KLAIPĖDA UNIVERSITY
FACULTY OF MARINE TECHNOLOGY AND NATURAL SCIENCES
DEPARTMENT OF NATURAL SCIENCES

MODELING OF EUTROPHICATION PROCESSES IN THE CURONIAN LAGOON

Master's Thesis in Ecology and Environmental Studies

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EUTROFIKACIJOS PROCESŲ MODELIAVIMAS KURŠIŲ MARIOSE

Ekologijos ir aplinkotyros studijų programos magistro baigiamasis darbas

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SANTRAUKA

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Raktažodžiai: eutrofikacija, Kuršių marios, ekologinis modeliavimas, ESTAS-AQUABC, priekrantės lagūnos.

Eutrofikacija tai procesas, kurio metu padidėja maistinių medžiagų prietaka į ekosistemą (Boeykens ir kt., 2017; Gamitos ir kt., 2005). Šis procesas dažniausiai nustatomas didėjant neorganinių maistinių medžiagų kiekiui vandens ekosistemoje. Azotas ir fosforas yra du pagrindiniai elementai atsakingi už spartų maistinių medžiagų didėjimą ir vandens augalų augimą vandens telkinyje (Boeykens ir kt., 2017; Yang ir kt., 2008; Gamitos ir kt., 2005).

Vandens ekosistemoje dumblių gamyba yra reikalinga, kaip pirmasis maisto grandinės ryšys, tačiau per didelis dumblių augimas, esant eutrofinėms sąlygoms, gali pakenkti vandens telkinio sistemai (Boeykens ir kt., 2017; Gamitos ir kt., 2005). Dažnai dumblių augimo didėjimas sukelia biologinės struktūros pokyčius visoje ekosistemoje. Esant dideliai maistinių medžiagų prietakai, jūros dumbliai ir lėtai augantys makrofitai pakeičiami sparčiai augančiais makrofitais ir fitoplanktonu, o galiausiai fitoplanktonas tampa dominuojančia augmenija ekosistemoje (Gamitos ir kt., 2005). Todėl azoto ir fosforo elementų patekimas į vandens sistemą pagreitina eutrofikacijos procesą (Boeykens ir kt., 2017; Gamitos ir kt., 2005).

Fosforas tai elementas, kuris natūraliai atsiranda vandenyje, tačiau tam tikra antropogeninė veikla labai prisideda prie jo kaupimosi vandens telkiniuose (Boeykens ir kt., 2017; Yang ir kt., 2008; Sperling, 2007). Natūrali fosforo kilmės priežastis vandens telkiniuose yra dirvožemio junginių ištirpimas, organinių medžiagų skilimas ir mikroorganizmų ląstelių skaidymas, o antropogeninis fosforo šaltinis susijęs su buitinėmis ir pramoninėmis nuotėkomis, plovikliais, gyvūnų ekskrementais ir trąšomis (Boeykens ir kt., 2017; Yang ir kt., 2008; Sperling, 2007).

Lagūna laikoma eutrofikuota, kai vandens stulpe aptinkama didelė maistinių medžiagų koncentracija. Fitoplanktono biomasė ir gamyba, skatinama maistinių medžiagų, yra labai drumsto vandens priežastis. Kai galiausiai fitoplanktono biomasė tampa pakankamai tanki, tai apriboja šviesos patekimą į vandens telkinio dugną ir užkerta kelią bentoso augalijos augimui (Gamitos ir kt., 2005). Tuomet bentoso augalija susitelkia seklesnėse vietose, o gilesniuose sluoksniuose beveik išnyksta (Gamitos ir kt., 2005). Deguonies suvartojimas dėl organinės medžiagos skilimo padidėja, ypač nuosėdose, o tai sąlygoja anoksinius periodus (Boeykens ir kt., 2017; Gamitos ir kt., 2005). Deguonies trūkumas ir toksiškų dujų susidarymas, tokių kaip vandenilio sulfidas, dėl nuosėdų anaerobinės būsenos, daro žalingą poveikį dugne gyvenantiems organizmams bei rūšių gausumui, ypač žuvų ir vėžiagyvių, kurie į lagūną patenka lervų pavidalu ir/ar jauniklio stadijoje (Gamitos ir kt., 2005).

Modeliavimas tai būdas, padedantis išspręsti realias problemas gamtoje (Grigoryev, 2016; Pilkauskas, 2011). Ekologiniai modeliai yra supaprastinti gamtos vaizdavimai ir jie gali būti naudojami tiek sprendžiant ekologines problemas, tiek stebint ir tvarkant įvairias teritorijas (Pereira ir kt., 2008). Šiuose modeliuose yra būdingos savybės (fizikiniai, cheminiai, biogeocheminiai prcesai), būtinos sprendžiant ar apibūdinant esamą situaciją (Pereira ir kt., 2008).

Ekologiniai modeliai yra labai naudingi tiriant bei bandant išsaugoti estuarijų ir pakrančių ekosistemas. Tinkamai pritaikyti vandens telkiniams, šie modeliai gali padėti suprasti vykstančius procesus, nustatyti ekosistemos būklę bei prognozuoti jos evoliuciją, arba įvertinti galimus pokyčius (Rodrigues ir kt., 2009).

Ekologiniai modeliai apima fizikinius, cheminius ir biologinius procesus, siekiant apibūdinti pagrindines ekosistemos ypatybes analizuojamoje teritorijoje (Pereira ir kt., 2008). Vandens ekosistemų modeliuose fizikiniai procesai apima srauto ir cirkuliacijos modelius, masės ir šilumos maišymąsi bei sklaidą, vandens temperatūrą, planktoninių organizmų ir suspenduotų medžiagų nusėdimą, Saulės radiaciją ir šviesos įsiskverbimą (Pereira ir kt., 2008). Šių procesų modeliavimas yra labai svarbus, kuriant visos ekosistemos modelį (Pereira ir kt., 2008).

Šio darbo tikslas – naudojant ESTAS-AQUABC modelį, sumodeliuoti eutrofikacijos procesus Kuršių mariose.

Uždaviniai:

1. Sukalibruoti ir pritaikyti ESTAS-AQUABC modelį Kuršių marioms.
2. Įvertinti pagrindinių parametrų, sukeliančių eutrofikaciją, erdvinį pasiskirstymą Kuršių mariose.
3. Įvertinti atmosferinio azoto fiksaciją, pasitelkiant modeliuotus ir išmatuotus duomenis.

Tyrimo objektas

Kuršių marios (3 pav.) yra didžiausia (1584 km^2) priekrantės lagūna Europoje, kuri su jūra ribojas siauru Klaipėdos sąsiauriu (Remeikaitė-Nikienė ir kt., 2017; Gasiūnaitė ir kt., 2008; Trimonis ir kt., 2003; Schernewski et. al., 2002; Žaromskis, 1996). Vidutinis marių gylis yra apie 3,8 m (Gasiūnaitė ir kt., 2008; Gudelis, 1998; Žaromskis, 1996),tačiau nepaisant Kuršių marių seklumo, vandens temperatūra baseine pasiskirsto tolygiai (Gudelis, 1998). Paviršinio Kuršių marių vandens temperatūra priklauso nuo oro temperatūros. Aukščiausia vandens temperatūra mariose dažniausiai fiksuojama rugpjūčio mėnesį ir siekia +23 °C, o žemiausia – žiemą ir siekia iki +1,3 °C (Gudelis, 1998). Deguonis atlieka svarbų vaidmenį Kuršių marių vandens dujiniame režime (Žilius ir kt., 2012; Gudelis, 1998). Jo koncentracija ir pasiskirstymas nėra vienodi dėl skirtingo vandens druskingumo laipsnio, temperatūros, bangavimo ir vandens maišymosi, deguonį gaminančių organizmų veiklos, biocheminių bei cheminių redukcinių procesų ir kt. (Žilius ir kt., 2012; Gudelis, 1998).

Nemuno upė atneša 96-98% visos gėlo vandens nuotėkio ir į Kuršių marias patenka centrinėje jų dalyje, taip padalindamas jas į dvi dalis (šiaurinę ir pietinę) (Remeikaitė-Nikienė ir kt., 2017; Gasiūnaitė ir kt., 2008; Daunys ir kt., 2006). Šiaurinėje marių dalyje didžiausią įtaką vandens dinamikai daro Nemuno upės nuotėkis ir vandens srautai iš jūros (Gasiūnaitė ir kt., 2008; Daunys ir kt., 2006). Pietinė Kuršių marių dalis pasižymi santykinai uždara cirkuliacijos sistema ir mažesniais srovių greičiais, kuriems didžiausią įtaką daro vyraujantys vėjai (Gasiūnaitė ir kt., 2008; Daunys ir kt., 2006). Dėl šių priežasčių pietinėje Kuršių marių dalyje vyksta pagrindiniai sedimentaciniai procesai (Daunys ir kt., 2006).

Kuršių marios apibūdinamos kaip eutrofinis arba hipereutrofinis vandens telkinys su pasikartojančiais diatominių dumblių žydėjimais pavasarį ir melsvabakterių žydėjimu vasaros metu (Remeikaitė-Nikienė ir kt., 2017; Vaičiūtė ir kt., 2015; Zilius ir kt., 2012). Antroje XX a. pusėje žemės ūkis ir pramonė tapo pagrindiniais azoto ir fosforo šaltiniais, reikšmingai prisidėjusiais prie eutrofikacijos procesų (Vaičiūtė ir kt., 2015; Aleksandrov, 2010). Padidėjusi maistinių medžiagų prietaka į marias, didina NO_3-N koncentraciją (iki 100 μM), palaiko aukštą fitoplanktono priminės produkcijos gamybą bei didina chlorofilo a koncentraciją (iki 50 μg/l) (Bresciani ir kt., 2012).

ESTAS-AQUABC modelis

ESTAS-AQUABC yra ekologinis modelis sukurtas Klaipėdos universiteto Jūros tyrimų institute, bendradarbiaujant su Stambulo universitetu (Ertur ir kt., ruoš.; Paškauskas ir kt., 2016). ESTAS-AQUABC programinio kodo lygmenyje yra susietas su hidrodinaminiu modeliu SHYFEM (Umgiesser 2009) ir naudoja pastarojo hidrodinaminių ir termodinaminių kintamųjų skaičiavimus (Ertur ir kt., ruoš.; Paškauskas ir kt., 2016). Modelis turi pelaginių procesų submodelius. Pelaginės dalies modelio būsenos kintamųjų sąrašas pateiktas 1-oje lentelėje.

Pelaginis modelis aprašo šias pagrindines procesų grupes (Ertur ir kt., ruoš.; Paškauskas ir kt., 2016):

- keturių pagrindinių fitoplanktono grupių (diatomai, N nefiksuojančios melsvabakterės, N fiksuojančios melsvabakterės ir žaliadumbliai) augimas, kvėpavimas, ekskrecija, mirtis ir išėdimas (zooplanktono);
- zooplanktono augimas ir mirtis;
- azotą fiksuojančių bakterijų N_2 fiksacija;
- NH_4+ nitrifikacija;
- detritinės dalelinės organinės medžiagos tirpimas;
- ištirpusios organinės medžiagos mineralizacija;
- skendinčių dalelių sedimentacija;
- visų modeliuojamų medžiagų pernaša dėl advekcijos ir turbulencinės difuzijos.

Modelio kalibravimas

Šio modelio kalibravimui buvo naudojami 2015 metais Jūros tyrimų instituto (Klaipėdos universiteto) Nidos stotyje matuoti duomenys. Kalibravimo proceso metu buvo lyginami modeliuoti ir išmatuoti duomenys, siekiant geriausio duomenų atitikimo.

ESTAS-AQUABC modelio kalibravimui buvo naudojamas bandymų ir klaidų metodas (8 ir 9 pav.). Taip pat buvo sukurtas R programos skriptas, kuris leido pasirinkti modelio konstantą, simuliacijų skaičių ir atvaizduoti rezultatus grafine išraiška. Siekiant užtikrinti vizualios analizės patikimumą, kiekvienam kalibruojamam parametrui buvo apskaičiuota determinacijos koeficiento (R^2) reikšmė.

Erdvinė analizė

Modelis naudoja 25 sritis (angl. boxes), t.y. Kuršių marios yra suskirstytos į 25 sritis, tačiau matuoti duomenys yra tik 14 srities (Nidos stoties) (6 pav.). Erdvinei analizei buvo naudojami modeliuoti duomenys iš visų 25 sričių. Duomenys buvo suskirstyti sezonais – žiemos, pavasario, vasaros ir rudens. Tam kad būtu žinoma koks yra erdvinis kalibruotų parametrų koncentracijų pasiskirstymas, apskaičiuoti kiekvieno sezono vidutines parametrų reikšmes.

Kadangi ESTAS-AQUABC modelis Kuršių marias dalija į 25 sritis, t. y. kiekvienas modelio elementas yra pateikiamas kaip stačiakampis langelis, įprastas interpoliacijos būdas erdvinei analizei nėra tinkamas. Todėl šiuo atveju buvo naudojamas klasifikavimo metodas, pasitelkiant QGIS 3.4 programą (10-12, 15 ir 17 pav.).

Rezultatai

Modelio kalibravimui buvo naudojami 2015 metų Nidos stotyje matuoti biogeocheminiai duomenys (Zilius ir kt., 2018; Petkuviene ir kt., ruoš.). Kalibravimo proceso metu buvo lyginami modeliuoti ir išmatuoti duomenys, siekiant geriausio duomenų atitikimo.

ESTAS-AQUABC modelio kalibravimui taikytas „bandymų ir klaidų“ vizualaus atitikimo metodas. Taip pat buvo sukurtas R programos skriptas, kuris leido pasirinkti modelio konstantą, simuliacijų skaičių ir atvaizduoti rezultatus grafine išraiška. Siekiant užtikrinti vizualios analizės patikimumą, kiekvienam kalibruojamam parametrui buvo apskaičiuota determinacijos koeficiento (R^2) reikšmė.

Remiantis išmatuotais biologinio azoto fiksavimo greičiais yra pastebėtas reikšmingas azoto padidėjimas pietinėje Kuršių marių dalyje vasaros laikotarpiu. Tačiau azoto fiksacijos greičių matavimai yra ganėtinai reti, pasižymi dideliu reikšmių kintamumu bei yra riboti erdvinėje skalėje (Zilius ir kt., 2018). Šiam tyrimui naudotas modelis leidžia įvertinti azoto fiksacijos procesą erdvinėje (10 pav.) ir laiko skalėse bei padeda suprasti veiksnius, reguliuojančius šį procesą, gerai sumaišytose estuarijų aplinkose. Buvo apskaičiuota, jog modeliuojami rezultatai kokybiškai sutampa su stebėjimų duomenimis (R^2=0.295, $p<0.05$) (9 pav.). Taip pat buvo patikrinta ir patvirtinta prielaida, remiantis matavimų duomenimis, susijusi su azoto fiksacija prie santykinio viso ištirpusio azoto (TDN) kiekio (NH_4^++NO_3^-+DON), kurio išeikvojimas lemia atmosferinio azoto asimiliaciją, ir viso azotą fiksuojančių melsvabakterių gausumo (R^2= 0.926, $p < 0.05$). Remiantis matavimų duomenimis pastebėta, kad azoto fiksacijos greičiai padidėja, kai TDN koncentracija neviršija < 0.8 mg N L^{-1}. Viso ištirpusio azoto (TDN) dinamika yra susijusi su upės nuotėkiu, taip pat priklauso nuo kritulių kiekio, temperatūros kitimo ir vegetacijos aktyvumo upės baseino teritorijoje (Vybernaite-Lubiene ir kt., 2018). Visi šie veiksniai yra įtraukti į modeliavimo sistemą, kaip išorinės įvesties duomenys.

Pirminės produkcijos erdvinis pasiskirstymas (11 pav.) suteikia galimybę stebėti fitoplanktono procesų heterogeniškumą Kuršių mariose. Gauti pirminio pirminės produkcijos rezultatai rodo didžiausią produkcijos greitį vasarą (0.96±0.45 g C m^{-2} d^{-1}) ir rudenį (0.13±0.07 g C m^{-2} d^{-1}). Didžiausi pirminės produkcijos greičiai buvo pastebėti pietinėje Kuršių marių dalyje, kurie atitinka ankstesnius matavimus (Zilius ir kt., 2014).

NH_4-N koncentracija, analizuojamoje 14 srityje – Nidos stotyje (6 pav.), svyruoja nuo mažiausios 0,018 mg N · L^{-1} sausį iki didžiausios 0,054 mg N · L^{-1} balandį. Analizuojant sezoniškumą, pastebėta, jog didžiausia NH_4-N koncentracija yra pavasarį (~0,045 mg N · L^{-1}) ir rudenį (~0,041 mg N · L^{-1}). Didžiausios koncentracijos kaupimasis buvo pastebėtas pietinėje Kuršių marių dalyje (12 pav.). Taip pat buvo nustatytas didelis NH_4-N koncentracijos kaupimasis Nemuno upės žiotyse žiemos metu, kai upės nuotėkis buvo didžiausias (~507 m^3/s) (14 pav.).

NO_3-N koncentracija tiriamoje Nidos stotyje svyravo nuo mažiausios 0,00024 mg N · L^{-1} liepą iki didžiausios 2,04 mg N · L^{-1} gegužę. Sezoniškai didžiausia NO_3-N koncentracija pastebėta pavasario metu (~1,97 mg N · L^{-1}), o mažiausia rudenį (~0,0097 mg N · L^{-1}). Remiantis NO_3-N koncentracijos erdvinio pasiskirstymo rezultatais pastebima, kad didžiausios koncentracijos telkiasi centrinėje ir pietinėje Kuršių marių dalyse (15 pav.). Taip pat matomas ryšys tarp NO_3-N

koncentracijos ir Nemuno upės nuotėkio (16 pav.). Remiantis modeliuotais ir išmatuotais (Kuršių mariose ir Nemuno upėje) duomenimis, stebimas NO_3-N koncentracijos padidėjimas pavasario sezonu, kai Nemuno upės nuotėkis yra ~489 m^3/s. Taip pat tarp išmatuotų duomenų Nemuno upėje ir Kuršių mariose fiksuojama panaši tendencija, siejama su nuotėkiu, žiemos-pavasario metu (16 pav.).

PO_4-P koncentracija tiriamoje 14 srityje (Nidos stotyje) svyravo nuo mažiausios 0,0004 mg P · L^{-1} gegužę iki didžiausios 0,021 mg N · L^{-1} gruodį. Analizuojant sezoninius svyravimus, matoma, jog didžiausia PO_4-P koncentracija yra žiemą (~ 0,013 mg P · L^{-1}), o mažiausia pavasarį (~ 0,0009 mg P · L^{-1}). Remiantis erdviniu PO_4-P koncentracijos pasiskirstymu, stebimas didžiausių koncentracijų telkimasis Nemuno upės žiotyse visais metų laikais (17 pav.). Pagrindinis koncentracijos telkimasis stebimas centrinėje ir pietinėje Kuršių marių dalyje. Analizuojant ryšį tarp PO_4-P koncentracijos ir Nemuno upės nuotėkio, pastebėta, kad didžiausios PO_4-P koncentracijos išmatuojamos upės nuotėkiui esant nuo 400 iki 600 m^3/s (18 pav.).

Upės nuotėkis priklauso nuo kritulių rūšies/intensyvumo, evapotranspiracijos/kaupimosi gruntiniuose vandenyse, temperatūros svyravimų, lemiančių sniego/ledo tirpsmą ar vandens užšalimą (Vybernaite-Lubiene ir kt., 2018). Todėl temperatūra reguliuoja upės nuotėkį, o šis lemia maistinių medžiagų patekimą iš upės į marias (Vybernaite-Lubiene irk t., 2018).

Išvados

1. Pasitelkus R programą, modelio kalibravimui buvo sukurta GUI programa, kuri padeda vartotojui kalibruoti modelį ir atvaizduoti modelio rezultatus grafine išraiška. Dauguma modeliuotų ir išmatuotų duomenų neatitikimų gali būti priskirti dabartinio modelio nesugebėjimui imituoti bentoso ir bento-pelaginių jungčių, įskaitant diatominių dumblių nusėdimą, resuspenciją ir kitų elementų nusėdimą.
2. Erdvinė analizė vaizduoja maistinių medžiagų pasiskirstymą Kuršių mariose skirtingais metų sezonais (žiemą, pavasarį, vasarą ir rudenį). Taip pat įrodo, jog didžiausias dalelių kaupimasis vyksta pietinėje Kuršių marių dalyje – pasirinkti modeliuoti parametrai daugiausia kaupiasi centrinėje ir/ar pietinėje Kuršių marių dalyje. Šis reiškinys siejamas su mažesne Nemuno upės bei vandens pasikeitimo su Baltijos jūra įtaka, taip pat lėtesniu vandens srovių greičiu.
3. Dauguma modeliuotų ir išmatuotų duomenų neatitikimų gali būti priskirta dabartinio modelio nesugebėjimui simuliuoti nuosėdinių procesų. Be to, yra vis daugiau įrodymų, jog atmosferinį azotą gali fiksuoti ne tik melsvabakterės, bet ir heterotrofiniai vienaląsčiai mikroorganizmai (Bentzon-Tilia ir kt., 2015). Todėl jie turi būti įtraukti į modeliavimo procesą (kaip būsenos kintamieji), reprezentuojantys atskirą atmosferinį azotą fiksuojančią grupę.

SUMMARY

Ilona Šakurova

MODELING OF EUTROPHICATION PROCESSES IN THE CURONIAN LAGOON

Master thesis in Ecology and Environmental Sciences

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Eutrophication is a global problem in many lakes and marine coastal areas (Gürevin et al., 2016; Bresciani et al., 2012; Gasiūnaitė et al., 2005). This process could lead to hypoxia and anoxia in bottom waters, intense growth of phytoplankton and other aquatic plants (Aleksandrov et al., 2018; Gürevin et al., 2016; McGlathery et al., 2007; Gasiūnaitė et al., 2005). Nitrogen and phosphorus are two key elements that cause the increase of nutrients and growth of aquatic plants (Boeykens et al., 2017; Yang et al., 2008; Gamitos et al., 2005).

Coastal lagoons are highly vulnerable to eutrophication (Vaikutienė et al., 2017; Gürevin et al., 2016; McGlathery et al., 2007) and the Curonian lagoon is a good example of that. To understand and quantify the processes occurring in coastal lagoons, we can use simulation models (ecological modeling methods) (Gürevin et al., 2016). Modeling is a useful tool for coastal lagoons management (Gürevin et al., 2016; Jørgensen, 2008), to evaluate the potential impacts of external forcing and to understand the system function (Paškauskas et al., 2016).

In this study, the ESTAS-AQUABC model was used, which was calibrated and adapted to the Curonian Lagoon. The modelled seasonal dynamics of inorganic nutrient concentrations were not followed perfectly, mostly due to the absence of bentho-pelagic exchange processes. For the spatial distribution, an analysis was used QGIS 3.4 program where calibrated data were analyzed and were created spatial distribution maps of the model's state variables (NH_4-N, NO_3-N, PO_4-P).

Table of Tables

Lentelių sąrašas

Table of Figures

Paveikslų sąrašas

Contents

INTRODUCTION

Coastal lagoons are highly vulnerable to eutrophication (Vaikutienė et al., 2017; Gürevin et al., 2016; McGlathery et al., 2007). Eutrophication is a global problem (Bresciani et al., 2012; Gasiūnaitė et al., 2005) characterized by high levels of nitrogen and phosphorus in water bodies, which causes intense growth of phytoplankton and other aquatic plants (Gürevin et al., 2016; Aleksandrov, 2010; Jašinskaitė, 2008).

