models such as PISCES-NEMO, DARWIN-  
376 MITgcm, and TOPAZ-NEMO have shown well representation of surface nutrients distribution in the global oceans  
377 with  $r$  ( $> 0.9$  for P and N;  $\sim 0.85$  for S),  $> 0.9$  for all nutrients, and  $> 0.95$  for all nutrients respectively. Both TOPAZ  
378 and PISCES have represented: (i) similar distribution of nutrients over global oceans, (ii) an overestimation in the  
379 Southern Pacific Ocean bias of  $\geq 4.5 \mu\text{mol kg}^{-1}$ ,  $\sim 0.32 \mu\text{mol kg}^{-1}$ , and  $\geq 16 \mu\text{mol kg}^{-1}$  for nitrate, phosphate, and  
380 silicate respectively, (iii) higher positive bias of nitrate ( $\geq 0.16 \mu\text{mol kg}^{-1}$ ) and silicate ( $\geq 8 \mu\text{mol kg}^{-1}$ ) in the central  
381 and southern Pacific, and the Southern Ocean and (iv) underprediction of phosphate (bias  $\sim -0.8 \mu\text{mol kg}^{-1}$ ) at the  
382 middle and higher latitudes in the Northern Hemisphere (Jung et al., 2019). The discrepancies in both models can be  
383 attributed to the low resolution, weak North Atlantic deep waters, and strong ventilation in the Antarctica waters.  
384 However, the improvement of the optical constituents by increasing the absorption of the optical constituents resulting  
385 in a reduction in the size of oligotrophic regions in the subtropical gyres could be a solution as proposed by  
386 (Dutkiewicz et al., 2015) using DARWIN-MITgcm. This has led to an enhancement of lateral nutrients supplies caused  
387 by a decrease of productivity in high latitude. Furthermore, skill assessment of 21 regional and global coupled  
388 biogeochemical models based on functional group approach including (PISCES, PlankTOM, COBALT, TOPAZ,  
389 HAMOCC, BIOMASS, MEDUSA, ERSEM, PELAGOS, PISCES, NOBM) were conducted for the Arctic region  
390 studies in order to investigate the capability of these models in representing the observed nitrate, mixed layer depth,  
391 as well as euphotic layer depth. Most of the models have shown positive bias for the depth averaged nitrate explaining  
392 the overestimation of nitrate in the upper layer ( $r \leq 0.68$ ) and none of these models were able to well represent the



393 variability in the field measurements. However, RECoM is applied and has shown to have a good performance for  
394 DIN and silicate ( $r = 0.75$ ) when coupled to a high resolution setup in the Arctic regions (Schourup-Kristensen et al.,  
395 2018).

### 396 **3.3 Micronutrients (Fe)**

397

398 Low iron concentrations were simulated in the North and North Central Pacific, North Atlantic, and Antarctic whereas  
399 in the North and Equatorial Indian and North Central Atlantic high levels were predicted using NOBM. The  
400 overestimation has resulted in  $r \sim 0.86$  and the reason of the iron overprediction is attributed to the lack of scavenging,  
401 excessive remineralization, and slow detritus sinking rate. However, PISCES-NEMO has shown a significant  
402 underestimation for the spatial variability of iron in the global ocean with  $r = 0.75$  suggesting a need to increase or  
403 make the sediment source of iron highly variable since it is too small in the model (Aumont et al., 2015). It is also  
404 suggested that iron supply to the surface layer is highly driven by eddies using a simplified version of DARWIN  
405 biogeochemical model of two species as described in (Dutkiewicz et al., 2009) coupled to a flat bottom zonally re-  
406 entrant MITgcm model (Uchida et al., 2019). So, a better representation of the iron fluxes in the Southern Ocean  
407 requires correct energetics of the mesoscale field which can be done by resolving and parametrizing the inverse energy  
408 cascade caused by baroclinic instabilities of meso and sub-mesoscale (Person et al., 2019). Hence, (Jiang et al., 2019)  
409 applied a modified version of Chai model coupled to ROMS which involved two phytoplankton groups (small  
410 phytoplankton and diatoms), two zooplankton groups (micro and meso zooplankton), nutrients (nitrogen, silicate,  
411 iron) indicating that dominant iron sources in the Scotia Sea are derived from sediments in the Antarctic Peninsula  
412 shelf along with the South Orkney Plateau. In addition to these sources, the Antarctic Circumpolar Current, the  
413 northern side of the Weddell Gyre, upwelling, atmospheric dust deposition, and icebergs are the common sources of  
414 iron in the Southern Ocean (Jiang et al., 2019). The iron levels estimated by the modified Chai model have shown an  
415 average overestimation by 0.26 nM deviated from the observed average value of 0.35 nM resulting in  $r = 0.76$ .

