

## Appendix A. Model equations

### A.1 TA equations

As mentioned in Section 2.1, TA increases (decreases) due to processes that produce (consume)  $\text{NH}_4^+$  or consume (produce)  $\text{NO}_3^-$ . Therefore, TA in the model increases due to new primary production, remineralization of LDON and RDON, water column denitrification, and sediment fluxes of  $\text{NH}_4^+$ ; it decreases due to regenerated primary production, water column nitrification, and sediment fluxes of  $\text{NO}_3^-$ . The equation for TA follows (note that the factor 14 represents the conversion of grams of nitrogen to moles of nitrogen; i.e., 14 g N = 1 mol N):

$$\frac{\partial TA}{\partial t} = PP_{new} - PP_{reg} - Nitr_{TA} + R_{LDON} + R_{RDON} + Den_{TA} + P_{predTA} + P_{lossTA} + Sed_{TA}$$

where each term represents the following:

$$PP_{new} = \text{New primary production} = \sum_{i=1}^2 (1 - PNi) * Pi * ANCi * Bi / 14$$

$$PP_{reg} = \text{Regenerated primary production} = \sum_{i=1}^2 PNi * Pi * ANCi * Bi / 14$$

where the subscripts  $i = 1, 2$  represent diatoms and dinoflagellates, respectively. The preferential uptake of  $\text{NH}_4^+$  is  $PNi = \text{NH}_4 \left( \frac{\text{NO}_3}{(KhNi + \text{NH}_4) * (KhNi + \text{NO}_3)} + \frac{KhNi}{(\text{NO}_3 + \text{NH}_4) * (KhNi + \text{NO}_3)} \right)$  as in Thomann and Fitzpatrick (1982).  $Bi$  is the algal biomass in  $\text{g C m}^{-3}$  and the coefficient  $ANCi$  is the nitrogen-to-carbon ratio for each type of phytoplankton.  $Pi$  is the total phytoplankton growth, given by  $Pi = PMi * FTi * Fli * \min(NLi, PLi) / CCHLi$ , where the temperature dependence term  $FTi$  is  $e^{-KTg1i*(T-TMPi)^2}$  if temperature  $< TMPi$  and  $e^{-KTg2i*(T-TMPi)^2}$  otherwise. The light limitation term is  $Fli = Iavg / \sqrt{(Pi/ai)^2 + Iavg^2}$  (Jassby and Platt, 1976), where  $Iavg$  is the average irradiance in each cell (incoming irradiance undergoes an exponential decay with depth). The nutrient limitation terms for nitrogen and phosphorus are  $NLi = \frac{\text{NH}_4 + \text{DIN} - PNi * \text{DIN}}{KhNi + \text{NH}_4 + \text{DIN} - PNi * \text{DIN}}$  and  $PLi = \frac{\text{PO}_4}{KhPi + \text{PO}_4}$ , respectively, where  $\text{DIN} = \text{NH}_4^+ + \text{NO}_3^-$ . The values of the coefficients  $PMi$  (maximum growth rate in  $\text{d}^{-1}$ ),  $CCHLi$  (carbon-to-chlorophyll ratio in  $\text{g C g Chl}^{-1}$ ),  $ANCi$ ,  $KhNi$  (half saturation concentration for nitrogen uptake in  $\text{g N m}^{-3}$ ),  $KhPi$  (half saturation concentration for phosphorus uptake in  $\text{g P m}^{-3}$ ),  $KTg1i$ ,  $KTg2i$ , and  $ai$  (photosynthesis vs. irradiance slope) are inputs to the model and can be found in Table A1.