The Curonian Lagoon is the large Baltic Sea lagoon connected to the sea by the narrow Klaipėda strait (Gasiūnaitė et al., 2008; Schernewski et al., 2002). Eutrophication is one of the main problems of the Curonian Lagoon (Aleksandrov, 2010; Gasiūnaitė et al., 2005). By the end of the 1980s, the nutrient inputs to the water body exceeded the permissible levels many times, which was one of the reasons why the lagoon was strongly eutrophic (HELCOM, 2018; Aleksandrov, 2010). Eutrophication in the Curonian Lagoon affects all trophic levels, in particular, the intensity of phytoplankton development (Aleksandrov, 2010).

To understand and quantify the processes occurring in coastal lagoons, we can use simulation models (ecological modeling methods) (Gürevin et al., 2016). Modeling is a useful tool for coastal lagoons management (Gürevin et al., 2016; Jørgensen, 2008), to evaluate the potential impacts of external forcing and to understand the system function (Paškauskas et al., 2016; Gürevin et al., 2016).

In this study, the ecological modeling method ESTAS-AQUABC (Paškauskas et al., 2016; Erturk et al., in prep.) was chosen to assess nutrient concentrations caused by eutrophication in the Curonian lagoon. This method used to interpolate data in spatial scale and time between measuring points. The ESTAS-AQUABC model is developed for coastal lagoons, therefore it allows to evaluate the nutrient input in the Curonian lagoon with Nemunas river runoff. Also, using the ESTAS-AQUABC model, the eutrophication level can be estimated with different concentrations of nutrients. Such assessment will allow making recommendations on permitted concentrations of nutrients in Curonian Lagoon with Nemunas River runoff. To prepare this thesis, the team of modellers was working. Author of this work used the model and R script to prepare the results and interpret them.

This work aims to model eutrophication processes in the Curonian Lagoon using ESTAS-AQUABC modeling software.

The main tasks:

1. Calibrate and apply the ESTAS-AQUABC model to the Curonian Lagoon.
2. Analyze the spatial distribution of eutrophication process parameters in the Curonian lagoon.
3. Follow the nitrogen cycle related processes in a shallow coastal lagoon and estimate it input through biological N_2-fixation from the atmosphere.

I. LITERATURE REVIEW

1.1. Eutrophication processes

Eutrophication can be described as the sum of the consequences of excessive phytoplankton growth, resulting in unbalanced primary and secondary productivity, and a faster consistency phase, an excessive phase of consistency caused by nutrient enrichment through leakage that carries excess fertilizer from agro-ecosystems and/or releases human waste from settlements (Boeykens et al., 2017; Yang et al., 2008; Gamitos et al., 2005). Water eutrophication can be accelerated by human activity, which increases the amount of nutrients in the water body (Boeykens et al., 2017; Wijnen et al., 2015; Yang et al., 2008). Nitrogen (N) and phosphorus (P) are the two key elements responsible for the rapid increase of nutrients and the growth of aquatic plants in the water body (Boeykens et al., 2017; Yang et al., 2008; Gamito et al., 2005).

The physical and chemical evaluation parameters were used to assess water eutrophication, mainly nutrient concentration (N and P), algal chlorophyll, water transparency and dissolved oxygen (Yang et al., 2008). Although there are many different assessment parameters, the concentrations of total nitrogen and phosphorus are the two basic ones (Yang et al., 2008). Water eutrophication causes degradation of a healthy aquatic ecosystem, therefore the assessment methods and parameters should reflect the extents of aquatic ecosystem health (Boeykens et al., 2017; Yang et al., 2008).

Generally speaking, the main harmfulness of water eutrophication is that it can break out the intrinsic equilibrium of the aquatic ecosystem and lead to the damage of the water ecosystem and the gradual degeneration of its functions (Yang et al., 2008). It can affect water quality and make transparency of water become worse than ever (Yang et al., 2008). Thus, little sunlight can penetrate water body and photosynthesis of plants under the water will be weakened or even stopped (Yang et al., 2008). Water eutrophication can also cause the super-saturation or lack of dissolved oxygen in water, which will be dangerous to aquatic animals and cause great death to them (Boeykens et al., 2017; Yang et al., 2008). Eutrophic systems tend to accumulate large amounts of organic carbon causing a shift in organic matter biochemical composition (Yang et al., 2008). Because of water eutrophication, a mass of algae, mainly Cyanophyta and green algae (Bresciani et al., 2012), bloom and form a thick layer of "green scum" on the water surface (Bresciani et al., 2012; Yang et al., 2008). Algae can release toxins and render the organic matters in water to be decomposed into harmful gases, which will poison the fish and seashell (Bresciani et al., 2012; Yang et al., 2008).

Water eutrophication in rivers occurs worldwide (Yang et al., 2008). During the past several decades, catastrophic losses in seagrass meadows have occurred worldwide (Yang et al., 2008; Zaldivar et al., 2008), especially in flushed estuaries, coastal embayments and lagoons where nutrient loads are both large and frequent (Yang et al., 2008). Coastal marine ecosystems of Northern Europe

are under pressure from global change which threatens these resources (Yang et al., 2008; Zaldivar et al., 2008).

River–estuarine and associated coastal systems are among the most productive areas on earth due to nutrient enrichment from land runoff, the usually shallow nature of the receiving system, and natural energy supplements in the form of wind, tidal currents, and thermohaline circulation (Yang et al., 2008; Livingstone, 2001). Phytoplankton and benthic microalgae represent one of the primary sources of organic carbon in river-dominated estuaries (Livingstone, 2001). Because of high diversity, taxonomic complexity, and rapid reproduction rates, community interactions of coastal microalgae are poorly understood even though such organisms form the basis of many coastal food webs (Yang et al., 2008; Livingstone, 2001). The food web structure of natural aquatic systems is molded by the eutrophication process, with complex interactions that depend largely on multiple biological processes of the primary producers and highly evolved feeding strategies of the consumers (Livingston, 2001). In addition to being highly productive, many temperate, river-dominated estuarine and coastal systems are known for rapid changes in the physical habitat that contribute to stress-induced changes in food web response (Livingstone, 2001). The many incompatibilities of the eutrophication process in coastal systems reflect varying combinations of nutrient loading and response mechanisms in habitats that change seasonally and interannually (Livingstone, 2001). Variation of the trophic organization of estuarine systems is an important part of the eutrophication process (Gamito et al., 2005; Livingstone, 2001).

There is growing evidence that human activities increasingly affect the quantitative and qualitative aspects of nutrient loading and phytoplankton response (i.e., bloom formation) in coastal systems around the world (Vaikutienė et al., 2017; Yang et al., 2008; Livingstone, 2001). Most of the estuaries studied were affected by human influence although only 14% of the affected estuaries had correspondingly high nitrogen inputs (Livingstone, 2001). More than half of these estuaries had a high capacity to retain nutrients (Livingstone, 2001). It was predicted that eutrophic conditions would worsen in 86 estuaries by the year 2020 (Livingstone, 2001). The authors emphasized that better data are needed in terms of estimators of anthropogenous forms of nutrient pressure and nutrient inputs by source (Yang et al., 2008; Livingstone, 2001).

Nutrient enrichment also adversely affects seagrass beds through changes associated with stimulation of micro- and macroalgae (Livingstone, 2001). The emphasis on shallow systems highlights the importance of sediments in the nutrient loading and accumulation process (Livingstone, 2001). Sediment resuspension as a product of water column dynamics can be a factor in nutrient storage and loading processes (Yang et al., 2008; Livingstone, 2001), although such effects are not always associated with hypereutrophication (Livingstone, 2001). The timed release and bioavailability of sediment nutrients, as modified by resuspension, remobilization, and regeneration

through biotic activity, remain poorly understood even though such processes could have an important effect on the response of benthic microalgae and macrophytes (Yang et al., 2008; Livingstone, 2001). The lack of information regarding non-point-source nutrient loading due to urban and agricultural runoff is another consideration when reviewing the causes of hypereutrophication (Yang et al., 2008; Livingstone, 2001). There are also the positive and negative effects of increased nutrient loading (Livingstone, 2001). There can be initial increases of secondary production and fisheries output with increased nutrient loading (Livingstone, 2001). However, prolonged increases often end in plankton blooms and accompanying declines of coastal populations that are often not discovered until there is an advanced state of hypereutrophication (Gamito et al., 2005; Livingstone, 2001). The complex processes associated with the interaction and competition of microphytes and macrophytes often complicate a uniform response of different estuaries to increased anthropogenous nutrient loading (Livingstone, 2001). However, in most of these studies, there is a general lack of detailed data concerning how phytoplankton blooms are initiated and how changes in the phytoplankton community structure actually affect secondary production (Yang et al., 2008; Livingstone, 2001). Despite a lot of studies concerning hypereutrophication in estuarine and coastal systems, the processes involved in nutrient loading that ultimately lead to altered phytoplankton populations and associated food web changes remain largely undefined (Yang et al., 2008; Livingstone, 2001).

Excess nutrients on coastal systems has led to increased algal biomass, excessive concentrations of sometimes toxic algae in the form of harmful brown and red tides, reduced seagrass and coral reef habitat, altered marine biodiversity, hypoxia/anoxia, and the loss of commercial fisheries (Yang et al., 2008; Gasiūnaitė et al., 2005; Livingstone, 2001). The recommendations of eutrophication management included expansion of monitoring programs, development of ways to reduce non-point sources of nitrogen and phosphorus, an increased public role in eutrophication issues, development of a classification scheme for management of nutrient over-enrichment, improvement of comprehensive assessments of environmental quality and associated modeling efforts, and expansion of our knowledge concerning eutrophication questions (Livingstone, 2001).

There are a lot of factors related to eutrophication, but the mechanism of their influencing algal bloom are not fully understood (Yang et al., 2008; McGlathery et al., 2007; Livingstone, 2001). Algal blooms occur in some seasons or years, when the environmental conditions are favorable (Yang et al., 2008). These factors directly govern the growth, diversity and density of the biotic components (Yang et al., 2008). The impact of algal bloom on any one or some of these factors indirectly influences the structure and characteristics of the water bodies (Yang et al., 2008).

Temperature and salinity are the two important factors to induce alga bloom (Yang et al., 2008). The variation of temperature and salinity also affect algal bloom, and an important condition for algal

bloom is that temperature increases and salinity decreases faster than ever in short time (Yang et al., 2008). Statistical analysis shows that the influence of temperature on algal growth rate is the largest, followed by salinity and their interaction (Yang et al., 2008). Research shows that salinity is negatively related with NO3-N, and PO4-P, but positively related with NH4-N, and however, it is not very related with NO2-N (Yang et al., 2008).

Carbon dioxide level is one of major factors controlling water eutrophication (Yang et al., 2008). Cyanophytes are more capable of utilizing low levels of carbon dioxide and become more buoyant at low levels of carbon dioxide and high pH (Yang et al., 2008). The reduction of light reaching the lake floor also inhibits submerged and rooted macrophytes, and sediments become anoxic as large amounts of planktonic biomass are added to them (Yang et al., 2008). The fluctuations in free carbon dioxide values correspond directly with the fluctuation in the standing crop of phytoplankton (Yang et al., 2008). As the diversity and density of phytoplanktons increase through various months, the amount of free carbon dioxide for photosynthetic activity becomes limiting (Yang et al., 2008). The pH changes in these ponds are governed by the amount of free carbon dioxide, carbon trioxide, and bicarbonate (Yang et al., 2008).

Light plays an important role in the growth, diversity and density of aquatic flora (Yang et al., 2008). As eutrophication progresses, a decline of submerged macrophytes occurs in many shallow water bodies, probably due to low light intensity caused by algal blooming (Yang et al., 2008). The light has been almost completely absorbed by the plankton of the top few meters, so that too little light penetrates to the thermocline and beyond to support photosynthesis (Yang et al., 2008). Eutrophication in an estuary is a complex process, and climate change is likely to affect each estuary differently due to interactions with nutrient loading and physical circulation (Yang et al., 2008). Hence, it is essential to consider the effects of climate change on the context of individual estuarine function to successfully manage eutrophication (Yang et al., 2008; Livingstone, 2001).

There are other factors like pH and dissolved oxygen affecting water eutrophication (Yang et al., 2008). The direct relationship between phytoplankton and dissolved oxygen content has been observed by a number of researchers (Yang et al., 2008). pH is a plant growth limiting factor, the change in pH is directly related to the availability and absorption of nutrients from solution (Yanh et al., 2008).

Figure 1. Eutrophication in Klaipėda Port, summer 2018
1 pav. Eutrofikacija Klaipėdos uoste, 2018 m. vasara

Nitrogen (N) is one of the key nutrients that cause water eutrophication and one of the main fertilizer using in agriculture (Monteny, 2001; Goodchild, 1998). Runoff is one of the main sources of N in waterbodies from agriculture activities (Ondersteijn et al., 2002; Monteny, 2001). Furthermore, nitrogen can cause not only environmental problems but can affect human health when polluted water is used for drinking water purposes (Ondersteijn et al., 2002; Monteny, 2001).

It is observed that agriculture-related nitrogen impact to EU aquatic environment has increased after World War II (Monteny, 2001; Goodchild, 1998). To reduce nitrogen impact from agriculture to the ground- and surface waters, the EU Nitrates Directive was initiated (Ondersteijn et al., 2002; Monteny, 2001). The directive aims to reduce nitrate concentration in the ground- and surface waters to values below 50 mg/l (Ondersteijn et al., 2002; Monteny, 2001; Goodchild, 1998).

The hydrochemical regime of the Curonian Lagoon determining by shallowness, wind currents, river runoff, water mixing and water exchange with the Baltic Sea (Aleksandrov et al., 2018). The Curonian lagoon and its catchment area are under a lot of pressure of human activities (the inflow rivers drain urban areas, in the northern part of the lagoon seaport is located) that cause intense eutrophication process (Aleksandrov et al., 2018; Vaikutienė et al., 2017). In the recent publication of Aleksandrov et al. (2018), researchers mentioned that the maximum concentration of nutrients occurs in winter and early spring, before the development of diatom algae. At the beginning of summer nitrate concentration decrease that leads the rapid regeneration and increase of phosphorus (Aleksandrov et al., 2018). This makes nitrogen to phosphorus ratio favorable for the cyanobacteria

bloom (Aleksandrov et al., 2018). Expansion of cyanobacteria over the lagoon start at the end of June – the beginning of July and continues till the end of October (Aleksandrov et al., 2018). The spatial and temporal concentration of dissolved oxygen in the Curonian lagoon during the bloom period very differs, that could result anoxic conditions at a high temperature and low wind speed (Aleksandrov et al., 2018; Gasiūnaitė et al., 2005). The impact of eutrophication and cyanobacteria blooming on the coastal zone of the Curonian Lagoon is very strong and intensive (Aleksandrov et al., 2018).

1.2.Ecological modelling

The dynamics of shallow estuaries and coastal waters are generally very difficult in the sense that its environmental conditions depend on hydrodynamic and ecological processes and their interactions (Saraiva et al., 2007). Hydrodynamics determines the availability of nutrients through transport processes, light penetration through transport and sediment deposition/erosion, and, above all, determines how long the water mass will remain in a particular location, in other words, water residence time (Saraiva et al., 2007). Ecological processes, such as primary production, only occur when appropriate conditions are found (eg light, nutrients, temperature) and if there is enough time for the organisms to become active (Saraiva et al., 2007). Systems with long residence times are particularly susceptible to blooms of developing algae when nutrient loads increase, and strong water currents usually prevent eutrophication by flushing out nutrients from waterbody (Saraiva et al., 2007). Therefore, assessment of the effects of nutrients on coastal systems requires an overall analysis of the hydrodynamic and environmental conditions of that particular system (Saraiva et al., 2007). The complex interaction of these different processes and the need to quantify these interactions lead to the development of digital models that can calculate the evolution of several properties in terms of space and time (Saraiva et al., 2007).

Ecological modeling is a way to simplify views of nature and solve real problems that occur in different ecosystems (Grigoryev, 2016; Gürevin et al., 2016; Pereira et al., 2008). These models contain only characteristic features that are essential to solve or describe the problem (Pereira et al., 2008).

Ecological models include physical, chemical and biological processes that characterize key ecosystem features in the analysis (Jørgensen, 2009; Pereira et al., 2008). The description of the physical, chemical and biological processes and the structure of the system do not take into account all the details (Jørgensen, 2009; Pereira et al., 2008). Warily designed models, which include principle processes and parameters, still exclude details that are not important to the object under consideration (Pereira et al., 2008). However, these excluded data can have a significant impact on the predicted output of these models (Pereira et al., 2008).

In aquatic ecological models, physical processes include flow and circulation patterns, mixing and dispersion of mass and heat, water temperature, settling of planktonic organisms and suspended matter, insulation and light penetration (Pereira et al., 2008). The modeling of these processes is very important for creating a good holistic ecosystem model (Pereira et al., 2008). One of the most important compromises is finding the optimal time and space scales of the model (Pereira et al., 2008). Spatial grids that are acceptable for physical and chemical processes (10 to 100 meters) are very detailed for biological processes, and time scales (minutes or hours) that are acceptable for physical and chemical processes may not be appropriate for biological processes (Pereira et al., 2008). The time scale of days and months could be appropriate for biotic components of an ecosystem (Pereira et al., 2008).

The simplest geometric imaging is a zero-dimensional (0D) model that simulates the system as a point and all changes depend on time (Pereira et al., 2008). One-dimensional (1D) imaging models assume that the system is characterized by a one-way flow (horizontal or vertical), and system properties vary with that direction and time (Pereira et al., 2008). When the system is large enough to be expressed sensitive features a vertical and/or horizontal direction is required and two or three dimensions (2D or 3D) are more common (Pereira et al., 2008).

Unlike chemical and physical parameters, which are almost known as exact values, biological parameters usually are not known as exact values and almost all literature present this parameters as approximate values or intervals (Pereira et al., 2008). Taking this into account, it is obvious that the parameter estimation approach is necessary for most biological parameters (Pereira et al., 2008). Therefore, the need for calibration is “essential” for ecological models (Pereira et al., 2008).

The researchers are particularly concerned with coastal lagoons and ecosystems that are located between land and sea (Pereira et al., 2008). These ecosystems receive fresh water, which is rich in organic and mineral nutrients from urban, agricultural and industrial wastewater and domestic wastewater (Pereira et al., 2008). In addition, coastal ecosystems are under severe anthropogenic pressure due to tourism and shellfish farming, these factors lead to significant ecosystem changes characterized by eutrophic conditions, algal blooms, oxygen depletion and more (Pereira et al., 2008).

Traditional eutrophication models describe the nutrient cycle and algal growth (Jørgensen, 2008; Koelmans et al., 2001). They are designed to assess the nutrient and algae biomass in the water column and are mostly used to simulate the impact of control measures to reduce the impact of eutrophication (Jørgensen, 2008; Koelmans et al., 2001).

Eutrophication models include nutrient and oxygen cycles and simulate phytoplankton growth (Koelmans et al., 2001). Eutrophication models are a very wide spectrum of complexity (i. e., the number of variables, the nutrients under consideration, the number of water body segments or number of water layers, whether constant stoichiometric or independent nutrient cycles have been used,

whether the model has been calibrated and validated, the number of case studies to which the model has been applied, etc.) (Koelmans et al., 2001).

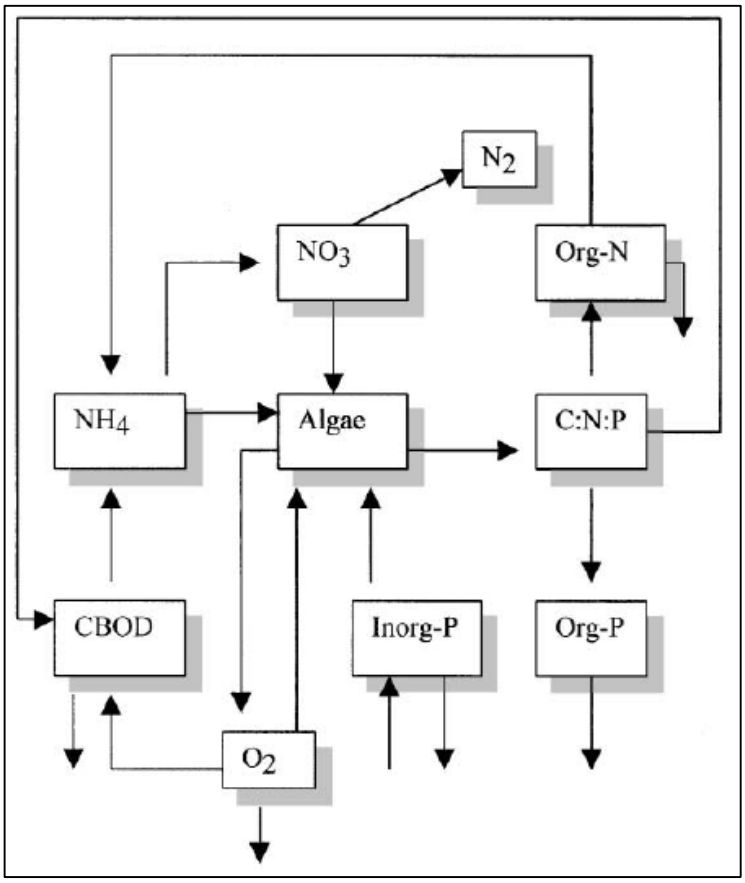

Figure 2. Processes typically described in eutrophication models (Koelmans et al., 2001)
2 pav. Eutrofikacijos modelių dažniausiai aprašomi procesai (Koelmans ir kt., 2001)

Jørgensen (2008) have mentioned that the dynamic models represent a wide range of complexity, therefore, the different models include a different number of sub-models. According to Jørgensen (2008) the 3 possible core sub-models that should be considered for inclusion in models of medium to high complexity are:

1. Phytoplankton growth with or without independent nutrient cycling;
2. Sediment-water exchange of nutrients;
3. Grazing and predation.

According to the characteristics of each case study, it should be decided whether these 3 sub-models should be included or not and with which level of complexity (Jørgensen, 2008, 2009). They reflect the typical choice of complexity of eutrophication models (Jørgensen, 2008, 2009).

Applying independent nutrient cycles inevitably increases the complexity of the model, as this situation requires that nitrogen, phosphorus, carbon, and possibly silicon dioxide be included as state variables at each trophic level (Jørgensen, 2008, 2009). However, in most models with independent nutrient cycles, only one variable applies to zooplankton and fish (Jørgensen, 2008, 2009). The use

of independent nutrient cycles means that phytoplankton growth is characterized as a two-stage process (Jørgensen, 2008):

- Phytoplankton nutrient uptake, according to Monod's kinetics;
- Phytoplankton growth determined by the internal substrate concentration.

This complication requires that the key data are of high quality and quantity (Jørgensen, 2008, 2009). The use of independent nutrient cycles is particularly important when the model is used for shallow, very eutrophic waterbodies (Jørgensen, 2008) like the Curonian Lagoon. On the other hand, this complication can be skipped due to deep, mesotrophic or oligotrophic waterbodies (Jørgensen, 2008, 2009).

Advantages of ecological models compared to other eutrophication assessment tools and methods are (Gürevin et al., 2016; Umgiesser, 2009):

- Models can spatially and temporally interpolate between measurement data points.
- Modeling allows for the testing of several hypotheses and investigating the outputs of different scenarios.
- Models can be used for "what if predictions" and to answer arising questions.

In addition to the advantages of ecological models, there are several disadvantages (Gürevin et al., 2016; Umgiesser, 2009):

- A good database is required to apply ecological models to specific ecosystems. The collection of these datasets may increase the study efforts and costs considerably.
- Complex ecological models that contain many parameters may be difficult to validate, requiring expertise to identify the key processes and extensive computational resources during the simulations repeated many times.
- There are generally accepted ecological/biogeochemical models for eutrophication analysis; however, these models are not always applicable to specific problems or ecosystems. Thus, scientists may need to develop their models, which may require extensive man-hours and increase study costs.