### 416 **3.4 Carbon**

417

418 Ocean carbon has been derived in different forms including the particulate organic and inorganic carbon (POC,  
419 PIC), partial pressure of CO<sub>2</sub> (pCO<sub>2</sub>) and dissolved inorganic carbon (DIC). A representation of the variable POC  
420 reactivity evolved from reactive continuum model suggested by (Boudreau and Ruddick, 1991) and was introduced





421 in PISCES with a coarse resolution NEMO for the global oceans (Aumont et al., 2017). With the POC introduction  
422 into the model, the POC levels in the ocean's interior increased by 1 to 2 orders of magnitude which has resulted from  
423 the slow sinking of small particles from the surface. In addition, an increase of higher than a factor of 2 of the carbon  
424 reaching the sediments has been attained showing better agreement with observations with Root Mean Squared Error  
425 (RMSE) of 0.14 (without continuum reactivity), and 0.08 (with continuum reactivity). In addition, PISCES-MITgcm  
426 has been used to qualitatively study the carbon cycle in the Arctic Ocean showing the capability in capturing the  
427 observed seasonal and regional trends of the dissolved pCO<sub>2</sub> (Manizza et al., 2011). However, the spring surface  
428 pCO<sub>2</sub> in the Canadian Archipelago is underestimated (~300 μatm) relative to observations (400-450 μatm) but able  
429 to capture the summer levels (200-250 μatm). The riverine POC and the impact of terrestrial carbon resulted from  
430 coastal erosion were neglected in the model hence caused the underprediction of carbon balance. Additionally, the  
431 sedimentation and resuspension processes were neglected by the model which may be important in the enrichment of  
432 the water column with carbon hence impacting air-sea gas exchange. In addition, the modelled surface DIC by  
433 PISCES-NEMO was comparable to observations with r of 0.91 (Aumont et al., 2015). With regard to the comparison  
434 conducted between PISCES-NEMO and TOPAZ-NEMO (Jung et al., 2019) for the surface DIC, TOPAZ-NEMO has  
435 represented similar agreement with observation (r > 0.95), and the zonal averaged surface content is better represented  
436 by TOPAZ-NEMO in the Northern Hemisphere (bias < 10 μmol kg<sup>-1</sup>). Similarly, compared to observations lower  
437 bias is shown for surface alkalinity by TOPAZ-NEMO than that of PISCES-NEMO in all oceans (e.g. Southern  
438 Hemisphere: negative bias ~ 80 μgmol kg<sup>-1</sup>, Equator: positive bias, mainly ≤ 16 μmol kg<sup>-1</sup>, Indian Ocean: negative  
439 bias, mainly < 32 μmol kg<sup>-1</sup>, Pacific: positive bias, mainly ≤ 16 μmol kg<sup>-1</sup>, Atlantic: negative bias, mainly < 64 μmol  
440 kg<sup>-1</sup>)

### 441 **3.5 Oxygen**

442

443 Surface oxygen level was estimated in the global oceans by PISCES-NEMO which has resolved the oxygen  
444 distribution with r ~ 0.97 because oxygen reach closely to its solubility level and hence is constrained by sea surface  
445 temperature (Aumont et al., 2015). Moreover, TOPAZ and PISCES coupled to NEMO (Jung et al., 2019) have shown  
446 comparable spatial distributions (r ~0.98) and zonal averages of surface dissolved oxygen (DO) to the observed data  
447 for DO in the global oceans but the overall was underestimated by TOPAZ (bias ~ -10 μmol kg<sup>-1</sup>) and a slight



448 overprediction of DO (bias  $\sim 10 \mu\text{mol kg}^{-1}$ ) was observed by PSICES except in polar regions. Because in polar regions  
449 (areas at  $60^\circ\text{N}$  or higher) the availability and quality of satellite data is limited.

