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Coastal General Ecosystem Model (CGEM)

GUIDE TO MODEL THEORY & FORMULATIONS VERSION 1.0

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Center for Environmental Measurement and Modeling

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Tables

1.0 Introduction

This guide presents a summary of state variables (Table 1), optional switches (Table 2), parameters (Tables 3 through 8), and formulations utilized in CGEM.

This guide is intended as a supplement to the user guide for understanding model theory.

2.0 CGEM State Variables and Formulations

2.1 State variables

CGEM has 36 state variables (Table 1 on page 23) represented by time-dependent differential equations. For all state variables, horizontal and vertical advection and sinking are implicit. These terms are not shown in this document.

Advection, diffusion, and temperature are hydrodynamic model results that are provided to CGEM at each model time step and point in the grid. Variables are presented in the order that they appear in Table 1 and are grouped by function in optics, phytoplankton, zooplankton, organic matter, nutrients, and oxygen and inorganic carbon dynamics.

2.1.1 Optics

Suspended Particulate Matter (*SPM* [g m^{-3}]) is calculated as the sum of the particulate organic matter represented in the model by

$$\frac{d}{dt}SPM = \frac{d}{dt}\left[\left(OM1\_A + OM1\_Z + \frac{OM1\_R}{CF\_SPMBC}\cdot\frac{12}{1000}\right)\right] \quad (A1)$$

where phytoplankton particulate organic matter (*OM1_A*), zooplankton fecal OM (*OM1_Z*), riverine particulate OM (*OM1_R*) and coastal ocean boundary and initial condition OM (*OM1_BC*) are described in equations (A9-A12). For *OM1_R*, *CF_SPM* is a conversion factor (default=1.8%) for adjusting OM1_R to river SPM, which is predominately inorganic material. The factor 12/1000 converts from mmol m^{-3} to g m^{-3}.

Chlorophyll-a (*Chl* [mg m^{-3}]) is tracked for use in the optical model and for comparison with observed chlorophyll-a, which is a routine measurement of phytoplankton biomass, with the equation

$$\frac{d}{dt}Chl = \sum_{i=1}^{6}(Chl{:}C)_i \cdot 12 \cdot Q_{C_i} \cdot \frac{d}{dt}A_i \quad (A2)$$

where *Chl:C* (chlorophyll:carbon, mg mg^{-1}) is calculated by equation (B4 or B5), *12* is a C conversion from mg to mmol , Q_C is the fixed C cell quota (mmol C $cell^{-1}$), and $\frac{d}{dt}A$ is the rate of change in phytoplankton cell abundance (*A,* cells m^{-3} d^{-1}) (described in equation A4).

Colored Dissolved Organic Matter *(CDOM* [ppb]) is considered to be of terrestrial origin and decays as

$$\frac{d}{dt}CDOM = -KGcdom \cdot CDOM \quad (A3)$$

where *KGcdom* is the decay rate (1% d^{-1}).

2.1.2 Phytoplankton

Phytoplankton abundance (*A*, cells m^{-3}) for X phytoplankton functional types (PFT, i = 1:X) are calculated as

$$\frac{d}{dt}A_i = Agrow_i - ArespTot_i - ZgrazA\_tot_i - AMort_i. \quad (A4)$$

where *Agrow* is phytoplankton population growth due to primary production (cells m^{-3} s^{-1}), *Aresp* (cells m^{-3} s^{-1}) is the respiration due to somatic and basal respiration, *ZgrazA_tot* (cells m^{-3} s^{-1}) is the total zooplankton grazing on A_i by the two zooplankton represented in the model, and *Amort* (cells m^{-3} s^{-1}) is the nongrazing mortality rate. *Agrow, Aresp, ZgrazA_tot, and Amort* are described in Appendix C, equations (C1), (C16), (C20), and (C23), respectively.

Phytoplankton internal quotas (*Q*, mmol $cell^{-1}$) of nitrogen (N) and phosphorus (P) are calculated as

$$\frac{d}{dt}Qn_i = vN_i - Qn_i \cdot uA_i - \frac{AexudN_i}{A_i} \quad (A5)$$

$$\frac{d}{dt}Qp_i = vP_i - Qp_i \cdot uA_i - \frac{AexudP_i}{A_i}. \quad (A6)$$

where *vN* and *vP* (mmol $cell^{-1}$ d^{-1}) are cellular uptake of nitrogen and phosphorus (described in Appendix C, equations C24-C28), $Q \cdot uA$ (mmol $cell^{-1}$ d^{-1}) is the utilization of *Q* to support the growth rate (*uA*, equation C2 or C3), and *AexudN and AexudP* are exudation of nitrogen and phosphorus, respectively, attributed to phytoplankton respiration (equations C18-C19) and divided by A_i to get a per cell exudation rate (mmol $cell^{-1}$ d^{-1}).

2.1.3 Zooplankton

Zooplankton (*Z*, ind m^{-3}) dynamics for X types (j = 1:X) are represented as

$$\frac{d}{dt}Z_j = Zgrow_j - Zresp_j - Zmort_j \quad (A7)$$

where zooplankton growth (*Zgrow*), respiration (*Zresp*), and mortality (*Zmort*) are described in Appendix D.

2.1.4 Organic matter

Particulate organic matter (*OM1*, mmol C m^{-3}) from phytoplankton (*OM1_A*), zooplankton (OM1_Z), rivers (*OM1_R*), and boundary conditions (*OM1_BC*) are calculated as

$$\frac{d}{dt}OM1\_A = ROM1\_A + \sum_{i=1}^{6}\left(Amort_i \cdot \frac{Q\,min\,N_i}{Qn_i} \cdot Qc_i\right) \quad (A8)$$

$$\frac{d}{dt}OM1\_Z = ROM1\_Z + ZegC_1 + ZunC_1 + ZmortC_1 + ZmortC_2 + (OM1\_Ratio \cdot ZslopC\_tot) \quad (A9)$$

$$\frac{d}{dt}OM1\_R = ROM1\_R \quad (A10)$$

$$\frac{d}{dt}OM1\_BC = ROM1\_BC \quad (A11)$$

In (A8), *ROM1* is the *OM1* remineralization rate and is a loss term for *OM1* (e.g., equation E39), *QminN* and *Qc* are parameters for the minimum cellular N quota and the fixed C quota per phytoplankton cell (Table 3 on page 25), respectively. In (A6), $ZegC_1$ is the Z_1 carbon in excess of growth requirements that is egested in fecal pellets (equation E18),

ZunC₁ is the *Z₁* ingested carbon that is unassimilated in the gut and also released in fecal pellets (equation D4), *ZslopC_tot* is the organic matter released during sloppy feeding by both *Z₁* and *Z₂* (equation D4), and *OM1_Ratio* (equation E19) is the fraction of organic matter derived from sloppy feeding that becomes *OM1_Z*.

Dissolved organic matter (*OM2*, mmol C m^{-3}) dynamics are represented by

$$\frac{d}{dt}OM2\_A = -ROM2\_A + \sum_{i=1}^{6}\left(Amort_i \cdot \frac{Qn_i - Q\,min\,N_i}{Qn_i} \cdot Qc_i\right), \quad (A12)$$

$$\frac{d}{dt}OM2\_Z = -ROM2\_Z + ZegC_2 + ZunC_2 + (OM2\_Ratio \cdot ZslopC) \quad (A13)$$

$$\frac{d}{dt}OM2\_R = -ROM2\_R \quad (A14)$$

$$\frac{d}{dt}OM2\_BC = -ROM2\_BC \quad (A15)$$

where *ROM2* is the *OM2* remineralization rate (e.g., equation E40) and other terms are described above.

NH4 (mmol m^{-3}) sources and sinks are attributed to OM remineralization, nitrification, phytoplankton uptake and exudation, and zooplankton excretion,

$$\frac{d}{dt}NH4 = RNH4 - AupN\frac{NH4}{NH4+NO3} + AexudN + ZexN + Sed \quad (A16)$$

where *RNH4* (equation 54) is the rate of change in *NH4* due to remineralization of organic matter and nitrification (equations E47 and E50, respectively), *AupN* is the phytoplankton uptake of dissolved inorganic nitrogen N, i.e. the sum $\sum_{i=1}^{6}(vN_i \cdot A)_i$, where vN_i is the uptake rate for group *i* (equation C24), *AexudN* is the phytoplankton exudation of N driven by respiration (equation C18), *ZexN* is the zooplankton excretion of N driven by respiration (equation D6), and *Sed* is the sediment-water exchange of *NH4*, which interacts with the bottom water that overlies the sediments.

Changes in *NO3* (mmol m^{-3}) are a function of nitrification-denitrification reactions and phytoplankton uptake,

$$\frac{d}{dt}NO3 = RNO3 - AupN\frac{NO3}{NO3+NH4} + Sed \quad (A17)$$

where *RNO3* (equation E53) is the rate of *NO3* change due to nitrification and denitrification (equation E50 and E45, respectively), and *AupN* is modified by the fraction to represent phytoplankton *NO3* uptake, and *Sed* is the sediment-water exchange of *NO3*.

PO4 (mmol m^{-3}) change is calculated as

$$\frac{d}{dt}PO4 = RPO4 - AupP + AexudP + ZexP + Sed \quad (A18)$$

where *RPO4* (equation E54) is the rate of *PO4* remineralization from organic matter (equation E46), *AupP* is phytoplankton uptake of *PO4*, *AexudP* is phytoplankton exudation of *PO4* driven by respiration (equation C19), *ZexP* is zooplankton excretion of *PO4* (equation D7), and *Sed* is the sediment-water exchange of *PO*.

Change in *Si* (mmol m^{-3}) is represented by

$$\frac{d}{dt}Si = RSi - AupSi + ZegSi + ZunSi + Sed\,. \quad (A19)$$

where *RSi* (equation E56) is the rate of *Si* change due to remineralization of organic matter, *AupSi* is the phytoplankton uptake of *Si*, *ZegSi* is the zooplankton egestion of *Si*, *ZunSi* is zooplankton unassimilated *Si*, and *Sed* is the sediment-water exchange.

O2 (mmol m^{-3}) and *DIC* (mmol m^{-3}) are represented by equations

$$\frac{d}{dt}O_2 = RO2 + Prim Prod - ArespC - ZrespC \pm Air - Sea\ Exchange \qquad (A20)$$

$$\frac{d}{dt}DIC = RDIC - Prim Prod + ArespC + ZrespC \pm Air - Sea\ Exchange \qquad (A21)$$

where *RO2* and *RDIC* rates are calculated by equations (E41) and (E42), *PrimProd* is the phytoplankton uptake rate of *DIC* to support organic matter production (equation E26), and other terms are described above.

The biogeochemical reactions affecting *ALK* (mmol m^{-3}) (Wolf-Gladrow et al. 2007) are represented by

$$\frac{d}{dt}ALK = RALK + AupN \cdot \frac{NO3}{NO3+NH4} - AupN \cdot \frac{NH4}{NO3+NH4} + AupP + 4.8 \cdot AupP \qquad (A22)$$

where *RALK* is attributed to anaerobic metabolism (equation 29) reactions, and other terms are phytoplankton uptake of nutrients. *AupN* of *NO3* and *NH4* is calculated assuming no preference by phytoplankton. *AupN-NO3* results in +1 mmol *ALK* and *AupN-NH4* results in -1 mmol *ALK*. *AupP* of 1 mmol *PO4* results in +1 mmol *ALK*. The *4.8·AupP* term in equation (A23) represents the change in *ALK* associated with phytoplankton uptake of sulfate (SO_4^{3-}), where SO_4^{3-} uptake is assumed to equal 2.4·*AupP* and each mmol uptake of SO_4^{3-} results in a 2 mmol increase in *ALK* (Wolf-Gladrow et al. 2007).

