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APPENDIX A – EQUATIONS OF THE NPZD MODEL

A.1 Nitrogen Cycle

Ammonia nitrogen (1st state variable) and nitrite+nitrate nitrogen (2nd state variable) are simulated using the Equation A.1 and Equation A.2 respectively,

$$\frac{\partial C_1}{\partial t} = N_{RESP,ZOOP} + N_{RESP,PHY\_G} + N_{RESP,PHY\_D} + N_{RESP,PHY\_C} + N_{DEG,ZOOP\_DIS\_DET} + N_{DEG,PHY\_G\_DIS\_DET} + N_{DEG,PHY\_D\_DIS\_DET} + N_{DEG,PHY\_C\_DIS\_DET} + N_{DEG,EX\_LAB\_DIS\_DET} + N_{DEG,EX\_REF\_DIS\_DET} - N_{NH4\_UPTAKE,PHY\_G} - N_{NH4\_UPTAKE,PHY\_D} - N_{NH4\_UPTAKE,PHY\_C} - N_{NITRIFICATION} \quad \text{(Equation A.1)}$$

$$\frac{\partial C_2}{\partial t} = N_{NITRIFICATION} - N_{DENITRIFICATION} - N_{NO3\_UPTAKE,PHY\_G} - N_{NO3\_UPTAKE,PHY\_D} - N_{NO3\_UPTAKE,PHY\_C} \quad \text{(Equation A.2)}$$

where C_1 is the concentration of ammonia nitrogen ($gN\cdot m^{-3}$), C_2 is the concentration of nitrate nitrogen ($gN\cdot m^{-3}$), $N_{RESP,ZOOP}$, N_{RESP,PHY_G}, N_{RESP,PHY_D} and N_{RESP,PHY_C} are the rates of ammonia nitrogen generation due to zooplankton, the other planktonic algae, diatoms and cyanobacteria respiration ($gN\cdot m^{-3}\cdot day^{-1}$); $N_{DEG,ZOOP\_DIS\_DET}$, $N_{DEG,PHY\_G\_DIS\_DET}$, $N_{DEG,PHY\_D\_DIS\_DET}$ and $N_{DEG,PHY\_C\_DIS\_DET}$ are the rates of ammonium nitrogen generation due to the degradation of zooplankton, other planktonic algae, diatoms and cyanobacteria based dissolved organic carbon ($gN\cdot m^{-3}\cdot day^{-1}$); $N_{DEG,EX\_LAB\_DIS\_DET}$ and $N_{DEG,EX\_REF\_DIS\_DET}$ the rates of ammonium nitrogen generation due to the degradation of labile and refractory external detritus ($gN\cdot m^{-3}\cdot day^{-1}$); N_{NH4_UPTAKE,PHY_G}, N_{NH4_UPTAKE,PHY_D}, N_{NH4_UPTAKE,PHY_C} are the rates of ammonia nitrogen uptake by other planktonic algae, diatoms and cyanobacteria ($gN\cdot m^{-3}\cdot day^{-1}$); N_{NO3_UPTAKE,PHY_G}, N_{NO3_UPTAKE,PHY_D}, N_{NO3_UPTAKE,PHY_C} are nitrate nitrogen uptake rates by the other planktonic algae, diatoms and cyanobacteria ($gN\cdot m^{-3}\cdot day^{-1}$); $N_{NITRIFICATION}$ is the rate of nitrification ($gN\cdot m^{-3}\cdot day^{-1}$) and is the rate of denitrification $N_{DENITRIFICATION}$ ($gN\cdot m^{-3}\cdot day^{-1}$).

Rates of ammonium nitrogen generation due to respiration are calculated using Equation A.3 to Equation A.6,

$$N_{RESP,ZOOP} = nc_{ZOOP}\, ZOOP_{RESP} \quad \text{(Equation A.3)}$$

$$N_{RESP,PHY\_G} = nc_{PHY\_G}\, PHY\_G_{RESP} \quad \text{(Equation A.4)}$$

$$N_{RESP,PHY\_D} = nc_{PHY\_D}\, PHY\_D_{RESP} \quad \text{(Equation A.5)}$$

$$N_{RESP,PHY\_C} = nc_{PHY\_C}\, PHY\_C_{RESP} \quad \text{(Equation A.6)}$$

where $ZOOP_{RESP}$, PHY_G_{RESP}, PHY_D_{RESP} and PHY_C_{RESP} are zooplankton, other planktonic algae, diatoms and cyanobacteria respiration rates (gC·m^{-3}·day^{-1}) and nc_{ZOOP}, nc_{PHY_G}, nc_{PHY_D} and nc_{PHY_C} are the nitrogen to carbon ratios for zooplankton, the other planktonic algae, diatoms and cyanobacteria. Nitrogen to carbon rations of the three phytoplankton groups are entered by the user. Nitrogen to carbon ratio of zooplankton are calculated using the nitrogen to carbon ratios for phytoplankton groups, external labile particulate detritus and food preference factors of zooplankton (Equation A.142).

Rates of ammonium nitrogen generation due to degradation of dissolved organic carbon are calculated using Equation A.7 to Equation A.12,

$$N_{DEG,ZOOP} = nc_{ZOOP} DD_{DEG,ZOOP}$$
(Equation A.7)

$$N_{DEG,PHY\_G} = nc_{PHY\_G} DD_{DEG,PHY\_G}$$
(Equation A.8)

$$N_{DEG,PHY\_D} = nc_{PHY\_D} DD_{DEG,PHY\_D}$$
(Equation A.9)

$$N_{DEG,PHY\_C} = nc_{PHY\_C} DD_{DEG,PHY\_C}$$
(Equation A.10)

$$N_{DEG,PHY\_C} = nc_{EX\_LAB} DD_{DEG,EX\_LAB}$$
(Equation A.11)

$$N_{DEG,PHY\_C} = nc_{EX\_REF} DD_{DEG,EX\_REF}$$
(Equation A.12)

where $DD_{DEG,ZOOP}$, DD_{DEG,PHY_G}, DD_{DEG,PHY_D} and DD_{DEG,PHY_C} are the degradation rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria based dissolved organic carbon (gC·m^{-3}·day^{-1}), DD_{DEG,EX_LAB} and DD_{DEG,EX_REF} are the degradation rates of labile and refractory dissolved organic carbon (gC·m^{-3}·day^{-1}).

Rates of ammonium nitrogen uptake by phytoplankton groups are calculated using Equation A.13 to Equation A.15,

$$N_{NH4\_UPTAKE,PHY\_G} = nc_{PHY\_G} PHY\_G_{NH4N\_PREF} PHY\_G_{GPP} \quad \text{(Equation A.13)}$$

$$N_{NH4\_UPTAKE,PHY\_D} = nc_{PHY\_D} PHY\_D_{NH4N\_PREF} PHY\_D_{GPP} \quad \text{(Equation A.14)}$$

$$N_{NH4\_UPTAKE,PHY\_C} = nc_{PHY\_C} PHY\_C_{NH4N\_PREF} PHY\_C_{GPP,NON\_FIX} \quad \text{(Equation A.15)}$$

where $PHY\_G_{NH4N\_PREF}$, $PHY\_D_{NH4N\_PREF}$, $PHY\_C_{NH4N\_PREF}$ are the ammonia nitrogen preference factors of the other planktonic algae, diatoms and cyanobacteria. PHY_G_{GPP} is the gross primary production rate of the other planktonic algae (gC·m^{-3}·day^{-1}), PHY_D_{GPP} is the gross primary production rate of diatoms (gC·m^{-3}·day^{-1}) and PHY_C_{GPP,NON_FIX} is the gross primary production rate of the cyanobacteria fraction that is not in nitrogen fixing state (gC·m^{-3}·day^{-1}).

Ammonia preference factors are calculated using Equation A.16 to Equation A.18

$$PHY\_G_{NH4N\_PREF} = C_1\left(\frac{C_2}{(K_{mN,PHY\_G}+C_1)(K_{mN,PHY\_G}+C_2)}\right)+ C_1\left(\frac{C_2}{(C_1+C_2)(K_{mN,PHY\_G}+C_2)}\right)$$

(Equation A.16)

$$PHY\_D_{NH4N\_PREF} = C_1\left(\frac{C_2}{(K_{mN,PHY\_D}+C_1)(K_{mN,PHY\_D}+C_2)}\right)+ C_1\left(\frac{C_2}{(C_1+C_2)(K_{mN,PHY\_D}+C_2)}\right)$$

(Equation A.17)

$$PHY\_C_{NH4N\_PREF} = C_1\left(\frac{C_2}{(K_{mN,PHY\_C}+C_1)(K_{mN,PHY\_C}+C_2)}\right)+ C_1\left(\frac{C_2}{(C_1+C_2)(K_{mN,PHY\_C}+C_2)}\right)$$

(Equation A.18)

where K_{mN,PHY_G} , K_{mN,PHY_G} and K_{mN,PHY_G} are inorganic nitrogen half saturation constants for the other planktonic algae, diatoms and cyanobacteria ($gN \cdot m^{-3}$).

Rates of nitrate nitrogen uptake by phytoplankton groups are calculated using Equation A.19 to Equation A.21.

$$N_{NO3\_UPTAKE,PHY\_G} = nc_{PHY\_G}(1 - PHY\_G_{NH4N\_PREF})PHY\_G_{GPP}$$

(Equation A.19)

$$N_{NO3\_UPTAKE,PHY\_D} = nc_{PHY\_D}(1 - PHY\_D_{NH4N\_PREF})PHY\_D_{GPP}$$

(Equation A.20)

$$N_{NO3\_UPTAKE,PHY\_C} = nc_{PHY\_C}(1 - PHY\_G_{NH4N\_PREF})PHY\_C_{GPP,NON\_FIX}$$

(Equation A.21)

Nitrification rate is calculated using Equation A.22,

$$N_{NITRIFICATION} = k_{NITR,20}\ \theta_{NITR}{}^{T-20}\ corr_{NITR,pH}\left(\frac{C_6}{C_6+KH_{NITR}}\right)C_1$$

(Equation A.22)

where T is the water temperature (°C), $k_{NITR,20}$ is the nitrification rate constant at 20°C (day^{-1}), θ_{NITR} is the Arrhenius temperature correction factor for nitrification, $corr_{NITR,pH}$ is the pH correction factor for nitrification, C_6 is the dissolved oxygen concentration ($gO_2 \cdot m^{-3}$) and KH_{NITR} is the half saturation constant for oxygen limitation of nitrification ($gO_2 \cdot m^{-3}$). The pH correction factor for nitrification is calculated using Equation A.23,

$$\begin{aligned}
&pH < pH_{NITR,OPT_MIN} &&\rightarrow\ corr_{NITR,pH} = e^{pH - pH_{NITR,OPT_MIN}}\\
&pH_{NITR,OPT_MIN} \le pH \le pH_{NITR,OPT_MAX} &&\rightarrow\ corr_{NITR,pH} = 1\\
&pH > pH_{NITR,OPT_MAX} &&\rightarrow\ corr_{NITR,pH} = e^{pH_{NITR,OPT_MAX} - pH}
\end{aligned} \qquad \text{(Equation A.23)}$$

where pH is the ambient pH, pH_{NITR,OPT_MIN} is the minimum pH of the optimal range for nitrification and pH_{NITR,OPT_MAX} is the maximum pH of the optimal range for nitrification.