In recent decade several models were applied to the Curonian lagoon. One of them 2D finite element model SHYFEM (Umgiesser, 2009; Umgiesser et al., 2016; Zemlys et al., 2008). SHYFEM is a model that could solve the shallow water hydrodynamic equations in lagoons, coastal seas, estuaries and lakes (Zemlys et al., 2008). This model that consist physical processes was combine with a eutrophication model EUTRO to develop an initial eutrophication model for the Curonian Lagoon (Zemlys et al., 2008). As authors Zemlys et al. (2008) of SHYFEM/EUTRO model application to the Curonian lagoon declareted: „SHYFEM/EUTRO version for the Curonian lagoon show that the model is an efficient computational tool to synthesise existing knowledge, to identify

the gaps to be covered and to foresee the directions for further field, experimental and modelling studies. However, formulation of the eutrophication module requires further improvement to account for the different phytoplankton groups as well as for the benthopelagic exchange processes ".

Also SHYFEM model was applied to the Curonian lagoon without combining with ecological models to represents the Curonian Lagoon and coastal area of the Baltic Sea (Umgiesser et al., 2016). These models consist of a finite element 3-D hydrodynamic model, a transport and diffusion model, and a radiation transfer model of heat at the water surface (Umgiesser et al., 2016).

Recently the Soil and Water Assessment Tool (SWAT) was used to assess the impact of climate-change scenarios on the run-off of the Nemunas River and the Minija River, which are located in the Curonian Lagoons drainage basin (Čerkasova et al., 2016). In particular study SWAT model was successfully calibrated and validated, and applied for the Curonian lagoon drainage basin (Čerkasova et al., 2016). Also authors mentioned that with additional calibration this model could be adapted to ecological, biogeochemical and sediment-transport models for the Curonian Lagoon (Čerkasova et al., 2016). It could support water-quality management studies of the Curonian Lagoon as well (Čerkasova et al., 2016).

II. MATERIAL AND METHODS

2.1. Study area

The Curonian Lagoon is a large (1584 km^2), shallow (average depth reaches 3.8 m) water body in the southeastern part of the Baltic Sea and connect to the sea by a narrow (0.4-1.1 km) strait of Klaipėda (Figure 3) (Jakimavičius et al., 2018; Remeikaitė-Nikienė et al., 2017; Vaičiūtė et al., 2015; Bresciani et al., 2012; Zilius et al., 2012; Dailidienė and Davulienė, 2008; Gasiūnaitė et al., 2008; Daunys et al., 2006; Žaromskis, 1996). As the lagoon has only one narrow connection to the sea, salinity ranges from 0 to 8 PSU (Dailidienė and Davulienė, 2008). The Nemunas River brings 96-98% of all freshwater runoff and entering the Curonian lagoon in its central part, dividing the water body into two parts (north and south) (Aleksandrov et al., 2018; Remeikaitė-Nikienė et al., 2017; Gasiūnaitė et al., 2008; Daunys et al., 2006). The northern part of the lagoon is mostly influenced by the Nemunas runoff and the inflow of water from the sea (Gasiūnaitė et al., 2008; Daunys et al., 2006). The southern part of the lagoon is characterized by relatively closed water circulation and lower current velocity, which is mostly influenced by wind (Gasiūnaitė et al., 2008; Daunys et al., 2006). Due to these factors, the southern part is a main depositional area of the Curonian lagoon (Daunys et al., 2006).

The Curonian Lagoon is also characterized as a eutrophic or hypereutrophic water body with repetitive diatoms blooms during the spring season and cyanobacteria blooms during the summer

period (Remeikaitė-Nikienė et al., 2017; Vaičiūtė et al., 2015; Zilius et al., 2012). In the second half of the 20th-century agriculture and urban activities have become the main sources of phosphorus and nitrogen, contributing significantly to eutrophication processes (Aleksandrov et al., 2018; Vaičiūtė et al., 2015; Aleksandrov, 2010). Every year, the Nemunas River brings about 98% of the particulate organic matter into the Curonian Lagoon (Vaičiūtė et al., 2015) and the deposition of phytoplankton blooms organic matter to the bottom forms the largest proportion of nutrient burial and sediment organic enrichment in the lagoon (Zilius et al., 2012). Also increased nutrient inflow to the lagoon increases NO3-N concentration (up to 100 μM), maintains high production of phytoplankton primary production, increases chlorophyll a concentration up to 50 μg/l (Bresciani et al., 2012).

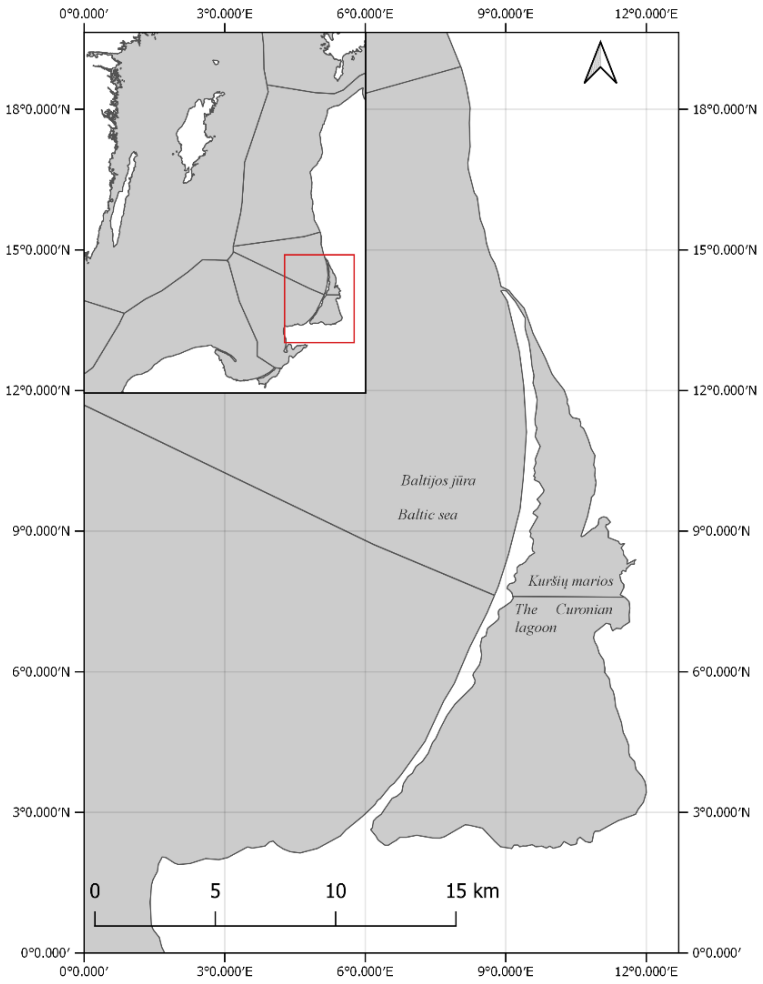

Figure 3. Study area – The Curonian Lagoon.
3 pav. Tyrimo objektas – Kuršių marios

2.2.ESTAS-AQUABC model

In this study was used ESTAS-AQUABC model for large highly eutrophic lagoons developed at the Klaipeda University's Marine Research Institute in collaboration with Istanbul University (Erturk et al., in prep; Paškauskas et al., 2016). The box model called ESTAS (Ecosystem and

Transport Simulator) solves the advection-diffusion using the box modeling approach as the spatial discretization, where the eutrophication kinetics are handled by AQUABC (Aquatic Biogeochemical Cycles) pelagic ecology model (Erturk et al., in prep). The model has the following characteristics (Erturk et al., in prep):

- The model is linked with SHYFEM hydrodynamic modeling framework that is discretizing the model domain with finite elements (Umgiesser, 2009). Since SHYFEM is running on an unstructured grid, ESTAS-AQUABC model boxes can also be of irregular shape and therefore represent water bodies that have irregular shapes and/or complex coastline with a reasonable number of computational elements.
- The box modeling type of spatial discretization utilized by ESTAS-AQUABC allows constructing model domains that can spatially varying spatial resolution.
- The eutrophication sub-model includes nutrients (C, N, P, Si) in both free inorganic form and organic (in case of N and P) or solid (in case of Si) bound form, non-conservative alkalinity, particulate organic matter, four groups of phytoplankton (Diatoms, Fixing cyanobacteria, Non-fixing cyanobacteria, and other planktonic algae) and zooplankton as state variables.
- ESTAS-AQUABC does not only provide state variables outputs but also provides outputs related to process rates with the aim of supporting a model validation step where the model calculated values corresponding to field measured process rates (for example primary production, nitrogen fixation, nitrification, etc.) could be checked for realism.

ESTAS-AQUABC is designed as a pelagic box model, where the boxes can be configured to generate spatially zero, one, three dimensional model domain representing small and well-mixed waterbodies, rivers, large and shallow water bodies and large and deep waterbodies to ensure flexibility and consequently wider applicability to different waterbodies and scientific problems (Figure 4) (Erturk et al., in prep).

The box model includes the following components, all of which as a tabular input data of time and space (Erturk et al., in prep):

- Advective transport field which is accounting the flows between the boxes.
- Diffusive transport field which is accounting the turbulent transport between the boxes.
- Settling which is accounting gain or loss of material between the boxes and losses from the pelagic system.
- Boundaries where the user can prescribe the water exchange between the model domain and its environment, and boundary concentrations on each open boundary.

- Mass loads into the system to represent zero order loads given in mass/time dimensions to account any prescribed load of state variables that do not have an attached water flux (such as small discharges, atmospheric deposition, etc.).
- Mass withdraws from the system to represent zero order negative loads given in mass/time dimensions to account any prescribed withdrawal of materials (as state variables) that do not have an attached water flux (such as the prescribed effect of bottom filtrators, prescribed fluxes because of diffusion into the sediments, etc).
- Kinetics that correspond to the biogeochemical cycles.
- Resuspension in two options, where it may either be directly prescribe as time series of resuspension velocities and resuspended concentrations corresponding to state variables or the simple approach utilizing the internal facilities in the model, which compare externally read shear stress time series and compare them with prescribe critical shear stress to switch on and off the settling process, when resuspension of the "fullfy layer" occurs (i. e., when the shear stress exceeds the critical shear stress).

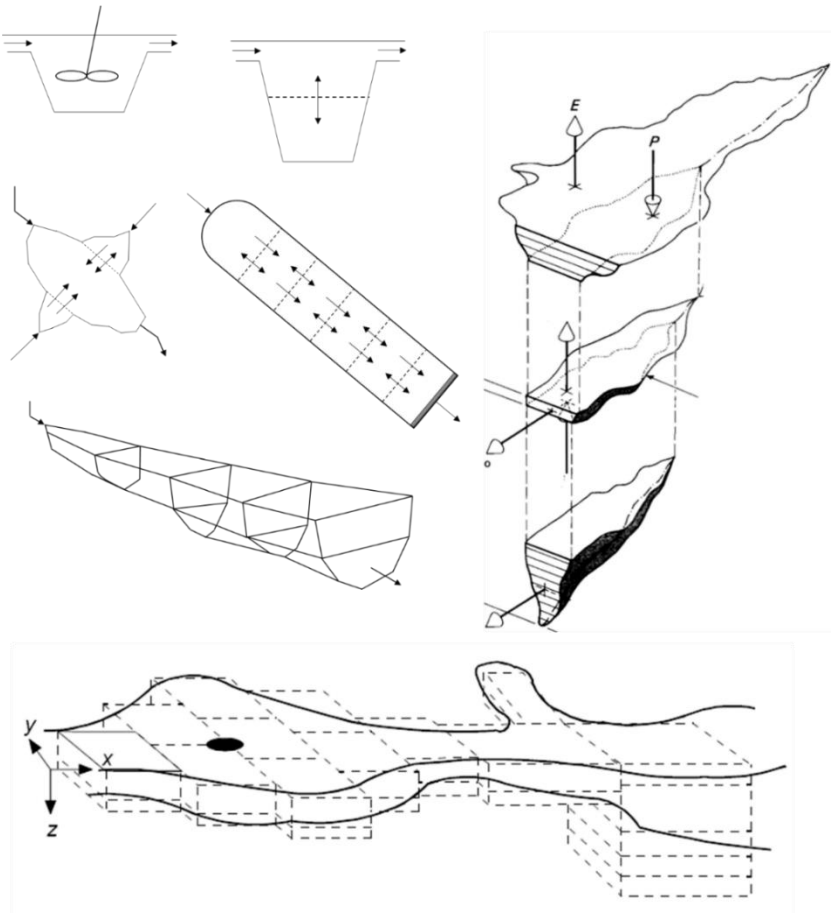

Figure 4. Possible box configurations for several waterbodies (Erturk et al., in prep)
4 pav. Galimos modelio konfiguracijos skirtingiems vandens telkiniams (Erturk ir kt., in prep)

The pelagic ecology model AQUABC is a fully featured eutrophication analysis model with nutrient cycles, primary production, organic matter mineralization and a zooplankton sub-model tracking the variable stoichiometry (Paškauskas et al., 2016). The pelagic part of the model describes the following main process groups (Paškauskas et al., 2016):

- growth, respiration, excretion, death and depletion (zooplankton) of four major phytoplankton groups (diatoms, N fixing cyanobacteria, N non-fixing cyanobacteria, other phytoplankton);
- zooplankton growth and death;
- N fixing bacteria‘s fixation of N_2;
- nitrification of NH_4^+;
- dissolution of detritus particulate organic matter;
- mineralization of dissolved organic matter;
- sedimentation of suspended particles;
- transfer of all modeled materials due to advection and turbulent diffusion.

The AQUABC model includes CO2SYS, which enables to describe the CO2 system (pH, dissolved inorganic carbon, alkalinity, water temperature, phosphate phosphorus, and salinity are used) (Erturk et al., in prep; Paškauskas et al., 2016).

All state variables that used in AQUABC model are measured and measurement data is used for calibration of model parameters (constants) and for model verification (Table 1) (Erturk et al., in prep; Paškauskas et al., 2016).

Table 1. State variables of pelagic model.
1 lentelė. Pelaginio modelio būsenos kintamieji.

State variable	Notation	Unit
Ammonia nitrogen	$[NH_4 - N]$	$gN \cdot m^{-3}$
Nitrate nitrogen	$[NO_3 - N]$	$gN \cdot m^{-3}$
Orthophosphate phosphorus	$[PO_4 - P]$	$gP \cdot m^{-3}$
Dissolved silicon	$[Si(OH)_4 - Si]$	$gSi \cdot m^{-3}$
Dissolved oxygen	$[O_2]$	$gO_2 \cdot m^{-3}$
Diatoms carbon	[Dia - C]	$gC \cdot m^{-3}$
Non-fixing cyanobacteria carbon	$[Cyn - C]_{NOFIX}$	$gC \cdot m^{-3}$
Fixing cyanobacteria carbon	$[Cyn - C]_{FIX}$	$gC \cdot m^{-3}$
Other planktonic algae carbon	[OPA - C]	$gC \cdot m^{-3}$
Zooplankton carbon	[Zoop - C]	$gC \cdot m^{-3}$
Zooplankton nitrogen	[Zoop - N]	$gN \cdot m^{-3}$
Zooplankton phosphorus	[Zoop - P]	$gP \cdot m^{-3}$
Detrital particulate organic carbon	$[POC]_{DET}$	$gC \cdot m^{-3}$
Detrital particulate organic nitrogen	$[PON]_{DET}$	$gN \cdot m^{-3}$
Detrital particulate organic phosphorus	$[POP]_{DET}$	$gP \cdot m^{-3}$
Particulate silica	[PSi]	$gSi \cdot m^{-3}$
Dissolved organic carbon	[DOC]	$gC \cdot m^{-3}$
Dissolved organic nitrogen	[DON]	$gN \cdot m^{-3}$
Dissolved organic phosphorus	[DOP]	$gP \cdot m^{-3}$
Dissolved inorganic carbon	[DIC]	$gC \cdot m^{-3}$
Alkalinity	[Alkalinity]	moles/L

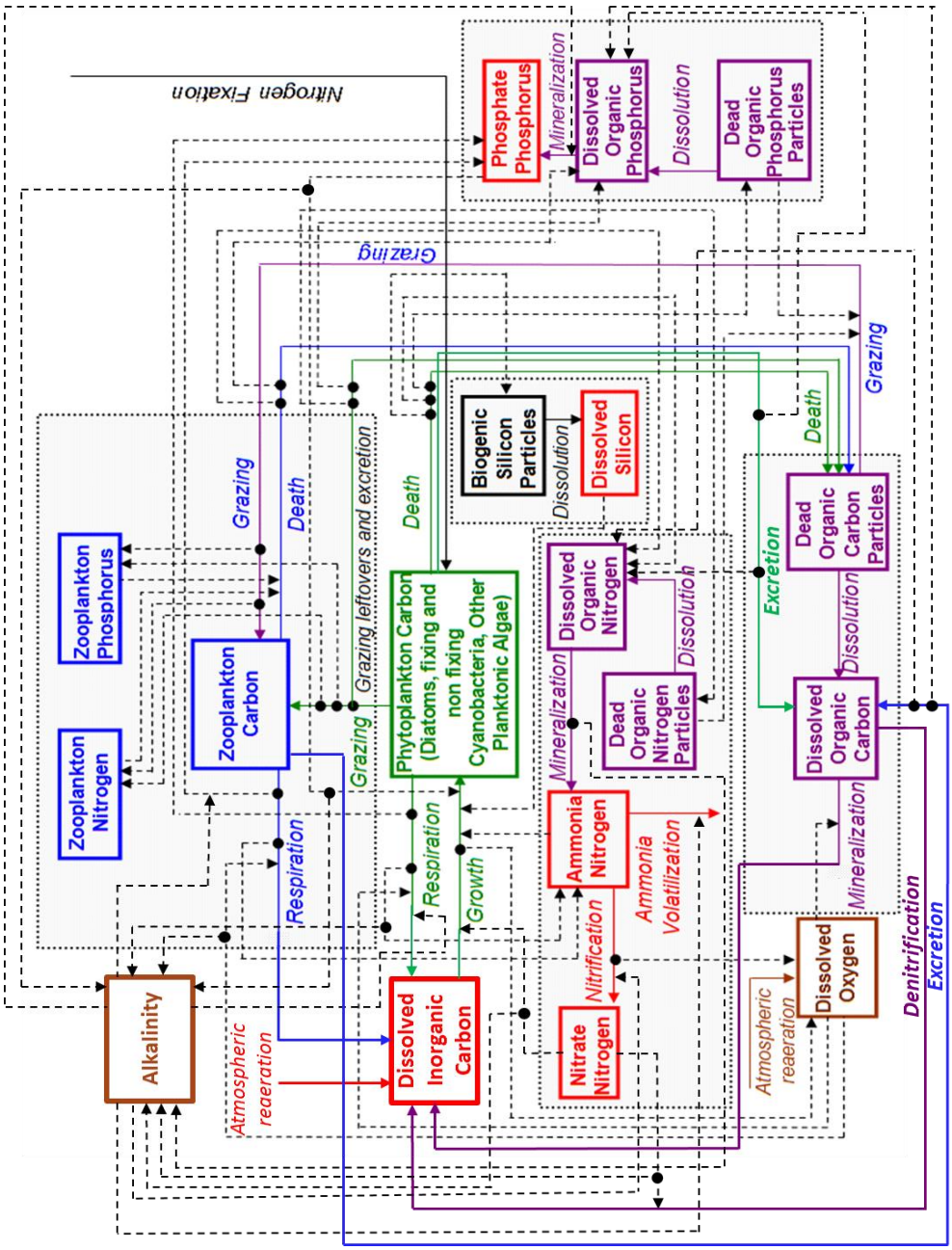

Figure 5. Conceptual diagram of pelagic AQUABC model
5 pav. Pelaginio AQUABC modelio koncepcinė schema

2.2.1. Calibration of the model

Calibration as a process defining appropriate values for each parameter in the simulation to approximate simulation results to the real situation (Pereira et al., 2008). Model calibration is performed by comparing observed data with predicted and is an important phase in the modeling process (Pereira et al., 2008).

For this model calibration was used available observation data measured at Nida station in 2015 by Marine Research Institute of Klaipeda University, Lithuania. As ESTAS-AQUABC model is a box model, for the calibration was used only one box – *box 14* (Figure 6), which overlaps with monitoring station. This station was chosen because of its location and resuspension effect. The Nida station located in the area where wind and currents have minimum effect for resuspension (Paškauskas et al., 2016) and therefore, this makes the calibration process more stable.

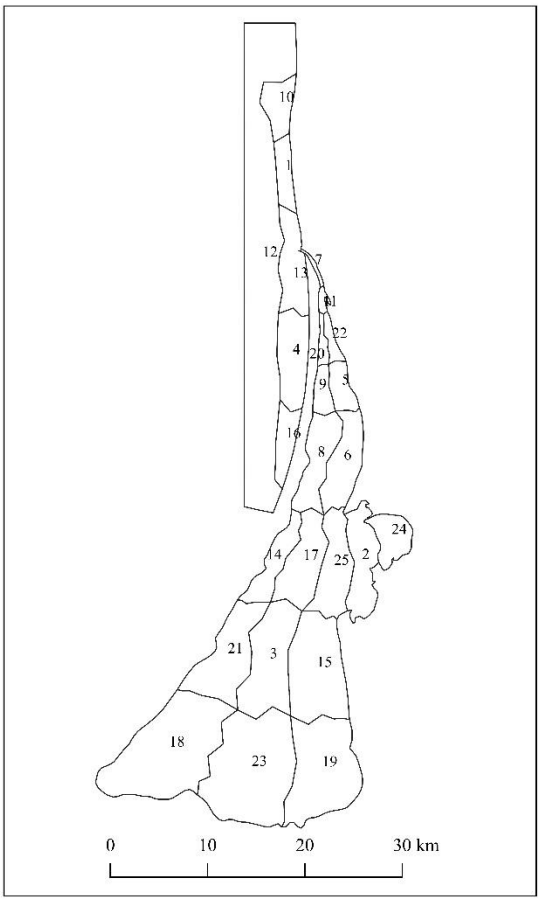

Figure 6. Boxes for ESTAS-AQUABC model
6 pav. 25 ESTAS-AQUABC modelio naudojamos sritys

In this case study, the model was calibrated through a trial and error method using R-squared statistics calculate between measured and modelled values as well as a visual fit. The calibrated model constants are given in Appendix B (altogether 183 constants). To simplify model calibration an R (R Core Team, 2019) based graphical user interface application was created (by Artūras Razinkovas-Baziukas) (Appendix C). The application allows to choose a model constant, that modeller prefers to calibrate, and the program produces as many simulations as modeller require. After the simulations with different constant values, the R application produces a graphical representations of state variables with both modelled and measured data (Figures 8-10). In order to ensure the reliability of visual analysis, the R^2 was calculated for each state variable. The state variables time series graphs represent the behaviour of the simulated versus measured eutrophication process parameters (NH_4-N, NO_3-N, PO_4-P, N_2-fixation, primary production). All the calibration graphs represent the box 14 (Nida station) for the entire year 2015 period.