2.2 Optical equations

A switch is available to select from two light attenuation models. Irradiance switch E1 uses inherent optical properties (IOPs) to calculate light attenuation (*k*). The main advantage of this approach is that the absorption (*a*) and backscattering (b_b) of light are calculated, which could facilitate comparison of modeled and observed IOPs as these observations become more common. This approach could also be extended to a multi-spectral treatment. *k* is calculated (Penta et al. 2008; 2009) as

$$PAR_z = PAR_0 e^{-k_{PAR}(z)z}$$
$$k_{PAR}(z) = k_1 + \frac{k_2}{(1+z)^{0.5}}$$
$$k_1 = \left[\chi_0 + \chi_1 (a_{490})^{0.5} + \chi_2 b_{b_{490}}\right](1 + \alpha_0 \sin\theta_a)$$
$$k_2 = \left[\zeta_0 + \zeta_1 (a_{490})^{0.5} + \zeta_2 b_{b_{490}}\right](\alpha_1 + \alpha_2 \cos\theta_a) \qquad (B1)$$

where E_z is irradiance at depth *z*, E_0 is the irradiance at the surface layer above *z*, model coefficients include χ, ζ, and α (Lee et al. 2005, Table 4 on page 27), and θ_a is the solar zenith angle calculated as a function of latitude and time. Absorption (a_{490}, m^{-1}) and backscattering ($b_{b_{490}}$, m^{-1}) are calculated (Penta et al., 2008) as

$$a_{490} = a_{Chl_{490}} + a_{CDOM_{490}} + a_{SPM_{490}} + a_{w_{490}} \qquad (B2)$$

where a_{Chl} is the absorption by chlorophyll (*Chl*), a_{CDOM} is the absorption by chromophoric dissolved organic matter (*CDOM*), a_{SPM} is the absorption by suspended particulate matter (*SPM*), and a_w is the absorption by seawater and is a model parameter. a_{Chl} is calculated as

$$a_{Chl_{490}} = astar490 \cdot Chl \qquad (B3)$$

where *astar490* (Table 4 on page 27) is *Chl* specific absorption and total *Chl* (mg m^{-3}) is calculated as

$$Chl = \sum_{i=1}^{6} (Chl{:}C)_i \cdot 12 \cdot Qc_i \cdot A_i \qquad (B4)$$

where *Chl:C* is the chlorophyll:carbon (mg mg^{-1}), 12 is a conversion from mg to mmol C, Q_C is the fixed C cell quota (mmol C $cell^{-1}$, Table 4), and *A* is the phytoplankton cell abundance (cells m^{-3} d^{-1}) (described in equation A4). *Chl:C* in equation (B4) may be calculated by two different methods as determined by a switch (Table 2 on page 24). With switch 1, *Chl:C* is calculated using Cloern et al.'s (1995) empirical equation

$$Chl{:}C_i = 0.003 + 0.0154 \cdot e^{0.050 \cdot T} \cdot e^{-0.0591 \cdot PAR} \cdot \mu_i \qquad (B5)$$

where *T* is the daily mean temperature (°C), *PAR* is mean daily irradiance (mol photons m^{-2} d^{-1}), and μ_i (d^{-1}) is the nutrient limited growth rate (i.e., $umax_i \cdot \min[func\_N_i, func\_P_i, func\_Si_i]$, described below) per A_i. With switch 2, *Chl* is calculated based on an empirically derived relationship between chlorophyll *a* and cell abundance (Murrell et al. 2013 data report). A regression relating these variables ($R^2 = 0.81$), with intercept set equal to zero, has the form

$$Chl = 3.0 \cdot 10^{-9} \cdot \sum_{i=1}^{6} A_i. \qquad (B6)$$

where $3.0 \cdot 10^{-9}$ is the slope of the observed relationship between chlorophyll-*a* and phytoplankton abundance (i.e. Chl:cell).

a_{CDOM} is based on *CDOM* (equation A13) loaded to the model domain from terrestrial sources. In the case of the Louisiana shelf, *CDOM* loaded from the rivers is derived from regression equations relating observed riverine CDOM and DOC concentrations. The Mississippi River time-series of observed DOC (mg l^{-1}) (USGS data) was converted to a_{CDOM} at wavelength 440 (m^{-1}) by the regression equation (Spencer et al. 2012)

$$a_{CDOM_{440}} = 1.10 \cdot DOC - 2.76. \qquad (B7)$$

Next, $a_{CDOM_{440}}$ was converted to $a_{CDOM_{312}}$ with the general $a_\lambda = a_{\lambda ref} \cdot e^{-S(\lambda - \lambda ref)}$, i.e.,

$$a_{CDOM_{312}} = a_{CDOM_{440}} \cdot e^{-S(312-440)} \qquad (B8)$$

where *S* is the spectral slope of *CDOM* (S = 0.016) (Spencer et al. 2012; D'Sa and Dimarco 2009). Then, $a_{CDOM_{312}}$ was converted to *CDOM* concentration using the regression equation (Conmy et al. 2004)

$$CDOM = 2.933 \cdot a_{CDOM_{312}} + 0.538 \qquad (B9)$$

Thus, in the model for the Louisiana shelf, first equations (B7-B9) are applied to riverine DOC measurements. *CDOM* concentration is then input by the rivers to the shelf model domain where it is decayed by equation (B5) and advected and mixed. $a_{CDOM_{490}}$ is required in equation (B2). Thus, *CDOM* is first back-transformed to $a_{CDOM_{312}}$ using the Conmy et al. (2004) equation, and then

$$a_{CDOM_{312}} \textit{ is converted to } a_{CDOM_{490}} \textit{ by}$$

$$a_{CDOM_{490}} = a_{CDOM_{312}} \cdot e^{-S(490-312)} . \qquad (B10)$$

a_{SPM} (m^{-1}) at 490 nm is calculated as the sum of absorption by the different types of *OM1* as

$$a_{SPM_{490}} = \begin{pmatrix} astarOMA \cdot OM1\_A + astarOMZ \cdot OM1\_Z + \\ astarOMR \cdot \frac{OM1\_R}{CF\_SPMBC} () \frac{12}{1000} \end{pmatrix} \qquad (B11)$$

where *astarOM* terms are parameters, *CF_SPM* is a conversion factor for adjusting OM1_R to river SPM. For the application of CGEM to the Louisiana shelf, *CF_SPM* = 1.8% was based on the average observed POC/SPM = 1.8% in the Mississippi and Atchafalaya rivers (USGS data). The factor 12/1000 converts from mmol m^{-3} to g m^{-3}.

Backscattering in equation (B1) was calculated (Penta et al. 2008; 2009) as a function of *Chl* as

$$b_{b,490} = 0.015 \cdot \left(0.3 \cdot Chl^{0.62} \cdot \left(\frac{550}{490}\right)\right). \quad (B12)$$

Using irradiance switch E2 (Table 2 on page 24), *k* is calculated from partial attenuation coefficients

$$k = k_W + k_{Chl} \cdot Chl + k_{SPM} \cdot SPM + k_{CDOM} \cdot CDOM \quad (B13)$$

where k_W is the absorption attributed to seawater (Table 4 on page 27), k_{Chl} is the partial attenuation coefficient for *Chl*, k_{CDOM} is the partial attenuation coefficient for *CDOM*, and k_{SPM} is the partial attenuation coefficient for *SPM*. Parameter values for partial attenuation coefficients are shown in Table 4. *SPM* is calculated as

$$SPM = \left(OM1\_A + OM1\_Z + \frac{OM1\_R}{CF\_SPMBC} \cdot \frac{12}{1000}\right) \quad (B14)$$

2.3 Phytoplankton equations

2.3.1 Phytoplankton growth

Algal growth (*Agrow*, cells m^{-3} d^{-1}) per PFT is calculated as

$$Agrow_i = \mu_{A_i} A_i \quad (C1)$$

where μ_A is the specific growth rate (d^{-1}) and *A* is the phytoplankton abundance (cells m^{-3}). *Agrow* is converted to units of carbon (mmol C m^{-3} d^{-1}) by the product $Agrow_i \cdot Q_{C_i}$, where Q_C is a fixed amount of carbon per cell (mmol C $cell^{-1}$) (Table 3 on page 25).

A code switch (Table 2) is available for three different ways to calculate the specific growth rate based on light, nitrogen, phosphorus, and silica dependent growth rates. Growth switch (1) uses Liebig's Law of the minimum (Table 2)

$$\mu_{A_i} = u_{max\,A_i} \cdot func\_T_i \cdot MIN[func\_E_i, func\_N_i, func\_P_i, func\_Si_i] \quad (C2)$$

where *func(T)*, *func(E)*, *func(N)*, *func(P)*, and *func(Si)* are limiting factors due to temperature, light, nitrogen, phosphorus, and silica, respectively (described below). Using growth switch (2) the specific growth rate is a product formulation of light and the minimum nutrient limiting factor

$$\mu_{A_i} = \mu_{max\,A_i} \cdot func\_T_i \cdot func\_E_i \cdot MIN[func\_E_i, func\_N_i, func\_P_i, func\_Si_i]. \quad (C3)$$

With growth switch (3), the light dependent growth rate is made a function of the nutrient-dependent growth rate (described below in equation C10), and, thus, the last term, i.e. *MIN* [*func_N, func_P, func_Si*], is omitted with switch (3).

2.3.2 Phytoplankton and zooplankton temperature-growth dependence

Temperature effects on growth rate are represented in three ways. Temperature switch (1) uses a sigmoidal function (Eldridge and Roelke 2010):

$$f0 = 0.1$$
$$r = 0.3$$
$$f1 = \frac{1}{f0} - 1$$
$$r1 = r \cdot \frac{46.5}{18}$$
$$denom = 1 + f1 \cdot e^{-r1 \cdot (T - Tref)}$$

$$func\_T = 0.3 \cdot \frac{1}{denom} + 0.7 \quad (C4)$$

where T_{ref} (Table 5 on page 28) is the mid-point between maximum and minimum *func_T* and *f0* and *r* are curve shape parameters. Currently, *f0* and *r* are not included in the parameter list file and, thus, may only be changed in the Fortran code. When using temperature switch 1, *umax* and *Zumax* should be adjusted to the maximum temperature.

Temperature switch (2) employs an optimum temperature threshold at which maximum growth rate is achievable (Cerco and Noel 2004):

$$func(T) = e^{-KTg_1(T-T_{ref2})^2}, \text{ when } T \leq T_{ref2} \quad (C5a)$$

$$func(T) = e^{-KTg_2(T_{ref2}-T)^2}, \text{ when } T \geq T_{ref2} \quad (C5b)$$

In this equation, T_{ref2} is the optimum temperature for growth (°C) and KTg_1 and KTg_2 (°C^2) specify the effect of temperature (T) below and above T_{opt}, respectively. This scheme has been employed to allow temperature driven seasonal succession in the phytoplankton community (Cerco and Noel 2004). When using temperature switch 2, *umax* and *Zumax* should be adjusted to the optimum temperature.

Temperature switch (3) takes the Arrhenius form (Geider et al. 1997):

$$func(T) = e^{-\frac{E_a}{R}\left[\left(\frac{1}{T}-\frac{1}{T_{ref3}}\right)\right]} \quad (C6)$$

where T_{ref3} is a reference temperature in degrees Kelvin (K) (conversion of *Tref* from Celsius to Kelvin is done internally in the code) and E_a/R (K) is the slope of an Arrhenius plot. Using switch (3), rate parameters should be adjusted to the reference temperature. All the parameters in eq. (C4-C6) can be specified uniquely for assigned phytoplankton and zooplankton functional types.