Denitrification rate is calculated using Equation A.24,

$$N_{DENITRIFICATION} = k_{DENITR,20}\ \theta_{DENITR}{}^{T-20}\ corr_{DENITR,pH}\left(\frac{KH_{DENITR}}{C_6 + KH_{DENITR}}\right)C_2 \qquad \text{(Equation A.24)}$$

where T is the water temperature (°C), $k_{DENITR,20}$ is the denitrification rate constant at 20°C (day^{-1}), θ_{DENITR} is the Arrhenius temperature correction factor for denitrification, $corr_{DENITR,pH}$ is the pH correction factor for denitrification, and KH_{DENITR} is the half saturation constant for oxygen limitation of denitrification ($gO_2 \cdot m^{-3}$). The pH correction factor for nitrification is calculated using Equation A.25,

$$\begin{aligned}
&pH < pH_{DENITR,OPT_MIN} &&\rightarrow\ corr_{DENITR,pH} = e^{pH - pH_{DENITR,OPT_MIN}}\\
&pH_{DENITR,OPT_MIN} \le pH \le pH_{DENITR,OPT_MAX} &&\rightarrow\ corr_{DENITR,pH} = 1\\
&pH > pH_{DENITR,OPT_MAX} &&\rightarrow\ corr_{DENITR,pH} = e^{pH_{DENITR,OPT_MAX} - pH}
\end{aligned} \qquad \text{(Equation A.25)}$$

where pH is the ambient pH, pH_{DENITR,OPT_MIN} is the minimum pH of the optimal range for denitrification and pH_{DENITR,OPT_MAX} is the maximum pH of the optimal range for denitrification.

A.2 Phosphorus Cycle

Phosphate phosphorus (3rd state variable) is simulated using the Equation A.26

$$\begin{aligned}
\frac{\partial C_3}{\partial t} = {} & P_{RESP,ZOOP} + P_{RESP,PHY_G} + P_{RESP,PHY_D} + P_{RESP,PHY_C} +\\
& P_{DEG,ZOOP_DIS_DET} + P_{DEG,PHY_G_DIS_DET} + P_{DEG,PHY_D_DIS_DET} +\\
& P_{DEG,PHY_C_DIS_DET} + P_{DEG,EX_LAB_DIS_DET} + P_{DEG,EX_REF_DIS_DET} -\\
& P_{UPTAKE,PHY_G} - P_{UPTAKE,PHY_D} - P_{UPTAKE,PHY_C}
\end{aligned} \qquad \text{(Equation A.26)}$$

where C_3 is the concentration of phosphate phosphorus ($gP \cdot m^{-3}$), $P_{RESP,ZOOP}$, P_{RESP,PHY_G}, P_{RESP,PHY_D} and P_{RESP,PHY_C} are the rates of phosphate phosphorus generation due to zooplankton, the other planktonic algae, diatoms and cyanobacteria respiration ($gP \cdot m^{-3} \cdot day^{-1}$); $P_{DEG,ZOOP\_DIS\_DET}$, $P_{DEG,PHY\_G\_DIS\_DET}$, $P_{DEG,PHY\_D\_DIS\_DET}$ and $P_{DEG,PHY\_C\_DIS\_DET}$ are the rates of phosphate phosphorus generation due to the degradation of zooplankton, the other planktonic algae, diatoms and cyanobacteria based dissolved organic carbon ($gP \cdot m^{-3} \cdot day^{-1}$);

$P_{DEG,EX\_LAB\_DIS\_DET}$ and $P_{DEG,EX\_REF\_DIS\_DET}$ the rates of phosphate phosphorus generation due to the degradation of labile and refractory external detritus (gP·m^{-3}·day^{-1}); $P_{UPTAKE,\ PHY\_G}$, $P_{UPTAKE,\ PHY\_D}$ and $P_{UPTAKE,\ PHY\_C}$ are rates of phosphate phosphorus uptake by the other planktonic algae, diatoms and cyanobacteria (gP·m^{-3}·day^{-1}).

Rates of phosphate phosphorus generation due to respiration are calculated using Equation A.27 to Equation A.30,

$$P_{RESP,ZOOP} = pc_{ZOOP}\, ZOOP_{RESP}$$
(Equation A.27)

$$P_{RESP,PHY\_G} = pc_{PHY\_G}\, PHY\_G_{RESP}$$
(Equation A.28)

$$P_{RESP,PHY\_D} = pc_{PHY\_D}\, PHY\_D_{RESP}$$
(Equation A.29)

$$P_{RESP,PHY\_C} = pc_{PHY\_C}\, PHY\_C_{RESP}$$
(Equation A.30)

where $ZOOP_{RESP}$, PHY_G_{RESP}, PHY_D_{RESP} and PHY_C_{RESP} are the rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria respiration (gC·m^{-3}·day^{-1}) and pc_{ZOOP}, pc_{PHY_G}, pc_{PHY_D} and pc_{PHY_C} are the phosphorus to carbon ratios for zooplankton, the other planktonic algae, diatoms and cyanobacteria. Phosphorus to carbon rations of the three phytoplankton groups are entered by the user. Phosphorus to carbon ratio of zooplankton are calculated using the phosphorus to carbon ratios for phytoplankton groups, external labile particulate detritus and food preference factors of zooplankton (Equation A.143).

Rates of phosphate phosphorus generation due to degradation of dissolved organic carbon are calculated using Equation A.31 to Equation A.36,

$$P_{DEG,ZOOP} = pc_{ZOOP}\, DD_{DEG,ZOOP}$$
(Equation A.31)

$$P_{DEG,PHY\_G} = pc_{PHY\_G}\, DD_{DEG,PHY\_G}$$
(Equation A.32)

$$P_{DEG,PHY\_D} = pc_{PHY\_D}\, DD_{DEG,PHY\_D}$$
(Equation A.33)

$$P_{DEG,PHY\_C} = pc_{PHY\_C}\, DD_{DEG,PHY\_C}$$
(Equation A.34)

$$P_{DEG,PHY\_C} = pc_{EX\_LAB}\, DD_{DEG,EX\_LAB}$$
(Equation A.35)

$$P_{DEG,PHY\_C} = pc_{EX\_REF}\, DD_{DEG,EX\_REF}$$
(Equation A.36)

where $DD_{DEG,ZOOP}$, DD_{DEG,PHY_G}, DD_{DEG,PHY_D} and DD_{DEG,PHY_C} are the degradation rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria based dissolved organic carbon (gC·m^{-3}·day^{-1}), DD_{DEG,EX_LAB} and DD_{DEG,EX_REF} are the degradation rates of labile and refractory dissolved organic carbon (gC·m^{-3}·day^{-1}).

Rates of phosphate phosphorus uptake by phytoplankton groups are calculated using Equation A.37 to Equation A.39,

$$P_{UPTAKE,\ PHY\_G} = pc_{PHY\_G}\ PHY\_G_{GPP}$$

(Equation A.37)

$$P_{UPTAKE,\ PHY\_D} = pc_{PHY\_D}\ PHY\_D_{GPP}$$

(Equation A.38)

$$P_{UPTAKE,\ PHY\_C} = pc_{PHY\_C}\ PHY\_C_{GPP}$$

(Equation A.39)

where PHY_G_{GPP} is the other planktonic algae (gC·m^{-3}·day^{-1}) gross primary production rate, PHY_D_{GPP} is the diatoms gross primary production rate (gC·m^{-3}·day^{-1}) and PHY_C_{GPP} is the cyanobacteria gross primary production rate (gC·m^{-3}·day^{-1}).

A.3 Silicon Cycle

Available silica silicon (10th state variable) is simulated using the Equation A.40,

$$\frac{\partial C_{10}}{\partial t} = Si_{RESP,ZOOP} + Si_{RESP,PHY\_D} + Si_{DEG,ZOOP\_DIS\_DET} + Si_{DEG,PHY\_D\_DIS\_DET} + Si_{DEG,EX\_LAB\_DIS\_DET} + Si_{DEG,EX\_REF\_DIS\_DET} - Si_{UPTAKE,PHY\_D}$$

(Equation A.40)

where C_{10} is the concentration of available silica silicon (gSi·m^{-3}), $Si_{RESP,ZOOP}$ and Si_{RESP,PHY_D} are the rates of available silica silicon generation due to zooplankton and diatoms respiration (gSi·m^{-3}·day^{-1}); $Si_{DEG,ZOOP\_DIS\_DET}$ and $Si_{DEG,PHY\_D\_DIS\_DET}$ are the rates of available silica silicon generation due to the degradation of zooplankton and diatoms based dissolved organic carbon (gSi·m^{-3}·day^{-1}); $Si_{DEG,EX\_LAB\_DIS\_DET}$ and $Si_{DEG,EX\_REF\_DIS\_DET}$ the rates of available silica silicon generation due to the degradation of labile and refractory external detritus (gSi·m^{-3}·day^{-1}); $Si_{UPTAKE,\ PHY\_D}$ is the rate of available silica silicon uptake by diatoms (gSi·m^{-3}·day^{-1}).

Rates of available silica silicon generation due to respiration are calculated using Equation A.41 and Equation A.42,

$$Si_{RESP,ZOOP} = sic_{ZOOP}\ ZOOP_{RESP}$$

(Equation A.41)

$$Si_{RESP,PHY\_D} = sic_{PHY\_D}\ PHY\_D_{RESP}$$

(Equation 3.42)

where $ZOOP_{RESP}$ and PHY_D_{RESP} are the rates of zooplankton and diatoms and respiration ($gC\cdot m^{-3}\cdot day^{-1}$); sic_{ZOOP} and sic_{PHY_D} are the silicon to carbon ratios for zooplankton and diatoms. Silicon to carbon ratio for diatoms is entered by the user. Silicon to carbon ratio of zooplankton is calculated using the silicon to carbon ratios for diatoms, external labile particulate detritus and food preference factors of zooplankton (Equation A.144).