$$Nitr_{TA} = \text{water column nitrification} = 2 * NT / 14$$

where  $NT = \frac{DO}{DO + KhOnt} * \frac{\text{NH}_4}{KhNnt + \text{NH}_4} * FT_{nt} * NTM$  is the nitrification rate in  $\text{g N m}^{-3} \text{d}^{-1}$ , with  $FT_{nt} = e^{-KTNT1*(TMNT-T[I,K])^2}$  if temperature  $< TMNT$  and  $FT_{nt} = e^{-KTNT2*(TMNT-T[I,K])^2}$  otherwise. The factor 2 represents that both the consumption of  $\text{NH}_4^+$  and the production of  $\text{NO}_3^-$  during

nitrification decrease TA (Wolf-Gladrow et al., 2007). The coefficients  $KhOnt$  (half saturation concentration for DO uptake during nitrification in  $g\ O_2\ m^{-3}$ ),  $KhNnt$  (half saturation concentration of  $NH_4^+$  required for nitrification in  $g\ N\ m^{-3}$ ),  $KTNT1$ ,  $KTNT2$ ,  $TMNT$ , and  $NTM$  (maximum nitrification rate in  $g\ N\ m^{-3}\ d^{-1}$ ) are given in Table A1.

$$R_{LDON} = \text{remineralization of LDON} = \frac{DO + AANOX * KhOdoc}{KhOdoc + DO} * KLDON * FTrm * \frac{LDON}{14}$$

$$R_{RDON} = \text{remineralization of RDON} = \frac{DO + AANOX * KhOdoc}{KhOdoc + DO} * KRDN * FTrm * \frac{RDON}{14}$$

where  $N = KLDN + KDNALG * (\sum_{i=1}^2 Bi) * \frac{KhNavg}{KhNavg + DIN}$ , with  $KhNavg = (KhN1 + KhN2)/2$ , and  $FTrm = e^{KTMNL*(T-TRMNL)}$ . The input coefficients  $KTMNL$ ,  $TRMNL$ ,  $AANOX$  (ratio of denitrification to oxic carbon respiration),  $KhOdoc$  (half saturation concentration of DO required for oxic respiration),  $KLDN$  (remineralization rate of LDON in  $d^{-1}$ ), and  $KRDN$  (remineralization rate of RDON in  $d^{-1}$ ) are found in Table A1.

$$Den_{TA} = \text{water column denitrification}$$

$$= ANDC * KLDON * FTrm * AANOX * \frac{KhOdoc}{KhOdoc + DO} * \frac{NO3}{KhNdn + NO3} * \frac{LDOC}{14}$$

where the input coefficients  $ANDC$  (mass of nitrate-nitrogen reduced per mass of dissolved organic carbon oxidized in  $g\ N\ g\ C^{-1}$ ) and  $KhNdn$  (half saturation concentration of  $NO_3^-$  required for denitrification in  $g\ N\ m^{-3}$ ) are given in Table A1.

$$P_{predTA} = P \text{ losses by predation} = \frac{1}{14} \sum_{i=1}^2 FNIP * BPRi * FTpr * ANCi$$

where  $FTpr = e^{KTPR*(T-TRPR)}$  is the temperature dependence and the input coefficients  $KTPR$ ,  $TRPR$ ,  $BPRi$  (predation rate at temperature  $TRPR$ , in  $d^{-1}$ ), and  $FNIP$  (fraction of inorganic nitrogen produced by predation), are provided in Table A1.

$$P_{lossTA} = P \text{ losses by basal metabolism and photorespiration}$$

$$= \frac{1}{14} \sum_{i=1}^2 FNii * ANCi * (Pi * PRSPi + BMi) * Bi$$

where  $BMi = BMRi * e^{KTBi*(T-TRi)}$  and the input coefficients  $KTBi$ ,  $TRi$ ,  $BMRi$  (metabolic rate at temperature  $TRi$ , in  $d^{-1}$ ),  $FNii$  (fraction of inorganic nitrogen produced by basal metabolism and photorespiration), and  $PRSPi$  (fraction of photosynthesis lost to photorespiration) can be found in Table A1.