2.3.3 Phytoplankton light-growth dependence

Light dependent growth is modeled as

$$\mu_{E_i} = u\,max_i \cdot func(E)_i, \quad (C7)$$

where func(E) may be represented with or without photoinhibition and may be given nutrient dependence (Table 2 on page 24). With photosynthesis switch (1), a light-dependent response curve with photoinhibition (Platt et al. 1980) is used

$$func(E) = \left(1 - e^{\frac{-alpha_i E}{u\,max_i}}\right) e^{\frac{-beta_i E}{u\,max_i}}. \quad (C8)$$

where *alpha* is the initial slope of the photosynthesis-irradiance curve (cm^2 s quanta^{-1} d^{-1}), *E* is photosynthetically available radiation (quanta cm^{-2} s^{-1}), and *beta* is the photoinhibition constant (cm^2 s quanta^{-1} d^{-1}).

The photoinhibition term may be excluded with photosynthesis switch (2)

$$func(E) = \left(1 - e^{\frac{-alpha_i E}{u\,max_i}}\right). \quad (C9)$$

If light photosynthesis (3) is selected, the *umax* in the denominator of the exponential is made nutrient dependent (Flynn 2003) such that

$$func(E) = \left(1 - e^{\frac{-alpha_i E}{u\,max_i \cdot min[func(N), func(P), func(Si)]}}\right). \quad (C10)$$

If light switch (3) is used, then growth switch (3) is automatically selected.

2.3.4 Phytoplankton nutrient-growth dependence

Nutrient-dependent phytoplankton growth rates are modeled based on available internal cell nutrient stores or quotas. A switch is provided in CGEM to allow for comparison of quota models of increasing complexity. With quota switch (1), the quota models for N and P are based on Droop (1973)

$$func(N) = \frac{Qn_i - Q\,min\,N_i}{Qn_i} \qquad (C11)$$

$$func(P) = \frac{Qp_i - Q\,min\,P_i}{Qp_i} \qquad (C12)$$

where Q_{min} is the minimum nutrient cell quota (mmol cell^{-1}) per phytoplankton group required for survival and Q is the cell quota (mmol cell^{-1}). As the models for N and P are the same, only the func(N) is shown for the remaining quota models. Quota switch (2) uses a quota model suggested by Nyholm (1978)

$$func(N) = \frac{Qn_i - Q\,min\,N_i}{Q\,max\,N_i - Q\,min\,N_i} \qquad (C13)$$

where Q_{max} is the maximum nutrient cell quota (mmol cell^{-1}) per phytoplankton group. Values for *Qmax*, were calculated as *vmax*/*umax* (Table 4 on page 27). Quota switch (3) is the model of Flynn (2003)

$$func(N) = \frac{(1+KQn_i)\cdot(Qn_i - Q\,min\,N_i)}{Qn_i - Q\,min\,N_i + KQn_i(QmaxN_i - QminN_i)} \qquad (C14)$$

where Flynn (2008) suggested *KQn* > 3 and *KQp* < 0.3 (approximately 5 and 0.2, respectively). Note that equation (C13), i.e. switch (2), is linear whereas the other two quota forms are hyperbolic.

Growth rate dependence on silica is modeled as a Monod function

$$func(Si) = \frac{Si}{Si + Ksi} \qquad (C15)$$

where *Si* is the modeled silica concentration (mmol m^{-3}) and *Ksi* is the half saturation concentration (mmol m^{-3}) of silica uptake.

2.3.5 Phytoplankton losses

Phytoplankton respiration (cells m^{-3} d^{-1}) is represented as a function of growth, cell abundance, and temperature

$$Aresp_i = respg_i \cdot Agrow_i + respb_i \cdot A_i \cdot func\_T \qquad (C16)$$

where *respg* is a respiration coefficient that scaled to growth rate and *respb* represents basal maintenance activities that scale to abundance. Phytoplankton respiration results in a loss of carbon from the cell (*ArespC*) and nutrient exudation (*Aexud*$_i$, mmol m^{-3} d^{-1}) as

$$ArespC = \sum_{i=1}^{6} ArespTot_i \cdot Qc_i \qquad (C17)$$

$$AexudN = \sum_{i=1}^{6} ArespTot_i \cdot Qn_i \qquad (C18)$$

$$AexudP = \sum_{i=1}^{6} ArespTot_i \cdot Qp_i. \qquad (C19)$$

Phytoplankton mortality (*Amort*, cells m^{-3} d^{-1}) is calculated by

$$Amort_i = A_i \cdot mA_i \qquad (C20)$$

where mA_i is the mortality rate (d^{-1}).

Phytoplankton sinking losses (cells m^{-3} d^{-1}) are applied implicitly in the advection and mixing routines with sinking velocities prescribed by the parameter *sink* (Table 3 on page 25).

Grazing losses (*ZgrazA_tot*, cells m^{-3} d^{-1}) are calculated as

$$ZgrazA\_tot_i = \sum_{j=1}^{2} \frac{Zgrazvol_{ji}}{volcell_i}. \quad (C21)$$

The term $Zgrazvol_{ji}$ is the grazing rate by each zooplankton (j=1:2) on each phytoplankton (i=1:6) in units of biovolume (µm3 m^{-3} d^{-1}) and is calculated by

$$Zgrazvol_{ji} = Z_j \cdot Zu\,max_j \cdot monodZ_{ji} \quad (C22)$$

where $Zumax_j$ is the maximum growth rate of the zooplankton in terms of volume of prey (Table 6 on page 29) and $monodZ_{ij}$ is a hyperbolic function represented by

$$monodZ_{ij} = \frac{(Abiovol_i - Athresh_i \cdot volcell_i) \cdot ediblevector_i}{ZKa_j + \sum_{i=1}^{6}(Abiovol_i \cdot ediblevector_i)}. \quad (C23)$$

In equation (C23), *Abiovol* (= $A_i \cdot volcell_i$) is the biovolume, *Athresh* is the threshold abundance (cells m^{-3}) below which grazing of A_i does not occur, *ediblevector* is a vector expressing prey edibility (unitless, possible range = 0 to 1), and *ZKa* is the grazing half-saturation (Table 6).

Phytoplankton mortality (cells m^{-3} d^{-1}) is

$$Amort_i = A_i \cdot mA_i \quad (C24)$$

where mA_i is the mortality rate (d^{-1}).

2.3.6 Phytoplankton uptake and utilization of N, P, and Si

Nutrient uptake by the modeled phytoplankton only occurs during the day. For the limiting nutrient substrate (*S*), which is determined as the min[*f_N, f_P, f_Si*], the nutrient uptake rate (*vS*, mmol cell $^{-1}$ d^{-1}) by a PFT is calculated as

$$vS_i = vmaxS_i \cdot \frac{S}{(S+K_{S_i})} \cdot Q10 \cdot func\_Qs_i vS_i = vmaxS_i \cdot \frac{S}{(S+K_{S_i})} \cdot Q10 \cdot func\_Qs_i \quad (C25)$$

where $v_{max}S$ is the maximum uptake rate (mmol cell $^{-1}$ d^{-1}), K_S is the half-saturation concentration (mmol m^{-3}), *Q10* is the temperature adjustment factor such that a doubling of the rate occurred for a 10°C change in temperature, and *func_Qs* is a quota model. The *func_Qs* models are different from the quota models used to calculate nutrient-growth dependence (Table 2 on page 24). Here, CGEM implements three *func_Qs* switches. Nutrient uptake switch U1 reduces the equation to Michaelis-Menten kinetics (Dugdale and Goering 1967) by setting

$$func\_Qs = 1 \quad (C26)$$

Switch (2) uses the treatment proposed by Lehman et al. (1975) and Geider et al. (1998)

$$func\_Qs = \left(\frac{QmaxS_i - Qs_i}{Q\,max\,S_i - Q\,min\,S_i}\right)^{nfQs_i} \quad (C27)$$

where *nfQs* = 1 is the Lehman et al (1975) treatment.

Switch (3) uses a form that allows for scaling of *vmaxS* based on internal quotas (Roelke 2000) in the form

$$func\_Qs_i = \frac{QmaxS_i}{Qs_i} \quad (C28)$$

For *Si*, only uptake case (1) is implemented.

If *S* is not the rate limiting nutrient, the PFT uptake is modified by an additional limitation term as

$$vS_i = vmaxS_i \cdot \frac{S}{\left(S+K_{S_i}\right)} \cdot Q10 \cdot func\_Qs_i \cdot \frac{RLN}{RLN+a_S \cdot K_{RLN_i}} \quad (C29)$$

where *RLN* is the substrate concentration of the rate limiting nutrient (*RLN*), K_{RLN} is the half-saturation concentration of the *RLN*, and a_S is a scaling factor (Roelke et al. 1999).

The total phytoplankton uptake of nutrient (shown here for nitrogen, i.e. *AupN*) is then

$$AupN = \sum_{i=1}^{6}(vN_i \cdot A)_i. \quad (C30)$$

2.4 Zooplankton equations

Zooplankton growth rates (individuals m^{-3} d^{-1}) are modeled as

$$Zgrow_j = Tadj \cdot MIN\left(\frac{ZinN_j}{ZQn_j}, \frac{ZinP_j}{ZQp_j}\right). \quad (D1)$$

where *ZinN* and *ZinP* are zooplankton ingestion rates of nitrogen and phosphorus (mmol m^{-3} d^{-1}), and Z*Qn* and Z*Qp* are zooplankton N and P quota parameters, respectively, (mmol per individual, Table 6 on page 29). *ZinN*, *ZinP,* zooplankton ingestion of carbon (*ZinC*) are calculated similarly. For brevity, only *ZinN* equations are shown.

$$ZgrazN_j = \sum_{i=1}^{6} ZgrazA_{ij} \cdot Qn_i \quad (D2)$$

$$ZslopN_j = Zslop_j \cdot ZgrazN_j \quad (D3)$$

$$ZunN_j = \left(1 - Zeffic_j\right) \cdot \left(ZgrazN_j - ZslopN_j\right) \quad (D4)$$

$$ZinN_j = ZgrazN_j - ZslopN_j - ZunN_j \quad (D5)$$

where *ZgrazN* (mmol N m^{-3} d^{-1}) is the grazing in units of nitrogen, *ZgrazA* is described in equations (C20 and C21), *ZslopN* is sloppy feeding (mmol N m^{-3} d^{-1}), *Zslop* is a sloppy feeding parameter (possible range = 0 to 1, Table 6), and *ZunN* (mmol N m^{-3} d^{-1}) is the amount of zooplankton unassimilated nitrogen, which is a function of the assimilation efficiency (*Zeffic*, Table 6) of each zooplankton.