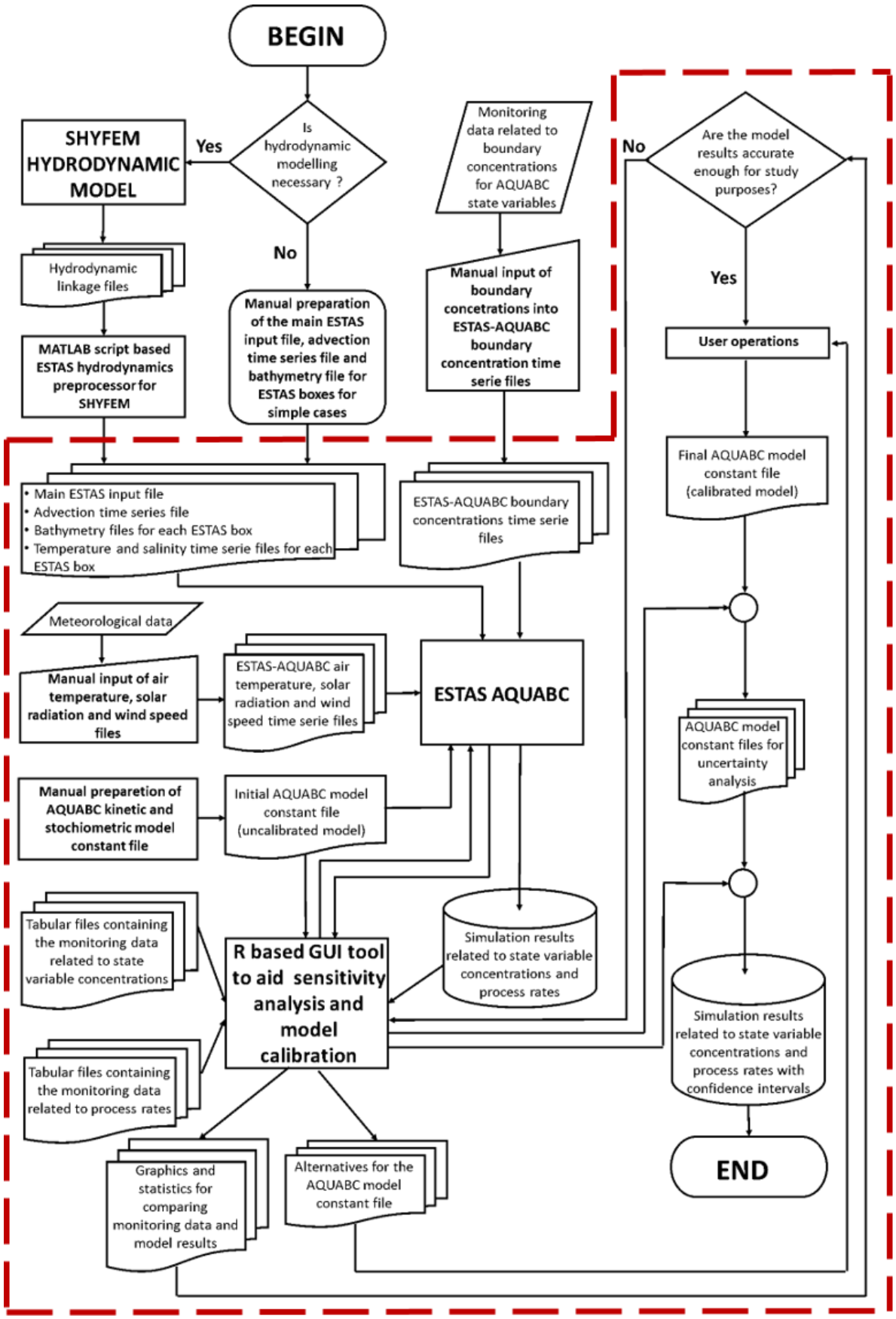

Figure 7. The modeling framework (Erturk et al., in prep). Red dotted line shows which part of the modeling was used while preparing this master thesis

7 pav. Modeliavimo schema (Erturk ir kt., in prep). Raudona punktyrinė linija žymi modeliavimo dalį, naudotą ruošiant šį darbą

2.3. Spatial analysis

Spatial analysis is the process of converting raw data into useful information by depicting it on the map (Blyth et al., 2008). Using spatial analysis, we can observe how the selected parameters change in space. To find out the spatial distribution of simulated data (NH_4-N, NO_3-N, PO_4-P, O_2, etc.) in the Curonian Lagoon, we used the QGIS 3.4 program.

In ESTAS-AQUBC box model, where each box is represented as a completely mixed reactor, where there wouldn't be any internal spatial concentration gradients, the typical interpolation methods such as kriging are not appropriate. For the spatial analysis, based on the modelled data of each 25 boxes, values were arranged by seasons: winter (January–February), spring (March–May), summer (June–August), and autumn (September–November). For the spatial representation of N_2-fixation and net primary production in the Curonian lagoon (19 boxes out of 25 boxes in the model domain) were used sum of season values of each box, while for the nutrient concentration were used average of season values of each box, and was used classification method using QGIS 3.4 program (Figures 11-13, 16, 18). The rates of N_2-fixation were negligible in winter and spring, according to both, monitoring and modelling results, therefore it was excluded from further discussion (Figure 11).

III. RESULTS

Prediction of dissolved inorganic forms of nitrogen and phosphorus was agreeable (Figure 8), but the model was not capable to capture increase in NH_4^+ and DIP concentrations observed in the late summer, while NO_3^- concentrations in spring were underestimated. We assume that the absence of benthic compartment in the modelling framework and missing benthic-pelagic exchange processes could account for this mismatch. Since the Curonian Lagoon is shallow system, biogeochemical processes within sediments is expected to be important regulating nutrient dynamic in overlaying water column, especially summer when water residence time is longer (Zilius et al., 2014; Petkuviene et al., 2016).

Since DIN (in this case NH_4-N and NO_3-N) and PO_4-P are the main factors that cause eutrophication (Li et al. 2018), we mainly analyzed the spatiotemporal variations of NH_4-N, NO_3-N and PO_4-P in the Curonian lagoon.

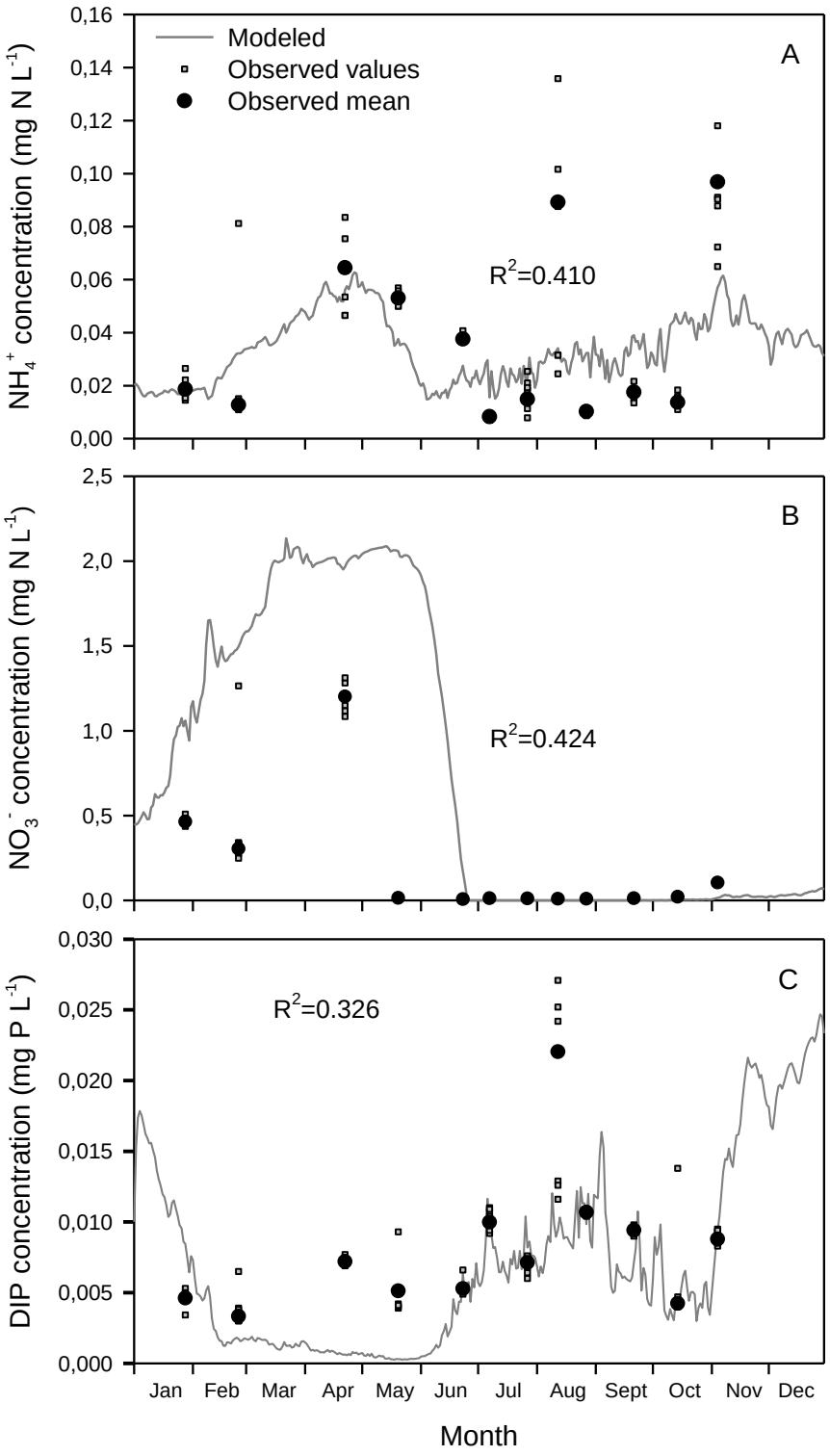

Figure 8. Modeled (line) and observed (closed circle and square) concentrations of dissolved ammonia (A), nitrogen (B) and inorganic phosphorus (C) at the Nida station in 2015

8 pav. Modeliuotų (linija) ir išmatuotų (taškai) ištirpusio amonio (A), azoto (B) ir neorganinio fosforo (C) koncentracijos Nidos stotyje 2015 m.

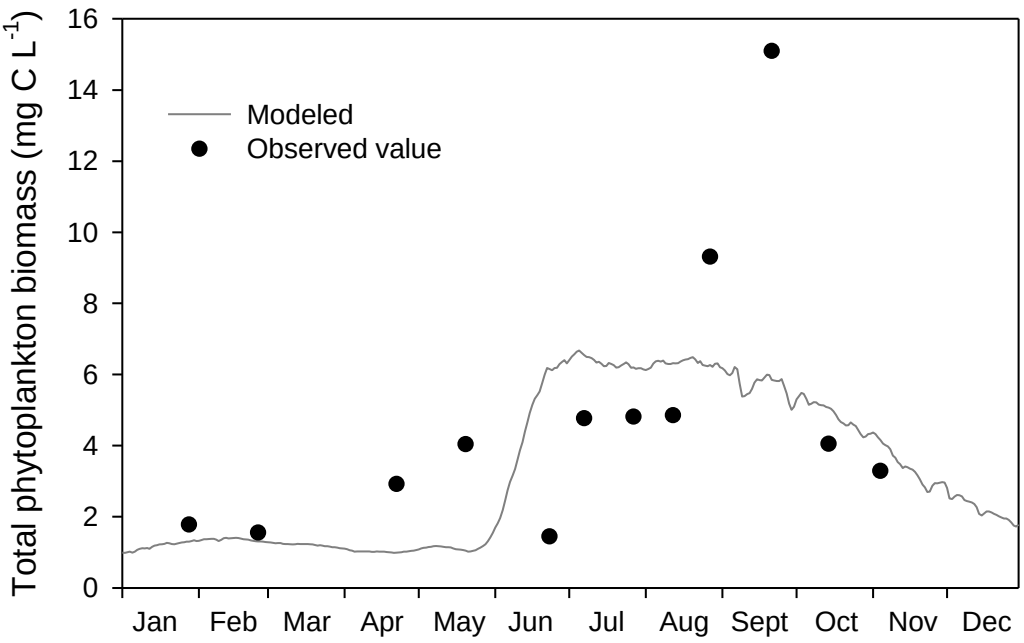

Figure 9. Modelled (line) and observed (closed circle) total phytoplankton biomass at the Nida station in 2015
9 pav. Modeliuoto (linija) ir išmatuoto (taškai) bendro fitoplanktono biomasė Nidos stotyje 2015 m.

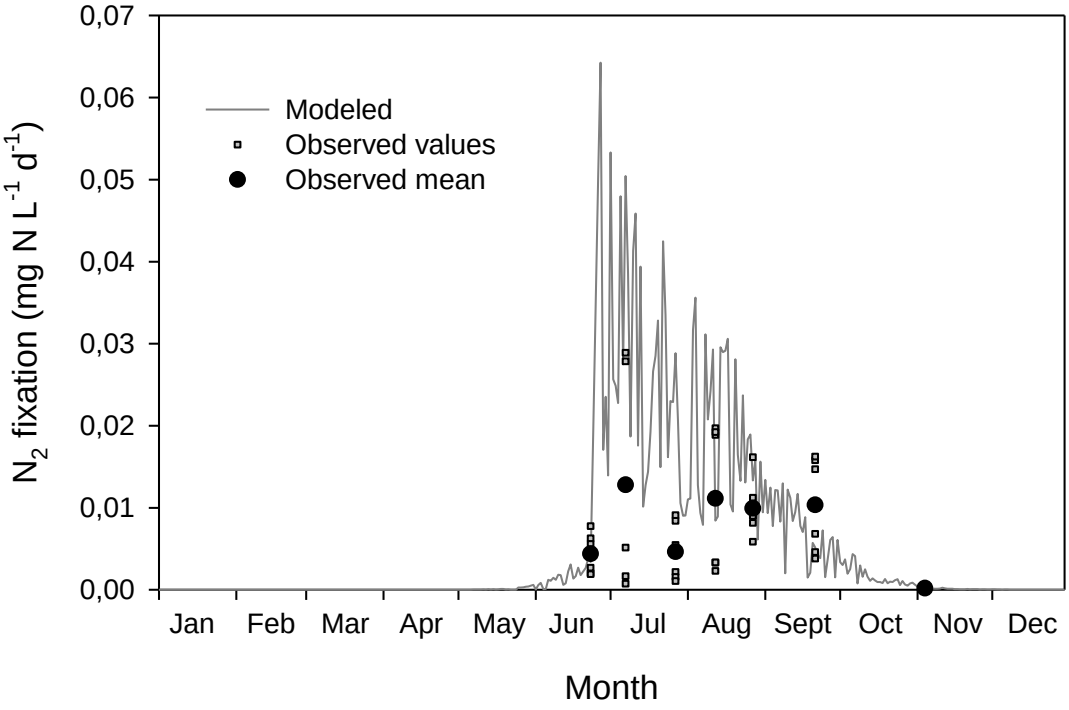

Figure 10. Modelled (line) and measured (closed circle and square) atmospheric nitrogen at the monitoring site in the Curonian Lagoon in 2015
10 pav. Modeliuotas (linija) ir išmatuotas (taškai) atmosferinis azotas Nidos stotyje 2015 m.

Although models are frequently constrained by uncertainties and/or requires further improvements but they could provide an invaluable tool for mass calculations over temporal and spatial patterns. We attempted to upscale N_2-fixation and net primary production processes to the spatial scale of the lagoon. Mean N_2-fixation rates varied by one order of magnitude among boxes

with mean rates of 0.026±0.008 g N m^{-2} d^{-1} and 0.002±0.001 m^{-2} d^{-1} in summer and autumn, respectively.

In general, results from upscaling show that mean daily contribution of biological N_2-fixation 50 % exceeded one provided by riverine inputs (0.013 g N m^{-2} d^{-1}) in summer. This indicates the importance of atmospheric N fixation, particularly during summer when the riverine discharges are lowest. In addition, we estimated (R^2= $p < 0.05$) the net primary production (PP) which is sum of gross primary production and respiration. The spatial patterns of net primary production distribution (Figure 12) provided better understanding heterogeneity of phytoplankton based processes in the Curonian lagoon. Obtained results indicates highest production rates observed in summer (0.96±0.45 g C m^{-2} d^{-1}) and autumn (0.13±0.07 g C m^{-2} d^{-1}). The highest PP rates were observed in southern part of the lagoon which is in line with previous measurements (Zilius et al., 2014). Obtained results for net primary production allows estimation of biological nitrogen assimilation by using measured carbon and nitrogen ratio. Our calculated mean assimilative nitrogen uptake values vary from <0.01 to 0.19 g C m^{-2} d^{-1} with peak in summer. There is clear decoupling between assimilative nitrogen uptake and supply in time, the latter being the highest in in spring. Using the model we could trace the further fate of assimilated nitrogen – whether it is remineralized to support autotrorophic phytoplankton development later.

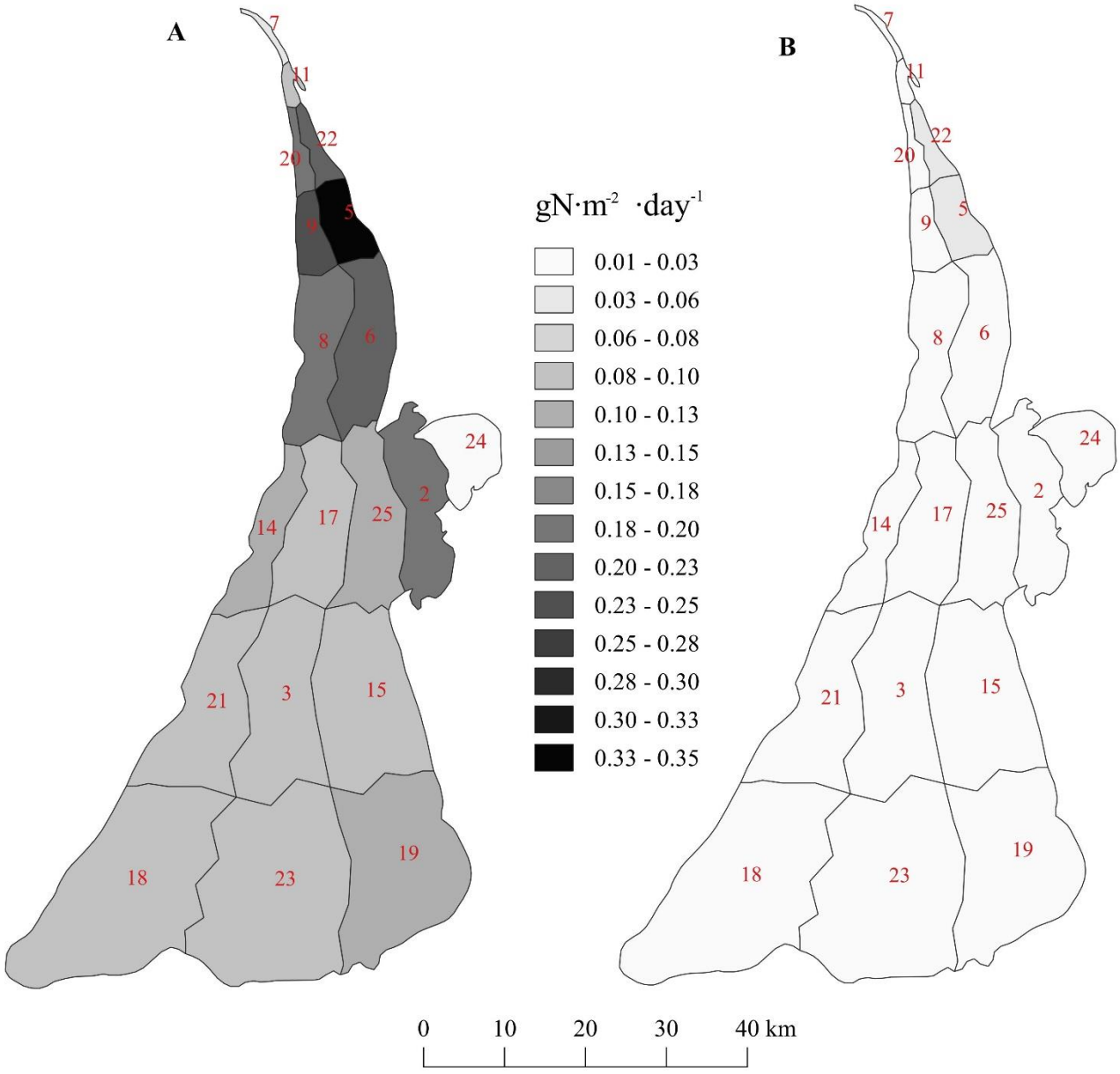

Figure 11. Spatial distribution of atmospheric nitrogen fixation in the Curonian lagoon in summer (A) and autumn (B) periods

11 pav. Atmosferinio azoto fiksacijos erdvinis pasiskirstymas vasarą (A) ir žiemą (B) Atmosferinio azoto erdvinis pasiskirstymas Kuršių mariose vasarą (A) ir rudenį (B)

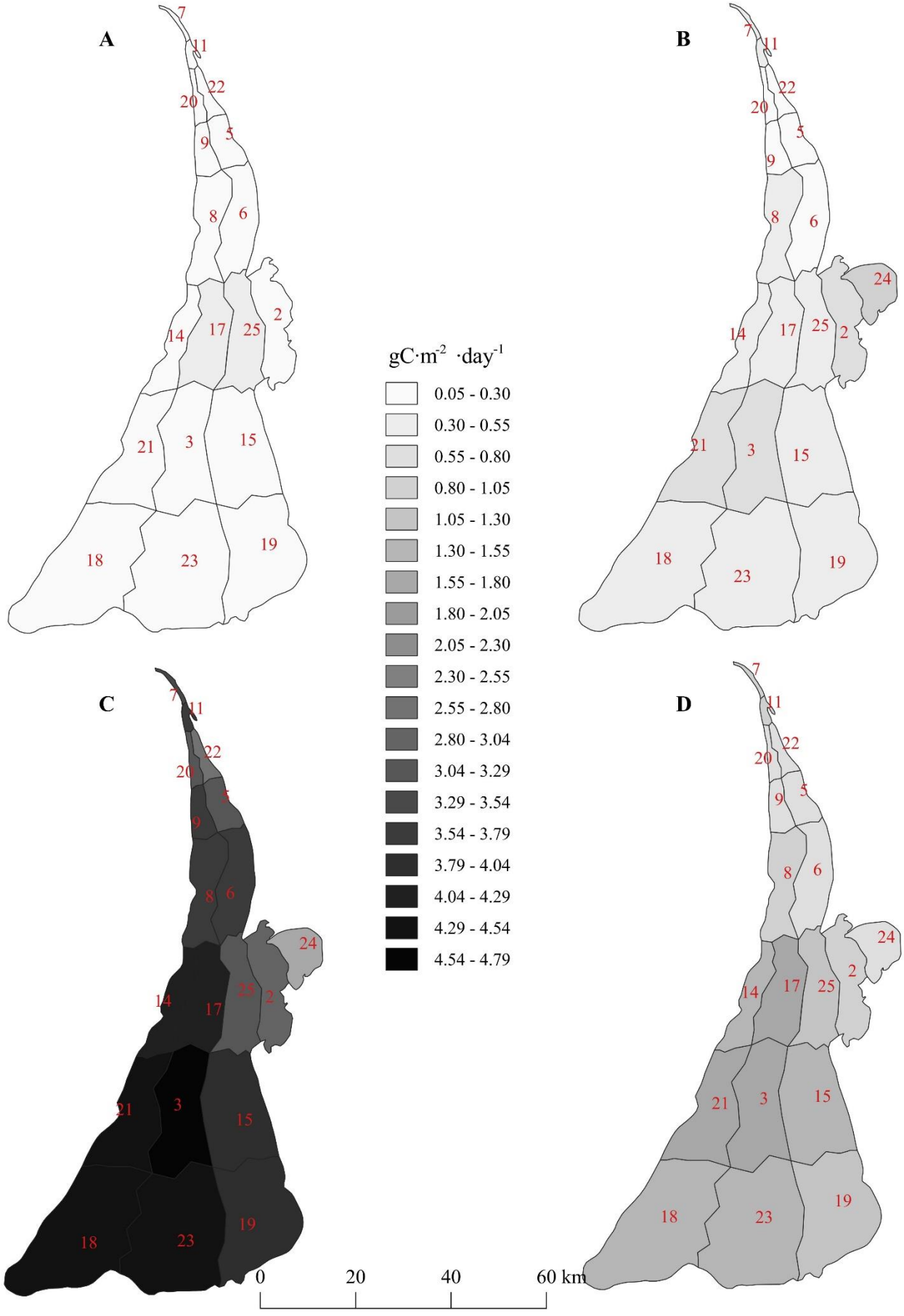

Figure 12. Spatial distribution of net primary production in the Curonian lagoon in winter (A), spring (B), summer (C), and autumn (D)

12 pav. Pirminės produkcijos erdvinis pasiskirstymas Kuršių mariose žiemą (A), pavasarį (B), vasarą (C) ir rudenį (D)

Spatially were estimated seasonal concentrations of NH_4-N, NO_3-N, PO_4-P (Figures 13, 16, 18). Modelled concentration of NH_4-N, in analyzed box 14 (Nida station), variate from minimum ~0.018 mg $\cdot N \cdot l^{-1}$ (in January) till maximum ~0.054 mg $\cdot N \cdot l^{-1}$ (in April). Seasonal variation showed that the highest concentration of NH_4-N observing in spring (~0.045 mg $\cdot N \cdot l^{-1}$), and then again increase in autumn (~0.041 mg $\cdot N \cdot l^{-1}$). The second peak of NH_4-N concentration in autumn overlapping with the lowest discharge of the Nemunas river (190.17 m^3/s). The lowest concentration of NH_4-N was in summer (~0.025 mg $\cdot N \cdot l^{-1}$) (Figure 13).