450 Both models have shown negative bias ( $\sim 25 \mu\text{mol kg}^{-1}$ ) in deep waters which was caused by the weak North Atlantic  
451 deep waters represented by the physical model. TOPAZ-NEMO has also shown a better representation of the oxygen  
452 minimum zone in the Pacific Ocean. ERSEM coupled to a 1D Princeton/Mellor–Yamada and GOTM physical models  
453 respectively were also implemented to study the global oxygen minimum zone. ERSEM-Princeton/Mellor–Yamada  
454 lacks horizontal advective processes which could be enhanced through considering the diurnal physical processes  
455 while ERSEM-GOTM ignores the episodic intrusion of oxygen within the oxygen minimum zone (Sankar et al., 2018)  
456 (Sankar et al., 2018) (Blackford and Burkill, 2002). Thus, the models have shown contradictions between the estimates  
457 and climatological seasonal cycles of oxygen at depths which might be attributed to the lack of lateral circulation in  
458 the model. Further studies on the oxygen minimum zone in the Arabian Sea were conducted by (Lachkar et al., 2017,  
459 2019, 2020) using Fasham model coupled to ROMS indicating that the primary productivity and oxygen minimum  
460 zone are highly impacted by monsoon wind intensification with an overall high  $r \sim 0.93$  for oxygen (both seasons) in  
461 the upper layer. Nevertheless, the model was incapable of resolving the full eddy spectrum because the resolution was  
462 overly coarse. The model has considered the nitrogen as a limiting nutrient neglecting iron, phosphate, and silicate  
463 which are the major nutrients limiting phytoplankton growth which may have led to amplify the impact of  
464 denitrification on the nitrogen budgets in the Arabian Sea (Lachkar et al., 2017) thus overpredicting the oxygen  
465 minimum zone.

466

## 467 **5 Conclusions**

468

469 This review presents the common biogeochemical models applied on various ecosystems of the world's ocean. These  
470 models are evaluated through reviewing the studies that have been conducted to estimate biochemical parameters such  
471 as chlorophyll-a, nutrients as well as carbon and oxygen components. Therefore, applications of biogeochemical  
472 models on different ecosystems have shown different performances depending on the complexity of these ecosystems  
473 and the governing equations. PFT's model approach has proven to be a good estimate of surface nutrients such as  
474 nitrogen (N), phosphorous (P), and silica (S) in global oceans with  $r \geq 0.85$ ,  $\geq 0.9$ , and  $\geq 0.78$  with some



475 inconsistencies apparent if coupled with the low-resolution physical component. NPZD models, for example Fasham,  
476 are capable of accurately estimating N, P, and oxygen (O) with  $R^2 > 0.9$  (for N, P), and  $> 0.9$  (for O) in the Indian and  
477 Pacific ecosystems. In contrast, the most effective prediction of iron with  $r$  is obtained between 0.7 and 0.86,  
478 particularly for models using the functional group approach. In comparison, the reported performance for chlorophyll-  
479  $a$  varies between models and  $r$  can range from 0.55 to 0.9. These varying reported performances for these  
480 biogeochemical parameters are dependent on the features of the ecosystems and reliability of the physical model.  
481 Therefore, when developing the biogeochemical model, it is necessary to take into consideration the most appropriate  
482 physical models.

#### 483 **6 Author contribution**

484 Kaltham Ismail and Maryam R. Al Shehhi defined the content of the manuscript. Kaltham Ismail prepared the  
485 manuscript and Maryam R. Al Shehhi contributed in revisions and improvements.

#### 486 **7 Competing interests**

487 The authors declare no conflict of interest.

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777 Table 1. Typical functional forms of phytoplankton response to irradiance  $I$ . These functional forms can be multiplied  
 778 by the maximum photosynthesis rate termed as  $P_{\max}$  in some processes. Adapted from (Franks P, 2002).

Functional Form	Definition
$\frac{I}{I_o}$	Linear response to incident light
$\frac{I}{I_o + I}$	Saturating response
$1 - \exp\left(-\frac{I}{I_o}\right)$	Saturating response
$\tanh\left(-\frac{I}{I_o}\right)$	Saturating response
$\frac{I}{I_o} \exp\left(1 - \frac{I}{I_o}\right)$	Saturating and photo-inhibiting response. $I_o$ represent the maximum photosynthesis rate.

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780 Table 2. Some of the commonly used functional forms of phytoplankton nutrient uptake. Adapted from (Leles et al.,  
 781 2016)

Functional Form*	Description
$\frac{V_{\max} \cdot N}{k + N}$	Michaelis-Menten/Monod; hyperbolic
$\mu_{\max} \frac{1 - \frac{Q_{\min}}{Q}}{1 - \frac{Q_{\min}}{Q_{\max}}}$	Quota Curve; hyperbolic
$\mu_{\max} \frac{Q - Q_{\min}}{(Q - Q_{\min}) + K}$	Quota Curve; rectangular- hyperbolic
$\mu_{\max} \frac{(1 + KQ) \cdot (Q - Q_{\min})}{(Q - Q_{\min}) + KQ \cdot (Q_{\max} - Q_{\min})}$	Normalized Quota equation; rectangular-hyperbolic

782 \*  $V_{\max}$ : maximum utilization rate of nutrient;  $k$ : affinity constant for nutrient uptake;  $Q_{\min}$ : minimum nutrient quota;  
 783  $Q_{\max}$ : maximum nutrient quota;  $Q$ : nutrient quota;  $K$ : half saturation constant for quota curve.