Zooplankton respiration loss (individuals m^{-3} d^{-1}) is represented with two terms

$$Zresp_j = Zrespg_j \cdot Zgrow_j + Zrespb_j \cdot Z_i \cdot func\_T \quad (D6)$$

where *Zrespg* and *Zrespb* are respiration coefficients (Table 6) on zooplankton growth and basal metabolism. Zooplankton excretion of nutrients (*Zex*, mmol m^{-3} d^{-1}) is used to mass balance zooplankton respiratory loss of CO_2 by

$$ZexN = \sum_{j=1}^{2} ZrespTot_j \cdot ZQn_j \quad (D7)$$

$$ZexP = \sum_{j=1}^{2} ZrespTot_j \cdot ZQp_j. \quad (D8)$$

Zooplankton mortality (individuals m^{-3} d^{-1}) is treated as a quadratic function of zooplankton abundance (Cerco and Noel 2004) and is assumed to represent mainly predation from higher trophic levels

$$Zmort_j = Zm_j {Z_j}^2 \quad (D9)$$

where *Zm* is the zooplankton mortality coefficient (Table 6)

2.5 Organic matter production and remineralization

2.5.1 Organic matter types and stoichiometry

Eight classes of organic matter representing phytoplankton, zooplankton, river, and boundary condition *OM* are tracked in the model in both particulate (*OM1*) and dissolved (*OM2*) forms and with variable stoichiometry $C_xN_yP_z$. *OM1* and *OM2* are created (mmol m^{-3} d^{-1}) in the model by phytoplankton and zooplankton mortality, zooplankton sloppy feeding, zooplankton egestion, and unassimilated *OM* that passes through the zooplankton (equations A13 and A14). The mechanisms controlling the partitioning of OM1 and OM2 by the processes are not well understood. Though, there is evidence to suggest that partitioning of to *OM1_A* and *OM2_A* is dictated by nutrient depletion such that more dissolved organic matter may accumulate when phytoplankton are nutrient stressed (Ittekot et al. 1981; Goldman et al. 1992). Thus, CGEM uses the internal nitrogen cell quota as a means to partition phytoplankton mortality by

$$OM1\_CA = \sum_{i=1}^{6}\left(Amort_i \cdot \frac{Q\,min\,N_i}{Qn_i} \cdot Qc_i\right) \quad (E1)$$

$$OM1\_NA = \sum_{i=1}^{6}(Amort_i \cdot Q\,min\,N_i) \quad (E2)$$

$$OM1\_PA = \sum_{i=1}^{6}(Amort_i \cdot Q\,min\,P_i) \quad (E3)$$

$$OM2\_CA = \sum_{i=1}^{6}\left(Amort_i \cdot \frac{Qn_i - Q\,min\,N_i}{Qn_i} \cdot Qc_i\right) \quad (E4)$$

$$OM2\_NA = \sum_{i=1}^{6}\left(Amort_i \cdot (Qn_i - Q\,min\,N_i)\right) \quad (E5)$$

$$OM2\_PA = \sum_{i=1}^{6}\left(Amort_i \cdot (Qp_i - Q\,min\,P_i)\right). \quad (E6)$$

Dynamic stoichiometric ratios ($C_xN_yP_z$) of *OM1_A* and *OM2_A* are tracked as

$$stoich\_x1A = \frac{(OM1\_CA + OM1\_A)}{OM1\_PA + \frac{1}{stoich\_x1A}} \quad (E7)$$

$$stoich\_y1A = \frac{\left(OM1\_NA + \frac{stoich\_y1A}{stoich\_x1A} \cdot OM1\_A\right)}{OM1\_PA + \frac{1}{stoich\_x1A} \cdot OM1\_A} \quad (E8)$$

$$stoich\_x2A = \frac{(OM2\_CA + OM2\_A)}{OM2\_PA + \frac{1}{stoich\_x2A}} \quad (E9)$$

$$stoich\_y2A = \frac{\left(OM2\_NA + \frac{stoich\_y2A}{stoich\_x2A} \cdot OM2\_A\right)}{OM2\_PA + \frac{1}{stoich\_x2A} \cdot OM2\_A} \quad (E10)$$

$$stoich\_z1A = stoich\_z2A = 1 \quad (E11)$$

Organic matter C, N, and P derived from zooplankton are calculated as

$$OM1\_CZ = ZegC_1 + ZunC_1 + ZmortC_1 + ZmortC_2 + (OM1\_Ratio \cdot ZslopC) \quad (E12)$$

$$OM1\_NZ = ZegN_1 + ZunN_1 + ZmortN_1 + ZmortN_2 + (OM1\_Ratio \cdot ZslopN) \quad (E13)$$

$$OM1\_PZ = ZegP_1 + ZunP_1 + ZmortP_1 + ZmortP_2 + (OM1\_Ratio \cdot ZslopP) \quad (E14)$$

$$OM2\_CZ = ZegC_2 + ZunC_2 + (OM2\_Ratio \cdot ZslopC) \quad (E15)$$

$$OM2\_NZ = ZegN_2 + ZunN_2 + (OM2\_Ratio \cdot ZslopN) \quad (E16)$$

$$OM2\_PZ = ZegP_2 + ZunP_2 + (OM2\_Ratio \cdot ZslopP) \quad (E17)$$

where *Zun* and *Zslop* equations are presented in Appendix D and zooplankton egestion (*Zeg*) is calculated as follows. *Zeg* in the model is governed by an optimal nutrient ratio of the zooplankton, i.e. *ZQn/ZQp*, such that

$$if ZinN_j > \frac{ZQn_j}{ZQp_j} \cdot ZinP_j$$

$$ZegN_j = ZinN_j - ZinP_j \cdot \frac{ZQn_j}{ZQp_j}$$

$$ZegC_j = ZinC_j - \frac{ZinP_j}{ZQp_j} \cdot ZQc_j$$

$$ZegP_j = 0$$

$$else$$

$$ZegP_j = ZinP_j - ZinN_j \cdot \frac{ZQp_j}{ZQn_j}$$

$$ZegC_j = ZinC_j - \frac{ZinN_j}{ZQn_j} \cdot ZQc_j$$

$$ZegP_j = 0. \quad (E18)$$

Similar to how the OM derived from mortality of phytoplankton cells is split into OM1_A and OM2_A, OM from sloppy feeding on phytoplankton cells is split into particulate and dissolved OM fractions based on the calculated *OM1_Ratio* and *OM2_Ratio* as

$$OM1\_Ratio = \frac{\sum_{i=1}^{6} A_i \cdot \frac{Q\,min\,N_i}{Qn_i}}{\sum_{i=1}^{6} A_i} \quad (E19)$$

$$OM2\_Ratio = \frac{\sum_{i=1}^{6} A_i \cdot \frac{Qn_i - Q\,min\,N_i}{Qn_i}}{\sum_{i=1}^{6} A_i} \quad (E20)$$

C, N, and P stoichiometry of *OM1_Z* and *OM2_Z* are tracked as

$$stoich\_x1Z = \frac{(OM1\_CZ + OM1\_Z)}{OM1\_PZ + \frac{1}{stoich\_x1Z} \cdot OM1\_Z} \quad (E21)$$

$$stoich\_y1Z = \frac{\left(OM1\_NZ + \frac{stoich\_y1Z}{stoich\_x1Z} \cdot OM1\_Z\right)}{OM1\_PZ + \frac{1}{stoich\_x1Z} \cdot OM1\_Z} \quad (E22)$$

$$stoich\_x2Z = \frac{(OM2\_CZ + OM2\_Z)}{OM2\_PZ + \frac{1}{stoich\_x2Z} \cdot OM2\_Z} \quad (E23)$$

$$stoich\_y2Z = \frac{\left(OM2\_NZ + \frac{stoich\_y2Z}{stoich\_x2Z} \cdot OM2\_Z\right)}{OM2\_PZ + \frac{1}{stoich\_x2Z} \cdot OM2\_Z} \quad (E24)$$

$$stoich\_z1Z = stoich\_z2Z = 1. \quad (E25)$$

2.5.2 Reactions

Primary production (*PrimProd)* of organic matter by phytoplankton is

$$Prim Prod = \sum_{i=1}^{6} Agrow_i \cdot Qc_i \quad (E26)$$

and proceeds according to the photosynthesis reaction

$$xCO_2 + yDIN + zDIP \overset{uptake}{\rightarrow} C_xN_yP_z + xO_2 \quad (E27)$$

where CO_2 (DIC), dissolved inorganic nitrogen (DIN) and dissolved inorganic phosphorus (DIP) are taken up to produce organic matter with C:N:P stoichiometry of *x:y:z*.

Organic matter oxidation by aerobic respiration is represented by

$$C_xN_yP_z + xO_2 \xrightarrow{R1} xCO_2 + yNH_4 + zPO_4 \quad (E28)$$

where *R1* is

$$R1 = \frac{O2}{KO2+O2} \quad (E29)$$

and *KO2* is the Monod half-saturation constant (Table 7 on page 30).

The organic matter reaction during denitrification uses the reaction equation of Van Cappellen and Wang (1996)

$$C_xN_yP_z + \left(\frac{4x+3y}{5}\right)NO3 \xrightarrow{R2} \left(\frac{2x+4y}{5}\right)N2 + \left(\frac{x-3y+10z}{5}\right)CO2 + \left(\frac{4x+3y-10z}{5}\right)HCO3 + zPO4 \quad (E30)$$

where

$$R2\ is R2 = \frac{NO3}{KNO3+NO3}\frac{KstarO2}{KstarO2+O2} \quad (E31)$$

and KNO3 is a Monod half-saturation constant (Table 7), and *KstarO2* is an *O2* based inhibition constant (Table 7) that limits denitrification when *O2* concentrations approach and exceed *KstarO2*.

Reaction rates (R) are determined for organic matter remineralization (*ROM*, mmol C m^{-3} d^{-1}), *DIC* production (*RDIC*, mmol C m^{-3} d^{-1}), *O2* utilization (*RO2*, mmol O_2 m^{-3} d^{-1}), nitrification and denitrification (*RNO3*, mmol N m^{-3} d^{-1}), and remineralization of *PO4* (*RPO4*, mmol P m^{-3} d^{-1}), *NH4* (*RNH*4, mmol C m^{-3} d^{-1}), *Si* (*RSi*, mmol C m^{-3} d^{-1}), , and *ALK* (*RALK*, mmol m^{-3} d^{-1}). The remineralization equations are identical for the four sources of OM and for brevity are only shown for OM_A.

Organic matter decay coefficients are adjusted for temperature by a Q10 relation

$$KG1\_Q10 = 10^{RQ1} \quad (E32)$$

$$KG2\_Q10 = 10^{RQ2}. \quad (E33)$$

where *RQ1* and *RQ2* are intermediate variables calculated as

$$RQ1 = LOG10(KG1) - FACTOR \quad (E34)$$

$$RQ2 = LOG10(KG2) - FACTOR \quad (E35)$$

and

$$FACTOR = LOG10(2) \cdot 0.1 \cdot (TQ1 - TQ2) \quad (E36)$$

where *TQ1* is the reference temperature of 25 °C and *TQ2* is the temperature of the reaction (i.e. the temperature obtained from a model or specified).

The temperature adjusted reaction (RCT) rates for *OM1_A* and *OM2_A* are then calculated as

$$RCT1\_A = KG1\_Q10 \cdot OM1\_A \quad (E37)$$

$$RCT2\_A = KG2\_Q10 \cdot OM2\_A. \quad (E38)$$

ROM1_A and *ROM2_A* are calculated as

$$ROM1\_A = -(RCT1\_A \cdot R1 + RCT1\_A \cdot R2) \quad (E39)$$

$$ROM2\_A = -(RCT2\_A \cdot R1 + RCT2\_A \cdot R2). \quad (E40)$$

The *DIC* production associated with *OM* remineralization is calculated based on the reaction stoichiometry in equation (E28 and E30). Thus,

$$RDIC\_A = -(ROM1\_A + ROM2\_A). \quad (E41)$$

$$RO2\_A = (RCT1\_A + RCT2\_A) \cdot R1 \quad (E42)$$

and

$$RDIC = RDIC\_A + RDIC\_Z + R\,D\,IC\_R + R\,D\,IC\_BC \quad (E43)$$

$$RO2 = RO2\_A + RO2\_Z + RO\,2\,\_R + RO\,2\,\_BC - 2 \cdot R\_1\,1 \quad (E44)$$

where *R_11* is the nitrification rate, which is an additional O2 sink (see equations E46 and E47).