Rates of available silica silicon generation due to degradation of dissolved organic carbon are calculated using Equation A.43 to Equation A.46,

$$Si_{DEG,ZOOP} = sic_{ZOOP} DD_{DEG,ZOOP}$$
(Equation A.43)

$$Si_{DEG,PHY\_D} = sic_{PHY\_D} DD_{DEG,PHY\_D}$$
(Equation A.44)

$$Si_{DEG,PHY\_C} = sic_{EX\_LAB} DD_{DEG,EX\_LAB}$$
(Equation A.45)

$$Si_{DEG,PHY\_C} = sic_{EX\_REF} DD_{DEG,EX\_REF}$$
(Equation A.46)

where $DD_{DEG,ZOOP}$ and DD_{DEG,PHY_D} are the degradation rates of zooplankton and diatoms based dissolved organic carbon ($gC\cdot m^{-3}\cdot day^{-1}$), DD_{DEG,EX_LAB} and DD_{DEG,EX_REF} are the labile and refractory dissolved organic carbon degradation rates ($gC\cdot m^{-3}\cdot day^{-1}$).

The rate of available silica silicon is calculated using Equation A.47,

$$Si_{UPTAKE,PHY\_D} = sic_{PHY\_D} PHY\_D_{GPP}$$
(Equation A.47)

where PHY_G_{GPP} is the gross primary production rate of diatoms ($gC\cdot m^{-3}\cdot day^{-1}$).

A.4 Carbon Cycle

External labile dissolved organic carbon (5^{th} state variable), external labile particulate detritus carbon (7^{th} state variable), external refractory dissolved organic carbon (8^{th} state variable) and external refractory particulate detritus carbon (11^{th} state variable) are modelled using Equations A.48 to A.51. The autochthonous detritus carbon is simulated using the other planktonic algae based dissolved organic carbon (15^{th} state variable), other planktonic algae based particulate detritus (16^{th} state variable), diatoms based dissolved organic carbon (17^{th} state variable), diatoms based particulate detritus (18^{th} state variable), cyanobacteria based dissolved organic carbon (19^{th} state variable), cyanobacteria based particulate detritus (20^{th} state variable), zooplankton based dissolved organic carbon (21^{st} state variable) and zooplankton based particulate detritus (22^{nd} state variable) using Equations A.52 to A.59. Inorganic carbon is simulated using carbon dioxide carbon (14^{th} state variable) (Equation A.60).

$$\frac{\partial C_5}{\partial t} = PD_{DISS,EX\_LAB} - DD_{DEG,EX\_LAB}$$
(Equation A.48)

$$\frac{\partial C_7}{\partial t} = - PD_{DISS,EX\_LAB} - ZOOP_{GRAZ,PD\_EX\_LAB}$$
(Equation A.49)

$$\frac{\partial C_8}{\partial t} = PD_{DISS,EX\_REF} - DD_{DEG,EX\_REF}$$
(Equation A.50)

$$\frac{\partial C_{11}}{\partial t} = -PD_{DISS,EX\_REF}$$
(Equation A.51)

$$\frac{\partial C_{15}}{\partial t} = PD_{DISS,PHY\_G} + PHY\_G_{EXCR} - DD_{DEG,PHY\_G}$$
(Equation A.52)

$$\frac{\partial C_{16}}{\partial t} = -PD_{DISS,PHY\_G} + PHY\_G_{DEAD} - ZOOP_{GRAZ,PHY\_G\_PDET} \quad \text{(Equation A.53)}$$

$$\frac{\partial C_{17}}{\partial t} = PD_{DISS,PHY\_D} + PHY\_D_{EXCR} - DD_{DEG,PHY\_D} \quad \text{(Equation A.54)}$$

$$\frac{\partial C_{18}}{\partial t} = -PD_{DISS,PHY\_G} + PHY\_G_{DEAD} - ZOOP_{GRAZ,PHY\_D\_PDET} \quad \text{(Equation A.55)}$$

$$\frac{\partial C_{19}}{\partial t} = PD_{DISS,PHY\_C} + PHY\_C_{EXCR} - DD_{DEG,PHY\_C} \quad \text{(Equation A.56)}$$

$$\frac{\partial C_{20}}{\partial t} = -PD_{DISS,PHY\_C} + PHY\_C_{DEAD} - ZOOP_{GRAZ,PHY\_C\_PDET} \quad \text{(Equation A.57)}$$

$$\frac{\partial C_{21}}{\partial t} = PD_{DISS,ZOOP} + ZOOP_{EXCR} - DD_{DEG,ZOOP}$$
(Equation A.58)

$$\frac{\partial C_{22}}{\partial t} = -PD_{DISS,ZOOP} + ZOOP_{DEAD}$$
(Equation A.59)

$$\begin{aligned}\frac{\partial C_{14}}{\partial t} = {} & ZOOP_{RESP} + PHY\_G_{RESP} + PHY\_D_{RESP} + PHY\_C_{RESP} + \\ & DD_{DEG,ZOOP} + DD_{DEG,PHY\_G} + DD_{DEG,PHY\_D} + DD_{DEG,PHY\_C} + \\ & DD_{DEG,EX\_LAB} + DD_{DEG,EX\_REF} + IC_{ATMO} - PHY\_G_{GPP} - \\ & PHY\_D_{GPP} - PHY\_C_{GPP}\end{aligned} \quad \text{(Equation A.60)}$$

where C_5 is the concentration of external labile dissolved organic carbon (gC·m^{-3}), C_7 is the concentration of external labile particulate detritus carbon (gC·m^{-3}), C_8 is the concentration of external refractory dissolved organic carbon (gC·m^{-3}), C_{11} is the concentration of external refractory particulate detritus carbon (gC·m^{-3}), C_{15} is the concentration of the other planktonic algae based dissolved organic carbon (gC·m^{-3}), C_{16} is the concentration of the other planktonic algae based particulate detritus carbon (gC·m^{-3}), C_{17} is the concentration of diatoms based dissolved organic carbon (gC·m^{-3}), C_{18} is the concentration of diatoms based particulate detritus carbon (gC·m⁻³), C_{19} is the concentration of cyanobacteria based dissolved organic carbon (gC·m⁻³), C_{20} is the concentration of cyanobacteria based particulate detritus carbon (gC·m⁻³), C_{21} is the concentration of zooplankton based dissolved organic carbon (gC·m⁻³), C_{22} is the concentration of zooplankton based particulate detritus carbon (gC·m⁻³), C_{14} is the concentration of inorganic carbon (gC·m⁻³), PD_{DISS,EX_LAB}, PD_{DISS,EX_REF}, $PD_{DISS,ZOOP}$, PD_{DISS,PHY_G}, PD_{DISS,PHY_D} and PD_{DISS,PHY_C} are the dissolution rates for external labile particulate detritus carbon, external refractory particulate detritus carbon, zooplankton based particulate detritus carbon, the other planktonic algae based particulate detritus carbon, diatoms based particulate detritus carbon and cyanobacteria based particulate detritus carbon (gC·m⁻³·day⁻¹); $DD_{DEG,ZOOP}$, DD_{DEG,PHY_G}, DD_{DEG,PHY_D} and DD_{DEG,PHY_C} are the degradation rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria based dissolved organic carbon (gC·m⁻³·day⁻¹), DD_{DEG,EX_LAB} and DD_{DEG,EX_REF} are the degradation rates of labile and refractory dissolved organic carbon (gC·m⁻³·day⁻¹); $ZOOP_{GRAZ,PD\_EX\_LAB}$ is the grazing rate of zooplankton on external labile particulate zooplankton carbon; $ZOOP_{GRAZ,PHY\_G\_PDET}$, $ZOOP_{GRAZ,PHY\_D\_PDET}$ and $ZOOP_{GRAZ,PHY\_C\_PDET}$ are the grazing rates of zooplankton on other planktonic algae, diatoms and cyanobacteria based detritus (gC·m⁻³·day⁻¹); $ZOOP_{DEAD}$, PHY_G_{DEAD}, PHY_D_{DEAD} and PHY_C_{DEAD} are death rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria (gC·m⁻³·day⁻¹); $ZOOP_{EXCR}$, PHY_G_{EXCR}, PHY_D_{EXCR} and PHY_C_{EXCR} are the excretion rates of zooplankton, the other planktonic algae, diatoms and cyanobacteria (gC·m⁻³·day⁻¹); PHY_G_{GPP}, PHY_D_{GPP} and PHY_C_{GPP} are the gross primary production rates of the other planktonic algae, the diatoms and cyanobacteria (gC·m⁻³·day⁻¹) and IC_{ATMO} is the exchange rate of inorganic carbon (gC·m⁻³·day⁻¹) between the water and the atmosphere.

The dissolution rates for particulate detritus carbon components are calculated using Equation A.61 to Equation A.66,

$$PD_{DISS,EX\_LAB} = k_{DISS,PD\_EX\_LAB,20}\ \theta_{DISS,PD\_EX\_LAB}^{T-20} C_7$$
(Equation A.61)

$$PD_{DISS,EX\_REF} = k_{DISS,PD\_EX\_REF,20}\ \theta_{DISS,PD\_EX\_REF}^{T-20} C_{11}$$
(Equation A.62)

$$PD_{DISS,ZOOP} = k_{DISS,PD\_ZOOP,20}\ \theta_{DISS,PD\_ZOOP}^{T-20} C_{22}$$
(Equation A.63)

$$PD_{DISS,PHY\_G} = k_{DISS,PD\_PHY\_G,20}\ \theta_{DISS,PD\_PHY\_G}^{T-20} C_{16}$$
(Equation A.64)

$$PD_{DISS,PHY\_D} = k_{DISS,PD\_PHY\_D,20}\ \theta_{DISS,PD\_PHY\_D}^{T-20} C_{18}$$
(Equation A.65)

$$PD_{DISS,PHY\_C} = k_{DISS,PD\_PHY\_C,20}\ \theta_{DISS,PD\_PHY\_C}^{T-20} C_{20}$$
(Equation A.66)

where $k_{DISS,PD\_EX\_LAB,20}$, $k_{DISS,PD\_EX\_REF,20}$, $k_{DISS,PD\_ZOOP,20}$, $k_{DISS,PD\_PHY\_G,20}$, $k_{DISS,PD\_PHY\_D,20}$ and $k_{DISS,PD\_PHY\_C,20}$ are the dissolution rate constants for external labile particulate detritus carbon, external refractory particulate detritus carbon, zooplankton based particulate detritus carbon, the other planktonic algae based particulate detritus carbon, diatoms based particulate detritus carbon and cyanobacteria based particulate detritus carbon at 20°C (day^{-1}) and θ_{DISS,PD_EX_LAB}, θ_{DISS,PD_EX_REF}, θ_{DISS,PD_ZOOP}, θ_{DISS,PD_PHY_G}, θ_{DISS,PD_PHY_D} and θ_{DISS,PD_PHY_C} are the Arrhenius constants of temperature correction factors for the dissolution of external labile particulate detritus carbon, external refractory particulate detritus carbon, zooplankton based particulate detritus carbon, the other planktonic algae based particulate detritus carbon, diatoms based particulate detritus carbon and cyanobacteria based particulate detritus carbon.