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788 Table 3. some of the commonly used functional forms of phytoplankton zooplankton grazing. Adapted from: (Leles  
 789 et al., 2016)

Functional Form*	Description
$a \cdot P$	Holling Type I: linear
$\frac{a \cdot P}{1 + a \cdot h \cdot P}$	Holling Type II: Hyperbolic
$\frac{I_{max} \cdot P}{k_1 + P}$	Michaelis-Menten/Monod Hyperbolic
$\frac{a \cdot P^2}{1 + a \cdot h \cdot P^2}$	Type III: sigmoidal
$\frac{I_{max} \cdot P^2}{k_1^2 \cdot P^2}$	Michaelis-Menten/Monod Sigmoidal
$\frac{a_i \cdot P_i}{1 + \sum_1^n a_r \cdot h_r \cdot P_r}$ where n is the number of preys	Type II; hyperbolic. multiple preys
$\frac{I_{max} \cdot \sum C_{pi}}{k_1 + \sum C_{pi}}$ where $C_{pi} = C_{ri} \cdot P_i$	Monod; hyperbolic; prey selectivity

790 \***a**: attack rate; P = phytoplankton availability; h = handling time;  $I_{max}$ : maximum ingestion rate;  $k_1$ : half saturation  
 791 constant for ingestion; i: subscript for prey type; r = subscript relative to prey type weight;  $C_{pi}$ : potential capture rate;  
 792  $C_{ri}$ : capture rate.

793

794 Table 4. Some of the functional forms for mortality rate of both phytoplankton and zooplankton. Adapted from:  
 795 (Franks P, 2002; Leles et al., 2016)

Functional form of i(P)	Description
$m$	Linear
$mP$	Quadratic non- linear
Functional form of j(Z)	Description
$m \cdot Z$	Linear
$\frac{m \cdot Z}{k_2 + Z}$	Hyperbolic
$\frac{m \cdot Z^2}{k_2^2 + Z^2}$	Sigmoidal
$\frac{m \cdot Z \cdot c}{k_2 + Z \cdot c}$	Hyperbolic- intraguild predation

796 **m**: mortality rate of zooplankton;  $k_2$ : half saturation constant for zooplankton closure term; **c**: zooplankton fraction  
 797 foe which closure terms acts.



798 Table 5. Biochemical models applied in the global ocean ecosystems including performance, physical  
 799 model and model resolution.

Ocean	Model approach	Resolution (grid size)	Key biochemical variables <sup>a</sup>	Physical model	Performance <sup>b</sup>	Ref.
Global	Moore	2-D global grid (100 X 116 grid-points); Longitudinal resolution of 3.6° and variable latitudinal resolution from 1–2° with higher resolution near the equator	Fe	NCAR	Bias: Fe = 265 pM (July-North Pacific) Fe = 14 pM (June-Equatorial Pacific) Fe = 121 pM (May-North Atlantic) Fe = 4514 pM (September/August-Arabian Sea) Fe = 2362 pM (November-Southern Ocean)	(Moore et al., 2001)
Global	NOBM	3-D; 2/3° latitude and 1.25° longitude with 14 layers	Fe, Chl-a	GCM	Fe: $r = 0.86$ & $R^2 = 0.74$ chl-a: $r > 0.7$	(Gregg et al., 2003)
Global	HAMOCC5	3-D; horizontal resolution is uniformly 3.5 by 3.5 degrees with 22 vertical layers	Fe, Chl-a	LSG	Bias: Fe = 0.15 nM (at depth of 3000 m) chl-a = 0.24mg/m <sup>3</sup>	(Aumont et al., 2003)
Global	ERSEM	1-D water column	Chl-a	GOTM	-	(Blackford et al., 2004)
Global	Moore	3-D 100 X 116 horizontal grid points with a resolution of 3.6° longitude and 0.9°-2° latitude	Fe	CCSM	Refer to Moore et al., 2001	(Moore et al., 2004)
Global	Moore	3-D; 3.6° in longitude; 0.9°–2° degree in latitude	IC, Fe	NCAR CCSM3	Refer to Moore et al., 2001	(Moore et al., 2006)
Global	Moore	3-D; 3.6° in longitude and 0.8° to 1.8° latitude and 25 levels in the vertical	Fe	CCSM	Refer to Moore et al., 2001	(Moore & Doney, 2007)