RNO3 is comprised of nitrification and denitrification (equation E30) reactions. Nitrification proceeds as a function of *NH4* and *O2* concentration (Van Cappellen and Wang 1996) as

$$NH_4^{+} + 2O_2 + 2HCO_3^{-} \xrightarrow{R\_11} NO_3^{-} + 2CO_2 + 3H_2O \quad (E45)$$

where *R_11* is the reaction rate defined as

$$R\_11 = k11\left[NH_4^{+}\right][O_2] \quad (E46)$$

with *k11* being a parameter rate constant (Table 7 on page 30) that is adjusted by a Q10 factor in the same way as described above for Q10 adjustment of *KG1* and *KG2* in equations (E37 and E38). For the denitrification reaction (equation E30), reaction stoichiometry is taken into account in intermediate variables (*GAM14* and *GAM24*) calculated as

$$GAM14 = \frac{4 \cdot stoich\_x1A + 3 \cdot stoich\_y1A}{\frac{5}{stoich\_x1A}} \quad (E47)$$

$$GAM24 = \frac{4 \cdot stoich\_x2A + 3 \cdot stoich\_y2A}{\frac{5}{stoich\_x2A}} \quad (E48)$$

where the coefficients 4, 3, and 5 are the coefficients to *NO3* in equation (E3). Then *RNO3* using *OM1_A* and *OM2_A* as electron donors is represented by

$$RNO3\_A = -(GAM14 \cdot RCT1\_A + GAM24 \cdot RCT2\_A()). \quad (E49)$$

Then, RNO3 is

$$RNO3 = R\_1\,1 + RNO3\_A + RNO3\_Z + R\,N\,O3\_R + R\,N\,O3\_BC. \quad (E50)$$

Remineralizaton of *PO4* during the *OM* oxidation reactions is calculated as

$$RPO4 = RPO4\_A + RPO4\_Z + R\,P\,O4\_R + R\,P\,O4\_BC \quad (E51)$$

with

$$RPO4\_A = ROM1\_A \cdot \frac{stoich\_z1A}{stoich\_x1A} + ROM2\_A \cdot \frac{stoich\_z2A}{stoich\_x2A}. \quad (E52)$$

Remineralization of *NH4* is

$$RNH4 = -R\_11 + RNH4\_A + RNH4\_Z + RNH4\_R + RNH4\_BC \quad (E53)$$

with

$$RNH4\_A = \left(RCT1\_A \cdot \frac{stoich\_y1A}{stoich\_x1A} + RCT2\_A \cdot \frac{stoich\_y2A}{stoich\_x2A}\right) \cdot R1 \quad (E54)$$

The rate of *Si* remineralization is

$$RSi = RSi\_A + RSi\_Z + RSi\_R + RSi\_BC \quad (E55)$$

with Si stoichiometrically linked to remineralization of N as Si:N = 1 such that

$$RSi\_A = ROM1\_A \cdot \frac{stoich\_y1A}{stoich\_x1A} + ROM2\_A \cdot \frac{stoich\_y2A}{stoich\_x2A}. \quad (E56)$$

The rate of *ALK* change is

$$RALK = -2 \cdot R\_11 + RALK\_A + RALK\_Z + RALK\_R + RALK\_BC. \quad (E57)$$

For *RALK_A*, the denitrification reaction stoichiometry (equation E30) is taken into account in two intermediate variables (*A14* and *A24*) calculated as

$$A14 = \frac{4 \cdot stoich\_x1A + 3 \cdot stoich\_y1A - 10 \cdot stoich\_z1A}{\frac{5}{stoich\_x1A}} \quad (E58)$$

$$A24 = \frac{4 \cdot stoich\_x2A + 3 \cdot stoich\_y2A - 10 \cdot stoich\_z2A}{\frac{5}{stoich\_x2A}} \quad (E59)$$

$$RALK\_A = (A14 \cdot RCT1\_A + A24 \cdot RCT2\_A()). \quad (E60)$$

2.6 Sediment-water exchanges

CGEM provides a number of switches for representing the sediment (Table 2 on page 24). These representations range in complexity from no sediment to a vertically resolved sediment model (Soetaert et al. 2000). In the default mode, when all of the sediment switches are set to 0, OM sinks to the bottom layer where it is subjected to the remineralization equations described in Appendix E and to advection. Sediment switches to turn on sediment models include 1. sediment O_2 consumption (SOC), 2. microphytobenthos production of O_2 and consumption of DIC, 3. sediment nutrient fluxes, 4. instantaneous remineralization of OM that sinks to the bottom, and 5. a full sediment diagenesis model. As classified by Soetaert et al. (2000), switches 1-4 are representative of reflective models which simply describe sediment fluxes as a function of bottom-water concentrations. Switch 5 employs a highly vertically resolved (> 400 layers) sediment diagenesis model that provides a realistic mass balance accounting of sediment fluxes and sediment organic matter remineralization (Eldridge and Morse 2008).

When the sediment oxygen consumption switch is set to 1, the sediment boundary consumes *O2* as a function of the bottom-water *O2* concentration (Murrell and Lehrter 2011) and temperature (Fennel et al. 2013)

$$SOC = -0.0235 \cdot O2 \cdot 2^{T/10^{\circ}C}. \quad (F1)$$

Also with this switch, sediment DIC flux (*DICFlux*) is modeled as

$$DICFlux = 16.6 \quad (F2)$$

where *16.6* mmol m^{-2} d^{-1} is an imposed DIC flux that was the average of observations (Lehrter et al. 2012).

For the microphytobenthos production, there are several empirical models relating microphytobenthos production to available light. Here, three empirical formulations are included. Setting this switch = 1, microphytobenthos production (MPB, mmol O_2 m^{-2} d^{-1}) is modeled with the relationship of Gatusso et al. (2006)

$$MPB\ O2\ Production = 120.82 \cdot \left(1 - e^{\frac{E_{sed}}{2.09}}\right) \quad (F3)$$

where E_{sed} is the irradiance (mol photons m^{-2} d^{-1}) calculated at the bottom of the water-column (i.e. the sediment-water interface). Setting the switch = 2, the relationship of Jahnke et al. (2008) is used

$$MPB\ O2\ Production = \left(\frac{1}{12}\right) \cdot 132 \cdot E_{sed}{}^{1.45}. \quad (F4)$$

With this switch = 3, a power function fit to the data of Lehrter et al. (2014) is used

$$MPB\ O2\ Production = 0.33 \cdot E_{sed}{}^{2.93}. \quad (F5)$$

A sediment switch is available to turn on sediment-water nutrient exchanges (mmol m^{-2} d^{-1}) that are calculated based on empirical relationships obtained from observed sediment exchanges (Lehrter et al. 2012).

$$NO3Flux = 0.0057 \cdot O2 - 0.52 \quad (F6)$$

$$NH4Flux = -1.55 \cdot NO3Flux + 0.69 \quad (F7)$$

$$PO4Flux = 0.094 \cdot NH4Flux - 0.0125 \quad (F8)$$

$$SiFlux = 1.68 \quad (F9)$$

Note that *SiFlux* is treated as a constant flux (out of the sediment) boundary condition. Also, note that a strict model mass balance is compromised for state variables *O2*, *DIC*, *NO3*, *NH4*, *PO4*, and *Si* when the empirical sediment equations above are used. However, the mass balance should be approximately correct for the range of observed conditions used to derive the empirical equations. For application of CGEM outside of the Louisiana shelf, the empirical equations would need to be altered to reflect local, site-specific relationships.

Sediment-water fluxes calculated by instantaneous remineralization of OM sinking to the bottom layer of the modeled water-column preserve mass balance, but at the expense of realistic lag times associated with sediment diagenesis. In this treatment, the parameter *KG_bot* (Table 7 on page 30) is used and is set to a large value (92,000 y^{-1}) such that all *OM1_A*, *OM2_A*, *OM1_Z*, and *OM2_Z* are instantaneously remineralized when they sink to the bottom layer. *OM* remineralization proceeds as described in Appendix E.

Caution is advised in using combinations of these switches. For example, the empirical nutrient flux equations described in equations (F6) to (F9) were based on experiments conducted in the dark and, thus, may not be appropriate if the MPB case is turned on. Similarly, if the sediment diagenesis model is turned on, the switches for SOC and nutrients should not be on since the diagenesis model calculates the sediment-water fluxes of *O2*, *DIC*, and nutrients.

2.7 Air-sea fluxes

Air-sea exchanges of *O2* and *CO2* were modeled based on concentration gradients and wind speed (Liss and Merlivat 1986; Whitfield and Turner 1986; Justić et al., 1996;

Eldridge and Cifuentes 2000). O_2 flux at the air-sea interface (*O2_atF*, mmol O_2 m^{-2} s^{-1}) was modeled (Justić et al., 1996) as

$$O2\_atF = Vtrans \cdot (O2\_sfc - alpha\_O2 \cdot Op) \quad (G1)$$

where *Vtrans* is the O2 transfer velocity (m s^{-1}), *O_2_sfc* is the O2 concentration in the surface layer of a model grid cell, *alpha_O2* is a parameter that is set equal to 1.025, and *Op* is the saturation O2 concentration (mmol m^{-3}) calculated as a function of surface layer temperature and salinity. *Vtrans* is calculated as a function of wind speed (*Wsp*) as

$$\text{if } Wsp < 3.6\ m\ s^{-1} \text{ then}$$

$$Vtrans = 5.9 \cdot (0.17 \cdot Wsp) \cdot Sc^{-\frac{2}{3}} \cdot \frac{1}{SDay}$$

$$\text{else if } Wsp \leq 13$$

$$Vtrans = 5.9 \cdot (2.85 \cdot Wsp\text{-}9.65) \cdot Sc^{-\frac{1}{2}} \cdot \frac{1}{SDay}$$

$$\text{else}$$

$$Vtrans = 5.9 \cdot (5.9 \cdot Wsp\text{-}49.3) \cdot Sc^{-\frac{1}{2}} \cdot \frac{1}{SDay} \quad (G2)$$

where *Sc* is the Schmidt number calculated as a function of surface salinity and temperature and *SDay* is the number of seconds per day. *Wsp* for the CGEM implementation on the Louisiana shelf were obtained from the U.S. Navy COAMPS model (9km scale estimates) and adjusted by +5% to account for a bias between COAMPS and observed winds (Lehrter et al. 2013).

CO2 flux at the air-sea interface (*CO2_atF*, mmol CO2 m^{-2} s^{-1}) was modeled (Eldridge and Cifuentes 2000) as

$$CO2\_atF = \frac{DZ \cdot (ATM\_CO2 - H2CO3)}{H \cdot 100} \quad (G3)$$

where *DZ* = 0.005 cm s^{-1} is a velocity transfer similar to *Vtrans* in equation (G2), *ATM_CO2* is the air CO_2 concentration (mmol C m-3, calculated as a function of pCO2 and Henry's constant), *H2CO3* is the carbonic acid concentration in the surface layer (calculated as a function of *DIC* and *pH*) and *H* (m) is the thickness of the surface layer. Air *pCO_2* in the model was set as a model parameter at 401 ppm (Table 8 on page 31). *pH* and *H2CO3* are calculated as a function of *DIC* and *ALK*, described in Appendix H.

Atmospheric nitrogen is fluxed into the model domain in oxidized and reduced forms using modeled N deposition loads derived from the Community Multi-Scale Air Quality (CMAQ) model. These fluxes may be turned on with a switch (Table 2 on page 24).

2.8 CO2 system

DIC and *ALK* are used to calculate pH, pCO2, and other carbonate system parameters with the code mocsy v2.0 (Orr and Epitalon 2015). The mocsy code computes the CO2 system variables with inputs of atmospheric pressure, depth, latitude, temperature, salinity, *ALK*, *DIC*, *Si*, and *PO4*. mocsy has been designed for use in ocean models and offers an efficient Fortran 95 code and current best constants and approximations to calculate the CO2 system. CGEM uses the mocsy INPUT options; optCON: 'mol/m3', optT: 'Tinsitu', optP: 'm', optB: 'u74', optK1K2: 'l', optKf: 'pf', optGAS: 'Pzero'.