Spatial distribution of NH_4-N concentration showed the highest concentrations (in spring and autumn seasons) occurs in the southern part of the Curonian lagoon. In winter season was observed the high concentration of NH_4-N in 24^{th} (~0.081 – 0.089 mg $\cdot N \cdot l^{-1}$) and 2^{nd} (~0.046 – 0.054 mg $\cdot N \cdot l^{-1}$) boxes that represent the mouth of the Nemunas river (Figure 13). In this season was observed the highest discharge of the Nemunas river (507 m^3/s) (Figure 15). During the 2015 period, total load of NH_4^+ to the Nemunas river from the watershed was 808 t $\cdot yr^{-1}$ (Vybernaite-Lubiene et al., 2018).

Relationship of concentration of NH_4-N with the discharge was negligible (Figure 14). Except for winter period when high concentration of NH_4-N occurs in the mouth of the Nemunas river area (Figure 13). It has been noticed the relationship between the concentration of NH_4-N and net primary production. According to spatial distribution of net primary production, the highest concentration in the Curonian lagoon observed in the summer period (Figure 12), while the concentration of NH_4-N was lowest (Figure 13).

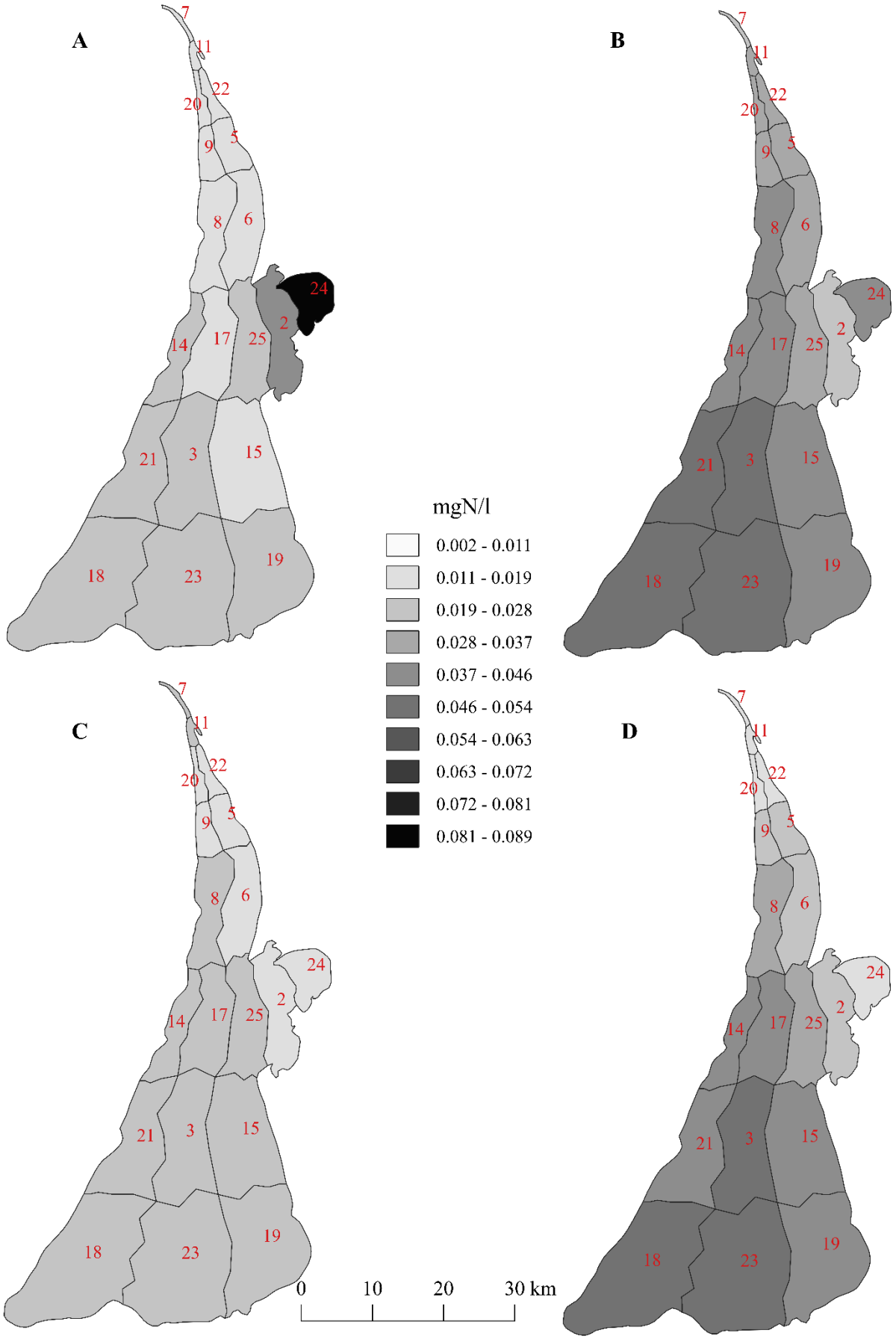

Figure 13. Spatial distribution of NH_4-N average seasonal concentration in the Curonian lagoon in winter (A), spring (B), summer (C), and autumn (D)

13 pav. NH_4-N vidutinės sezoninės koncentracijos erdvinis pasiskirstymas Kuršių mariose žiemą (A), pavasarį (B), vasarą (C) ir rudenį (D)

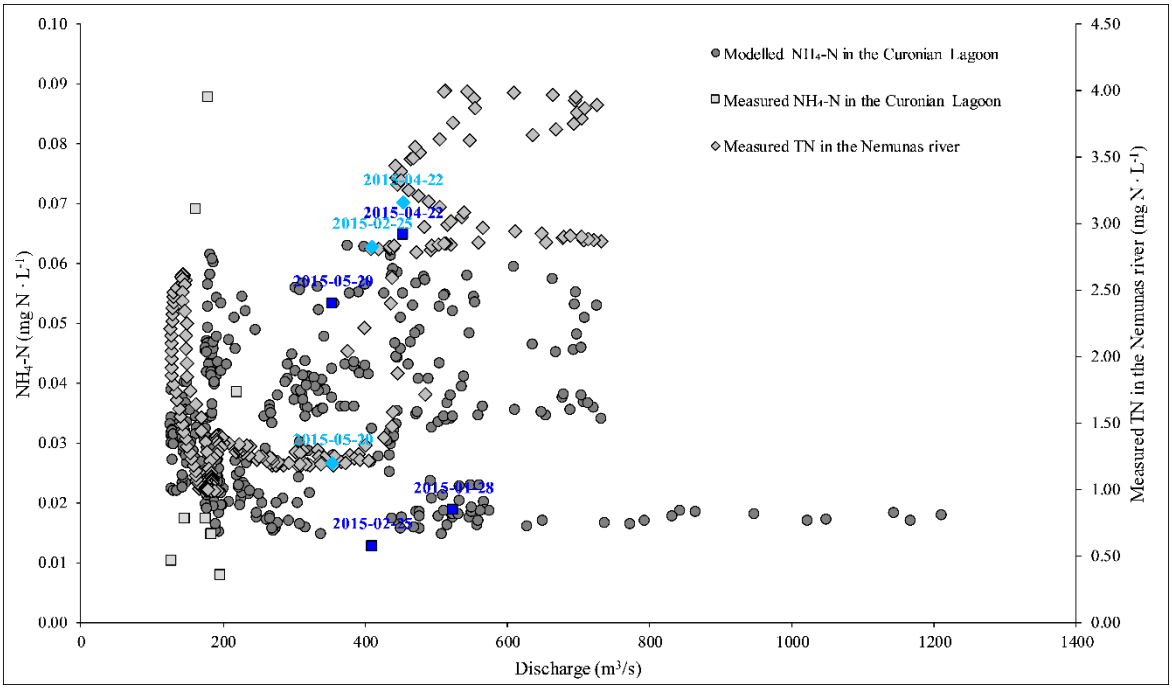

Figure 14. The relationship between NH_4-N and discharge (light blue diamonds represent the measured N_2 in the Nemunas river in the winter-spring season, darker blue squares represent measured NH_4-N in the Curonian lagoon in the winter-spring season)

14 pav. Ryšys tarp NH_4-N koncentracijos ir Nemuno upės nuotėkio (šviesiai mėlyni rombai atspindi Nemuno upėje išmatuotą N_2 koncentraciją žiemos-pavasario sezonu, tamsiai mėlyni kvadratai atspindi Kuršių mariose išmatuotą NH_4-N koncentraciją)

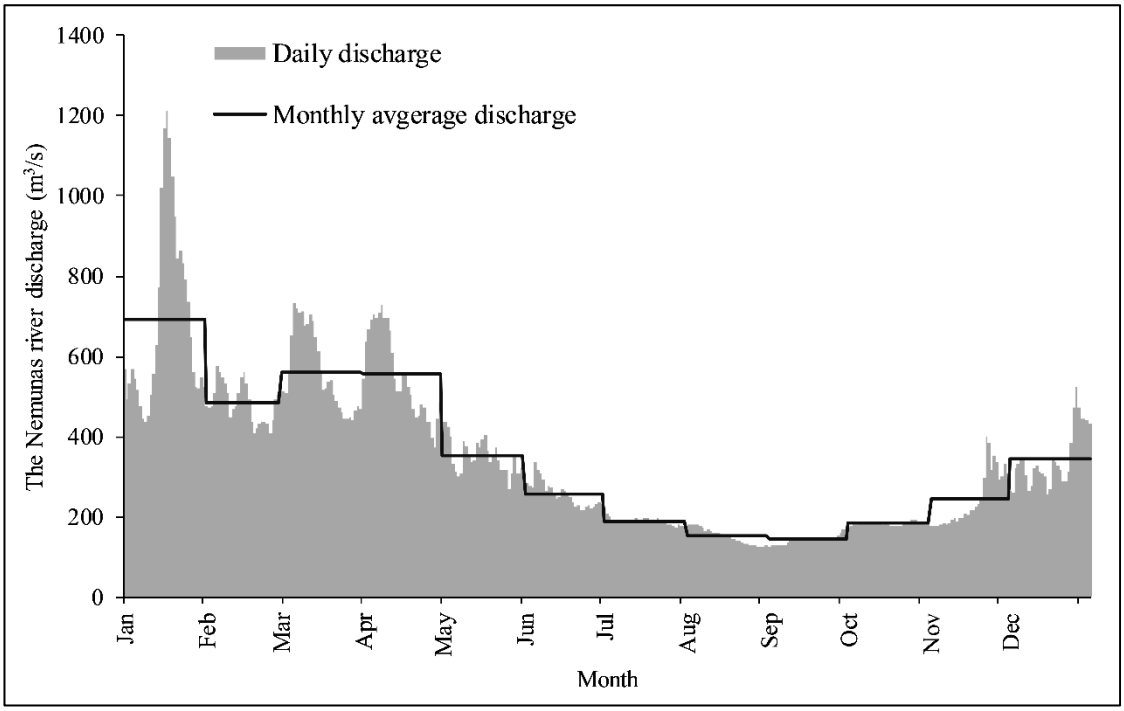

Figure 15. Discharge of the Nemunas river, during 2015 period

15 pav. Nemuno upės nuotėkis 2015 m.

The modelled concentration of NO_3-N, in analyzed box 14 (Nida station), variate from minimum ~0.00024 mg ·N · l^{-1} (in July) till maximum ~2.04 mg ·N · l^{-1} (in May), when average discharge was of the Nemunas river was 351.79 m^3/s. Seasonal variation showed that the highest concentration of NO_3-N was ~1.97 mg ·N · l^{-1} in spring, with mean discharge of 489.08 m^3/s. The lowest concentration of NO_3-N observed in autumn (~0.0097 mg ·N · l^{-1}), while the discharge of the Nemunas river was lowest (190.17 m^3/s).

The concentration of NO_3-N in the autumn season was negligible, therefore it do not represent the NO_3-N concentration variation over the boxes (Figure 16). In winter season was observed the highest concentration of NO_3-N in the mouth of the Nemunas river, that variate from ~2.14 mg ·N · l^{-1} till ~4.01 mg ·N · l^{-1}, while the discharge of the Nemunas river in this season was highest – 507 m^3/s. The spatial distribution of NO_3-N concentration in different seasons showed that it mostly accumulates in the central and/or southern part of the Curonian lagoon (Figure 16). In the spring season was captured the highest average concentration of NO_3-N (~1.51 mg ·N · l^{-1}) over 19 boxes (the Curonian lagoon), while the average concentration of NO_3-N in the 14^{th} box (Nida station) was ~1.97 mg ·N · l^{-1}. The highest concentration of NO_3-N occurs in the mouth of the Nemunas river when discharge was 489 m^3/s. In summer, when discharge was 200 m^3/s, the concentration of NO_3-N accumulates in southern part of the Curonian lagoon, and variate from ~0.01 mg ·N · l^{-1} till ~0.31 mg ·N · l^{-1} (Figure 16).

The seasonal concentrations of NO_3-N variate with the seasonal cycle of freshwater input in the Curonian lagoon. Relationship of concentration of NO_3-N with discharge showed that both modelled and measured (in the Curonian lagoon and the Nemunas river) concentrations were highest in spring season when average discharge was 489 m^3/s. Furthermore, between measured data from the Nemunas river and the Curonian lagoon, was captured the same trend of variation of concentration related to discharge (Figure 17). Total NO_3^- load to the Nemunas river during the 2015 period was 23.792 t · yr^{-1}, and it was the main form of the total nitrogen (TN) load (Vybernaite-Lubiene et al., 2018).

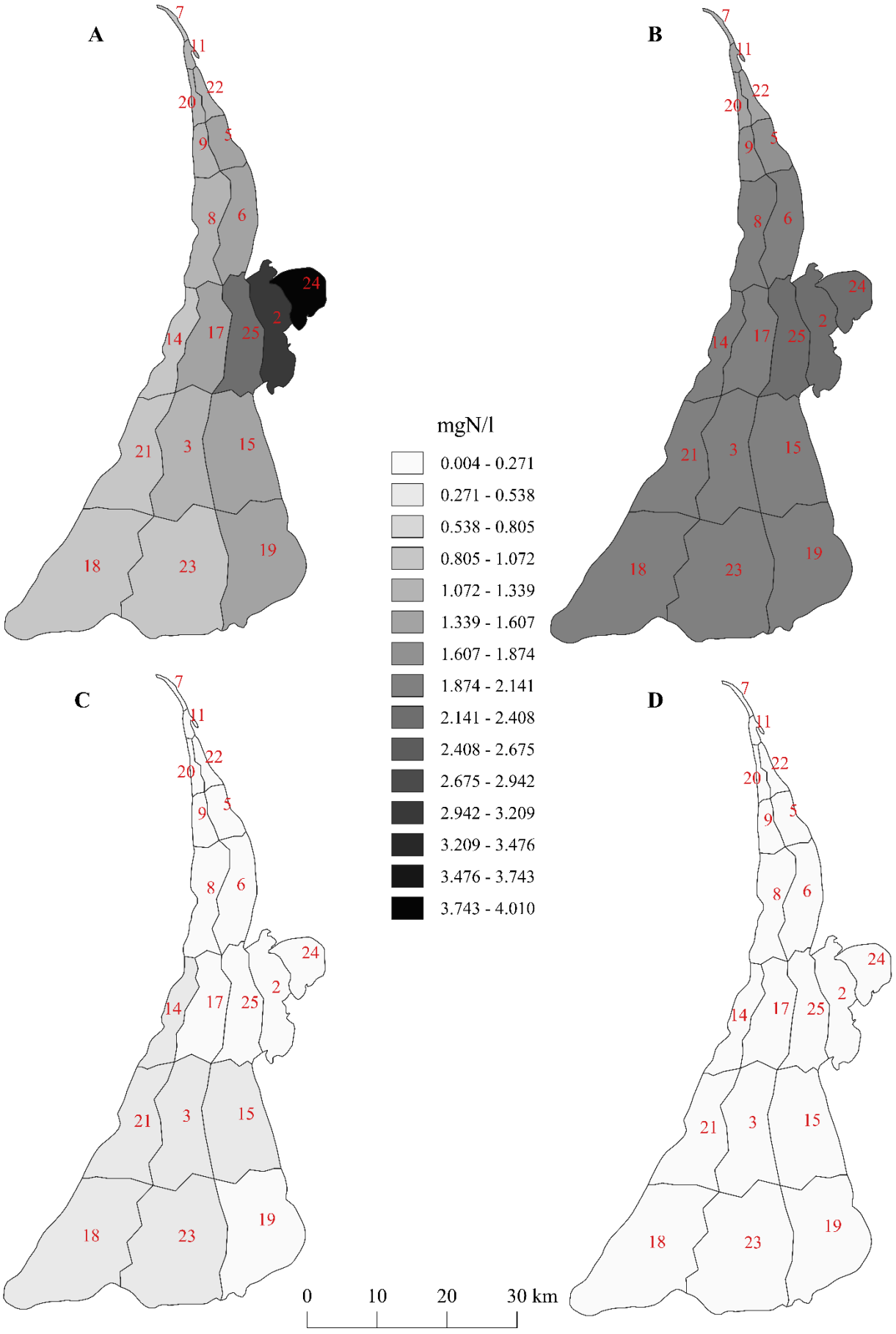

Figure 16. Spatial distribution of NO_3-N average seasonal concentration in the Curonian lagoon in winter (A), spring (B), summer (C), and autumn (D)

16 pav. NO_3-N vidutinės sezoninės koncentracijos erdvinis pasiskirstymas Kuršių mariose žiemą (A), pavasarį (B), vasarą (C) ir rudenį (D)

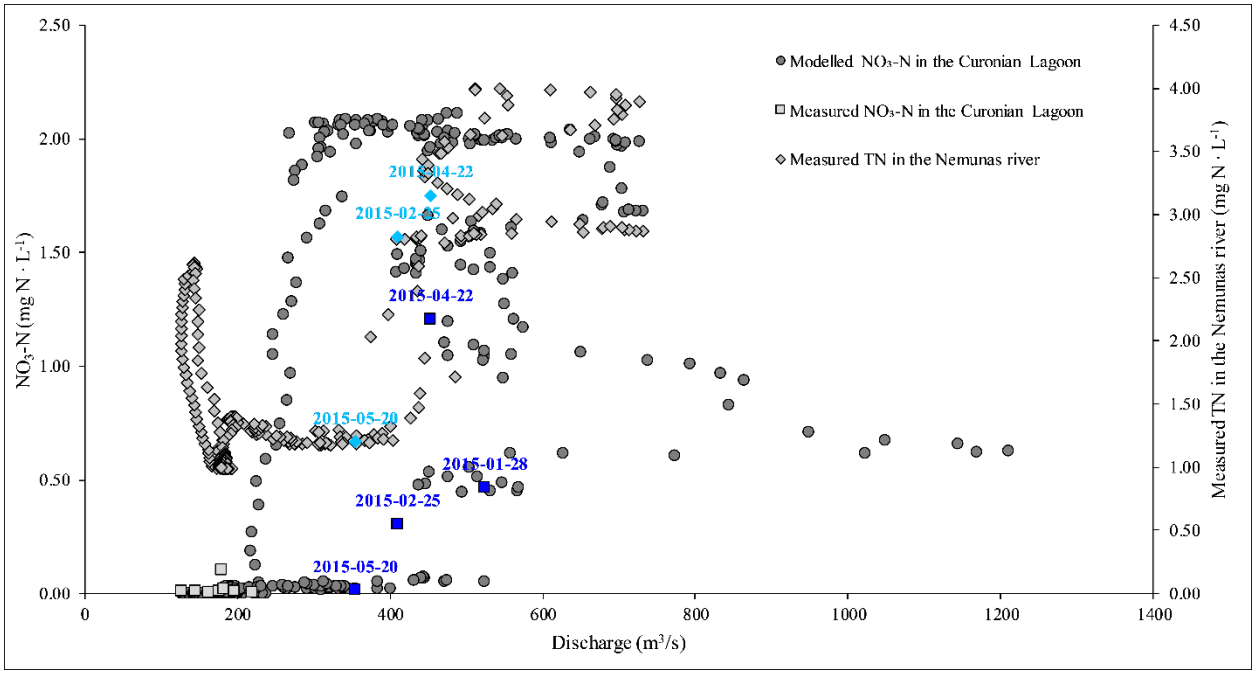

Figure 17. The relationship between NO_3-N concentration and discharge (light blue diamonds represent the measured N_2 in the Nemunas river in the winter-spring season, darker blue squares represent measured NO_3-N in the Curonian lagoon in the winter-spring season)

17 pav. Ryšys tarp NO_3-N koncentracijos ir Nemuno upės nuotėkio (šviesiai mėlyni rombai atspindi Nemuno upėje išmatuotą N_2 koncentraciją žiemos-pavasario sezonu, tamsiai mėlyni kvadratai atspindi Kuršių mariose išmatuotą NO_3-N koncentraciją)

The modelled concentrations of PO_4-P in analyzed box 14 (Nida station) variate from minimum ~0.0004 mg ·P · l^{-1} (in May) till maximum ~0.021 mg ·P · l^{-1} (in December). Seasonal variation showed that highest concentration of PO_4-P observed in winter (~0.013 mg ·P · l^{-1}), when the discharge of the Nemunas river was highest (507 m^3/s), and lowest concentration of PO_4-P observed in spring (~0.0009 mg ·P · l^{-1}).

According to the spatial distribution of PO_4-P, the highest concentrations occurred in the mouth of the Nemunas river over all four (winter, spring, summer, and autumn) seasons (Figure 18). The main accumulation of concentration of PO_4-P occurs in the central and southern part of the Curonian lagoon.