Global	PlankTOM	3-D; 2° in longitude, 1.1° average in latitude with 31 vertical levels	Chl-a	NEMO	RSS = -13%	(Buitenhuis et al., 2013)
Global	PISCES	3-D; 2° by 2°cosΦ (where Φ is the latitude) with a focusing of the meridional resolution to 0.5° in the equatorial domain. 30 vertical layers	IC, P, N, Fe, Alk, O, S	NEMO	r: C = 0.91 P = ~0.91 N = 0.95 Fe = 0.75 Alk = ~0.8 O = 0.97 S = ~0.85	(Aumont et al., 2015)
Global	DARWIN	3-D; horizontal resolution of 1° x 1° with 23 levels	P, N, S, Chl-a	MITgcm	r: P,N,S > 0.9 Chl-a ~ 0.55	(Dutkiewicz et al., 2015)
Global	PlankTOM	3-D; zonal resolution of 2° and a meridional resolution of 2°×cos(latitude) with 30 z levels	O	NEMO	-	(Andrews et al., 2017)
Global	PISCES	3D; 2° by 2°cos(φ) (where φ is the latitude) with an increased meridional resolution to 0.5° in the equatorial domain. 30 vertical layers	POC	NEMO	RMSE: No Reactivity Continuum (RC) = 0.14 With RC = 0.08	(Aumont et al., 2017)
Global	Moore	2-D; horizontal resolution of 0.27°–0.53°	S, N, P, O, DIC flux, Chl-a	NCAR-CSM1	r: S = 0.8 N = 0.95 P = 0.92 O = 0.85 DIC = 0.75 Chl-a = 0.6 (Doney et al., 2009)	(Pant et al., 2018)
Global	Moore	3D; 60 vertical levels, was run at the nominal one-degree resolution	IC & coccolithophores	CESM	Refer to Moore et al., 2001	(Krumhardt et al., 2019)
Global	TOPAZ & PISCES	3-D; horizontal resolution of 2° × 2° (182 × 149 grid points) and meridional resolution of 0.5° with 31 levels	Chl-a, N, P, S, O, IC, Alk	NEMO	r: chl-a :0.6-0.9 (both models) N, P, O, & S, DIC & Alk > 0.95 (Both models)	(Jung et al., 2019a)





Atlantic	Fasham	3-D; 2° horizontal resolution and 25 vertical levels	Chl-a, nutrients	MOM	RMSD = 0.97 (for detrital sinking rate of 10 m d <sup>-1</sup> ) & 0.77 (detrital sinking rate of 1 m d <sup>-1</sup> ) Based on Fasham et al, 1990 metrics Chl-a	(Oschlies & Garçon, 1999)
Atlantic	Fasham	3-D; horizontal resolution is 10 km, and 30 sigma levels	Chl-a	ROMS	Winter: r = 0.75 Spring: r = 0.72 Summer: r = 0.85 Fall: r = 0.83 Bias:	(Fennel et al., 2008)
Atlantic	Fasham	3-D; 10-km horizontal resolution and 30 terrain-following vertical levels	Chl-a	ROMS	Chl-a (with DOM) = 4 mgchl/m <sup>3</sup> Chl-a (without DOM) = 6 mgchl/m <sup>3</sup>	(Druon et al., 2010)
Atlantic	Fasham	3-D; horizontal resolution of 5 km, and 36 vertical terrain-following layers	Chl-a	ROMS	r: chl-a = Spring: 0.6 Summer: 0.65 Fall: 0.53 Winter: 0.45	(Xue et al., 2013)
Atlantic	ERSEM	3-D; 1/8° horizontal resolution with 43 vertical levels	P, N	OGCM-MED16	r > 0.6	(Lazzari et al., 2016)
Atlantic	ERSEM	3-D; resolution of 1/10° X 1/10° (~10 X10 Km) in the horizontal axis and 24 sigma-levels in the vertical axis	Chl-a, P,N	POM	r: chl-a = 0.64 P = 0.02 mmolP/m <sup>3</sup> N = 0.55 mmolN/m <sup>3</sup>	(Kalaroni et al., 2019)
Atlantic	ERSEM	3-D; resolution of 1/10° x 1/10° (~10 X10 Km) in the horizontal axis and 24 sigma-levels in the vertical axis	Chl-a, P	POM	Refer to Kalaroni et al., 2019	(Kalaroni et al., 2020)
Indian	Fasham	3-D; 1° resolution in latitude and longitude with 10 vertical levels	Chl-a, N	OGCM	Bias: Chl-a = 0.1 N = -11 mmolN/m <sup>3</sup>	(Ryabchenko et al., 1998)
Indian	ERSEM	1-D; grid size of approximately 20 km with 40 vertical layers	N	Princeton/Mellor -Yamada	Bias: N = 9 mmol/m <sup>3</sup>	(Blackford & Burkill, 2002)