2.9 References

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2.10 Tables

Table 1. *State variables. Number of possible functional types for phytoplankton (i) and zooplankton (j) are noted*

Symbol	State Variable	Units
A	phytoplankton abundance (i = 1:6)	cells m^{-3}
Qn	cell nitrogen quota (i = 1:6)	mmol N $cell^{-1}$
Qp	cell phosphorus quota (i = 1:6)	mmol P $cell^{-1}$
Z	zooplankton (j = 1:2)	individuals m^{-3}
OM1_A	particulate organic matter from phytoplankton	mmol m^{-3}
OM1_Z	particulate organic matter from zooplankton fecal pellets	mmol m^{-3}
OM1_R	particulate organic matter from rivers	mmol m^{-3}
OM1_BC	particulate organic matter from lateral boundaries	mmol m^{-3}
OM2_A	dissolved organic matter from phytoplankton	mmol m^{-3}
OM2_Z	dissolved organic matter from zooplankton	mmol m^{-3}
OM2_R	dissolved organic matter from rivers	mmol m^{-3}
OM2_BC	dissolved organic matter from lateral boundaries	mmol m^{-3}
CDOM	colored dissolved organic matter	ppb
NH4	ammonium	mmol m^{-3}
PO4	phosphate	mmol m^{-3}
Si	silica	mmol m^{-3}
NO3	nitrate	mmol m^{-3}
O2	oxygen	mmol m^{-3}
DIC	dissolved inorganic carbon	mmol m^{-3}
Alk	alkalinity	mmol m^{-3}

Table 2. *CGEM model switch option representing biogeochemical processes. Multiple cases per process are provided for evaluating uncertainty related to equations used.*

Switch Category: Fluxes	Description
O2 surface exchange	on (1) off (0)
DIC surface exchange	on (1) off (0)
Sediment Oxygen Consumption	[1] linear (Murrell and Lehrter 2010); [2] hyperbolic (Hetland and DiMarco 2008); [3] logistic; (4) diagenetic (Eldridge and Morse 2008)
Microphytobenthos	on (1) off (0)
Sediment Nutrient Fluxes	on (1) off (0)
Atmospheric Nutrient Deposition	on (1) off (0)
Bottom Instant Remineralization	on (1) off (0)
Sediment Diagenesis Model	on (1) off (0)

Switch Category: Other	Description
Temperature	Sigmoidal (1); Optimum Temperature Threshold (2); Arrenhius (3)
Nutrient Uptake	Michaelis-Menten (1); Geider (2); Roelke (3)
Nutrient Dependent Growth	Dropp (1); Nyholm (2); Flynn (3)
Optical Properties	Inherent Optical Properties (1); Apparent Optical Properties (2)
C:Chla	user defined fixed C:Chla (1); Cloern Chl:C (2)
Photosynthesis	photoinhibition (1); without photoinhibiton (2); nutrient dependent (3)
Phytoplankton Growth	minimum (1); product formulation (2); nutrient dependent μmax (3)
Solar Radiation	Model calculated solar radiation (0); Read file solar radiation (1)
Initialization	Regression Input (0); Regular Restart (1); Restart from Crash (2); User defined restart (3)

Table 3. *Phytoplankton parameters*

Symbol	Parameter (switch)	Units	Value
volcell	biovolume per cell	μm^3	[33693 2569 77429 513 547 87]
Qc	carbon per cell	10^{-7} mmol C $cell^{-1}$	[13.5 1.68 26.5 0.454 0.478 0.108]
umax	maximum growth rate at 20 °C	d^{-1}	[0.41 0.76 0.34 1.12 1.10 1.72]
alpha	initial slope of the photosynthesis versus irradiance curve	10^{-16} cm^2 s $quanta^{-1}d^{-1}$	[0.842 2.18 0.619 3.96 3.87 0.763]
beta	photoinhibition (P1)	10^{-18} cm^2 s $quanta^{-1}d^{-1}$	[1.1 1.1 1.1 1.1 1.1 1.1]
respg	growth dependent respiration	dimensionless	[0.1 0.1 0.1 0.1 0.1 0.1]
respb	basal respiration	d^{-1}	[0.02 0.02 0.02 0.02 0.02 0.02]
QminN	minimum N cell-quota	10^{-9} mmol N $cell^{-1}$	[6.08 0.632 12.7 0.153 0.162 0.0321]
QminP	minimum P cell-quota	10^{-10} mmol P $cell^{-1}$	[6.19 0.510 13.9 0.107 0.114 0.0191]
QmaxN	maximum N cell-quota (Q2)	10^{-7} mmol N $cell^{-1}$	[2.04 0.253 4.01 0.0685 0.0722 0.0162]
QmaxP	maximum P cell-quota (Q2)	10^{-8} mmol P $cell^{-1}$	[1.28 0.158 2.50 0.0428 0.0451 0.0102]
Kn	half saturation coefficient for N uptake	mmol N m^{-3}	[4.51 1.93 5.93 1.13 1.16 0.63]
Kp	half saturation coefficient for P uptake	mmol P m^{-3}	[2.86 1.00 4.02 0.51 0.53 0.25]
Ksi	half saturation coefficient for Si uptake	mmol Si m^{-3}	[4.51 1.93 5.93 1.13 1.16 0.63]
KQn	Qn constant (Q3)	mmol N m^{-3}	[5 5 5 5 5 5]
KQp	Qp constant (Q3)	mmol P m^{-3}	[0.2 0.2 0.2 0.2 0.2 0.2]
nfQs	exponent for switch (U2)	dimensionless	[1 1 1 1 1 1]
vmaxN	N-uptake rate at mumax	10-8 mmol N cell-1d-1	[4.10 0.497 8.11 0.133 0.140 0.0309]
vmaxP	P-uptake rate at mumax	10-8 mmol P cell-1d-1	[2.68 0.204 6.15 0.0407 0.0434 0.00691]

Symbol	Parameter (switch)	Units	Value
vmaxSi	Si-uptake rate at mumax	10-8 mmol si cell-1d-1	[4.10 0.497 8.11 0.133 0.140 0.0309]
aN	coefficient for non-limiting nutrient	dimensionless	[1 1 1 1 1 1]
Athresh	phytoplankton threshold for zooplankton grazing	107 cells m-3	[7 7 7 7 7 7]
ediblevector	edibility of phytoplankton	dimensionless	[0.25 0.5 0.25 0.5 0.6 1]
sink	sinking rate	m d-1	[1.49 0.55 2.07 0.29 0.29 0.15]
mA	mortality of phytoplankton	d-1	[0.041 0.076 0.034 0.11 0.11 0.17]

Table 4. *Light attenuation parameters*

IOP Light Attentuation Scheme (optical properties switch 1)

Symbol	Parameter	Unit	Value
chi0, chi1, chi2	coefficients	dimensionless	-0.057, 0.482, 4.221
zeta0, zeta1, zeta2	coefficients	dimensionless	0.183, 0.702, -2.567
alpha0, alpha1, alpha2	coefficients	dimensionless	0.090, 1.465, -0.67
astar490	Chla specific absorption (490 nm)	$m^{-1}(mg\ Chla\ m^{-3})^{-1}$	0.020
aw490	water absorption (490 nm)	m^{-1}	0.005
astarOMA	OM1_A specific absorption (490 nm)	$m^{-1}(g\ OM1\_A\ m^{-3})^{-1}$	0.1
astarOMZ	OM1_Z specific absorption (490 nm)	$m^{-1}(g\ OM1\_Z\ m^{-3})^{-1}$	0.1
astarOMR	OM1_R specific absorption (490 nm)	$m^{-1}(g\ OM1\_R\ m^{-3})^{-1}$	0.1
astarOMBC	OM1_BC specific absorption (490 nm)	$m^{-1}(g\ OM1\_BC\ m^{-3})^{-1}$	0.1
CF_SPM	percentage of river SPM that is OM1_R	%	1.8

AOP light attenuation scheme (optical properties switch 2)

Symbol	Parameter	Unit	Value
k_w	light attenuation due to water	m^{-1}	0.146
k_{cdom}	light attenuation due to CDOM	$m^{-1}\ (ppb\ CDOM)^{-1}$	0.001
k_{spm}	light attenuation due to SPM	$m^{-1}\ (g\ SPM\ m^{-3})^{-1}$	0.029
k_{chla}	light attenuation due to Chla	$m^{-1}\ (mg\ Chla\ m^{-3})^{-1}$	0.024

Table 5. *Temperature parameters for phytoplankton and zooplankton (nospA = 6 + nospZ =2).*

T1, T2, and T3 denote the three temperature switches available for representing growth rate as a function of temperature. The curve shape parameters (f_0,r) for T1 are hard-coded and may only be changed in the Fortran code. For switch T3, Tref is converted to Kelvin in the code.

Symbol	Parameter	Unit	Value
Tref	reference temperature (T1, T2, T3)	C	[22 22 17 17 26 29 22 26]
f_0, r	curve shape parameters (T1)	dimensionless	0.1, 0.3
KTg1	curve shape parameters (T2)	10^{-3} dimensionless	[3.5 3.5 3.5 3.5 3.5 3.5 3.5 3.5]
KTg2	temperature switch (T2)	10^{-2} dimensionless	[3 4 2 3 6 6 3 6]
Ea_R	Arrenhius slope (T3)	10^{3} dimensionless	[8.4 6.0 8.4 6.0 10 10]

Table 6. *Zooplankton parameters*

Symbol	Parameter	Units	Value
Zvolcell	volume per individual	μm^3 $individual^{-1}$	[2.98e+7 6.74e+5]
ZQc	carbon per individual	mmol C $individual^{-1}$	[3.13e-4 7.08e-7]
ZQn	N per individual	mmol N $individual^{-1}$	[6.95e-5 1.57e-7]
ZQp	P per individual	mmol P $individual^{-1}$	[3.77e-6 8.53e-9]
Zslop	sloppy feeding coefficient	dimensionless	[0.25 0]
Zeffic	assimilation efficiency as a fraction of ingestion	dimensionless	[0.4 0.4]
ZKa	grazing half saturation coefficient	μm^3 m^{-3}	[1.12e+12 1.12e+12]
Zrespg	growth dependent respiration	dimensionless	[0.2 0.3]
Zrespb	biomass (basal) dependent respiration	d^{-1}	[0.1 0.416]
Zumax	maximum growth rate in terms of volume of prey	μm^3 ind^{-1} d^{-1}	[9.45e+8 2.98e+7]
Zm	zooplankton mortality constant for quadratic mortality	m^6 ind^{-2} d^{-1}	[0.00072 0.00072]