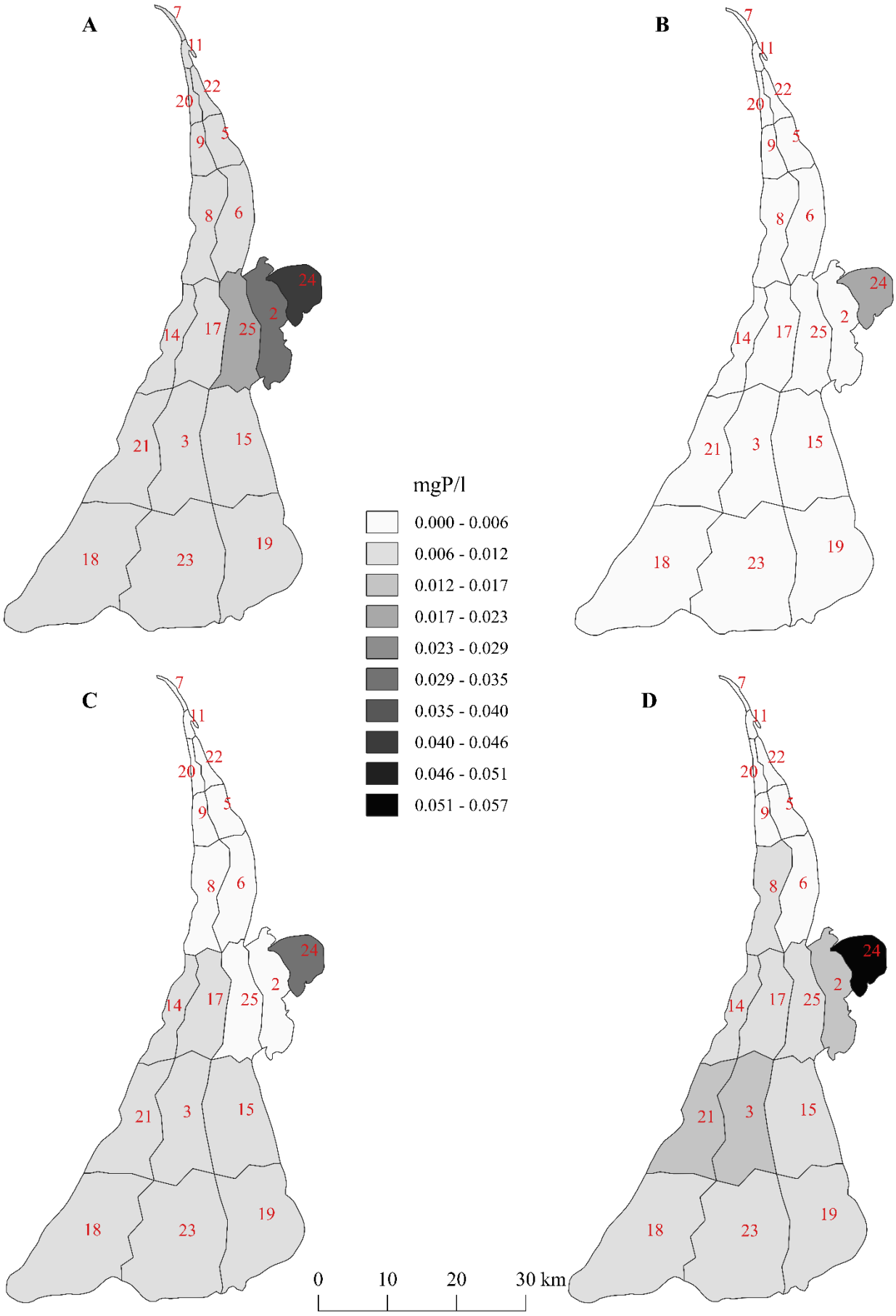

Figure 18. Spatial distribution of PO_4-P average seasonal concentration in the Curonian lagoon in winter (A), spring (B), summer (C), and autumn (D)

18 pav. PO_4-P vidutinės sezoninės koncentracijos erdvinis pasiskirstymas Kuršių mariose žiemą (A), pavasarį (B), vasarą (C) ir rudenį (D)

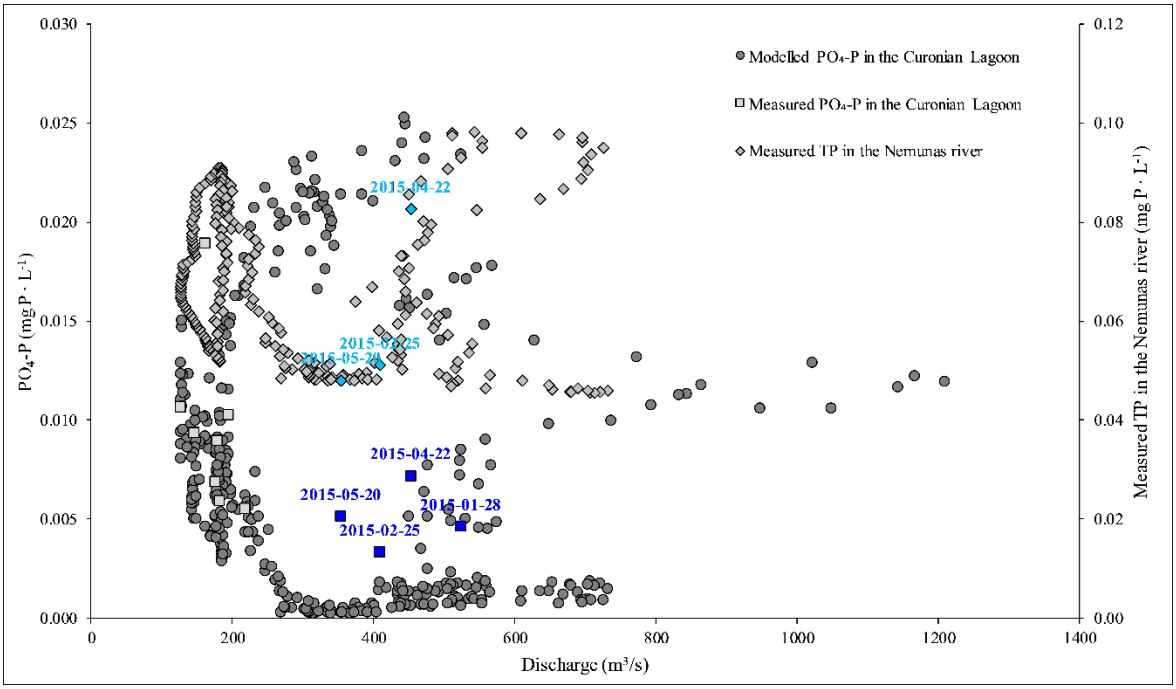

Figure 19. The relationship between PO4-P concentration and discharge (light blue diamonds represent the measured P_2 in the Nemunas river in the winter-spring season, darker blue squares represent measured PO_4-P in the Curonian lagoon in the winter-spring season)

19 pav. Ryšys tarp PO_4-P koncentracijos ir Nemuno upės nuotėkio (šviesiai mėlyni rombai atspindi Nemuno upėje išmatuotą P_2 koncentraciją žiemos-pavasario sezonu, tamsiai mėlyni kvadratai atspindi Kuršių mariose išmatuotą PO_4-P koncentraciją)

Relationship of concentration of PO_4-P with discharge showed that the highest concentrations of both measured and modelled data occur when discharge is between 400 and 600 m^3/s. Also, between measured data from the Nemunas river and the Curonian lagoon, was captured the similar trend of variation of concentration in winter and early spring period (Figure 19). In 2015 period the total DIP (dissolved inorganic phosphorus) load to the Nemunas river was 442 $t \cdot yr^{-1}$ (Vybernate-Lubiene et al., 2018).

IV. DISCUSSION

A new, open source, biogeochemical modelling software package focused on nutrient cycles and eutrophication was used. The software package consists of three main components:

- R-based GUI application that acts as a workbench helping the users to calibrate the model and view the model results with some simple post-processing.
- MATLAB based scripts that read the information written by SHYFEM and built most of the model inputs automatically.

- The computational engine of the model developed in FORTRAN modularly, with two sub-components: i) a transport component that solves the advection-diffusion-reaction equation discretized as the box model domain, and therefore handles the material fluxes between the boxes, and ii) a kinetic component that provides the transport component with reaction rates in each model box. This design allows the modeller to create new models for different aquatic ecosystems just by modifying the kinetic component or removing it completely and writing a new subroutine to simulate a different type of ecosystem.

The model was applied to the Curonian Lagoon on a fairly complex model domain that consists of 25 model boxes (Figure 6). The Curonian Lagoon case study represents an attempt to capture patterns of pelagic biogeochemical and biological processes in a coastal lagoon dominated by freshwater inputs from a large river and occasionally brackish water intrusions. The Curonian Lagoon is characterized by a strong spatial heterogeneity in both chemical and physical parameters as well as bottom sediment characteristics (Ferrarin et al., 2008; Petkuviene et al., 2016; Umgiesser et al., 2016; Zilius et al., 2018) affecting in turn seasonal and spatial patterns of biological and chemical processes. The hydraulic transport calculated using high resolution finite element model (http://www.ismar.cnr.it/shyfem) as fluxes between boxes allowed us to follow closely the seasonal circulation patterns in the lagoon including discharges from the Nemunas River and exchange with Baltic Sea, where the boundary conditions were set up. As the Curonian Lagoon is mostly well-mixed vertically (Umgiesser et al., 2016), the absence of vertical resolution in the modelled boxes is an acceptable simplification of transport processes existing in the lagoon. Thus each simulation for a one-year period during ESTAS-AQUABC calibration took 75 seconds on a standard personal computer using the configuration shown in Figure 5. The calibrated model constants are given in Appendix B.

The benthic fluxes of NH_4^+, NO_3^- and DIP measured in the same period (Zilius et al., 2018; Petkuviene et al., prep.) could account for at least 50 % of ammonia concentration mismatch between modelled and observed data. Sediments were always a NH_4^+ source, particularly during the summer when intensive mineralization occurred (Zilius et al., 2018). Although sediments in the lagoon could be considered as a sink for NO_3^-, the measured fluxes explain only 2 % of difference between modelled and observed concentrations. Zilius et al. (2018) demonstrated that assimilative uptake by benthic and pelagic diatoms is the most important mechanism regulating nitrate concentrations in overlaying water. However, in absence of benthic compartment in the model, this flux left unaccounted as well. There is no clear explanation of the fact that model underestimates DIP concentrations in the late summer, as the measured DIP flux from the sediments was negative. However, it is known that even local hypoxia developed during summer due to short-term thermal stratification (which could be easily missed during measurement campaigns) and intensive respiration

could trigger intensive phosphorus release from sediments (Petkuviene et al., 2016). Moreover, even as we tried to mimic some effects of resuspension by introduction of relationship between bottom shear stress and settling velocities (zero values when critical shear stress is exceeded), vast majority of resuspension related processes were left unaccounted.

Spatial distribution of nutrients concentration and net primary production shows the highest accumulation in central and southern parts of the Curonian Lagoon, what proves previous studies of this area (Aleksandrov, 2010). The environmental conditions in this area were favourable because of absence of the sea water intusion, slow water exchange, fresh water ineraction (Aleksandrov, 2010; Dailidienė and Davulienė, 2008). Also it was noticed the seasonal variability of nutrients and net primary production, as well as, N_2 fixation (Figure 11-13, 16, 18). The hydrological and hydrochemical conditions affect seasonality of nutients concentration in the Curonian Lagoon (Zilius et al., 2018; Aleksandrov, 2010). It is known that water temperature is one of the key factors determining the seasonal variation of the primary production and abundance of phytoplankton (Zilius et al., 2018; Aleksandrov, 2010; Pilkaityte and Razinkovas. 2006).

In this study we assumed to estimate the relationship between nutrient concentration and the Nemunas river discharge (Figure 14, 17, 19). According to the results, relationship between concentration of NH_4-N and discharge was negligible (Figure 14). We assume that the relationship between primary production and concentration of NH_4-N is stronger. According to previous studies, it is known that the main source of NH_4^+ is sediments (Zilius et al., 2018). NH_4^+ efflux from silty sediments in the southern part of the Curonian Lagoon was 6.6 mmol $m^{-2} \cdot day^{-1}$ (Zilius et al., 2018).

The relationship between concentration of NO_3-N and discharge was noticeable (Figure 17). We captured the concentration of NO_3-N peak during winter-spring season while discharge was highest, and minima concentration during summer-autumn, while discharge was lowest (Figure 16). This is line with previous works (Vybernaite-Lubiene et al., 2018). During colder period of the year, NO_3-N loss from the watershed is higher, as biogeochemical processes that are able to transform NO_3^- into organic or molecular N via uptake or denitrification are limited, while retention is reduced by snow melting and precipitation (Vybernaite-Lubiene et al., 2018). Also we captured the same trend between measured data from the Nemunas river and the Curonian Lagoon at the winter-spring period (Figure 17).

Inorganic phosphorus (PO_4-P) concentrations were highest during winter season when the discharge of the Nemunas river was also the highest (Figure 18-19). However, according to previous studies the total phosphorus concentrations are associated with Chl-a concentration and (Staehr et al., 2017; Petkuviene et al., 2016; Petkuviene, 2015).

The discharge is affected by a combination of precipitation patterns/intensities, evapotranspiration/accumulation in groundwater, and steep changes in temperature that drive

snow/ice melt or water freezing (Vybernaite-Lubiene et al., 2018). Therefore, the air temperature co-regulates river discharge, and the discharge affects the pattern of nutrient delivery from the river to the lagoon (Vybernate-Lubiene et al., 2018).

CONCLUSIONS

1. For the model calibration was created R-based GUI application that acts as a workbench helping the users to calibrate the model and view the model results with some simple post-processing. A test aimed case study was conducted on the Curonian Lagoon, with an acceptable level of preliminary calibration which provided satisfactory results for the dynamics of inorganic nutrient and, particularly pelagic nitrogen fixation.
2. Spatial analysis showed the distribution of nutrients in the Curonian lagoon of different seasons. Modelled data spatial distribution showed that most selected parameters (NH_4-N, NO_3-N, PO_4-P) accumulate in the central and southern parts of the study area. The spatial patterns of the net primary production distribution provided better understanding of the heterogeneity of phytoplankton based processes in the Curonian lagoon.
3. Most of the discrepancy between modelled and measured data could be attributed to the incapability of present model to simulate benthic compartment and bento-pelagic coupling, including the resuspension, settling and burial of diatoms. This knowledge gives us clear direction where and how to improve the model to provide better prediction power and capacity. Apart from these necessary enhancements there is an increasing evidence that not only filamentous cyanobacteria, but also heterotrophic unicellular microorganisms are capable to fix N_2 (e.g. Bentzon-Tilia et al., 2015), which must be reflected in the future by adding additional state variable as different size groups of N_2-fixers in the kinetic part of the modelling framework.

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APPENDICES

APPENDIX A.

A.1 PHYTOPLANKON KINETICS

Fixed stochiometry is assumed for phytoplankton so, there are no state variables such as "diatoms nitrogen" or "cyanobacteria phosphorus". All phytoplankton undergo the same five main processes; where growth results in uptake of the relevant nutrients and incorporate them into phytoplankton biomass; where

- Death converts the phytoplankton biomass to detrital particulate organic matter (in case of diatoms Biogenic Silicon in particulate form)
- Excreion converts the phytoplankton biomass to dissolved organic matter
- Respiration converts the phytoplankton biomass to inorganic nutrients
- Grazing converts the phytoplankton biomass to zooplankton biomass

A.1.1 Diatoms

The main kinetic derivative for phytoplankton is given in Equation A.1.1.1

$$\frac{d[DIA-C]}{dt} = \underbrace{R_{DIA,GROWTH}}_{Diatoms\ growth} - \underbrace{R_{DIA,TOT,RESP}}_{Diatoms\ total\ respiration} - \underbrace{R_{DIA,EXCR}}_{Diatoms\ excretion} - \underbrace{R_{DIA,DEATH}}_{\substack{Diatoms\ death\ not\ related\ to \\ zooplankton\ grazing}} - \underbrace{R_{ZOO,GRAZ,DIA}}_{Zooplankton\ grazing\ on\ diatoms}$$

(Equation A.1.1.1)

where each of the process rates will be further described in the equations given in the following subsections except the zooplankton grazing rate on diatoms, which will be discussed in Section A.2.

A.1.1.1 Diatom Growth

The growth rate of diatoms is given in Equation A.1.1.2

$$R_{DIA,GROWTH} = k_{G,DIA,MAX} \cdot lim_{k,G,DIA} \cdot [DIA-C] \quad \text{(Equation A.1.1.2)}$$

The notation of Equation A.1.1.2 is given below:

$R_{DIA,GROWTH}$: Growth rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{G,DIA,MAX}$: Growth rate constant for diatoms at optimum conditions (day^{-1})

$lim_{k,G,DIA}$: Limitation factor for diatom growth (dimensionless)

Limitation factor for diatom growth is given in Equation A.1.1.3

$$lim_{k,G,DIA} = lim_{k,G,DIA,TEMP} \cdot lim_{k,G,DIA,LIGHT} \cdot \min\left(lim_{k,G,DIA,DOXY}, lim_{k,G,DIA,NUTR}\right)$$

(Equation A.1.1.3)

The notation of Equation A.1.1.3 is given below:

$\lim_{k,G,DIA,TEMP}$: Temperature limitation factor for diatom growth (dimensionless)

$\lim_{k,G,DIA,LIGHT}$: Light limitation factor for diatom growth (dimensionless)

$\lim_{k,G,DIA,DOXY}$: Limitation factor related to the lack of dissolved oxygen for diatom growth (dimensionless)

$\lim_{k,G,DIA,NUTR}$: Nutrient limitation factor for diatom growth (dimensionless)

Calculation details of the temperature limitation factor for diatom growth is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

The limitation factor is given in Equation A.1.1.4

$$\lim_{k,G,DIA,LIGHT} = \frac{2.718 \cdot f_{DAY}}{k_E \cdot H} \cdot \left(\exp\left(-\frac{I_A}{I_{S,DIA}} \cdot \exp(-1 \cdot k_E \cdot H) \right) - \exp\left(-\frac{I_A}{I_{S,DIA}} \right) \right)$$

(Equation A.1.1.4)

The notation of Equation A.1.1.4 is given below:

H : Depth (m)
k_E : Light extinction coefficient (m^{-1}) (calculation details given in Section A.1.5)
f_{DAY} : Fraction of daylight in a particular day (dimensionless)
I_A : Available light at the water surface (langleys)
$I_{S;DIA}$: Light saturation constant for diatoms (langleys)

Limitation factor related to the lack of dissolved oxygen for diatom growth is given in Equation A.1.1.5

$$\lim_{k,G,DIA,DOXY} = \frac{[O_2]}{k_{HS,O2,DIA} + [O_2]}$$

(Equation A.1.1.5)

The notation of Equation A.1.1.5 is given below:

$k_{HS,O2,DIA}$: Monod type half-saturation concentration of diatom growth for dissolved oxygen ($gO_2 \cdot m^{-3}$)

Nutrient limitation factor for diatom growth is given in Equation A.1.1.6 – A.1.1.9

$\lim_{k,G,DIA,NUTR} = \min\left(\lim_{k,G,DIA,N}, \lim_{k,G,DIA,P}, \lim_{k,G,DIA,DISS,Si}\right)$ (Equation A.1.1.6)

$$\lim_{k,G,DIA,N} = \frac{[NH4-N] + [NO3-N]}{k_{HS,DIN,DIA} + [NH4-N] + [NO3-N]}$$

(Equation A.1.1.7)

$$\lim_{k,G,DIA,P} = \frac{[PO4 - P]}{k_{HS,DIP,DIA} + [PO4 - P]}$$

(Equation A.1.1.8)

$$\lim_{k,G,DIA,DISS,Si} = \frac{Si_{DISS}}{k_{HS,DSi,DIA} + Si_{DISS}}$$

(Equation A.1.1.9)

The notation of Equation A.1.1.6 - A.1.1.9 is given below:

$k_{HS,DIN,DIA}$: Monod type half-saturation concentration of diatom growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$k_{HS,DIP,DIA}$: Monod type half-saturation concentration of diatom growth for dissolved inorganic phosphorus ($gP \cdot m^{-3}$)

$k_{HS,DSi,DIA}$: Monod type half-saturation concentration of diatom growth for dissolved inorganic silicon ($gSi \cdot m^{-3}$)

A.1.1.2 Diatom Total Respiration

The growth rate of diatoms is given in Equation A.1.1.10

$$R_{DIA,TOT,RESP} = R_{DIA,INT,RESP} + R_{DIA,MET,RESP}$$ (Equation A.1.1.10)

The notation of Equation A.1.1.10 is given below:

$R_{DIA,TOT,RESP}$: Total respiration rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,INT,RESP}$: Internal (dark) respiration rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,MET,RESP}$: Respiration rate of diatoms due to metabolic activities ($gC \cdot m^{-3} \cdot day^{-1}$)

Internal (dark) respiration rate of diatoms given in Equation A.1.1.11.

$$R_{DIA,INT,RESP} = k_{R,DIA,20} \cdot \theta_{k,R,DIA}^{(TEMP-20)} \cdot \lim_{k,G,DIA,DOXY} \cdot [DIA - C]$$ (Equation A.1.1.11)

The notation of Equation A.1.1.11 is given below:

$k_{R,DIA,20}$: Dark respiration rate constant of diatoms at 20˚C (day^{-1})

$\theta_{k,R,DIA,20}$: Arrhenius-type temperature correction coefficient for dark respiration rate constant of diatoms (dimensionless)

$\lim_{k,G,DIA,DOXY}$: Limitation factor related to the lack of dissolved oxygen for diatom growth (dimensionless)

Respiration rate of diatoms due to metabolic activities is given in Equation A.1.1.12

$$R_{DIA,MET,RESP} = (1 - frac_{DIA,EXCR}) \cdot R_{DIA.MET,WASTE}$$ (Equation A.1.1.12)

The notation of Equation A.1.1.12 is given below:

$R_{DIA.MET,WASTE}$: Metabolic waste production rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{DIA,EXCR}$: Fraction of metabolic waste excreted as DOC (dimensionless)

Metabolic waste production rate of diatom is given in Equation A.1.1.13.

$$R_{DIA,MET,WASTE} = R_{DIA,GROWTH} \cdot (1 - eff_{DIA,GROWTH})$$ (Equation A.1.1.13)

The notation of Equation A.1.1.13 is given below:

$R_{DIA,GROWTH}$: Growth rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)
$eff_{DIA,GROWTH}$: Efficiency of diatom growth (dimensionless)

A.1.1.3 Diatom Excretion

The excretion rate of diatoms is given in Equation A.1.1.14

$$R_{DIA,MET,RESP} = frac_{DIA,EXCR} \cdot R_{DIA.MET,WASTE}$$ (Equation A.1.1.14)

The notation of Equation A.1.1.14 is given below:

$R_{DIA.MET,WASTE}$: Metabolic waste production rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{DIA,EXCR}$: Fraction of metabolic waste excreted as DOC by diatoms (dimensionless)

A.1.1.4 Diatom Death

The death rate of diatoms is given in Equation A.1.1.15

$$R_{DIA,DEATH} = k_{D,DIA,20} \cdot \theta_{k,D,DIA}^{(TEMP-20)} \cdot FAC_{HYPOX,DIA,D} \cdot [DIA - C]$$ (Equation A.1.1.15)

The notation of Equation A.1.1.15 is given below:

$R_{DIA.DEATH}$: Death rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{D,DIA,20}$: Death rate constant of diatoms at 20˚C (day^{-1})

$\theta_{k,D,DIA,20}$: Arrhenius-type temperature correction coefficient for death rate constant of diatoms (dimensionless)

$FAC_{HYPOX,DIA,D}$: Acceleration factor of hypoxia on diatom death (dimensionless)

Calculation details of the acceleration factor of hypoxia on diatom death is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

A.1.2 Non-Nitrogen Fixing Cyanobacteria

The main kinetic derivative for phytoplankton is given in Equation A.1.2.1

$$\frac{d[CYN-C]_{NOFIX}}{dt} = \underbrace{R_{NOFIX,CYN,GROWTH}}_{\substack{Non-nitrogen\ fixing\\ cyanobacteria\ growth}} - \underbrace{R_{NOFIX,CYN,TOT,RESP}}_{\substack{Non-nitrogen\ fixing\\ cyanobacteria\ total\\ respiration}} - \underbrace{R_{NOFIX,CYN,EXCR}}_{\substack{Non-nitrogen\ fixing\\ cyanobacteria\ excretion}} - \underbrace{R_{NOFIX,CYN,DEATH}}_{\substack{Non-nitrogen\ fixing\ cyanobacteria\\ death\ not\ related\ to\\ zooplankton\ grazing}} - \underbrace{R_{ZOO,GRAZ,NOFIX,CYN}}_{\substack{Zooplankton\ grazing\ on\\ non-nitrogen\ fixing\ cyanobacteria}}$$

(Equation A.1.2.1)

where each of the process rates will be further described in the equations given in the following subsections except the zooplankton grazing rate on non-nitrogen fixing cyanobacteria, which will be discussed in Section A.2.