$$Sed_{TA} = \text{sediment flux of TA to water} = \frac{(BenthicFlux_{NH4} - BenthicFlux_{NO3})}{14} * \frac{1000}{dz_{bott}}$$

where  $dz_{bott}$  is the thickness of the bottom layer of the water column and  $BenthicFlux_{NH_4}$  and  $BenthicFlux_{NO_3}$  are the fluxes of  $NH_4^+$  and  $NO_3^-$  from the top sediment layer to the water column (units are  $g\ N\ m^{-2}\ d^{-1}$ , such that the factor 1000/14 converts them to  $mmol\ N\ m^{-2}\ d^{-1}$ ). They are calculated as  $BenthicFlux_C = SDV * (C_{TopSediment} - C_{BottomSeawater})$ , where  $C$  stands for the concentrations of either  $NH_4^+$  or  $NO_3^-$  and  $SDV$  represents the surface diffusion velocity (in  $m\ d^{-1}$ ):  $SDV = SOD/DO_{BottomSeawater}$ , where  $SOD$  stands for Sediment Oxygen Demand ( $g\ O_2\ m^{-2}\ d^{-1}$ ) and is divided by the DO concentration in the bottom layer of the water column ( $g\ O_2\ m^{-3}$ ). The calculation of  $SOD$ ,  $S$ , and the benthic fluxes follows an iterative approach described in Roberts et al. (2015) and Di Toro (2001).  $Sed_{TA}$  is only added to the bottom layer of water column.

## A.2 DIC equations

The processes that consume DIC are primary production and water column nitrification, while production of DIC occurs through remineralization of LDOC and RDOC, water column denitrification, phytoplankton losses by predation, basal metabolism and photorespiration, and sediment fluxes. Air-sea  $CO_2$  fluxes can either increase or decrease DIC depending on whether the atmospheric  $pCO_2$  is higher or lower than the seawater  $pCO_2$ . The equation for the temporal rate of change in DIC is represented by

$$\frac{\partial DIC}{\partial t} = -PP - Nitr_{DIC} + R_{LDOC} + R_{RDOC} + Den_{DIC} + P_{predDIC} + P_{lossDIC} + GasEx + Sed_{DIC}$$

where each term represents the following (please refer to Appendix A.1 for indices, functions, and parameters that were already defined there):

$$PP = \text{primary production} = \sum_{i=1}^2 Pi * Bi$$

$$Nitr_{DIC} = \text{water column nitrification} = \frac{NT}{14 * 11}$$

where the factor 14 transforms the nitrification rate  $NT$  (in  $g\ N\ m^{-3}\ d^{-1}$ ) to  $mol\ m^{-3}\ d^{-1}$  and the factor 11 is the ratio of  $mol\ N$  to  $mol\ C$  (Wezernak and Gannon, 1967; Billen, 1976).

$$R_{LDOC} = \text{remineralization of LDOC} = KLDOC * FTrm * \frac{DO}{KhOdoc + DO} * LDOC$$

$$R_{RDOC} = \text{remineralization of RDOC} = KRDOC * FTrm * \frac{DO}{KhOdoc + DO} * RDOC$$

$$\begin{aligned} Den_{DIC} &= \text{water column denitrification} \\ &= KLDOC * FTrm * AANOX * \frac{DO}{KhOdoc + DO} * \frac{NO3}{KhNdn + NO3} * LDOC \end{aligned}$$

$$P_{predDIC} = \text{P losses by predation} = \sum_{i=1}^2 FDOP * BPRi * FTpr * \frac{DO}{KhRi + DO}$$

where FDOP (fraction of inorganic carbon produced by predation) and  $KhRi$  (half saturation concentration for LDOC excretion, in  $\text{g O}_2 \text{ m}^{-3}$ ) are given in Table A1. The main difference between  $P_{predDIC}$  and  $P_{predTA}$  is the oxygen dependence term in  $P_{predDIC}$ . When DO becomes scarce (DO close to or lower than  $KhRi$ ), the fraction of inorganic carbon produced by predation decreases while the excretion of LDOC increases by a factor  $1 - DO/(KhRi + DO)$ .