Table 7. *Organic Matter parameters*

Symbol	Parameter	Units	Value
KG1	decay rate of OM1_A and OM1_G	y^{-1}	30
KG2	decay rate of OM2_A and OM2_G	y^{-1}	30
KG1_R	decay rate of OM1_R	y^{-1}	11
KG2_R	decay rate of OM2_R	y^{-1}	3.7
KG1_BC	decay rate of OM1_BC	y^{-1}	1
KG2_BC	decay rate of OM2_BC	y^{-1}	1
KG_bot	decay rate of OM when instantaneous remineralization is used	y^{-1}	92,000
k11	rate constant for nitrification	$(mmol\ m^{-3})^{-1}\ y^{-1}$	5
KO2	half-saturation constant for O_2 uptake	$mmol\ m^{-3}$	10
KstarO2	inhibition constant for denitrification	$mmol\ m^{-3}$	10
KNO3	half-saturation constant for denitrification	$mmol\ m^{-3}$	10
stoich_x1R	initial C:P stoichiometry of OM1_R	mol/mol	51
stoich_y1R	initial N:P stoichiometry of OM1_R	mol/mol	4.5
stoich_x2R	initial C:P stoichiometry of OM2_R	mol/mol	700
stoich_y2R	initial N:P stoichiometry of OM2_R	mol/mol	50
stoich_x1BC	initial C:P stoichiometry of OM1_BC	mol/mol	106
stoich_y1BC	initial N:P stoichiometry of OM1_BC	mol/mol	16
stoich_x2BC	initial C:P stoichiometry of OM2_BC	mol/mol	106
stoich_y2BC	initial N:P stoichiometry of OM2_BC	mol/mol	16
sink_OM1_A	sinking rate of OM1_A	$m\ d^{-1}$	10
sink_OM2_A	sinking rate of OM2_A	$m\ d^{-1}$	0
sink_OM1_Z	sinking rate of OM1_Z	$m\ d^{-1}$	10
sink_OM2_Z	sinking rate of OM2_Z	$m\ d^{-1}$	0
sink_OM1_R	sinking rate of OM1_R	$m\ d^{-1}$	10
sink_OM2_R	sinking rate of OM2_R	$m\ d^{-1}$	0
sink_OM1_BC	sinking rate of OM1_BC	$m\ d^{-1}$	10
sink_OM2_BC	sinking rate of OM2_BC	$m\ d^{-1}$	0
sink_CDOM	sinking rate of CDOM	$m\ d^{-1}$	0
Kcdom_decay	decay rate of CDOM	d^{-1}	0.01
K	Q10 coefficient such that a 10 °C increase results in a 2-fold increase in OM remineralization	dimensionless	0.07

Table 8. *Miscellaneous parameters*

Symbol	Parameter	Units	Value
a	air-sea exchange transfer velocity coefficient	non-dimensional	2.85
b	air-sea exchange transfer velocity coefficient	non-dimensional	-9.65
pCO2	atmospheric CO2	ppm	380

Appendix A: Differential equations describing state variables

The change in photosynthetically available radiation is expressed by

$$\frac{dE_z}{dt} = E_0 \int_z^0 (absorption + backscattering) \quad (A1)$$

The rate change in chla is

$$\frac{dChl}{dt} = Chl{:}Cell \times (Growth_{\phi_i} - Respiration_{\phi_i} - Mortality_{\phi_i} - Grazing_{\phi_i} \pm Advection_{\phi_i} \pm Sinking_{\phi_i}) \quad (A2)$$

where Chl:Cell is the chla to phytoplankton cell ratio determined empirically and the remaining terms are phytoplankton gains and losses calculated as changes in phytoplankton cell abundance (ϕ, shown below) . Other state variables used in the light attenuation schemes are as follows

$$\frac{dCDOM}{dt} = -Remineralization - Advection \quad (A3)$$

$$\frac{dSPM}{dt} = -Remineralization - Advection - Sinking \quad (A4)$$

$$\frac{d\,a_{490}}{dt} = \frac{d\,a_{490}Chl}{dt} + \frac{d\,a_{490}CDOM}{dt} + \frac{d\,a_{490}SPM}{dt} \quad (A5)$$

$$\frac{d\,b_{b_{490}}}{dt} = \frac{d\,b_{b_{490}}Chl}{dt} + \frac{d\,b_{b_{490}}CDOM}{dt} + \frac{d\,b_{b_{490}}SPM}{dt}. \quad (A6)$$

Rates of change of phytoplankton abundances for types (i = 1:X) are determined as

$$\frac{d\phi_i}{dt} = Growth_{\phi_i} - Respiration_{\phi_i} - Mortality_{\phi_i} - Grazing_{\phi_i} \pm Advection_{\phi_i} \pm Sinking_{\phi_i} \quad (A7)$$

Phytoplankton cell internal nitrogen and phosphorus quotas are calculated by

$$\frac{dQ_{\phi_i|N}}{dt} = Uptake_{\phi_i|N} - Utilization_{\phi_i|N} \quad (A8)$$

$$\frac{dQ_{\phi_i|P}}{dt} = Uptake_{\phi_i|P} - Utilization_{\phi_i|P}. \quad (A9)$$

The zooplankton rate of change for two types (j = 1:2) are expressed by

$$\frac{dG_j}{dt} = Growth_{G_j} - Respiration_{G_j} - Mortality_{G_j} \pm Advection_{G_j} \quad (A10)$$

Rates of change to DIN (NO_3^-+NH_4^+) and DIP (PO_4^{3-}) are as follows

$$\frac{dDIN}{dt} = -Uptake_{\phi N} + Exudation_{\phi N} + Sloppy_{G_1|N} + Excretion_{G|N} + Egestion_{G|N} + Mortality_{G|N} + Remineralization_{OM|N} + Sediment_N + Advection_{\phi,G|N} \quad (A11)$$

$$\frac{dDIP}{dt} = -Uptake_{\phi|P} + Exudation_{\phi|P} + Sloppy_{G_1|P} + Excretion_{G|P} + Egestion_{G|P} + Mortality_{\phi|P} + Remineralization_{OM|P} \pm Sediment_P \pm Advection_{\phi,G|P} \quad (A12)$$

Organic matter rate of changes is calculated by

$$\frac{dPOC}{dt} = Egestion_{G_1} + Unassimilated_{\phi,G} - Remineralization_{POC} \pm Advection_{POC} \pm Sinking_{POC} \quad (A13)$$

$$\frac{dDOC}{dt} = Egestion_{G_1} + Unassimilated_{\phi,G|} - Remineralization_{POC} \pm Advection_{POC} \pm Sinking_{POC} \quad (A14)$$

Dissolved O_2 and dissolved inorganic carbon are modeled by

$$\frac{dO_2}{dt} = Photosynthesis_{\phi} - Respiration_{\phi_i} - Respiration_{G_j} - Remineralization_{OM} - Sediment \pm Air - Sea\ Exchange \pm Advection \quad (A15)$$

$$\frac{dDIC}{dt} = -Photosynthesis_{\phi} + Respiration_{\phi_i} + Respiration_{G_j} + Remineralization_{OM} + Sediment \pm Air - Sea\ Exchange \pm Advection \quad (A16)$$

Appendix B: Phytoplankton equations

Phytoplankton growth (cells m^{-3} d^{-1}) per PFT are calculated as

$$Growth_{\phi} = \mu_{\phi_i}\phi_i \quad (B1)$$

where μ_{ϕ} is the specific growth rate (d^{-1}) and ϕ is the phytoplankton abundance (cells m^{-3}). The specific growth rate is calculated from the light-, nitrogen-, and phosphorus-dependent growth rates ($V_{\phi|E}$, $\mu_{\phi|N}$, $\mu_{\phi|P}$, respectively) using Liebig's Law of the minimum

$$\mu_{\phi} = MIN\left(V_{\phi|E}, \mu_{\phi|N}, \mu_{\phi|P}\right) \quad (B2)$$

or by a product formulation

$$\mu_{\phi} = V_{\phi|E} \times MIN\left(\mu_{\phi|N}, \mu_{\phi|P}\right).$$

The light dependent growth rate is calculated without photoinhibition as

$$V_{\phi_i} = V_{max,\phi_i}\left(1 - e^{-A_{\phi_i}}\right) \quad (B3)$$

where V_{max} is the maximum light-dependent growth rate and A is

$$A_{\phi_i} = \frac{\alpha_{\phi_i} E}{V_{max,\phi_i}} \quad (B4)$$

where α is the initial slope of the photosynthesis-irradiance curve and all other variables have been previously defined. Including photoinhibition (default, Table 4 on page 27) resulted in

$$V_{\phi_i} = V_{max,\phi_i}\left(1 - e^{-A_{\phi_i}}\right)e^{-B_{\phi_i}} \quad (B5)$$

where

$$B_{\phi_i} = \frac{\beta_{\phi_i} E}{V_{max,\phi_i}} \quad (B6)$$

and β is photoinhibition.

A Droop (1968) formula is used to describe nutrient-dependent growth rate

$$\mu_N = \mu\phi|N\left(1 - \frac{Q_{min\,\phi|N}}{Q_{\phi|N}}\right)_{max} \quad (B7)$$

$$\mu_P = \mu\phi|P\left(1 - \frac{Q_{min\,\phi|P}}{Q_{\phi|P}}\right)_{max} \quad (B8)$$

where Q_{min} is the minimum nutrient cell quota per phytoplankton group required for survival, μ_{max} is the maximum nutrient-dependent growth rate per functional type, and Q is the cell quota determined as the balance of nutrient uptake and utilization (eqns A8 and A9).

The nutrient uptake rate (ρ, mmol cell $^{-1}$ d^{-1}) is determined from

$$\rho = \rho\frac{S}{(S+k_s)_{max}} \quad (B9)$$

where ρ is the nutrient uptake rate, ρmax is the nutrient uptake rate, S is the concentration of the growth rate limiting substrate (mmol m^{-3}), and k_s, is the half-saturation constant for nutrient uptake (mmol m^{-3}). Under N-limiting conditions the equation for N uptake is

$$\rho_N = \rho_{max\,N}\frac{N}{(N+k_N)}\frac{Q_{maxN}}{Q_N} \quad (B10)$$

where ρ_N is the N-uptake rate (mmol cell $^{-1}$ d^{-1}), ρ_{maxN} is the N-uptake rate measured at μ_{max}, N is the seawater dissolved inorganic nitrogen concentration (mmol m^{-3}), k_N is the nitrogen half-

saturation constant, Q_{maxN} is the cell-quota for N measured at μ_{max}, and Q_N is the cell-quota for N.

The equation that described P uptake under N-limiting conditions is

$$\rho_P = \rho_{max} \frac{P}{(P+k_P)} \frac{Q_{maxP}}{Q_P} \frac{N}{N+a_N k_N} \quad (B11)$$

where ρ_P is the P-uptake rate (µmol cell $^{-1}$ d^{-1}), ρ_{maxP} is the P-uptake rate measured at μ_{max}, P is the seawater dissolved inorganic phosphorus concentration (mmol m^{-3}), k_P is the phosphorus half-saturation constant, Q_{maxP} is the cell-quota for P measured at μ_{max}, Q_P is the cell-quota for P, a_N is a scaling factor, and other variables are previously defined.

Under P-limiting conditions, N and P uptake are described by

$$\rho_N = \rho_{maxN} \frac{N}{(N+k_N)} \frac{Q_{maxN}}{Q_N} \frac{e^{\mu t}-1}{e^{\mu_{max} P t}-1} \quad (B12)$$

$$\rho_P = \rho_{maxP} \frac{P}{(P+k_P)} \frac{Q_{maxP}}{Q_P} \quad (B13)$$

where t = 1 d and all other symbols are as previously described.

N and P utilization for growth are determined as

$$Utilization_N = \mu Q_{Ni} \quad (B14)$$

$$Utilization_P = \mu Q_{Pi} \quad (B15)$$

Phytoplankton respiration (cells m^{-3} d^{-1}) is represented as a function of growth

$$Respiration_{\phi_i} = r_{\phi_i} Growth_{\phi_i} \quad (B16)$$

where r is a PFT specific linear respiration coefficent.

Phytoplankton mortality (cells m^{-3} d^{-1}) is

$$Mortality_{\phi_i} = m_{\phi} \phi_i \quad (B17)$$

where m is a specific loss rate applied to the group cell abundance. Phytoplankton mortality represented death by processes other than grazing.

Grazing losses (cells m^{-3} d^{-1}) are specified as

$$Grazing_{\phi_i} = \sum_{j=1}^{2} \frac{\gamma_{ji} G_{ji}}{Q_{fixv,\phi_i}} \quad (B18)$$

where grazing is a function of γ, the zooplankton group specific growth rate in terms of prey volume, and the zooplankton number density.

Advection and sinking losses are specified as

$$Advection_{\phi_i} = uA\phi_i + vA\phi_i \quad (B19)$$

$$Sinking_{\phi_i} = wA\phi_i + \omega A\phi_i \quad (B20)$$

where u and v and are horizontal advection (m s^{-1}) and w and ω are vertical advection and sinking, respectively (m s^{-1}), normal to a flow face with area (A, m^2).