A.1.2.1 Non-N fixing Cyanobacteria Growth

The growth rate of Non-nitrogen fixing cyanobacteria is given in Equation A.1.2.2

$$R_{NOFIX,GROWTH} = k_{G,NOFIX,CYN,MAX} \cdot lim_{k,G,NOFIX,CYN} \cdot [CYN-C]_{NOFIX}$$

(Equation A.1.2.2)

The notation of Equation A.1.2.2 is given below:

$R_{NOFIX,CYN,GROWTH}$: Growth rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{G,NOFIX,CYN,MAX}$: Growth rate constant for Non-nitrogen fixing cyanobacteria at optimum conditions (day^{-1})

$lim_{k,G,NOFIX,CYN}$: Limitation factor for Non-nitrogen fixing cyanobacteria growth (dimensionless)

Limitation factor for non-nitrogen fixing cyanobacteria growth is given in Equation A.1.2.3

$$lim_{k,G,NOFIX,CYN} = lim_{k,G,NOFIX,CYN,TEMP} \cdot lim_{k,G,NOFIX,CYN,LIGHT} \cdot \min\left(lim_{k,G,NOFIX,CYN,DOXY}, lim_{k,G,NOFIX,CYN,NUTR}\right)$$

(Equation A.1.2.3)

The notation of Equation A.1.2.3 is given below:

$lim_{k,G,NOFIX,CYN,TEMP}$: Temperature limitation factor for non-nitrogen fixing cyanobacteria growth (dimensionless)

$lim_{k,G,NOFIX,CYN,LIGHT}$: Light limitation factor for non-nitrogen fixing cyanobacteria growth (dimensionless)

$lim_{k,G,NOFIX,CYN,DOXY}$: Limitation factor related to the lack of dissolved oxygen for

non-nitrogen fixing cyanobacteria growth (dimensionless)

$\lim_{k,G,NOFIX,CYN,NUTR}$: Nutrient limitation factor for non-nitrogen fixing cyanobacteria growth (dimensionless)

Calculation details of the temperature limitation factor for Non-nitrogen fixing cyanobacteria growth is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

The light limitation factor for non-nitrogen fixing cyanobacteria growth is given in Equation A.1.2.4

$$\lim_{k,G,NOFIX,CYN,LIGHT} = \frac{2.718 \cdot f_{DAY}}{k_E \cdot H} \cdot \left(\exp\left(-\frac{I_A}{I_{S,NOFIX,CYN}} \cdot \exp(-1 \cdot k_E \cdot H) \right) - \exp\left(-\frac{I_A}{I_{S,NOFIX,CYN}} \right) \right)$$

(Equation A.1.2.4)

The notation of Equation A.1.2.4 is given below:

H : Depth (m)

k_E : Light extinction coefficient (m^{-1}) (calculation details given in Section A.1.5)

f_{DAY} : Fraction of daylight in a particular day (dimensionless)

I_A : Available light at the water surface (langleys)

$I_{S;NOFIX,CYN}$: Light saturation constant for non-nitrogen fixing cyanobacteria (langleys)

Limitation factor related to the lack of dissolved oxygen for non-nitrogen fixing cyanobacteria growth is given in Equation A.1.2.5

$$\lim_{k,G,NOFIX,CYN,DOXY} = \frac{[O_2]}{k_{HS,O2,NOFIX,CYN} + [O_2]}$$

(Equation A.1.2.5)

The notation of Equation A.1.2.5 is given below:

$k_{HS,O2,NOFIX,CYN}$: Monod type half-saturation concentration of Non-nitrogen fixing cyanobacteria growth for dissolved oxygen ($gO_2 \cdot m^{-3}$)

Nutrient limitation factor for Non-nitrogen fixing cyanobacteria growth is given in Equation A.1.2.6 – A.1.2.8

$$\lim_{k,G,NOFIX,CYN,NUTR} = \min\left(\lim_{k,G,NOFIX,CYN,N}, \lim_{k,G,NOFIX,CYN,P}\right)$$ (Equation A.1.2.6)

$$\lim_{k,G,NOFIX,CYN,N} = \frac{[NH4-N] + \left([DON] \cdot f_{avail,DON}\right) + [NO3-N]}{k_{HS,DIN,NOFIX,CYN} + [NH4-N] + \left([DON] \cdot f_{avail,DON}\right) + [NO3-N]}$$

(Equation A.1.2.7)

$$\lim_{k,G,NOFIX,CYN,P} = \frac{[PO4 - P]}{k_{HS,DIP,NOFIX,CYN} + [PO4 - P]}$$

(Equation A.1.2.8)

The notation of Equation A.1.2.6 - A.1.2.8 is given below:

$k_{HS,DIN,NOFIX,CYN}$: Monod type half-saturation concentration of non-nitrogen fixing cyanobacteria growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$f_{avail,DON}$: Fraction of DON available to non-nitrogen fixing cyanobacteria as nitrogen source for growth

$k_{HS,DIP,NOFIX,CYN}$: Monod type half-saturation concentration of non-nitrogen fixing cyanobacteria growth for dissolved inorganic phosphorus ($gP \cdot m^{-3}$)

A.1.2.2 Non-Nitrogen Fixing Cyanobacteria Total Respiration

The growth rate of Non-nitrogen fixing cyanobacteria is given in Equation A.1.2.9

$$R_{NOFIX,CYN,TOT,RESP} = R_{NOFIX,CYN,INT,RESP} + R_{NOFIX,CYN,MET,RESP}$$ (Equation A.1.2.9)

The notation of Equation A.1.2.9 is given below:

$R_{NOFIX,CYN,TOT,RESP}$: Total respiration rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,INT,RESP}$: Internal (dark) respiration rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,MET,RESP}$: Respiration rate of non-nitrogen fixing cyanobacteria due to metabolic activities ($gC \cdot m^{-3} \cdot day^{-1}$)

Internal (dark) respiration rate of non-nitrogen fixing cyanobacteria given in Equation A.1.2.10.

$$R_{NOFIX,CYN,INT,RESP} = k_{R,NOFIX,CYN,20} \cdot \theta_{k,R,NOFIX,CYN}^{(TEMP-20)} \cdot \lim_{k,G,NOFIX,CYN,DOXY} \cdot [CYN - C]_{NOFIX}$$

(Equation A.1.2.10)

The notation of Equation A.1.2.10 is given below:

$k_{R,NOFIX,CYN,20}$: Internal respiration rate constant of non-nitrogen fixing cyanobacteria at 20˚C (day^{-1})

$\theta_{k,R,NOFIX,CYN,20}$: Arrhenius-type temperature correction coefficient for dark respiration rate constant of non-nitrogen fixing cyanobacteria (dimensionless)

$\lim_{k,G,NOFIX,CYN,DOXY}$: Limitation factor related to the lack of dissolved oxygen for

non-nitrogen fixing cyanobacteria growth (dimensionless)

Respiration rate of non-nitrogen fixing cyanobacteria due to metabolic activities is given in Equation A.1.2.11

$$R_{NOFIX,CYN,MET,RESP} = \left(1 - frac_{NOFIX,CYN,EXCR}\right) \cdot R_{NOFIX,CYN.MET,WASTE}$$

(Equation A.1.2.11)

The notation of Equation A.1.2.11 is given below:

$R_{NOFIX,CYN.MET,WASTE}$: Metabolic waste production rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{NOFIX,CYN,EXCR}$: Fraction of metabolic waste excreted as DOC by non-nitrogen fixing cyanobacteria (dimensionless)

Metabolic waste production rate of non-nitrogen fixing cyanobacteria is given in Equation A.1.2.12.

$$R_{NOFIX,CYN,MET,WASTE} = R_{NOFIX,CYN,GROWTH} \cdot \left(1 - eff_{NOFIX,CYN,GROWTH}\right)$$

(Equation A.1.2.12)

The notation of Equation A.1.2.12 is given below:

$R_{NOFIX,CYN,GROWTH}$: Growth rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-2} \cdot day^{-1}$)

$eff_{NOFIX,CYN,GROWTH}$: Efficiency of non-nitrogen fixing cyanobacteria growth (dimensionless)

A.1.2.3 Non-Nitrogen Fixing Cyanobacteria Excretion

The excretion rate of non-nitrogen fixing cyanobacteria is given in Equation A.1.2.13

$$R_{NOFIX,CYN,MET,RESP} = frac_{NOFIX,CYN,EXCR} \cdot R_{NOFIX,CYN.MET,WASTE}$$ (Equation A.1.2.13)

The notation of Equation A.1.2.13 is given below:

$R_{NOFIX,CYN.MET,WASTE}$: Metabolic waste production rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{NOFIX,CYN,EXCR}$: Fraction of metabolic waste excreted as DOC (dimensionless)

A.1.2.4 Non-Nitrogen Fixing Cyanobacteria Death

The death rate of non-nitrogen fixing cyanobacteria is given in Equation A.1.2.14

$$R_{NOFIX,CYN,DEATH} = k_{D,NOFIX,CYN,20} \cdot \theta_{k,D,NOFIX,CYN}^{(TEMP-20)} \cdot FAC_{HYPOX,NOFIX,CYN,D} \cdot [CYN - C]_{NOFIX}$$

(Equation A.1.2.14)

The notation of Equation A.1.2.14 is given below:

$R_{NOFIX,CYN.DEATH}$: Death rate of Non-nitrogen fixing cyanobacteria ($gC \cdot m^{-2} \cdot day^{-1}$)

$k_{D,NOFIX,CYN,20}$: Death rate constant of Non-nitrogen fixing cyanobacteria at 20˚C (day^{-1})

$\theta_{k,D,\mathrm{NOFIX,CYN,20}}$: Arrhenius-type temperature correction coefficient for death rate constant of Non-nitrogen fixing cyanobacteria (dimensionless)

$\mathrm{FAC_{HYPOX,NOFIX,CYN,D}}$: Acceleration factor of hypoxia on non-nitrogen fixing cyanobacteria death (dimensionless)

Calculation details of the acceleration factor of hypoxia on non-nitrogen fixing cyanobacteria death is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

A.1.3 Other Planktonic Algae

The main kinetic derivative for phytoplankton is given in Equation A.1.3.1

$$\frac{\mathrm{d[OPA-C]}}{\mathrm{dt}} = \underbrace{\mathrm{R_{OPA,GROWTH}}}_{\substack{Other\ planktonic\\ algae\ growth}} - \underbrace{\mathrm{R_{OPA,TOT,RESP}}}_{\substack{Other\ planktonic\ algae\\ total\ respiration}} - \underbrace{\mathrm{R_{OPA,EXCR}}}_{\substack{Other\ planktonic\\ algae\ excretion}} - \underbrace{\mathrm{R_{OPA,DEATH}}}_{\substack{Other\ planktonic\ algae\\ death\ not\ related\ to\\ zooplankton\ grazing}} - \underbrace{\mathrm{R_{ZOO,GRAZ,OPA}}}_{\substack{Zooplankton\ grazing\ on\\ Other\ planktonic\ algae}}$$

(Equation A.1.3.1)

where each of the process rates will be further described in the equations given in the following subsections except the zooplankton grazing rate on other planktonic algae, which will be discussed in Section A.2.

A.1.3.1 Other Planktonic Algae Growth

The growth rate of Other planktonic algae is given in Equation A.1.3.2

$$\mathrm{R_{OPA,GROWTH}} = \mathrm{k_{G,OPA,MAX}} \cdot \mathrm{lim_{k,G,OPA}} \cdot \mathrm{[OPA-C]}$$ (Equation A.1.3.2)

The notation of Equation A.1.3.2 is given below:

$\mathrm{R_{OPA,GROWTH}}$: Growth rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$\mathrm{k_{G,OPA,MAX}}$: Growth rate constant for other planktonic algae at optimum conditions (day^{-1})

$\mathrm{lim_{k,G,OPA}}$: Limitation factor for other planktonic algae growth (dimensionless)

Limitation factor for other planktonic algae growth is given in Equation A.1.3.3

$$\mathrm{lim_{k,G,OPA}} = \mathrm{lim_{k,G,OPA,TEMP}} \cdot \mathrm{lim_{k,G,OPA,LIGHT}} \cdot \min\left(\mathrm{lim_{k,G,OPA,DOXY}}, \mathrm{lim_{k,G,OPA,NUTR}}\right)$$

(Equation A.1.3.3)

The notation of Equation A.1.3.3 is given below:

$\mathrm{lim_{k,G,OPA,TEMP}}$: Temperature limitation factor for other planktonic algae growth (dimensionless)

$\mathrm{lim_{k,G,OPA,LIGHT}}$: Light limitation factor for other planktonic algae growth (dimensionless)

$\lim_{k,G,OPA,DOXY}$: Limitation factor related to the lack of dissolved oxygen for other planktonic algae growth (dimensionless)

$\lim_{k,G,OPA,NUTR}$: Nutrient limitation factor for other planktonic algae growth (dimensionless)

Calculation details of the temperature limitation factor for Other planktonic algae growth is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

The light limitation factor for other planktonic algae growth is given in Equation A.1.3.4

$$\lim_{k,G,OPA,LIGHT} = \frac{2.718 \cdot f_{DAY}}{k_E \cdot H} \cdot \left(\exp\left(-\frac{I_A}{I_{S,OPA}} \cdot \exp(-1 \cdot k_E \cdot H) \right) - \exp\left(-\frac{I_A}{I_{S,OPA}} \right) \right)$$

(Equation A.1.3.4)

The notation of Equation A.1.3.4 is given below:

H : Depth (m)
k_E : Light extinction coefficient (m^{-1}) (calculation details given in Section A.1.5)
f_{DAY} : Fraction of daylight in a particular day (dimensionless)
I_A : Available light at the water surface (langleys)
$I_{S,OPA}$: Light saturation constant for other planktonic algae (langleys)

Limitation factor related to the lack of dissolved oxygen for other planktonic algae growth is given in Equation A.1.3.5

$$\lim_{k,G,OPA,DOXY} = \frac{[O_2]}{k_{HS,O2,OPA} + [O_2]}$$

(Equation A.1.3.5)

The notation of Equation A.1.3.5 is given below:

$k_{HS,O2,OPA}$: Monod type half-saturation concentration of other planktonic algae growth for dissolved oxygen ($gO_2 \cdot m^{-3}$)

Nutrient limitation factor for other planktonic algae growth is given in Equation A.1.3.6 – A.1.3.8

$$\lim_{k,G,OPA,NUTR} = \min\left(\lim_{k,G,OPA,N}, \lim_{k,G,OPA,P}\right)$$

(Equation A.1.3.6)

$$\lim_{k,G,OPA,N} = \frac{[NH4-N] + [NO3-N]}{k_{HS,DIN,OPA} + [NH4-N] + [NO3-N]}$$

(Equation A.1.3.7)

$$\lim_{k,G,OPA,P} = \frac{[PO4-P]}{k_{HS,DIP,OPA} + [PO4-P]}$$

(Equation A.1.3.8)

The notation of Equation A.1.3.6 - A.1.3.8 is given below:

$k_{HS,DIN,OPA}$: Monod type half-saturation concentration of other planktonic algae

growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$k_{HS,DIP,OPA}$: Monod type half-saturation concentration of other planktonic algae growth for dissolved inorganic phosphorus ($gP \cdot m^{-3}$)

A.1.3.2 Other Planktonic Algae Total Respiration

The growth rate of Other planktonic algae is given in Equation A.1.3.9

$$R_{OPA,TOT,RESP} = R_{OPA,INT,RESP} + R_{OPA,MET,RESP} \quad \text{(Equation A.1.3.9)}$$

The notation of Equation A.1.3.9 is given below:

$R_{OPA,TOT,RESP}$: Total respiration rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,INT,RESP}$: Internal (dark) respiration rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,MET,RESP}$: Respiration rate of other planktonic algae due to metabolic activities ($gC \cdot m^{-3} \cdot day^{-1}$)

Internal (dark) respiration rate of other planktonic algae given in Equation A.1.3.10.

$$R_{OPA,INT,RESP} = k_{R,OPA,20} \cdot \theta_{k,R,OPA}^{(TEMP-20)} \cdot lim_{k,G,OPA,DOXY} \cdot [OPA - C] \quad \text{(Equation A.1.3.10)}$$

The notation of Equation A.1.3.10 is given below:

$k_{R,OPA,20}$: Internal respiration rate constant of non-nitrogen fixing cyanobacteria at 20˚C (day^{-1})

$\theta_{k,R,OPA,20}$: Arrhenius-type temperature correction coefficient for dark respiration rate constant of other planktonic algae (dimensionless)

$lim_{k,G,OPA,DOXY}$: Limitation factor related to the lack of dissolved oxygen for other planktonic algae growth (dimensionless)

Respiration rate of other planktonic algae due to metabolic activities is given in Equation A.1.3.11

$$R_{OPA,MET,RESP} = (1 - frac_{OPA,EXCR}) \cdot R_{OPA.MET,WASTE} \quad \text{(Equation A.1.3.11)}$$

The notation of Equation A.1.3.11 is given below:

$R_{OPA.MET,WASTE}$: Metabolic waste production rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{OPA,EXCR}$: Fraction of metabolic waste excreted as DOC (dimensionless)

Metabolic waste production rate of other planktonic algae is given in Equation A.1.3.12.

$$R_{OPA,MET,WASTE} = R_{OPA,GROWTH} \cdot \left(1 - eff_{OPA,GROWTH}\right)$$ (Equation A.1.3.12)

The notation of Equation A.1.3.12 is given below:

$R_{OPA,GROWTH}$: Growth rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$eff_{OPA,GROWTH}$: Efficiency of other planktonic algae growth (dimensionless)

A.1.3.3 Other Planktonic Algae Excretion

The excretion rate of other planktonic algae is given in Equation A.1.3.13

$$R_{OPA,MET,RESP} = frac_{OPA,EXCR} \cdot R_{OPA.MET,WASTE}$$ (Equation A.1.3.13)

The notation of Equation A.1.3.13 is given below:

$R_{OPA.MET,WASTE}$: Metabolic waste production rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{OPA,EXCR}$: Fraction of metabolic waste excreted as DOC by other planktonic algae (dimensionless)

A.1.3.4 Other Planktonic Algae Death

The death rate of other planktonic algae is given in Equation A.1.3.14

$$R_{OPA,DEATH} = k_{D,OPA,20} \cdot \theta_{k,D,OPA}^{(TEMP-20)} \cdot FAC_{HYPOX,OPA,D} \cdot [OPA - C]$$ (Equation A.1.3.14)

The notation of Equation A.1.3.14 is given below:

$R_{OPA.DEATH}$: Death rate of Other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{D,OPA,20}$: Death rate constant of other planktonic algae at 20˚C (day^{-1})

$\theta_{k,D,OPA,20}$: Arrhenius-type temperature correction coefficient for death rate constant of other planktonic algae (dimensionless)

$FAC_{HYPOX,OPA,D}$: Acceleration factor of hypoxia on other planktonic algae death (dimensionless)

Calculation details of the acceleration factor of hypoxia on other planktonic algae death is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

A.1.4 Nitrogen Fixing Cyanobacteria

The main kinetic derivative for phytoplankton is given in Equation A.1.4.1

$$\frac{d[CYN-C]_{FIX}}{dt} = \underbrace{R_{NON,FIX,CYN,GROWTH}}_{\substack{Nitrogen\ fixing \\ cyanobacteria\ growth}} - \underbrace{R_{FIX,CYN,TOT,RESP}}_{\substack{Nitrogen\ fixing\ cyanobacteria \\ total\ respiration}} - \underbrace{R_{FIX,CYN,EXCR}}_{\substack{Nitrogen\ fixing \\ cyanobacteria \\ excretion}} - \underbrace{R_{FIX,CYN,DEATH}}_{\substack{Nitrogen\ fixing\ cyanobacteria \\ death\ not\ related\ to \\ zooplankton\ grazing}} - \underbrace{R_{ZOO,GRAZ,FIX,CYN}}_{\substack{Zooplankton\ grazing\ on \\ nitrogen\ fixing\ cyanobacteria}}$$

(Equation A.1.4.1)

where each of the process rates will be further described in the equations given in the following subsections except the zooplankton grazing rate on nitrogen fixing cyanobacteria, which will be discussed in Section A.2.