Indian	McCreary	1-D; with 4 vertical layers	Chl-a, N	Four-layer model	Bias: Chl-a = 2 mg chl-a/m <sup>3</sup> N = 5 molN/kg	(Hood et al., 2003)
Indian	Fasham	3-D; horizontal resolution of 1/3° both meridionally and zonally with 35 levels	Chl-a, N	MOM	Bias: Chl-a = 0.40 (scale: 0-2 mg/m <sup>3</sup> ) N = 15 (depth of 75 m) (0-30 mmolN/m <sup>3</sup> )	(Kawamiya & Oschlies, 2003)
Indian	PISCES	3-D; mean horizontal resolution of 0.5° by 0.5° cos $\phi$ (where $\phi$ is the latitude) with 30 vertical layers	Chl-a	NEMO	-	(Koné et al., 2009)
Indian	PISCES	3-D; resolution 1/12° (~9 km) horizontal grid with 46 vertical layers	Chl-a, Fe	NEMO	Bias: Fe = 0.15 nM (at depth of 3000 m) chl-a = 0.24mg/m <sup>3</sup>	(Resplandy et al., 2011)
Indian	McCreary	1-D; 6 vertical layers	Chl-a	Six-layer model	Bias: Chl-a = 2 mgchl-a/m <sup>3</sup>	(McCreary et al., 2013)
Indian	Fasham	3-D; 1/12° horizontal resolution with 32 vertical sigma layers	Chl-a, N, O	ROMS	Chl-a: r between 0.69 (summer);0.74(winter) N: r = 0.88 O: r = 0.93	(Lachkar et al., 2017)
Indian	ERSEM	1-D; 100 vertical levels	S, P, N, O	GOTM	r > 0.9 for S,P,N,O	(Sankar et al., 2018)
Indian	Fasham	3-D; horizontal resolution of 1/24° and a vertical grid made of 32 levels	Chl-a, N, O	ROMS	Chl-a: r between 0.69-0.74 N: r = 0.88 O: r = 0.93	(Lachkar et al., 2019)
Indian	PISCES	3-D; grid resolution of 1/10° with 32 vertical layers	Fe	ROMS	Refer to Aumont et al., 2015	(Guiou et al., 2019)
Indian	NOBM	3-D; 1.25° longitude by 2/3° latitude with 14 vertical layers	N, S, Chl-a	OGCM	r: N = 0.9-0.96 S ~ 0.95 Chl-a = 0.78 (in situ) & 0.618 (SeaWiFS)	(Das et al., 2019)



Indian	TOPAZ	3D; 1° horizontal resolution with 1/3° resolution near the equator; 50 vertical layers	Fe	MOM	Bias: Fe = 1.5 nMol/m <sup>3</sup>	(Sharada et al., 2020)
Indian	Fasham	3-D; 1/10° horizontal resolution with 32 sigma-coordinate vertical layers	Chl-a, N, O	ROMS	r: N & O = 0.9; Chl-a = 0.42 (winter) ,0.67 (fall)	(Lachkar et al., 2020)
Southern	PlankTOM	3-D; 2° of longitude and a mean resolution of 1.5° of latitude with 30 vertical levels	Chl-a, N, S, P	NEMO	r: Chl-a ~ 0.8(PlankTOM6) Chl-a ~ 0.81(PlankTOM10) P ~ 0.9 (PlankTOM6) P ~ 0.92(PlankTOM10) N ~ 0.9 (PlankTOM6) N ~ 0.85(PlankTOM10) S ~ 0.8(PlankTOM6) S ~ 0.78(PlankTOM10)	(Le Quéré et al., 2016)
Southern	NOBM	3-D; 2/3° latitude and 1 ¼ ° longitude with 14 vertical layers	PIC,N, S	OGCM	-	(Trull et al., 2018)
Southern	DARWIN	3D; three horizontal grid spacings are used: 20, 5, and 1 km with 76 vertical layers	Fe	MITgcm	No detailed skill analysis of the biological state variables against observations	(Uchida et al., 2019)
Southern	PISCES	3-D; 1° horizontal resolution on an isotropic mercator grid with a local meridional refinement up to 1/3° at the Equator with 75 levels	Fe	NEMO	Refer to Aumont et al., 2015	(Person et al., 2019)
Sothern	DARWIN	3-D; with mean horizontal spacing of 18 km and 50 vertical levels	Chl-a	MITgcm	MAE: 0.74 mg chl-a m <sup>-3</sup> (diatoms) 0.22 mg chl-a m <sup>-3</sup> (haptophytes)	(Lo et al., 2019)
Southern	Chai	3-D; horizontal scale of 2-3 km with 40 vertical layers	Fe	ROMS	r = 0.76	(Jiang et al., 2019)
Southern	TOPAZ	3-D; 1° × 1° horizontal resolution with increased resolution near the Equator and 50 unevenly spaced vertical levels in depth coordinates	DIC, N	ESM2M	-	(Bronselauer et al., 2020)