The dissolution rates for particulate detritus carbon components are calculated using Equation A.67 to Equation A.72,

$$DD_{DEG,EX\_LAB} = k_{DEG,DD\_EX\_LAB,20}\ \theta_{DISS,DD\_EX\_LAB}^{T-20}\ C_5$$
(Equation A.67)

$$DD_{DEG,EX\_REF} = k_{DEG,DD\_EX\_REF,20}\ \theta_{DISS,DD\_EX\_REF}^{T-20}\ C_8$$
(Equation A.68)

$$DD_{DEG,ZOOP} = k_{DEG,DD\_ZOOP,20}\ \theta_{DISS,DD\_ZOOP}^{T-20}\ C_{21}$$
(Equation A.69)

$$DD_{DEG,PHY\_G} = k_{DEG,DD\_PHY\_G,20}\ \theta_{DISS,DD\_PHY\_G}^{T-20}\ C_{15}$$
(Equation A.70)

$$DD_{DEG,PHY\_D} = k_{DEG,DD\_PHY\_D,20}\ \theta_{DISS,DD\_PHY\_D}^{T-20}\ C_{17}$$
(Equation A.71)

$$DD_{DEG,PHY\_C} = k_{DEG,DD\_PHY\_C,20}\ \theta_{DISS,DD\_PHY\_C}^{T-20}\ C_{19}$$
(Equation A.72)

$k_{DEG,DD\_EX\_LAB,20}$, $k_{DEG,DD\_EX\_REF,20}$, $k_{DEG,DD\_ZOOP,20}$, $k_{DEG,DD\_PHY\_G,20}$, $k_{DEG,DD\_PHY\_D,20}$ and $k_{DEG,DD\_PHY\_C,20}$ are the dissolution rate constants for external labile particulate detritus carbon, external refractory particulate detritus carbon, zooplankton based particulate detritus carbon, the other planktonic algae based particulate detritus carbon, diatoms based particulate detritus carbon and cyanobacteria based particulate detritus carbon at 20°C (day^{-1}) and θ_{DEG,DD_EX_LAB}, θ_{DEG,DD_EX_REF}, θ_{DEG,DD_ZOOP}, θ_{DISS,PD_PHY_G}, θ_{DEG,DD_PHY_D} and θ_{DEG,DD_PHY_C} are the Arrhenius constants of temperature correction factors for the dissolution of external labile particulate detritus carbon, external refractory particulate detritus carbon, zooplankton based particulate detritus carbon, the other planktonic algae based particulate detritus carbon, diatoms based particulate detritus carbon and cyanobacteria based particulate detritus carbon.

The atmospheric exchange rate of inorganic carbon is calculated using Equation A.73 to Equation A.76,

$$IC_{ATMO} = \frac{12}{44}\left(K_{liq,CO_2}\left(\left[CO_2\right]_{SAT} - \frac{44}{12}C_{14}\right)\right)$$

(Equation A.73)

$$K_{liq,CO_2} = K_{A,20}\theta_A{}^{T-20}\left(\frac{12}{44}\right)^{0.25}$$

(Equation A.74)

$$\left[CO_2\right]_{SAT} = K_{H,CO_2}\, p_{CO_2}$$

(Equation A.75)

$$K_{H,CO_2} = 44000\left(10^{\left(\frac{2385.73}{T+273.15} - 14.0184 + 0.0152642(T+273.15)\right)}\right)$$

(Equation A.76)

where K_{liq,CO_2} is the rate constant for CO_2 transfer into the water (day^{-1}), $\left[CO_2\right]_{SAT}$ is the saturation concentration of CO_2 ($gCO_2 \cdot m^{-3}$), $K_{A,20}$ is the rate constant for aeration at 20°C (day^{-1}), θ_A is the Arrhenius coefficient for temperature correction of aeration, K_{H,CO_2} is the Henry's law coefficient for CO_2 ($gCO_2 \cdot m^{-3} \cdot atm$) and p_{CO_2} is the partial pressure of CO_2 in the atmosphere that is assumed equal to 0.00035 atm by ALUKAS.

A.5 Dissolved Oxygen

Dissolved oxygen is simulated using the equation Equation A.77,

$$\begin{aligned}\frac{\partial C_6}{\partial t} = {} & K_{A,20}\theta_A{}^{T-20}\left(\left[O_2\right]_{SAT} - C_6\right) + \\ & oc_{PHY\_G}\, PHY\_G_{NH4\_PREF}\, PHY\_G_{GPP} + oc_{PHY\_D}\, PHY\_D_{NH4\_PREF}\, PHY\_D_{GPP} + \\ & oc_{PHY\_C}\, PHY\_C_{NH4\_PREF} PHY\_C_{GPP} - \\ & oc_{PHY\_G}\left(1 - PHY\_G_{NH4\_PREF}\right)PHY\_G_{GPP}\left(1 + \frac{48}{14}nc_{PHY\_G}\right) + \\ & oc_{PHY\_D}\left(1 - PHY\_D_{NH4\_PREF}\right)PHY\_D_{GPP}\left(1 + \frac{48}{14}nc_{PHY\_D}\right) + \\ & oc_{PHY\_C}\left(1 - PHY\_C_{NH4\_PREF}\right)PHY\_C_{GPP}\left(1 + \frac{48}{14}nc_{PHY\_C}\right) - \\ & oc_{ZOOP}\, ZOOP_{RESP} - oc_{PHY\_G}\, PHY\_G_{RESP} - oc_{PHY\_D}\, PHY\_D_{RESP} - \\ & oc_{PHY\_C}\, PHY\_C_{RESP} - oc_{ZOOP}\, DD_{DEG,ZOOP} - oc_{PHY\_G}\, DD_{DEG,PHY\_G} - oc_{PHY\_D}\, DD_{DEG,PHY\_D} - \\ & oc_{PHY\_C}\, DD_{DEG,PHY\_C} - oc_{DD\_EX\_LAB}\, DD_{DEG,EX\_LAB} - oc_{DD\_EX\_REF}\, DD_{DEG,EX\_REF} - \frac{64}{14}N_{NITRIFICATION}\end{aligned}$$

(Equation A.77)

where C_6 is the concentration of dissolved oxygen ($gO_2 \cdot m^{-3}$), $\left[O_2\right]_{SAT}$ is the saturation concentration of dissolved oxygen ($gO_2 \cdot m^{-3}$), $K_{A,20}$ is the rate constant for aeration at 20°C (day^{-1}), θ_A is the Arrhenius coefficient for temperature correction of aeration, oc_{ZOOP},

oc_{PHY_G}, oc_{PHY_D} and oc_{PHY_C} are the phosphorus to carbon ratios for zooplankton, the other planktonic algae, diatoms and cyanobacteria, $oc_{DD\_EX\_LAB}$ is the oxygen to carbon ratio for external labile dissolved organic carbon and $oc_{DD\_EX\_REF}$ is the oxygen to carbon ratio for external refractory dissolved organic carbon.

The aeration coefficient is calculated with the same method as explained in Appendix B. Dissolved oxygen saturation concentration is calculated using Equations A.78 to A.83. The saturation concentration of dissolved oxygen in saline water at sea level is calculated using Equation A.74.

$$\ln(o_{ss}) = \ln(o_{sf}) - S\left(1.7674\ 10^{-2} - \frac{1.0754\ 10^{1}}{T + 273.16} + \frac{2.1407\ 10^{3}}{(T + 273.16)^{2}}\right) \quad \text{(Equation A.78)}$$

where, o_{sf} is the saturation concentration of dissolved oxygen in saline water at sea level ($gO_2 \cdot m^{-3}$), S is the salinity (ppt), T is the water temperature (°C) and o_{sf} is the saturation concentration of dissolved oxygen in fresh water at sea level ($gO_2 \cdot m^{-3}$), which is calculated using Equation A.75.

$$\ln(o_{sf}) = -139.34411 + \frac{1.5757\ 10^{5}}{T + 273.16} - \frac{6.642308\ 10^{7}}{(T + 273.16)^{2}} + \frac{1.2438\ 10^{10}}{(T + 273.16)^{3}} - \frac{8.621949\ 10^{11}}{(T + 273.16)^{4}}$$

(Equation A.79)

In ALUKAS, the calculated dissolved oxygen concentration at sea level is adjusted to the water surface elevation using Equation A.76,

$$[O_2]_{SAT} = o_{ss}\left[\frac{\left(1 - \frac{P_w}{P}\right)(1 - \theta P)}{(1 - P_w)(1 - \theta P)}\right]$$

(Equation A.80)

where P is the atmospheric pressure (atm), P_w is the partial pressure of water vapour (atm) and θ is a temperature dependent parameter, which is calculated using Equation A.77.

$$\theta = 0.000975 - 1.426\ 10^{-5}T + 6.436\ 10^{-8}T^{2}$$

(Equation A.81)

Partial pressure of water vapour is estimated using Equation A.78.

$$P_w = \exp\left(11.8571 - \frac{3840.7}{T + 273.16} - \frac{216961}{(T + 273.16)^{2}}\right)$$

(Equation A.82)

Atmospheric pressure is estimated using Equation A.79,

$$P = 1 - 0.0875H$$

(Equation A.83)

where H is the water surface elevation with reference to the mean sea level (m). This algorithm provides the possibility to apply ALUKAS not only to estuaries at sea level but also river-estuarine ecosystems where the entire watershed may reach up to elevations of several thousands metres.

A.6 Phytoplankton Groups

The other planktonic algae (4th state variable), diatoms (12th state vairable) and cyanobacteria (13th state variable) are simulated using Equation A.84, Equation A.85 and Equation A.86,

$$\frac{\partial C_4}{\partial t} = PHYT\_G_{GPP} - PHYT\_G_{RESP} - PHYT\_G_{EXCR} - PHYT\_G_{DEAD} - ZOOP_{GRAZ,PHY\_G}$$

(Equation A.84)

$$\frac{\partial C_{12}}{\partial t} = PHYT\_D_{GPP} - PHYT\_D_{RESP} - PHYT\_D_{EXCR} - PHYT\_D_{DEAD} - ZOOP_{GRAZ,PHY\_D}$$

(Equation A.85)

$$\frac{\partial C_{13}}{\partial t} = PHYT\_C_{GPP} - PHYT\_C_{RESP} - PHYT\_C_{EXCR} - PHYT\_C_{DEAD} - ZOOP_{GRAZ,PHY\_C}$$

(Equation A.86)

where C_4, C_{12} and C_{13} are the concentrations of the other planktonic algae carbon, diatoms carbon and cyanobacteria carbon ($gC \cdot m^{-3}$); PHY_G_{GPP}, PHY_D_{GPP} and PHY_C_{GPP} are the gross primary production rates of the other planktonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$); PHY_G_{EXCR}, PHY_D_{EXCR} and PHY_C_{EXCR} are the excretion rates of the other planktonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$); PHY_G_{DEAD}, PHY_D_{DEAD} and PHY_C_{DEAD} are the death rates of the other planctonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$) and $ZOOP_{GRAZ,\ PHY\_G}$, $ZOOP_{GRAZ,\ PHY\_D}$ and $ZOOP_{GRAZ,\ PHY\_C}$ are the grazing rates of zooplankton for the other planktonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$).