Losses of nutrients from the phytoplankton are required to compensate for the loss of cells due to respiration and mortality. Phytoplankton nutrient exudation (mmol m^{-3} d^{-1}) is linked to respiration, and phytoplankton mortality contributed to the remineralization of phytoplankton nutrients (mmol m^{-3} d^{-1}) to the seawater pool.

$$Exudation_{\phi_{total}/N} = \sum_{i=1}^{6} Respiration_{\phi_i} Q_{\phi_i/N} \quad (B21)$$

$$Exudation_{\phi_{total}/P} = \sum_{i=1}^{6} Respiration_{\phi_i} Q_{\phi_i/P} \quad (B22)$$

$$Mortality_{\phi_{total}/N} = \sum_{i=1}^{6} Mortality_{\phi_i} Q_{\phi_i/N} \quad (B23)$$

$$Mortality_{\phi_{total}/P} = \sum_{i=1}^{6} Mortality_{\phi_i} Q_{\phi_i/P} \quad (B24)$$

Appendix C:Zooplankton equations

Zooplankton growth rates (individuals m^{-3} d^{-1}) are determined by applying Liebig's Law to quotients of nutrients ingested to fixed intracellular nutrient composition as

$$\text{Growth}_{G_j} = \text{MIN}\left(\frac{\text{Ingestion}_{G_j|N}}{Q_{fix,G_j\ |N}}, \frac{\text{Ingestion}_{G_j|P}}{Q_{fix,G_j\ |P}}\right) \quad (C1)$$

where the ingestion rates of N and P (mmol m^{-3} d^{-1}) are

$$\text{Ingestion}_{G_j\ |N} = \left(\sum_{i=1}^{6} \frac{\gamma_j G_j Q_{\phi_i|N}}{Q_{\text{fix}V,\phi_i}} + \frac{\gamma_j Q_{\text{fix},G_j|N}}{Q_{\text{fix}V,G_j}}\right)(1-\chi) \quad (C2)$$

$$\text{Ingestion}_{G_j\ |P} = \left(\sum_{i=1}^{6} \frac{\gamma_j G_j Q_{\phi_i|P}}{Q_{\text{fix}V,\phi_i}} + \frac{\gamma_j Q_{\text{fix},G_j|P}}{Q_{\text{fix}V,G_j}}\right)(1-\chi). \quad (C3)$$

where χ is a sloppy feeding coefficient and all other variables are previously defined. Thus, ingestion rates are a function of zooplankton specific growth rates and abundance, the nutritional status of the phytoplankton cells (i.e. the nutrient cell quotas), and the amount of sloppy feeding.

The zooplankton growth rate in terms of volume of prey (μm^3 $individual^{-1}$ d^{-1}) is a function of the phytoplankton cell volume and the body size of the zooplankton relative to the size of the prey.

$$\gamma_j = \sum_{i=1}^{6} \gamma_{max_j} \quad MIN\left(\left(\frac{\theta_i - \theta_{th_i}}{k_{G_j} + \theta_{Tot}}\right)(S_Z{:}S_P)_i\right) \quad (C4)$$

where γ_{max} is the maximum grazing rate (μm^3 $individual^{-1}$ d^{-1}), $S_{Z:}S_P$ is the relative prey size and

$$\theta_i = \phi_i Q_{fixV,\phi_i} \quad (C5)$$

$$\theta_{Tot} = \sum \theta_i \quad (C6)$$

Zooplankton respiration loss (individuals m^{-3} d^{-1}) is represented with two terms

$$Respiration_{G_j} = r^1{}_{G_j} Growth_{G_j} + r^2{}_{G_j} G_j \quad (C7)$$

such that for the first term respiration is a function of zooplankton growth rate (i.e. larger growth rate, larger respiration rate) and for the second term respiration is a function of the zooplankton biomass (i.e. a low-level metabolic loss attributed to cell maintenance and which is independent of the growth rate).

Similar to phytoplankton, zooplankton mortality loss (individuals m^{-3} d^{-1}) is treated as a function of zooplankton biomass.

$$Mortality_{G_j} = m_{G_j} G_j \quad (C8)$$

Zooplankton mortality is assumed to represent mainly predation from higher trophic levels.

Zooplankton excretion of nutrients (mmol m^{-3} d^{-1}) is used to mass balance losses due to zooplankton respiration in order to maintain the fixed zooplankton intracellular pools of N and P by

$$Excretion_{G_{total}/N} = \sum_{j=1}^{2} Respiration_{G_j} Q_{fix,G_j/N} \quad (C9)$$

$$Excretion_{G_{total}/P} = \sum_{j=1}^{2} Respiration_{G_j} Q_{fix,G_j/P} \quad (C10)$$

Similarly, zooplankton losses to mortality had to be mass balanced by

$$Mortality_{G_{total}/N} = \sum_{j=1}^{2} Mortality_{G_j} Q_{fix,G_j/N} \quad (C11)$$

$$Mortality_{G_{total}/P} = \sum_{j=1}^{2} Mortality_{G_j} Q_{fix,G_j/P} \quad (C12)$$

In the model, sloppy feeding (mmol m^{-3} d^{-1}) also provided a pathway for remineralization of zooplankton to N and P pools, but only for the macrozooplankton (G_1)

$$Sloppy_{G_1/P} = \chi Ingestion_{G_1/P} \quad (C13)$$

$$Sloppy_{G_1/N} = \chi Ingestion_{G_1/N} \quad (C14)$$

Also related to Ingestion is Egestion (mmol m^{-3} d^{-1}), which is necessary to maintain the fixed nutrient content of the zooplankton. Thus, Egestion removed the excess non-limiting nutrient brought into the cell during Ingestion.

$$Egestion_{G_{total}/P} = \sum_{j=1}^{2} Ingestion_{G_j/P} - Ingestion_{G_j/N} \left(\frac{Q_{fix,G_j/P}}{Q_{fix,G_j/N}} \right) \quad (C15)$$

$$Egestion_{G_{total}/N} = \sum_{j=1}^{2} Ingestion_{G_j/N} - Ingestion_{G_j/P} \left(\frac{Q_{fix,G_j/N}}{Q_{fix,G_j/P}} \right) \quad (C16)$$

Appendix D: Nutrient equations

Nutrients uptake and release equations related to phytoplankton are described in Appendix B and nutrient remineralization due to zooplankton processes are described in Appendix C. Nutrient remineralization is stoichiometrically linked (Table 7 on page 30) to carbon remineralization of POC and DOC (described below). Nitrification and denitrification in the model may proceed in the water-column at appropriate concentrations of O_2 and NO_3^- (Table 1 on page 23). In this version of CGEM we have simply parameterized sediment exchanges (mmol m^{-2} d^{-1}) of NO_3^-, NH_4^+, and PO_4^{3-} based on empirical relationships (Lehrter et al. 2012) as

$$NO_3^- \text{ Exchange} = 0.0057(O_2) - 0.52 \quad (D1)$$

$$NH_4^+ \text{ Exchange} = -1.55(NO_3^- \text{ Exchange}) + 0.69 \quad (D2)$$

$$PO_4^{3-} \text{ Exchange} = 0.094(NH_4^+ \text{ Exchange}) - 1.0125 \quad (D3)$$

where NO_3^-, NH_4^+, and PO_4^{3-} Exchanges are the exchange rates across the sediment-water interface (positive = flux to the water-column) and O_2 is the bottom-water O_2 concentration.

Appendix E: Organic matter equations

POC and DOC are created (mmol m^{-3} d^{-1}) in the model by phytoplankton mortality and the creation of zooplankton fecal pellets and are also transported into the model by riverine sources and boundary concentrations (equations A13 and A14).

$$POC\ sources = Phytoplankton\ Mortality + Zooplankton\ Fecal\ Pellet\ Production + River\ and\ Boundary\ Condition\ Loadings \quad (E1)$$

$$DOC\ sources = Phytoplankton\ Mortality + Zooplankton\ Fecal\ Pellet\ Production + River\ and\ Boundary\ Condition\ Loadings \quad (E2)$$

where all the terms on the right-hand side of the equations are in mmol m^{-3} d^{-1}. Zooplankton fecal pellets are created by egestion and the fraction (0.6) of material that is ingested by zooplankton but not assimilated in the zooplankton.

Sinks of POC and DOC are specified by

$$POC\ sinks = \omega POC_{\phi} + \omega POC_{fp} + \omega POC_{R} + K\_POC_{\phi}\ POC\phi + K\_POC_{fp}\ POC_{fp} + K\_POC_{R}\ POC_{R} \quad (E3)$$

$$DOC\ sinks = K\_DOC_{\phi}\ DOC\phi + K\_DOC_{fp}\ DOC_{fp} + K\_DOC_{R}\ DOC_{R} \quad (E4)$$

where for POC there is a sinking (mmol d^{-1}) and remineralization loss (mmol d^{-1}) for each POC type and for DOC there is only a remineralization loss. As carbon is remineralized, nutrients are released according to fixed C:N:P of the organic matter classes.

Appendix F: O_2 and DIC

During photosynthesis, respiration of phytoplankton and zooplankton, and remineralization of organic matter, O_2 and DIC stoichiometry is assumed to be 1:1. Thus, O_2 and DIC are linked stoichiometrically to carbon and nutrient cycling rates through the equations in Table 2 (page 24), the stoichiometries listed in Table 7 (page 30), and the fixed carbon content of phytoplankton (Table 3 on page 25) and zooplankton (Table 6 on page 29).

Sediments consumed O_2 based on an empirical relationship between sediment O_2 exchange and bottom-water O_2 concentration

$$O_2\ Exchange = 0.094[O_2]. \quad (F1)$$

The model also simulated photosynthetic O_2 production attributed to the microphytobenthos (MPB, mmol O_2 m^{-2} d^{-1}, C:O_2 = 1) (Gattuso et al., 2006) by

$$MPB\ O_2\ \ Pr\,o\,duction = 120.82 \times \left(1 - e^{-\frac{E_{sed}}{2.09}}\right) \quad (F2)$$

where E_{sed} is the irradiance calculated at the bottom of the water-column (i.e., the sediment-water interface).

Exchanges of O_2 across the air-sea interface are modeled based on O_2 concentration gradients from surface water to atmosphere and wind speed (Justić et al., 1996; Eldridge and Roelke, 2010), where wind speeds are obtained from the U.S. Navy COAMPS model. Vertical transports in the water-column are calculated based on diffusive and advective transport provided by the hydrodynamic model and modeled O_2 concentration gradients.

Sediment DIC fluxes are modeled as a dynamic ratio between the sediment DIC and sediment O_2 exchange rate as a function of O_2 (Lehrter et al. 2012). This empirically derived expression has the form

$$\frac{DIC}{O_2} Exchange = -3.7 \times O_2 + 19.4 \quad (F3)$$

where O_2 is the observed O_2 concentration and DIC/O_2 is the ratio of observed sediment DIC and O_2 exchanges. Once this ratio is calculated, the sediment DIC Exchange is simply calculated by multiplying by the O_2 exchange obtained from equation F1.

DIC exchanges of pCO_2 across the air-sea interface are modeled based on CO_2 concentration gradients from surface water to atmosphere and wind speed (Whitfield and Turner 1986; Eldridge and Cifuentes, 200), where wind speeds are obtained from the U.S. Navy COAMPS model. The inorganic carbon system is modeled exactly as described in Eldridge and Roelke (2010), with the assumption that alkalinity is a conservative property. Similar to O_2, vertical transports in the water-column are based on diffusive and advective transport provided by the hydrodynamic model and modeled DIC concentration gradients.