Arctic	PISCES	3-D; horizontal resolution with an average spacing of ~ 18 km and 50 levels	DIC	MITgcm	No detailed skill analysis available	(Manizza et al., 2011)
Arctic	21 coupled biogeochemical models with different physical systems <sup>c)</sup>	-	Majority includes N, P, S, Fe	-	r: see below the table <sup>d)</sup>	(Babin et al., 2016)
Arctic	REcoM2	3-D; resolution north of 60°N equals 4.5 km, between 40 and 60°N it is approximately 25 km, while a resolution of nominal 1° is used south of 40°N; 32 vertical levels	DIN, S, Chl-a	FESOM	r: DIN: 0.75 Si:0.75  Chl-a: 0.56 Bias: chl-a ≤ 0.1 mg/m <sup>3</sup> ; (Schourup-Kristensen et al., 2014)	(Schourup-Kristensen et al., 2018)
Arctic	BLING	3-D; horizontal resolution of 0.25° with 50 vertical levels	Chl-a, DIM	NEMO	R <sup>2</sup> : IC ≥ 0.93; Chl-a ≥ 0.76 except in BB & HB regions where R <sup>2</sup> = 0.1 & 0.4 respectively; DIM: 0.84, 0.82, 0.93 for BS, LS, BG respectively. Yet R <sup>2</sup> = -0.21 in BB	(Castro de la Guardia et al., 2019)
Arctic	DARWIN	3-D; 18 km of horizontal resolution with 50 vertical levels	DIC	MITgcm	No detailed skill analysis available	(Manizza, 2019)
Pacific	Leonard	1-D vertical ecosystem model; latitudinal resolution of (1/3)° near the equator	Chl-a	OGCM	r: chl-a = 0.55 & 0.93 if data from June-August 1998 are excluded	(Christian et al., 2001)
Pacific	Chai	3-D; horizontal resolution of 1/8 degree with 30 levels in the vertical direction	Chl-a	ROMS	Bias: Chl-a = 0.18 mg/m <sup>3</sup> (Scale: 0.05-0.4)	(Xiu & Chai, 2011)



Pacific	Fasham	3-D; 3 km horizontal grid size with 30 vertical levels	N, P	ROMS	RMSD = 0.97 (for detrital sinking rate of 10 m d <sup>-1</sup> ) & 0.77 (detrital sinking rate of 1 m d <sup>-1</sup> ) based on (Fasham et al., 1990)	(Gan et al., 2014)
Pacific	Fasham	3-D; (1/12) <sup>o</sup> × (1/12) <sup>o</sup> of horizontal resolution, 5 d of temporal resolution and 22 sigma levels	O, N	ROMS	R <sup>2</sup> : O = 0.88 N = 0.95	(Ji et al., 2017)
Pacific	PISCES	3D; resolution of 7.5 km and 32 sigma levels	Chl-a, Fe	ROMS	Bias: Chl-a = 12 mg/m <sup>3</sup> Fe = 2.5 nM	(Vergara et al., 2017)
Pacific	TOPAZ	1-D; single water column	Chl-a, O, N, P, S, CO <sub>2</sub>	GOTM	r: chl-a = 0.53 O = 0.47 N = 0.31 P = 0.16 S = 0.19 CO <sub>2</sub> = 0.94	(Jung et al., 2019b)
Pacific	Chai	1D; 100 layers in the vertical direction	Chl-a	ROMS	r > 0.6	(Ma et al., 2019)
Pacific	Fasham	3-D; horizontal resolution ranged from ~7 km in the north to ~10 km in the south with respect to a cylindrical map projection with 30 vertical levels	P & N	ROMS	R <sup>2</sup> > 0.9	(Lu et al., 2020)
Pacific	Kearney	3-D; 10km horizontal resolution with 30 depth levels	Chl-a	Bering 10K ROMS	No detailed skill analysis of the biological state variables against observations	(Kearney et al., 2020)

800 <sup>a)</sup> **N**: nitrogen (NO<sub>3</sub>, NH<sub>4</sub>); **P**: phosphorus; **S**: silicon; **C**: carbon; **O**: oxygen; **Chl**: chlorophyll; **DIC**:  
 801 dissolved inorganic carbon; **PIC**: particulate inorganic carbon; **DIN**: dissolved inorganic nitrogen; **DIC**:  
 802 dissolved inorganic carbon; **POC**: particulate organic carbon; **Alk**: Alkalinity; **TP**: total phosphorous;  
 803 **TN**: total nitrogen; **NOx**: nitrate+nitrite; **DO**: dissolved oxygen.