$$P_{lossDIC} = P \text{ losses by basal metabolism and photorespiration} \\ = \sum_{i=1}^2 FCLi * (Pi * PRSPi * BMi) * \frac{DO}{KhRi + DO} * Bi$$

where, again, a DO-dependence term means that the generation of inorganic carbon decreases as DO becomes closer to or less than  $KhRi$ .  $FCLi$  (fraction of inorganic carbon produced by basal metabolism and photorespiration) is not directly given as an input, but calculated as the remainder of all other fractions sourced to LDOC, RDOC, LPOC, and RPOC:  $FCLi = 1 - FCLDi - FCRDi - FCLPi - FCRPi$  (where all of the fractions other than  $FCLi$  are given as inputs, shown in Table A1).

$$GasEx = \text{air - sea CO}_2 \text{ exchange} = 0.251 * WMS^2 * \sqrt{\frac{600}{Sc}} * \frac{24}{100} * \frac{[CO_{2sat}^* - CO_{2surf}^*]}{dz_{surf}}$$

where 0.251 is the gas transfer velocity in  $\text{cm h}^{-1}$  (Wanninkhof, 2014),  $WMS$  is the wind speed ( $\text{m s}^{-1}$ ) provided as input to the model,  $Sc$  is the Schmidt number for  $\text{CO}_2$  (Wanninkhof, 2014), the factor  $24/100$  converts the units of the gas transfer velocity from  $\text{cm hr}^{-1}$  to  $\text{m d}^{-1}$ , and  $dz_{surf}$  is the thickness of the surface layer. When gaseous  $\text{CO}_2$  from the atmosphere dissolves in seawater, it first gets hydrated into aqueous form ( $\text{CO}_{2aq}$ ) and immediately reacts with water to form carbonic acid ( $\text{H}_2\text{CO}_3$ ) with the equilibrium reaction  $\text{CO}_{2aq} + \text{H}_2\text{O} \leftrightarrow \text{H}_2\text{CO}_3$ . As it is difficult to distinguish analytically between  $\text{CO}_{2aq}$  and  $\text{H}_2\text{CO}_3$ , a hypothetical species called  $\text{CO}_2^*$  expresses the sum of both concentrations. Therefore, the exchange of  $\text{CO}_2$  between air and sea depends on the difference between the seawater saturation concentration of  $\text{CO}_2^*$  ( $\text{CO}_{2sat}^*$ ) and the  $\text{CO}_2^*$  at surface ( $\text{CO}_{2surf}^*$ ). The latter is calculated from CO2SYS equations, and  $\text{CO}_{2sat}^*$  is calculated from the atmospheric  $\text{pCO}_2$  ( $\text{pCO}_{2atm}$ ) through Henry's Law:  $\text{CO}_{2sat}^* = K0 * \text{pCO}_{2atm}$ , where  $K0$  is the equilibrium constant of the reaction  $\text{CO}_{2(gas)} \leftrightarrow \text{CO}_2^*$  from Weiss (1974).  $GasEx$  is only added to the surface layer of the water column:

$$Sed_{DIC} = \text{sediment flux of DIC to water} = \frac{BenthicFlux_{CO2}}{dz_{bott}} * \frac{1000}{12}$$

where  $BenthicFlux_{CO2}$  is the flux of  $\text{CO}_2$  from the sediment layer to the water column (in  $\text{g C m}^{-2} \text{ d}^{-1}$ ) and the factor  $1000/12$  converts it to  $\text{mmol C m}^{-2} \text{ d}^{-1}$  (using a mole-to-gram ratio for carbon of  $12 \text{ g C mol C}^{-1}$ ).  $BenthicFlux_{CO2}$  is calculated as the sum of the  $\text{CO}_2$  produced by aerobic oxidation of organic matter in the sediments ( $CSOD$ ) and the  $\text{CO}_2$  produced by anoxic oxidation of dissolved organic carbon by denitrification ( $CDen$ ):  $BenthicFlux_{CO2} = (CSOD + CDen)/2.667$ , where  $CSOD$  and  $CDen$  have units of  $\text{g O}_2 \text{ m}^{-2} \text{ d}^{-1}$  and the denominator is the oxygen-to-carbon ratio ( $2.667 \text{ g O}_2 \text{ g C}^{-1}$ ). The calculation of

$CSOD$  and  $CDen$  follows an iterative approach described in Roberts et al. (2015) and Di Toro (2001).  $Sed_{DIC}$  is only added to the bottom layer of water column.