The gross primary production rates of the other planktonic algae and diatoms are calculated using Equation A.87 and Equation A.88,

$$PHY\_G_{GPP} = k_{MAX\_GROW,\ PHY\_G}\, LIM_{TEMP,\ PHY\_G}\, LIM_{NUTR\_AND\_LIGHT,\ PHY\_G}\, C_4 \quad \text{(Equation A.87)}$$

$$PHY\_D_{GPP} = k_{MAX\_GROW,\ PHY\_D}\, LIM_{TEMP,\ PHY\_D}\, LIM_{NUTR\_AND\_LIGHT,\ PHY\_D}\, C_{12} \quad \text{(Equation A.88)}$$

where $k_{MAX\_GROW,\ PHY\_G}$ and $k_{MAX\_GROW,\ PHY\_G}$ are the maximum growth rate constants of the other planktonic algae and diatoms (day^{-1}); $lim_{TEMP,\ PHY\_G}$ and $lim_{TEMP,\ PHY\_D}$ are the temperature limitation factors for the other planktonic algae and diatoms and

$lim_{NUTR\_AND\_LIGHT, PHY\_G}$ and $lim_{NUTR\_AND\_LIGHT, PHY\_D}$ are the nutrient and light limitation factors for the other planktonic algae and diatoms. The gross primary production rate of cyanobacteria is calculated using a different algorithm. ALUKAS assumes that the cyanobacteria switch to nitrogen fixation if the total inorganic nitrogen (ammonia nitrogen + nitrate nitrogen) is depleteA. However, switching from inorganic nitrogen uptake to nitrogen fixation is not described by a step function. It is a transition so that inorganic nitrogen uptake and nitrogen fixation can occur at the same time. At relatively high total inorganic nitrogen concentrations, ALUKAS calculates negligible rates for nitrogen fixation. Gross primary production rate of cyanobacteria is calculated using Equation A.89,

$$PHY\_C_{GPP} = PHY\_C_{GPP, NH4+NO3\_UPTAKE} + PHY\_C_{GPP, N\_FIXATION} \quad \text{(Equation A.89)}$$

where $PHY\_C_{GPP, NH4+NO3\_UPTAKE}$ is the gross primary production rate of non nitrogen fixing cyanobacteria growth ($gC \cdot m^{-3} \cdot day^{-1}$) and $PHY\_C_{GPP, N\_FIXATION}$ is the gross primary production rate of nitrogen fixing cyanobacteria growth ($gC \cdot m^{-3} \cdot day^{-1}$). $PHY\_C_{GPP, NH4+NO3\_UPTAKE}$ and $PHY\_C_{GPP, N\_FIXATION}$ are calculated using Equation A.90 and Equation A.91,

$$PHY\_C_{GPP, NH4+NO3\_UPTAKE} = k_{MAX\_GROW, PHY\_C} LIM_{TEMP, PHY\_C} LIM_{NUTR\_AND\_LIGHT, PHY\_C, NO\_NITR\_FIX} C_{13} \quad \text{(Equation A.90)}$$

$$PHY\_C_{GPP, N\_FIXATION} = k_{MAX\_GROW, PHY\_C} LIM_{TEMP, PHY\_C} LIM_{NUTR\_AND\_LIGHT, PHY\_C, NITR\_FIX} C_{13} \quad \text{(Equation A.91)}$$

where k_{MAX_GROW, PHY_C} is the maximum growth rate of cyanobacteria (day^{-1}) and lim_{TEMP, PHY_C} and lim_{TEMP, PHY_D} is the temperature limitation factor of cyanobacteria, $LIM_{NUTR\_AND\_LIGHT, PHY\_C, NO\_NITR\_FIX}$ is the nutrient and light limitation factor of cyanobacteia for non nitrogen fixing growth and $LIM_{NUTR\_AND\_LIGHT, PHY\_C, NITR\_FIX}$ is the nutrient and light limitation factor of cyanobacteia for nitrogen fixing growth.

Temperature limitations on the other planktonic algae, diatoms and cyanobacteria are simulated using Stroganov functions, which are summarized in Equation A.92 to Equation A.94,

$$LIM_{TEMP, PHY\_G} = f_{STROGANOV}\left(T, q_{10,PHY\_G}, T_{MAX, PHY\_G}, T_{OPT, PHY\_G}, XM_{PHY\_G}, K_{T\_ACC, PHY\_G}, T_{ACC\_REF, PHY\_G}\right) \quad \text{(Equation A.92)}$$

$$LIM_{TEMP,PHY\_D} = f_{STROGANOV}\left(T, q_{10,PHY\_D}, T_{MAX,PHY\_D}, T_{OPT,PHY\_D}, XM_{PHY\_D}, K_{T\_ACC,PHY\_D}, T_{ACC\_REF,PHY\_D}\right) \quad \text{(Equation A.93)}$$

$$LIM_{TEMP, PHY\_C} = f_{STROGANOV}\left(T, q_{10,PHY\_C}, T_{MAX, PHY\_C}, T_{OPT, PHY\_C}, XM_{PHY\_C}, K_{T\_ACC, PHY\_C}, T_{ACC\_REF, PHY\_C}\right) \quad \text{(Equation A.94)}$$

where T is the water temperature (°C); q_{10,PHY_G}, q_{10,PHY_D} and q_{10,PHY_C} are the change ratios of growth rates of the other planktonic algae, diatoms and cyanobacteria per 10°C;

T_{MAX, PHY_G}, T_{MAX, PHY_D} and T_{MAX, PHY_C} are the maximum temperatures at which the other planktonic algae, diatoms and cyanobacteria can grow (°C); T_{OPT, PHY_G}, T_{OPT, PHY_D} and T_{OPT, PHY_C} are the optimum growth temperatures for the other planktonic algae, diatoms and cyanobacteria (°C); XM_{PHY_G}, XM_{PHY_D}, and XM_{PHY_C} are the maximum shifts for acclimation temperatures of the other planktonic algae, diatoms and cyanobacteria (°C); K_{T_ACC, PHY_G}, K_{T_ACC, PHY_D} and K_{T_ACC, PHY_C} are the coefficients for decreasing acclimation as temperature approaches the reference temperatures for phytoplankton, diatoms and cyanobacteria acclimation and T_{ACC_REF, PHY_G}, T_{ACC_REF, PHY_D} and T_{ACC_REF, PHY_C} are the reference (minimum) temperatures for phytoplankton, diatoms and cyanobacteria acclimation (°C).

Light and nutrient limitations simulated using Equation A.95 to Equation A.98,

$$LIM_{NUTR\_LIGHT, PHY\_G} = \min\left(LIM_{LIGHT, PHY\_G}, LIM_{C, PHY\_G}, LIM_{N, PHY\_G}, LIM_{P, PHY\_C}\right)$$

(Equation A.95)

$$LIM_{NUTR\_LIGHT, PHY\_D} = \min\left(LIM_{LIGHT, PHY\_D}, LIM_{C, PHY\_D}, LIM_{N, PHY\_D}, LIM_{P, PHY\_D}, LIM_{Si, PHY\_D}\right)$$

(Equation A.96)

$$LIM_{NUTR\_AND\_LIGHT, PHY\_C, NO\_NITR\_FIX} = \min\left(LIM_{LIGHT, PHY\_C}, LIM_{C, PHY\_G}, LIM_{N, PHY\_C, NO\_FIX}, LIM_{P, PHY\_C}\right)$$ (Equation A.97)

$$LIM_{NUTR\_AND\_LIGHT, PHY\_C, NITR\_FIX} = \min\left(LIM_{LIGHT, PHY\_C}, LIM_{C, PHY\_G}, LIM_{N, PHY\_C, FIX}, LIM_{P, PHY\_C}\right)$$ (Equation A.98)

where LIM_{LIGHT, PHY_G}, LIM_{LIGHT, PHY_D} and LIM_{LIGHT, PHY_C} are the light limitation factors for the other planktonic algae, diatoms and cyanobacteria; LIM_{C, PHY_G}, LIM_{C, PHY_D} and LIM_{C, PHY_C} are the carbon factors for the other planktonic algae, diatoms and cyanobacteria; LIM_{P, PHY_G}, LIM_{P, PHY_D} and LIM_{P, PHY_C} are the phosphorus factors for the other planktonic algae, diatoms and cyanobacteria; LIM_{Si, PHY_D} is the silicon limitation factor for diatoms; LIM_{N, PHY_G} and LIM_{N, PHY_D} are the nitrogen limitation factors for the other planktonic algae and diatoms; LIM_{N, PHY_C, NO_FIX} is the nitrogen limitation factor for cyanobacteria for non nitrogen fixing growth and $LIM_{N, PHY\_C, FIX}$ is the nitrogen limitation factor for cyanobacteria for nitrogen fixing growth. The nutrient limitation factors are calculated using Equation A.99 to Equation A.109.