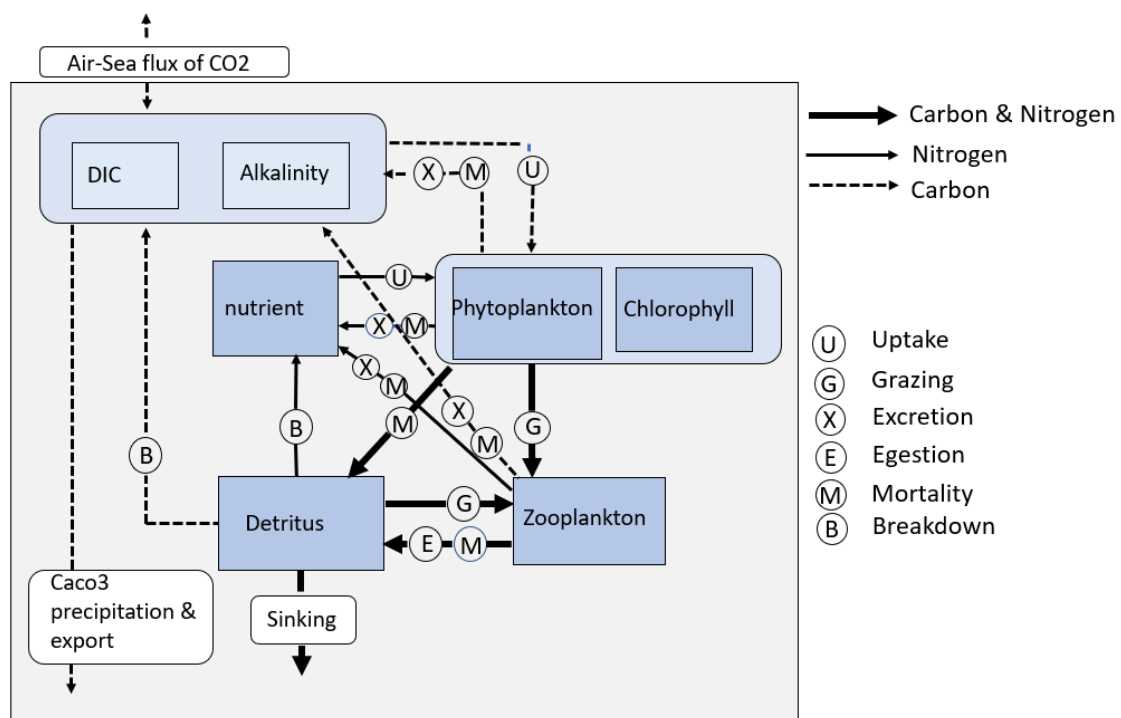
804 <sup>b)</sup> **r**: Pearson correlation coefficient; **R<sup>2</sup>**: coefficient of determination; **SCC** = Spearman correlation  
 805 coefficients; **RSS**: residual sum of squares; **RMSD/E**: root mean square difference/error; **MAE**: mean  
 806 absolute error.

807 <sup>c)</sup> 1. NEMO-PISCES; 2.NEMO-PlankTOM5.3; 3.NEMO-PlankTOM10; 4.MOM-COBALT; 5.MOM-  
 808 TOPAZ; 6.MICOM-HAMOCC; 7.POP-BIOMASS; 8.NEMO-MEDUSA; 9.NEMO-ERSEM; 10.NEMO-  
 809 updated configuration of ERSEM; 11.PELAGOS(NEMO-BFM); 12.POP-Moore; 13.NEMO-PISCES;  
 810 14.NEMO-PISCES; 15.NEMO-PISCES; 16.NorESM(HAMOCC); 17. GISS-E2-R-CC(NOBM); 18.MPI-  
 811 OM HAMOCC.

812 <sup>d)</sup> 0.46; -0.01; 0.28; 0.68; 0.66; -0.02; 0.05; 0.49; 0.27; 0.28; 0.57; 0.30; 0.46; 0.06; 0.56;



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 819 Figure 1. Schematic representation of the Hadley Centre Ocean Carbon model (HadOCC) which is an NPZD model  
 820 coupled with carbon cycle (Palmer & Totterdell, 2001). The labelled boxes nutrient, phytoplankton, zooplankton, and  
 821 detritus are representing the  
 822