## Appendix B. Riverine concentrations of pH and TA

### B.1 pH in rivers

Mohamedali et al. (2011) calculated pH as a function of river flow with a multilinear regression based on available data from US and Canadian rivers for the period 1998–2008. Our further analysis of observations from 21 US rivers showed that 99.9% of pH data was above 6.5, and 99.7% of pH data were below 8.5. Therefore, we decided to cap the pH values calculated from the flow regression between 6.5 and 8.5 for US rivers. For Canadian rivers, the previously established pH-flow relationships (Mohamedali et al., 2011) gave constant values for pH. For our study, we used observed pH values for Fraser, Cowichan, English, and Tsolum Rivers. As no pH data were available for Squamish, Clowhorn, or Harris Rivers, we assumed them to be the same as Cowichan River due to their similar flows.

### B.2 TA in rivers

TA observations in both US and Canadian rivers were separated according to their flows in five categories: little (flow  $< 1 \text{ m}^3 \text{ s}^{-1}$ ), small ( $1\text{--}10 \text{ m}^3 \text{ s}^{-1}$ ), medium ( $> 10\text{--}100 \text{ m}^3 \text{ s}^{-1}$ ), large ( $> 100\text{--}1000 \text{ m}^3 \text{ s}^{-1}$ ), and extra-large ( $> 1000 \text{ m}^3 \text{ s}^{-1}$ ). Only the Fraser River fell in the last category. The median TA in each category was used as the TA input in all rivers with flows corresponding to that category. From little to extra-large flows, the following were the median TA values: 1420, 740, 540, 480, and 1060  $\text{mmol m}^{-3}$ . One of the exceptions was the discharge from North Vancouver Island, which is made up of two small rivers but had low alkalinity: its TA median value was 200  $\text{mmol m}^{-3}$  for all months. When more than one river flowed into the same model node, the rivers were combined such that the resulting TA was the flow-weighted average of TA in each river.

### B.3 pH and TA in point sources

Data were obtained from 13 plants: Shelton, Tamoshan, Gig Harbor, Manchester, Port Orchard, Redondo, Lakota, Central Kitsap, Midway, Tacoma central, Chambers, West Point, and South King. From all of the available data, we calculated monthly-mean time series for pH and a median value for TA ( $2000 \text{ mmol m}^{-3}$ ) which were used for point sources.

**Table A1.** Biological model parameters from equations in Appendix A<sup>a</sup>.

Parameter	Description	Value <sup>b</sup>
$AANOX$	Ratio of denitrification to oxic carbon respiration	0.5
$ANCi$	Nitrogen-to-carbon ratio of algae group $i$	0.175, 0.175 $\text{g N g C}^{-1}$
$ANDC$	Mass of nitrate-nitrogen reduced per mass of dissolved organic carbon oxidized	0.933 $\text{g N g C}^{-1}$
$BMRi$	Metabolic rate at temperature $TRi$ of algae group $i$	0.1, 0.1 $\text{d}^{-1}$