$$LIM_{C, PHY\_G} = \frac{C_{14}}{K_{H, C, PHY\_G} + C_{14}}$$

(Equation A.99)

$$LIM_{C, PHY\_D} = \frac{C_{14}}{K_{H, C, PHY\_D} + C_{14}}$$

(Equation A.100)

$$LIM_{C,PHY\_C} = \frac{C_{14}}{K_{H,C,PHY\_C} + C_{14}}$$
(Equation A.101)

$$LIM_{P,PHY\_G} = \frac{C_3}{K_{H,P,PHY\_G} + C_3}$$
(Equation A.102)

$$LIM_{P,PHY\_D} = \frac{C_3}{K_{H,P,PHY\_D} + C_3}$$
(Equation A.103)

$$LIM_{P,PHY\_C} = \frac{C_3}{K_{H,P,PHY\_C} + C_3}$$
(Equation A.104)

$$LIM_{Si,PHY\_D} = \frac{C_{10}}{K_{H,Si,PHY\_D} + C_{10}}$$
(Equation A.105)

$$LIM_{N,PHY\_G} = \frac{(C_1 + C_2)}{K_{H,N,PHY\_G} + (C_1 + C_2)}$$
(Equation A.106)

$$LIM_{N,PHY\_D} = \frac{(C_1 + C_2)}{K_{H,N,PHY\_D} + (C_1 + C_2)}$$
(Equation A.107)

$$LIM_{N,PHY\_C,NO\_FIX} = \frac{(C_1 + C_2)}{K_{H,N,PHY\_C} + (C_1 + C_2)}$$
(Equation A.108)

$$LIM_{N,PHY\_C,FIX} = R_{N\_FIX,PHY\_C} \frac{K_{H,N\_FIX,PHY\_C}}{K_{H,N\_FIX,PHY\_C} + (C_1 + C_2)}$$
(Equation A.109)

where K_{H,C,PHY_G}, K_{H,C,PHY_D} and K_{H,C,PHY_C} are the half saturation concentrations of inorganic carbon for the other planktonic algae, diatoms and cyanobacteria growth (gC·m^{-3}); K_{H,P,PHY_G}, K_{H,P,PHY_D} and K_{H,P,PHY_C} are the half saturation concentrations of phosphate phosphorus for the other planktonic algae, diatoms and cyanobacteria growth (gP·m^{-3}); K_{H,Si,PHY_D} is the half saturation concentration for available silica silicon for diatoms growth (gSi·m^{-3}); K_{H,N,PHY_G} and K_{H,N,PHY_D} are the half saturation concentrations of inorganic nitrogen for the other planktonic algae and diatoms growth (gN·m^{-3}); K_{H,N,PHY_C} is the half saturation concentration of inorganic nitrogen for non nitrogen fixing cyanobacteria growth (gN·m^{-3}); K_{H,N_FIX,PHY_C} K_{H,N,PHY_C} is the half saturation concentration of inorganic nitrogen for nitrogen fixing cyanobacteria growth (gN·m^{-3}) and R_{N_FIX,PHY_C} is the ratio of maximum rates of non nitrogen fixing and nitrogen fixing cyanobacteria growths.

The light limitation factors are calculated in ALUKAS according to Smith approach (Smith, 1980), which is explained in Appendix B in detail.

The respiration rates of the other planktonic algae, diatoms and cyanobacteria are calculated using Equation A.110 to Equation A.112,

$$PHY\_G_{RESP} = PHY\_G_{RESP,DARK} + PHY\_G_{RESP,PHOTO}$$

(Equation A.110)

$$PHY\_D_{RESP} = PHY\_D_{RESP,DARK} + PHY\_D_{RESP,PHOTO}$$

(Equation A.111)

$$PHY\_C_{RESP} = PHY\_C_{RESP,DARK} + PHY\_C_{RESP,PHOTO}$$

(Equation A.112)

where $PHY\_G_{RESP,DARK}$, $PHY\_D_{RESP,DARK}$, $PHY\_C_{RESP,DARK}$ are the dark respiration rates for the other planktonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$) and $PHY\_G_{RESP,PHOTO}$, $PHY\_D_{RESP,PHOTO}$ and $PHY\_C_{RESP,PHOTO}$ are the photo respiration rates for the other planktonic algae, diatoms and cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$).

The dark respiration rates for the other planktonic algae, diatoms and cyanobacteria are calculated using Equation A.113 to Equation A.115,

$$PHY\_G_{RESP} = k_{RESP,PHY\_G,20} \theta_{RESP,PHY\_G}^{T-20} C_4$$

(Equation A.113)

$$PHY\_D_{RESP} = k_{RESP,PHY\_D,20} \theta_{RESP,PHY\_D}^{T-20} C_{12}$$

(Equation A.114)

$$PHY\_C_{RESP} = k_{RESP,PHY\_C,20} \theta_{RESP,PHY\_C}^{T-20} C_{13}$$

(Equation A.115)

where $k_{RESP,PHY\_G,20}$, $k_{RESP,PHY\_D,20}$ and $k_{RESP,PHY\_C,20}$ are the dark respiration rate coefficients of the other planktonic algae, diatoms and cyanobacteria at 20°C (day^{-1}) and θ_{RESP,PHY_G}, θ_{RESP,PHY_D} and θ_{RESP,PHY_C} is the Arrhenius coefficient for temperature correction for dark respiration rate coefficients of the other planktonic algae, diatoms and cyanobacteria.

The photo respiration rates for the other planktonic algae, diatoms and cyanobacteria are calculated using Equation A.116 to Equation A.118,

$$PHY\_G_{RESP,PHOTO} = f_{RESP,PHOTO,PHY\_G} PHY\_G_{GPP} \quad \text{(Equation A.116)}$$

$$PHY\_D_{RESP,PHOTO} = f_{RESP,PHOTO,PHY\_D} PHY\_D_{GPP} \quad \text{(Equation A.117)}$$

$$PHY\_C_{RESP,PHOTO} = f_{RESP,PHOTO,PHY\_C} PHY\_C_{GPP} \quad \text{(Equation A.118)}$$

where $f_{RESP,PHOTO,PHY\_G}$, $f_{RESP,PHOTO,PHY\_D}$ and $f_{RESP,PHOTO,PHY\_C}$ are the photo respiration ratios of the other planktonic algae, diatoms and cyanobacteria.

The excretion rates for the other planktonic algae, diatoms and cyanobacteria are calculated using Equation A.118 to Equation A.120,

$$PHY\_G_{EXCR} = k_{EXCR,PHY\_G,20}\,\theta_{EXCR,PHY\_G}^{\;T-20}\,C_4$$
(Equation A.118)

$$PHY\_D_{EXCR} = k_{EXCR,PHY\_D,20}\,\theta_{EXCR,PHY\_D}^{\;T-20}\,C_{12}$$
(Equation A.119)

$$PHY\_C_{EXCR} = k_{EXCR,PHY\_C,20}\,\theta_{EXCR,PHY\_C}^{\;T-20}\,C_{13}$$
(Equation A.120)

where $k_{EXCR,PHY\_G,20}$, $k_{EXCR,PHY\_D,20}$ and $k_{EXCR,PHY\_C,20}$ are the excretion rate coefficients of the other planktonic algae, diatoms and cyanobacteria at 20°C (day^{-1}) and θ_{EXCR,PHY_G}, θ_{EXCR,PHY_D} and θ_{EXCR,PHY_C} is the Arrhenius coefficient for temperature correction for excretion rate coefficients of the other planktonic algae, diatoms and cyanobacteria.

The death rates for the other planktonic algae, diatoms and cyanobacteria are calculated using Equation A.121 to Equation A.123,

$$PHY\_G_{DEAD} = k_{DEAD,PHY\_G,20}\,\theta_{DEAD,PHY\_G}^{\;T-20}\,C_4$$
(Equation A.121)

$$PHY\_D_{DEAD} = k_{DEAD,PHY\_D,20}\,\theta_{DEAD,PHY\_D}^{\;T-20}\,C_{12}$$
(Equation A.122)

$$PHY\_C_{DEAD} = k_{DEAD,PHY\_C,20}\,\theta_{DEAD,PHY\_C}^{\;T-20}\,C_{13}$$
(Equation A.123)

where $k_{DEAD,PHY\_G,20}$, $k_{DEAD,PHY\_D,20}$ and $k_{DEAD,PHY\_C,20}$ are the death rate coefficients of the other planktonic algae, diatoms and cyanobacteria at 20°C (day^{-1}) and θ_{DEAD,PHY_G}, θ_{DEAD,PHY_D} and θ_{DEAD,PHY_C} is the Arrhenius coefficient for temperature correction for death rate coefficients of the other planktonic algae, diatoms and cyanobacteria.

A.7 Zooplankton

Zooplankton carbon is simulated using Equation A.124,

$$\frac{\partial C_9}{\partial t} = eff_{GRAZ,ZOOP}\,ZOOP_{GRAZ} - ZOOP_{RESP} - ZOOP_{EXCR} - ZOOP_{DEAD} \quad \text{(Equation A.124)}$$

where C_9 is the zooplankton carbon concentration ($gC \cdot m^{-3}$), $eff_{GRAZ,\,ZOOP}$ is the grazing efficiency of zooplankton, $ZOOP_{GRAZ}$ is the grazing rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$), $ZOOP_{RESP}$ is the respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$), $ZOOP_{EXCR}$ is the excretion rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$) and $ZOOP_{DEAD}$ the death rate of zooplankton ($gC \cdot m^{-3} day^{-1}$). The grazing efficiency must be supplied by the user. The grazing rate of zooplankton is calculated using Equation A.125,

$$\begin{aligned}ZOOP_{GRAZ} = {} & ZOOP_{GRAZ,PHY\_G} + ZOOP_{GRAZ,PHY\_D} + \\ & ZOOP_{GRAZ,PHY\_C} + ZOOP_{GRAZ,PD\_EX\_LAB} + \\ & ZOOP_{GRAZ,PHY\_G\_PDET} + ZOOP_{GRAZ,PHY\_D\_PDET} + \\ & ZOOP_{GRAZ,PHY\_C\_PDET}\end{aligned}$$
(Equation A.125)

where $ZOOP_{GRAZ,\ PHY\_G}$, $ZOOP_{GRAZ,\ PHY\_D}$, $ZOOP_{GRAZ,\ PHY\_C}$, $ZOOP_{GRAZ,\ PD\_EX\_LAB}$ are the grazing rates of zooplankton on the other planktonic algae, diatoms, cyanobacteria and external labile particulate detritus (gC·m^{-3}·day^{-1}). The grazing rates are calculated using Equation A.126 to Equation A.129,

$$ZOOP_{GRAZ,\ PHY\_G} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_G}\ C_9 \quad \text{(Equation A.126)}$$

$$ZOOP_{GRAZ,\ PHY\_D} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_D}\ C_9 \quad \text{(Equation A.127)}$$

$$ZOOP_{GRAZ,\ PHY\_C} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_C}\ C_9 \quad \text{(Equation A.128)}$$

$$ZOOP_{GRAZ,\ PD\_EX\_LAB} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PD\_EX\_LAB}\ C_9 \quad \text{(Equation A.129)}$$

$$ZOOP_{GRAZ,\ PHY\_G\_PDET} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_G\_PDET}\ C_9 \quad \text{(Equation A.130)}$$

$$ZOOP_{GRAZ,\ PHY\_D\_PDET} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_D\_PDET}\ C_9 \quad \text{(Equation A.131)}$$

$$ZOOP_{GRAZ,\ PHY\_C\_PDET} = k_{MAX\_GRAZ,\ ZOOP}\ LIM_{TEMP,\ ZOOP}\ FF_{ZOOP,\ PHY\_C\_PDET}\ C_9 \quad \text{(Equation A.132)}$$

where $k_{MAX\_GRAZ,\ ZOOP}$ is the maximum grazing rate coefficient of zooplankton under optimal conditions (day^{-1}), is $LIM_{TEMP,\ ZOOP}$ the temperature limitation factor for zooplankton grazing, $FF_{ZOOP,\ PHY\_G}$, $FF_{ZOOP,\ PHY\_D}$, $FF_{ZOOP,\ PHY\_C}$ and $FF_{ZOOP,\ PD\_EX\_LAB}$ are the food factors for the other planktonic algae, diatoms, cyanobacteria and external labile particulate detritus grazing.

Temperature limitation on zooplankton is simulated using a Stroganov function, which is summarized in Equation A.133,

$$\begin{aligned}LIM_{TEMP,\ ZOOP} = f_{STROGANOV}\big(&T, q_{10,ZOOP}, T_{MAX,\ ZOOP}, T_{OPT,\ ZOOP}, \\ &XM_{ZOOP}, K_{T\_ACC,\ ZOOP}, T_{ACC\_REF,\ ZOOP}\big)\end{aligned} \quad \text{(Equation A.133)}$$

where T is the water temperature (°C); $q_{10,ZOOP}$ is the change ratio of zooplankton grazing rate per 10°C, $T_{MAX,\ ZOOP}$ is the maximum temperature at which zooplankton can graze (°C), $T_{OPT,\ ZOOP}$ is the optimum growth temperature for zooplankton grazing (°C), XM_{ZOOP} is the maximum shift for acclimation temperature of zooplankton (°C), $K_{T\_ACC,\ ZOOP}$, is the coefficient for decreasing acclimation as temperature approaches the reference temperature zooplankton and $T_{ACC\_REF,\ ZOOP}$ is the reference (minimum) temperature for zooplankton acclimation (°C). The food factors for the other planktonic algae, diatoms, cyanobacteria, external labile particulate detritus, the other planktonic algae based particulate detritus, diatoms based particulate detritus and cyanobacteria based particulate detritus grazing are calculated using Equation A.134 to Equation A.140,

$$FF_{ZOOP,PHY\_G} = \frac{pref_{ZOOP,GRAZ,PHY\_G}\left(C_4 - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$

(Equation A.134)

$$FF_{ZOOP,PHY\_D} = \frac{pref_{ZOOP,GRAZ,PHY\_D}\left(C_{12} - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$

(Equation A.135)

$$FF_{ZOOP,PHY\_C} = \frac{pref_{ZOOP,GRAZ,PHY\_C}\left(C_{13} - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$

(Equation A.136)

$$FF_{ZOOP,PD\_EX\_LAB} = \frac{pref_{ZOOP,GRAZ,PD\_EX\_LAB}\left(C_7 - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$ (Equation A.137)

$$FF_{ZOOP,PHY\_G\_PDET} = \frac{pref_{ZOOP,GRAZ,PHY\_G\_PDET}\left(C_{16} - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$ (Equation A.138)

$$FF_{ZOOP,PHY\_D\_PDET} = \frac{pref_{ZOOP,GRAZ,PHY\_D\_PDET}\left(C_{18} - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$ (Equation A.139)

$$FF_{ZOOP,PHY\_C\_PDET} = \frac{pref_{ZOOP,GRAZ,PHY\_C\_PDET}\left(C_{20} - food_{MIN,ZOOP}\right)}{food_{AVAIL,ZOOP} + K_{H,ZOOP,GRAZ}}$$ (Equation A.140)

where $pref_{ZOOP,\, GRAZ,\, PHY\_G}$, $pref_{ZOOP,\, GRAZ,\, PHY\_D}$ $pref_{ZOOP,\, GRAZ,\, PHY\_C}$ and $pref_{ZOOP,\, GRAZ,\, PD\_EX\_LAB}$ are the grazing preference factors of zooplankton for the other planktonic algae, diatoms, cyanobacteria and external labile particulate detritus; $food_{MIN,\, ZOOP}$ is the minimum amount of food required for zooplankton grazing, $K_{H,ZOOP,\, GRAZ}$ is the half saturation concentration of food for zooplankton ($gC{\cdot}m^{-3}$) and $food_{AVAIL,\, ZOOP}$, which is calculated using Equation A.141, is the total available food for zooplankton grazing ($gC{\cdot}m^{-3}$).

$$\begin{aligned} food_{AVAIL,ZOOP} = {} & \left(pref_{ZOOP,GRAZ,PHY\_G}C_4\right) + \left(pref_{ZOOP,GRAZ,PHY\_D}C_{12}\right) + \\ & \left(pref_{ZOOP,GRAZ,PHY\_C}C_{13}\right) + \left(pref_{ZOOP,GRAZ,PD\_EX\_LAB}C_7\right) + \\ & \left(pref_{ZOOP,GRAZ,PHY\_G}C_{16}\right) + \left(pref_{ZOOP,GRAZ,PHY\_D}C_{18}\right) + \\ & \left(pref_{ZOOP,GRAZ,PHY\_G}C_{20}\right) \end{aligned}$$ (Equation A.141)

ALUKAS assumes that zooplankton have a similar stochiometry to its food, which are calculated using Equation A.142, A.140 and A.144,

$$\begin{aligned} nc_{ZOOP} = {} & \left(FF_{ZOOP,PHY\_G}nc_{PHY\_G}\right) + \left(FF_{ZOOP,PHY\_D}nc_{PHY\_D}\right) + \\ & \left(FF_{ZOOP,PHY\_C}nc_{PHY\_C}\right) + \left(FF_{ZOOP,ZOOP,PD\_EX\_LAB}nc_{EX\_LAB}\right) + \\ & \left(FF_{ZOOP,PHY\_G\_PDET}nc_{PHY\_G}\right) + \left(FF_{ZOOP,PHY\_D\_PDET}nc_{PHY\_D}\right) + \\ & \left(FF_{ZOOP,PHY\_C\_PDET}nc_{PHY\_C}\right) \end{aligned}$$ (Equation A.142)

$$\begin{aligned} pc_{ZOOP} = {} & \left(FF_{ZOOP,PHY\_G}pc_{PHY\_G}\right) + \left(FF_{ZOOP,PHY\_D}pc_{PHY\_D}\right) + \\ & \left(FF_{ZOOP,PHY\_C}pc_{PHY\_C}\right) + \left(FF_{ZOOP,ZOOP,PD\_EX\_LAB}pc_{EX\_LAB}\right) + \\ & \left(FF_{ZOOP,PHY\_G\_PDET}pc_{PHY\_G}\right) + \left(FF_{ZOOP,PHY\_D}pc_{PHY\_D\_PDET}\right) + \\ & \left(FF_{ZOOP,PHY\_C\_PDET}pc_{PHY\_C}\right) \end{aligned}$$ (Equation A.143)

$$sic_{ZOOP} = (FF_{ZOOP,\,PHY\_D}\, sic_{PHY\_D}) + (FF_{ZOOP,\,ZOOP,\,PD\_EX\_LAB}\, sic_{EX\_LAB}) + (FF_{ZOOP,\,PHY\_D\_PDET}\, sic_{PHY\_D})$$ (Equation A.144)

where nc_{ZOOP} is the nitrogen to carbon ratio for zooplankton, np_{ZOOP} is the phosphorus to carbon ratio for zooplankton and sic_{ZOOP} is the silicon to carbon ratio for zooplankton, nc_{PHY_G}, nc_{PHY_D}, nc_{PHY_C} and nc_{EX_LAB} are the nitrogen to carbon ratios of the other planktonic algae, diatoms, cyanobacteria and external labile detritus; pc_{PHY_G}, pc_{PHY_D}, pc_{PHY_C} and pc_{EX_LAB} are the nitrogen to carbon ratios of the other planktonic algae, diatoms, cyanobacteria and external labile detritus; sic_{PHY_D} is the silicon to carbon ratio of diatoms and sic_{EX_LAB} is the silicon to carbon ratio of external labile detritus.

The respiration rate of zooplankton is calculated using Equation A.145,

$$ZOOP_{RESP} = k_{RESP,ZOOP,20}\, \theta_{RESP,ZOOP}{}^{T-20}\, C_9$$
(Equation A.145)

where $k_{RESP,\,ZOOP,20}$ is the zooplankton respiration rate coefficient at 20°C (day^{-1}) and $\theta_{RESP,\,ZOOP}$ is the Arrhenius coefficient for temperature correction for zooplankton respiration rate coefficient. The excretion rate of zooplankton is calculated using Equation A.146,

$$ZOOP_{EXCR} = k_{EXCR,ZOOP,20}\, \theta_{EXCR,ZOOP}{}^{T-20}\, C_9$$
(Equation A.146)

where $k_{EXCR,\,ZOOP,20}$ is the zooplankton excretion rate coefficient at 20°C (day^{-1}) and $\theta_{EXCR,\,ZOOP}$ is the Arrhenius coefficient for temperature correction for zooplankton excretion rate constant. The excretion rate of zooplankton is calculated using Equation A.147,

$$ZOOP_{DEAD} = k_{DEAD,ZOOP,20}\, \theta_{DEAD,ZOOP}{}^{T-20}\, C_9$$
(Equation A.147)

where $k_{DEAD,\,ZOOP,20}$ is the zooplankton excretion rate coefficient at 20°C (day^{-1}) and $\theta_{DEAD,\,ZOOP}$ is the Arrhenius coefficient for temperature correction for zooplankton excretion rate constant.

A.8 Temperature Limitation for Phytoplankton and Zooplankton Groups

To calculate the temperature limitation factors on growth of the three phytoplankton groups and the zooplankton group; ALUKAS uses a general algorithm (Stroganov), which represents the nonlinear and adaptive response of organisms to temperature changes. In This algorithm assumes that the growth rate increases as the temperature increase until an optimum temperature is reacheA. However growth rate decreases with increasing temperature if the optimum temperature is exceeded and will be equal to zero if the maximum temperature for growth or a higher temperature is reacheA. Equation A.148 is used to calculate the temperature limitation factor

$$T > T_{MAX} \quad \rightarrow \quad f_{STROGANOV} = 0$$
$$T \leq T_{MAX} \quad \rightarrow \quad f_{STROGANOV} = VT^{XT} \exp(XT(1 - VT))$$
(Equation A.148)

where VT is the ratio of the difference between the maximum temperature for growth and the ambient temperature over the difference between the maximum temperature for growth and the optimal temperature for growth and XT is the exponent factor. VT is calculated using the Equation A.149,

$$VT = \frac{(T_{MAX} + Acc) - T}{(T_{MAX} + Acc) - (T_{OPT} + Acc)}$$
(Equation A.149)

where T is the ambient temperature (°C), T_{MAX} is the maximum temperature for growth (°C), T_{OPT} is the optimum growth temperature for growth (°C) and Acc is the temperature acclimation (ºC) calculated using Equation A.150,

$$Acc = XM\left(1 - \exp\left(-K_{T\_ACC}\right)\left|T - T_{ACC\_REF}\right|\right)$$
(Equation A.150)

where XM is the maximum shift for acclimation temperature (°C), K_{T_ACC} , is the coefficient for decreasing acclimation as temperature approaches the reference temperature and T_{ACC_REF} is the reference (minimum) acclimation temperature (°C). The exponent factor XT is calculated using Equation A.151 to Equation A.153,

$$XT = \frac{WT^2\left(1 + \sqrt{1 + \frac{40}{YT}}\right)^2}{400}$$
(Equation A.151)

$$WT = \ln(q_{10})((T_{MAX} + Acc) - (T_{OPT} + Acc))$$
(Equation A.152)

$$XT = \ln(q_{10})((T_{MAX} + Acc) - (T_{OPT} + Acc) + 2)$$
(Equation A.153)

where q_{10} is the change ratio of growth rate per 10°C.