<i>BPRi</i>	Predation rate on algae group <i>i</i> at temperature <i>TRPR</i>	1.0, 0.5 d <sup>-1</sup>
<i>CCHLi</i>	Carbon-to-chlorophyll ratio of algae group <i>i</i>	37.0, 50.0 g C g Chl <sup>-1</sup>
<i>FCLDi</i>	Fraction of LDOC produced by predation of algae group <i>i</i>	0, 0
<i>FCLPi</i>	Fraction of LPOC produced by predation of algae group <i>i</i>	0, 0
<i>FCRDi</i>	Fraction of RDOC produced by predation of algae group <i>i</i>	0, 0
<i>FCRPi</i>	Fraction of RPOC produced by predation of algae group <i>i</i>	0, 0
<i>FDOP</i>	Fraction of inorganic carbon produced by predation	0
<i>FNli</i>	Fraction of inorganic nitrogen produced by basal metabolism and photorespiration of algae group <i>i</i>	0.55, 0.55
<i>FNIP</i>	Fraction of inorganic nitrogen produced by predation	0.4
<i>KhNdn</i>	Half saturation concentration of NO <sub>3</sub> <sup>-</sup> required for denitrification	0.1 g N m <sup>-3</sup>
<i>KhNi</i>	Half saturation concentration for nitrogen uptake by algae group <i>i</i>	0.06, 0.06 g N m <sup>-3</sup>
<i>KhNnt</i>	Half saturation concentration of NH <sub>4</sub> <sup>+</sup> required for nitrification	0.5 g N m <sup>-3</sup>
<i>KhOdoc</i>	Half saturation concentration of DO for oxidic respiration	0.5 g O <sub>2</sub> m <sup>-3</sup>
<i>KhOnt</i>	Half saturation concentration of DO required for nitrification	3.0 g O <sub>2</sub> m <sup>-3</sup>
<i>KhPi</i>	Half saturation concentration for phosphorus uptake by algae group <i>i</i>	0.02, 0.02 g P m <sup>-3</sup>
<i>KhRi</i>	Half saturation concentration for LDOC excretion by algae group <i>i</i>	0.5, 0.5 g O <sub>2</sub> m <sup>-3</sup>
<i>KLDN</i>	Minimum remineralization rate of LDON	0.05 d <sup>-1</sup>
<i>KRDN</i>	Remineralization rate of RDON	0.0025 d <sup>-1</sup>
<i>KTBi</i>	Effect of temperature on basal metabolism of algae group <i>i</i>	0.032, 0.032 °C <sup>-1</sup>
<i>KTG1i</i>	Effect of temperature below <i>TMPi</i> on growth of algae group <i>i</i>	0.008, 0.2 °C <sup>-1</sup>
<i>KTg2i</i>	Effect of temperature above <i>TMPi</i> on growth of algae group <i>i</i>	0.05, 0.0008 °C <sup>-1</sup>
<i>KTMNL</i>	Effect of temperature deviations from <i>TRMNL</i> on remineralization	0.092 °C <sup>-1</sup>
<i>KTNT1,2</i>	Effect of temperature below, above <i>TMNT</i> on	0.0045, 0.0045 °C <sup>-1</sup>

	nitrification	
<i>KTPR</i>	Effect of temperature in predation	0.069 °C <sup>-1</sup>
<i>NTM</i>	Maximum nitrification rate at optimal temperature	0.4 g N m <sup>-3</sup> d <sup>-1</sup>
<i>PMi</i>	Maximum growth rate of algae group <i>i</i>	300–525, 357–525 d <sup>-1</sup> 1 c
<i>PRSPi</i>	Fraction of photosynthesis lost to photorespiration by algae group <i>i</i>	0.25, 0.25
<i>TMNT</i>	Optimal temperature for nitrification	30.0 °C
<i>TMPi</i>	Optimal temperature for growth of algae group <i>i</i>	12.0, 18.0 °C
<i>TRi</i>	Reference temperature for metabolism by algae group <i>i</i>	20.0, 20.0 °C
<i>TRMNL</i>	Reference temperature for remineralization	20.0 °C
<i>TRPR</i>	Reference temperature for predation	20.0 °C
$\alpha_i$	Photosynthesis vs. irradiance slope for algae group <i>i</i>	6, 6 $\frac{\text{g C g Chl}^{-1} \text{ d}^{-1}}{\mu\text{E m}^{-2} \text{ s}^{-1}}$

<sup>a</sup>Coefficients that end with “*i*” represent two algal groups: diatoms (*i* = 1) and dinoflagellates (*i* = 2).

<sup>b</sup>Where two values are provided, the first corresponds to diatoms (*i* = 1) and the second to dinoflagellates (*i* = 2)

<sup>c</sup>Two values were set for each algal group, with the smaller one in the Puget Sound Central Basin.

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