APPENDIX B-Submodel for the Calculation of Reaeration Coefficient

The reaeration rate coefficient is a function of the average water velocity, depth, wind, and temperature. The user may specify single reaeration rate constant, or allow the model to calculate variable reaeration rates based upon flow or wind. Calculated reaeration follows either the flow-induced rate or the wind-induced rate, whichever is larger.

Flow induced reaeration is based on the Covar method (Covar, 1976). This method calculates reaeration as a function of velocity and depth by one of three formulas Owens (Equation B.1), Churchill (Equation B.2), or O'Connor-Dobbins (Equation B.3), respectively,

$$k_{qj,20} = 5.349\, v_j^{0.67} D_j^{-1.85}$$

(Equation B.1)

$$k_{qj,20} = 5.049\, v_j^{0.97} D_j^{-1.67}$$

(Equation B.2)

$$k_{qj,20} = 3.93\, v_j^{0.50} D_j^{-1.50}$$

(Equation B.3)

where $k_{qj,20}$ is the flow-induced reaeration rate constant at 20°C (day^{-1}), v_j is the average water velocity in segment j ($m \cdot s^{-1}$) and D_j is the average segment depth (m]).

The Owens formula is automatically selected for segments with depth less than 0.61 m (2 feet). For segments deeper than 0.61 m (2 feet), one of the O'Connor-Dobbins or Churchill formula is selected based on a consideration of depth and velocity. Deeper, slowly moving rivers require O'Connor-Dobbins; moderately shallow, faster moving streams require Churchill's formula. Temperature is used to adjust the temperature corrections are done for the flow-induced reparation coefficient using Equation B.4,

$$k_{qj} = k_{qj,20}\, \theta_a^{T-20}$$

(Equation B.4)

where T is the water temperature (°C), k_{qj} is the reaeration rate (day^{-1}) at temperature T and θ_a is the temperature correction coefficient for the flow-induced reaeration rate constant.

Wind-induced reaeration is calculated according to O'Connor (1983). This method calculates reaeration as a function of wind speed, air and water temperature, and depth using one of three formulas given in Equations B.5, B.6 and B.7,

$$k_{wj} = \frac{86400}{100\, D_j} \left(\frac{D_{OW}}{v_W} \right)^{2/3} \left(\frac{\rho_a}{\rho_W} \right)^{1/2} \frac{\kappa^{1/3}}{\Gamma} \sqrt{C_d}\, (100\, W)$$

(Equation B.5)

$$k_{wj} = \frac{86400}{100\,D_j}\left(\left(\left(\frac{D_{OW}}{v_W}\right)^{2/3}\left(\frac{\rho_a}{\rho_W}\right)^{1/2}\frac{\kappa^{1/3}}{\Gamma_u}\sqrt{C_d}\,100\,W\right)^{-1} + \left(\left(\frac{D_{OW}}{\kappa\, z_0}\frac{\rho_a\, v_a}{\rho_W\, v_W}\sqrt{C_d}\right)^{1/2}\right)^{-1}\sqrt{100\,W}\right)$$

(Equation B.6)

$$k_{wj} = \frac{86400}{100\,D_j}\left(\frac{D_{OW}}{\kappa\, z_e}\frac{\rho_a\, v_a}{\rho_W\, v_W}\sqrt{C_d}\right)^{1/2}\sqrt{100\,W}$$

(Equation B.7)

where k_{wj} is the wind-induced reaeration rate coefficient (day^{-1}), W is the wind speed at 10 cm above surface ($m \cdot s^{-1}$), T_a is the air temperature (°C), ρ_a is the density of air, a function of T_a ($g \cdot cm^{-3}$), ρ_w is the density of water assumed as 1.0 ($g \cdot cm^{-3}$), v_a is the viscosity of air as a function of T_a ($cm^2 \cdot s^{-1}$), v_W is the viscosity of water, a function of T ($cm^2 \cdot s^{-1}$), D_{OW} is the diffusivity of oxygen in water as a function of T ($cm^2 \cdot s^{-1}$), κ is the von Karman's coefficient, 0.4, v_t is the transitional shear velocity, set to 9, 10, and 10 for small, medium, and large scales ($cm^2 \cdot s^{-1}$), v_c is the critical shear velocity, set to 22, 11, and 11 for small, medium, and large scales ($cm^2 \cdot s^{-1}$), z_e is the equivalent roughness, set to 0.25, 0.35, and 0.35 for small, medium, and large scales (cm), z_0 is the effective roughness as a function of z_e, Γ, C_d, v_t, v_a, and W (cm), λ is the inverse of Reynolds number, set to 10, 3, and 3 for small, medium, and large scales, Γ is the non dimensional coefficient, set to 10, 6.5, and 5 for small, medium, and large scales, Γ_u is the non dimensional coefficient, a function of Γ, v_c, C_d, and W, C_d is the drag coefficient as a function of z_e, Γ, v_a, κ, v_t, and W. Equation B.5 is used for wind speeds less or equal to 6 $m \cdot s^{-1}$ where the interfacial conditions are smooth and momentum transfer is dominated by viscous forces. Equation B.7 is used for wind speeds over 20 $m \cdot s^{-1}$ At this wind speed, the interfacial conditions are rough and momentum transfer is dominated by turbulent eddies. Equation B.6 is used for wind speeds between 6 and 20 $m \cdot s^{-1}$ and represents a transition zone in which the diffusive sub layer decays and the roughness height increases.

APPENDIX C-Submodel for the Calculation of Light Limitation for Phytoplankton

Light limitation calculation according to Smith (1980) is presented in Equations C.1 to C.5,

$$X_{RI}(t) = \frac{e}{K_e D}\left(\exp\left(-\frac{I_0}{I_s}\exp(-K_e D)\right) - \exp\left(-\frac{I_0}{I_s}\right)\right) \qquad \text{(Equation C.1)}$$

$$0 \le t \le f \qquad \rightarrow \qquad I_0(t) = \left(\frac{\pi}{2}\frac{I}{f}\right)\sin\left(\frac{\pi t}{f}\right)$$

$$f < t \le 1 \qquad \rightarrow \qquad I_0(t) = 0$$

(Equation C.2)

$$I_s = \frac{k_{1c}\, X_{RT}\, \Theta_c\, e}{\Phi_{max}\, K_c\, f_u}$$

(Equation C.3)

$$K_e = K_e' + K_{e,shd}$$

(Equation C.4)

$$K_{e,shd} = 0.0088\,\text{chl - A} + 0.054(\text{chl - A})^{0.67}$$

(Equation C.5)

where I_o is the time variable incident light intensity just below the surface, assumed to follow a half sine function over daylight hours (ly·day^{-1}), Φ_{max} is the quantum yield expressed as mg carbon fixed per mole of light quanta absorbed, t is the fraction of the current day, K_c is the extinction coefficient per unit of chlorophyll (m^2·mg^{-1} chlorophyll-A), K_e is the light extinction coefficient (m^{-1}), f_u is the unit conversion factor (0.083, assuming 43% incident light is visible and 1 mole photons is equivalent to 52000 cal) (mole photons·m^{-2}ly^{-1}) and Θ_c is the ratio of carbon to chlorophyll in the phytoplankton. Equations C.1 to C.5 give a light limitation coefficient that varies over the day with incident light. This term is numerically integrated over the day to obtain daily average light limitation (Equation C.6).

$$\overline{X_{RI}} = \int_0^1 X_{RI}(t)\,dt$$

(Equation C.6)

A second feature incorporated into the model derived from Smith's work is the calculation of a variable carbon to chlorophyll ratio based on the assumption that adaptive changes in carbon to chlorophyll occur so as to maximize the specific growth rate for ambient conditions of light and temperature. Smith (1980) found that phytoplankton adjust chlorophyll composition so that I_s roughly equals 30% of the average available light (Ambrose et. al, 1993). The expression used to calculate the carbon to chlorophyll ratio is given in Equation C.7,

$$\Theta_c = 0.3\frac{\Phi_{max}\, K_c\, f_u}{k_{1c}\, X_{RT}\, e}\, I_a\left[\frac{1 - \exp(-K_e D)}{K_e D}\right]$$

(Equation C.7)

where the latter term is the average daily solar radiation within a segment during daylight hours, in (ly·day^{-1}). The light limitation approximation according to Steele (1962) is given light limitation formulation is given in Equation C.8 and Figure C.1

$$\varphi_L = \frac{ef}{k_e H}\left(\exp\left(-\frac{I_m\left(\frac{2}{\pi}\right)}{I_s}\exp\left(-k_e H_2\right)\right) - \exp\left(-\frac{I_m\left(\frac{2}{\pi}\right)}{I_s}\exp\left(-k_e H_1\right)\right)\right) \quad \text{(Equation C.8)}$$

where, H, H_1 and H_2 are illustrated in Figure C.1, I_m is the maximum light intensity during the day (ly) and the other terms on Equation C.8 are the same as Smith's formula.

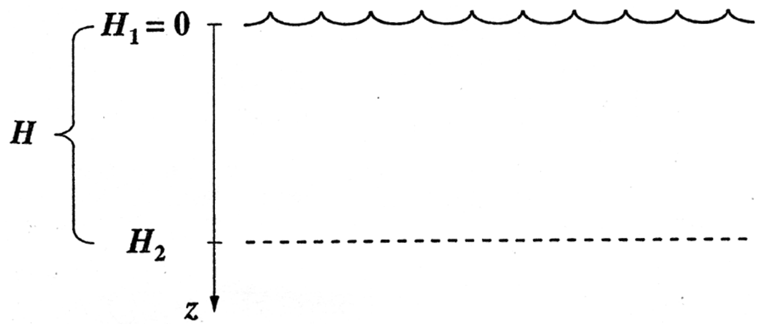

Figure C.1 **Representaion of depths for the light limitation (Chapra, 1997)**

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