A.1.4.1 Nitrogen Fixing Cyanobacteria Growth

The growth rate of nitrogen fixing cyanobacteria is given in Equation A.1.4.2. Growth rate of nitrogen fixing cyanobacteria is calculated as the sum of the growth in non-nitrogen fixing state (if enough useable nitrogen is present) and the nitrogen fixing state (if enough useable nitrogen is scarce).

$$R_{FIX,CYN,GROWTH} = R_{NON,FIX,CYN,GROWTH} + R_{FIX,FIX,CYN,GROWTH}$$ (Equation A.1.4.2)

The notation of Equation A.1.4.2 is given below:

$R_{FIX,CYN,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NON,FIX,CYN,GROWTH}$: Growth rate for nitrogen fixing cyanobacteria at non-nitrogen fixing state ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,FIX,CYN,GROWTH}$: Growth rate for nitrogen fixing cyanobacteria at nitrogen fixing state ($gC \cdot m^{-3} \cdot day^{-1}$)

Growth rate for nitrogen fixing cyanobacteria at non-nitrogen fixing state and the growth rate for nitrogen fixing cyanobacteria at nitrogen fixing state are given in Equation A.1.4.3 and Equation A.1.4.4.

$$R_{NON,FIX,CYN,GROWTH} = k_{G,FIX,CYN,MAX} \cdot lim_{k,G,NON,FIX,CYN} \cdot [CYN-C]_{FIX}$$ (Equation A.1.4.3)

$$R_{FIX,FIX,CYN,GROWTH} = k_{G,FIX,CYN,MAX} \cdot lim_{k,G,FIX,FIX,CYN} \cdot [CYN-C]_{FIX}$$ (Equation A.1.4.4)

The notation of Equation A.1.4.3 and Equation A.1.4.4 is given below:

$k_{G,NOFIX,CYN,MAX}$: Growth rate constant for nitrogen fixing cyanobacteria at optimum conditions (day^{-1})

$lim_{k,G,NON,FIX,CYN}$: Growth limitation factor for nitrogen fixing cyanobacteria at non-nitrogen fixing state (dimensionless)

$lim_{k,G,FIX,FIX,CYN}$: Growth limitation factor for nitrogen fixing cyanobacteria at

nitrogen fixing state (dimensionless)

Growth limitation factor for nitrogen fixing cyanobacteria at non-nitrogen fixing state and growth limitation factor for nitrogen fixing cyanobacteria at nitrogen fixing state are given in Equation A.1.4.5 and Equation A.1.4.6 respectively

$$\lim_{k,G,NON,FIX,CYN} = \lim_{k,G,FIX,CYN,TEMP} \cdot \lim_{k,G,FIX,CYN,LIGHT} \cdot \min\left(\lim_{k,G,FIX,CYN,DOXY}, \lim_{k,G,NON,FIX,CYN,NUTR}\right) \quad \text{(Equation A.1.4.5)}$$

$$\lim_{k,G,FIX,FIX,CYN} = \lim_{k,G,FIX,CYN,TEMP} \cdot \lim_{k,G,FIX,CYN,LIGHT} \cdot \min\left(\lim_{k,G,FIX,CYN,DOXY}, \lim_{k,G,FIX,FIX,CYN,NUTR}\right) \quad \text{(Equation A.1.4.6)}$$

The notation of Equation A.1.4.5 and Equation A.1.4.6 is given below:

$\lim_{k,G,FIX,CYN,TEMP}$: Temperature limitation factor for nitrogen fixing cyanobacteria growth (dimensionless)

$\lim_{k,G,FIX,CYN,LIGHT}$: Light limitation factor for nitrogen fixing cyanobacteria growth (dimensionless)

$\lim_{k,G,FIX,CYN,DOXY}$: Limitation factor related to the lack of dissolved oxygen for nitrogen fixing cyanobacteria growth (dimensionless)

$\lim_{k,G,NON,FIX,CYN,NUTR}$: Nutrient limitation factor for nitrogen fixing cyanobacteria growth at non nitrogen fixing state (dimensionless)

$\lim_{k,G,FIX,FIX,CYN,NUTR}$: Nutrient limitation factor for nitrogen fixing cyanobacteria growth at nitrogen fixing state (dimensionless)

Calculation details of the temperature limitation factor for nitrogen fixing cyanobacteria growth is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

The light limitation factor for nitrogen fixing cyanobacteria growth is given in Equation A.1.4.7

$$\lim_{k,G,FIX,CYN,LIGHT} = \frac{2.718 \cdot f_{DAY}}{k_E \cdot H} \cdot \left(\exp\left(-\frac{I_A}{I_{S,FIX,CYN}} \cdot \exp(-1 \cdot k_E \cdot H) \right) - \exp\left(-\frac{I_A}{I_{S,FIX,CYN}} \right) \right) \quad \text{(Equation A.1.4.7)}$$

The notation of Equation A.1.4.7 is given below:

H : Depth (m)

k_E : Light extinction coefficient (m^{-1})
(calculation details given in Section A.1.5)

f_{DAY} : Fraction of daylight in a particular day (dimensionless)

I_A : Available light at the water surface (langleys)

$I_{S;\,FIX,CYN}$: Light saturation constant for nitrogen fixing cyanobacteria (langleys)

Limitation factor related to the lack of dissolved oxygen for nitrogen fixing cyanobacteria growth is given in Equation A.1.4.8

$$\lim_{k,G,FIX,CYN,DOXY} = \frac{[O_2]}{k_{HS,O2,FIX,CYN} + [O_2]}$$

(Equation A.1.4.8)

The notation of Equation A.1.4.8 is given below:

$k_{HS,O2,FIX,CYN}$: Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved oxygen ($gO_2 \cdot m^{-3}$)

Nutrient limitation factor for nitrogen fixing cyanobacteria growth is given in Equation A.1.4.9 – A.1.4.12

$\lim_{k,G,NON,FIX,CYN,NUTR} = \min(\lim_{k,G,NON,FIX,CYN,N}, \lim_{k,G,FIX,CYN,P})$ (Equation A.1.4.9)

$\lim_{k,G,FIX,FIX,CYN,NUTR} = \min(\lim_{k,G,FIX,FIX,CYN,N}, \lim_{k,G,FIX,CYN,P})$ (Equation A.1.4.10)

$$\lim_{k,G,NON,FIX,CYN,N} = \frac{[NH4-N] + ([DON] \cdot f_{avail,DON}) + [NO3-N]}{k_{HS,DIN,FIX,CYN} + [NH4-N] + ([DON] \cdot f_{avail,DON}) + [NO3-N]}$$

(Equation A.1.4.11)

$$\lim_{k,G,FIX,FIX,CYN,N} = \frac{k_{HS,NFIX}}{k_{HS,NFIX} + [NH4-N] + ([DON] \cdot f_{avail,DON}) + [NO3-N]}$$

(Equation A.1.4.12)

$$\lim_{k,G,NOFIX,CYN,P} = \frac{[PO4-P]}{k_{HS,DIP,FIX,CYN} + [PO4-P]}$$

(Equation A.1.4.13)

The notation of Equation A.1.4.9 - A.1.4.13 is given below:

$k_{HS,DIN,FIX,CYN}$: Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$f_{avail,DON}$: Fraction of DON available to nitrogen fixing cyanobacteria as nitrogen source for growth

$k_{HS,NFIX}$: Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved inorganic nitrogen to continuously switch off the nitrogen fixation process ($gN \cdot m^{-3}$). This constant is used in a reversed way compared to standard Monod model. In this approach, increase of available nitrogen concentration for uptake will diminish nitrogen fixation.

$k_{HS,DIP,FIX,CYN}$: Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved inorganic phosphorus ($gP \cdot m^{-3}$)

A.1.4.2 Nitrogen Fixing Cyanobacteria Total Respiration

The growth rate of nitrogen fixing cyanobacteria is given in Equation A.1.4.14

$$R_{FIX,CYN,TOT,RESP} = R_{FIX,CYN,INT,RESP} + R_{FIX,CYN,MET,RESP}$$

(Equation A.1.4.14)

The notation of Equation A.1.4.14 is given below:

$R_{FIX,CYN,TOT,RESP}$: Total respiration rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,INT,RESP}$: Internal (dark) respiration rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,MET,RESP}$: Respiration rate of nitrogen fixing cyanobacteria due to metabolic activities ($gC \cdot m^{-3} \cdot day^{-1}$)

Internal (dark) respiration rate of nitrogen fixing cyanobacteria given in Equation A.1.4.15.

$$R_{FIX,CYN,INT,RESP} = k_{R,FIX,CYN,20} \cdot \theta_{k,R,FIX,CYN}^{(TEMP-20)} \cdot lim_{k,G,FIX,CYN,DOXY} \cdot [CYN - C]_{FIX}$$

(Equation A.1.4.15)

The notation of Equation A.1.4.15 is given below:

$k_{R,FIX,CYN,20}$: Internal respiration rate constant of nitrogen fixing cyanobacteria at 20˚C (day^{-1})

$\theta_{k,R,FIX,CYN,20}$: Arrhenius-type temperature correction coefficient for dark respiration rate constant of nitrogen fixing cyanobacteria (dimensionless)

$lim_{k,G,FIX,CYN,DOXY}$: Limitation factor related to the lack of dissolved oxygen for nitrogen fixing cyanobacteria growth (dimensionless)

Respiration rate of nitrogen fixing cyanobacteria due to metabolic activities is given in Equation A.1.4.16

$$R_{FIX,CYN,MET,RESP} = (1 - frac_{FIX,CYN,EXCR}) \cdot R_{FIX,CYN.MET,WASTE}$$

(Equation A.1.4.16)

The notation of Equation A.1.4.16 is given below:

$R_{FIX,CYN.MET,WASTE}$: Metabolic waste production rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{FIX,CYN,EXCR}$: Fraction of metabolic waste excreted as DOC by nitrogen fixing cyanobacteria (dimensionless)

Metabolic waste production rate of nitrogen fixing cyanobacteria is given in Equation A.1.4.17.

$$R_{FIX,CYN,MET,WASTE} = R_{FIX,CYN,GROWTH} \cdot \left(1 - eff_{FIX,CYN,GROWTH}\right) \quad \text{(Equation A.1.4.17)}$$

The notation of Equation A.1.4.17 is given below:

$R_{NOFIX,CYN,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$eff_{NOFIX,CYN,GROWTH}$: Efficiency of nitrogen fixing cyanobacteria growth (dimensionless)

A.1.4.3 Nitrogen Fixing Cyanobacteria Excretion

The excretion rate of nitrogen fixing cyanobacteria is given in Equation A.1.4.18

$$R_{NOFIX,CYN,MET,RESP} = frac_{NOFIX,CYN,EXCR} \cdot R_{NOFIX,CYN.MET,WASTE} \quad \text{(Equation A.1.4.18)}$$

The notation of Equation A.1.4.18 is given below:

$R_{FIX,CYN.MET,WASTE}$: Metabolic waste production rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{FIX,CYN,EXCR}$: Fraction of metabolic waste excreted as DOC (dimensionless)

A.1.4.4 Nitrogen Fixing Cyanobacteria Death

The death rate of nitrogen fixing cyanobacteria is given in Equation A.1.4.19

$$R_{NOFIX,CYN,DEATH} = k_{D,NOFIX,CYN,20} \cdot \theta_{k,D,NOFIX,CYN}^{(TEMP-20)} \cdot FAC_{HYPOX,NOFIX,CYN,D} \cdot [CYN - C]_{NOFIX} \quad \text{(Equation A.1.4.19)}$$

The notation of Equation A.1.4.19 is given below:

$R_{NOFIX,CYN.DEATH}$: Death rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{D,NOFIX,CYN,20}$: Death rate constant of nitrogen fixing cyanobacteria at 20˚C (day^{-1})

$\theta_{k,D,NOFIX,CYN,20}$: Arrhenius-type temperature correction coefficient for death rate constant of nitrogen fixing cyanobacteria (dimensionless)

$FAC_{HYPOX,NOFIX,CYN,D}$: Acceleration factor of hypoxia on nitrogen fixing cyanobacteria death (dimensionless)

Calculation details of the acceleration factor of hypoxia on nitrogen fixing cyanobacteria death is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

A.1.5 Light Extinction

The light extinction coefficient is given in Equation A.1.5.1

$$k_E = k_{B,E} + (8.8 \cdot 10^{-3} \cdot CHLA) + \left(5.4 \cdot 10^{-2} \cdot CHLA^{2/3}\right) \quad \text{(Equation A.1.5.1)}$$

The notation of Equation A.1.5.1 is given below:

k_E : Light extinction coefficient (m^{-1})

$k_{B,E}$: Background light extinction coefficient (m^{-1})

$CHLA$: Chlorophyll-A ($mg \cdot m^{-3}$)

Chlorophyll-A is given in Equation A.1.5.2

$$CHLA = \left(\frac{[DIA - C]}{C{:}\,CHLA_{DIA}} + \frac{[CYN - C]_{NOFIX}}{C{:}\,CHLA_{NOFIX,CYN}} + \frac{[OPA - C]}{C{:}\,CHLA_{OPA}} + \frac{[CYN - C]_{FIX}}{C{:}\,CHLA_{FIX,CYN}}\right) \cdot 1000 \quad \text{(Equation A.1.5.2)}$$

$C{:}\,CHLA_{DIA}$: Carbon to Chlorophyll-A value for diatoms

$C{:}\,CHLA_{NOFIX,CYN}$: Carbon to Chlorophyll-A value non-nitrogen fixing cyanobacteria

$C{:}\,CHLA_{OPA}$: Carbon to Chlorophyll-A value for other planktonic algae

$C{:}\,CHLA_{FIX,CYN}$: Carbon to Chlorophyll-A value for nitrogen fixing cyanobacteria

A.2 ZOOPLANKON KINETICS

Zooplankton is handled using three state variables; namely zooplankton carbon, zooplankton nitrogen and zooplankton phosphorus. This is necessary, because zooplankton is assumed to use five different food sources (four phytoplankton and detrital particulate matter) each with potentially different carbon to nutrients stoichiometry.

The main kinetic derivatives for zooplankton is given in Equation A.2.1 – A.2.3.

$$\frac{d[ZOOP-C]}{dt} = \underbrace{R_{ZOOP,GROWTH}}_{Zooplankton\ growth} - \underbrace{R_{ZOOP,TOT,RESP}}_{Zooplankton\ total\ respiration} - \underbrace{R_{ZOOP,EXCR}}_{Zooplankton\ excretion} - \underbrace{R_{ZOOP,DEATH}}_{Zooplankton\ death}$$

(Equation A.2.1)

$$\begin{aligned}\frac{d[ZOOP-N]}{dt} = {} & \underbrace{\left(R_{ZOOP,GRAZ,DIA}\cdot N{:}\,C_{DIA}\right)}_{Gain\ of\ zooplankton\ nitrogen\ by\ grazing\ on\ diatoms} + \underbrace{\left(R_{ZOOP,GRAZ,NON,FIX,CYN}\cdot N{:}\,C_{NON,FIX,CYN}\right)}_{Gain\ of\ zooplankton\ nitrogen\ by\ grazing\ on\ non-nitrogen\ fixing\ cyanobacteria} \\ & + \underbrace{\left(R_{ZOOP,GRAZ,FIX,CYN}\cdot N{:}\,C_{FIX,CYN}\right)}_{Gain\ of\ zooplankton\ nitrogen\ by\ grazing\ on\ nitrogen\ fixing\ cyanobacteria} + \underbrace{\left(R_{ZOOP,GRAZ,OPA}\cdot N{:}\,C_{OPA}\right)}_{Gain\ of\ zooplankton\ nitrogen\ by\ grazing\ on\ other\ planktonic\ algae} \\ & + \underbrace{\left(R_{ZOOP,GRAZ,POC}\cdot N{:}\,C_{POC}\right)}_{Gain\ of\ zooplankton\ nitrogen\ by\ grazing\ on\ detritus} - \underbrace{\left(R_{ZOOP,EXCR}\cdot N{:}\,C_{ZOOP}\right)}_{Conversion\ of\ zooplankton\ nitrogen\ to\ dissolved\ organic\ nitrogen\ by\ excretion} \\ & - \underbrace{\left(R_{ZOOP,TOT,RESP}\cdot N{:}\,C_{ZOOP}\right)}_{Conversion\ of\ zooplankton\ nitrogen\ to\ ammonia\ nitrogen\ by\ respiration} - \underbrace{\left(R_{ZOOP,DEATH}\cdot N{:}\,C_{ZOOP}\right)}_{Conversion\ of\ zooplankton\ nitrogen\ to\ particulate\ organic\ nitrogen\ by\ death}\end{aligned}$$

(Equation A.2.2)

$$\begin{aligned}\frac{d[ZOOP-P]}{dt} = {} & \underbrace{\left(R_{ZOOP,GRAZ,DIA}\cdot P{:}\,C_{DIA}\right)}_{\substack{Gain\ of\ zooplankton\\ phosphorus\ by\\ grazing\ on\ diatoms}} + \underbrace{\left(R_{ZOOP,GRAZ,NON,FIX,CYN}\cdot P{:}\,C_{NON,FIX,CYN}\right)}_{Gain\ of\ zooplankton\ phosphorus\ by\ grazing\ on\ non-nitrogen\ fixing\ cyanobacteria} \\ & + \underbrace{\left(R_{ZOOP,GRAZ,FIX,CYN}\cdot P{:}\,C_{FIX,CYN}\right)}_{Gain\ of\ zooplankton\ phosphorus\ by\ grazing\ on\ nitrogen\ fixing\ cyanobacteria} + \underbrace{\left(R_{ZOOP,GRAZ,OPA}\cdot P{:}\,C_{OPA}\right)}_{Gain\ of\ zooplankton\ phosphorus\ by\ grazing\ on\ other\ planktonic\ algae} \\ & + \underbrace{\left(R_{ZOOP,GRAZ,POC}\cdot P{:}\,C_{POC}\right)}_{Gain\ of\ zooplankton\ phosphorus\ by\ grazing\ on\ detritus} - \underbrace{\left(R_{ZOOP,EXCR}\cdot P{:}\,C_{ZOOP}\right)}_{Conversion\ of\ zooplankton\ phosphorus\ to\ dissolved\ organic\ phosphorus\ by\ excretion} \\ & - \underbrace{\left(R_{ZOOP,TOT,RESP}\cdot P{:}\,C_{ZOOP}\right)}_{\substack{Conversion\ of\ zooplankton\\ phosphorus\ to\\ phospate\ phosphorus\ by\ respiration}} - \underbrace{\left(R_{ZOOP,DEATH}\cdot P{:}\,C_{ZOOP}\right)}_{\substack{Conversion\ of\ zooplankton\\ phosphorus\ to\\ particulate\ organic\ phosphorus\ by\ death}}\end{aligned}$$

(Equation A.2.3)

The notation of Equation A.2.1 – A.2.3 is given below:

$N: C_{DIA}$: Nitrogen to carbon ratio for diatoms (dimensionless)

$P: C_{DIA}$: Phosphorus to carbon ratio for diatoms (dimensionless)

$N: C_{NOFIX,CYN}$: Nitrogen to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$P: C_{NOFIX,CYN}$: Phosphorus to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$N: C_{OPA}$: Nitrogen to carbon ratio for other planktonic algae (dimensionless)

$P: C_{OPA}$: Phosphorus to carbon ratio for other planktonic algae (dimensionless)

$N: C_{FIX,CYN}$: Nitrogen to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$P: C_{FIX,CYN}$: Phosphorus to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$N: C_{ZOOP}$: Nitrogen to carbon ratio for zooplankton (dimensionless)

$P: C_{ZOOP}$: Phosphorus to carbon ratio for zooplankton (dimensionless)

$N: C_{POC}$: Nitrogen to carbon ratio for detrital particulate organic matter (dimensionless)

$P: C_{POC}$: Phosphorus to carbon ratio for detrital particulate organic matter (dimensionless)

$N: C_{DIA}$, $P: C_{DIA}$, $N: C_{NOFIX,CYN}$, $P: C_{NOFIX,CYN}$, $N: C_{OPA}$, $P: C_{OPA}$, $N: C_{FIX,CYN}$, $P: C_{FIX,CYN}$ are user entered stoichiometric model constants, whereas $N: C_{ZOOP}$, $P: C_{ZOOP}$, $N: C_{POC}$, $P: C_{POC}$ are calculated internally by AQUABC given in Equation A.2.4 - Equation A.2.7.

$$N: C_{ZOOP} = \frac{[ZOOP - N]}{[ZOOP - C]}$$

(Equation A.2.4)

$$P: C_{ZOOP} = \frac{[ZOOP - P]}{[ZOOP - C]}$$

(Equation A.2.5)

$$N: C_{POC} = \frac{[PON]_{DET}}{[POC]_{DET}}$$

(Equation A.2.6)

$$P: C_{POC} = \frac{[POP]_{DET}}{[POC]_{DET}}$$

(Equation A.2.7)

A.2.1 Zooplankton Growth Rate

The main kinetic derivative for phytoplankton is given in Equation A.2.8.

$$R_{ZOO,GROWTH} = R_{ZOO,FEEDING,DIA} + R_{ZOO,FEEDING,NOFIX,CYN} + R_{ZOO,FEEDINGFIX,CYN} + R_{ZOO,FEEDING,OPA} + R_{ZOO,FEEDING,DET,PART}$$

(Equation A.2.8)

The notation of Equation A.2.8 is given below:

$R_{ZOO,GROWTH}$: Total growth rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,FEEDING,DIA}$: Feeding rate of zooplankton on diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,FEEDING,NOFIX,CYN}$: Feeding rate of zooplankton on non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,FEEDING,OPA}$: Feeding rate of zooplankton on nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,FEEDING,FIX,CYN}$: Feeding rate of zooplankton on other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,FEEDING,DET,PART}$: Feeding rate of zooplankton on particulate detritus ($gC \cdot m^{-3} \cdot day^{-1}$)

The feeding rates of zooplankton on different food-sources are given in Equations A.2.9 – A.2.13.

$$R_{ZOO,FEEDING,DIA} = k_{G,ZOO,MAX} \cdot lim_{k,G,ZOO,TEMP} \cdot lim_{k,G,ZOO,DOXY} \cdot mult_{k,G,ZOO,DIA} \cdot FF_{ZOO,DIA} \cdot [ZOOP - C]$$

(Equation A.2.9)

$$R_{ZOO,FEEDING,NOFIX,CYN} = k_{G,ZOO,MAX} \cdot lim_{k,G,ZOO,TEMP} \cdot lim_{k,G,ZOO,DOXY} \cdot mult_{k,G,ZOO,NOFIX,CYN} \cdot FF_{ZOO,NOFIX,CYN} \cdot [ZOOP - C]$$

(Equation A.2.10)

$$R_{ZOO,FEEDING,OPA} = k_{G,ZOO,MAX} \cdot lim_{k,G,ZOO,TEMP} \cdot lim_{k,G,ZOO,DOXY} \cdot mult_{k,G,ZOO,OPA} \cdot FF_{ZOO,OPA} \cdot [ZOOP - C]$$

(Equation A.2.11)

$$R_{ZOO,FEEDING,FIX,CYN} = k_{G,ZOO,MAX} \cdot lim_{k,G,ZOO,TEMP} \cdot lim_{k,G,ZOO,DOXY} \cdot mult_{k,G,ZOO,FIX,CYN} \cdot FF_{ZOO,FIX,CYN} \cdot [ZOOP - C]$$

(Equation A.2.12)

$$R_{ZOO,FEEDING,DET,PART} = k_{G,ZOO,MAX} \cdot lim_{k,G,ZOO,TEMP} \cdot lim_{k,G,ZOO,DOXY} \cdot mult_{k,G,ZOO,DET,PART} \cdot FF_{ZOO,DET,PART} \cdot [ZOOP - C]$$

(Equation A.2.13)

The notation of Equations A.2.9 – A.2.13. is given below:

$k_{G,ZOO,MAX}$: Growth rate constant zooplankton at optimum conditions (day^{-1})

$lim_{k,G,ZOO,TEMP}$: Temperature limitation factor for zooplankton growth (dimensionless)

$lim_{k,G,ZOO,DOXY}$: Limitation factor related to the lack of dissolved oxygen for zooplankton growth (dimensionless)

$mult_{k,G,ZOO,DIA}$: Zooplankton growth rate constant multiplier for diatoms as food source (dimensionless)

$FF_{ZOO,DIA}$: Food factor of diatoms for zooplankton grazing (dimensionless)

$mult_{k,G,ZOO,NOFIX,CYN}$: Zooplankton growth rate constant multiplier for non-nitrogen fixing cyanobacteria as food source (dimensionless)

$FF_{ZOO,NOFIX,CYN}$: Food factor of non-nitrogen fixing cyanobacteria for zooplankton grazing

$mult_{k,G,ZOO,OPA}$: Zooplankton growth rate constant multiplier for other planktonic algae as food source (dimensionless)

$FF_{ZOO,OPA}$: Food factor of other planktonic algae for zooplankton grazing (dimensionless)

$mult_{k,G,ZOO,FIX,CYN}$: Zooplankton growth rate constant multiplier for nitrogen fixing cyanobacteria as food source (dimensionless)

$FF_{ZOO,FIX,CYN}$: Food factor of nitrogen fixing cyanobacteria for zooplankton grazing (dimensionless)

$mult_{k,G,ZOO,DET,PART}$: Zooplankton growth rate constant multiplier for particulate detritus as food source (dimensionless)

$FF_{ZOO,DET,PART}$: Food factor of for particulate detritus for zooplankton grazing (dimensionless)

Calculation details of the temperature limitation factor for nitrogen fixing cyanobacteria growth is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

Limitation factor related to the lack of dissolved oxygen for zooplankton growth is given in Equation A.2.1.14.

$$lim_{k,G,ZOO,DOXY} = \frac{[O_2]}{k_{HS,O2,ZOO} + [O_2]}$$

(Equation A.2.1.14)

The notation of Equation A.2.1.14 is given below:

$k_{HS,O2,ZOO}$: Monod type half-saturation concentration of zooplankton growth for dissolved oxygen ($gO_2 \cdot m^{-3}$)

$mult_{k,G,ZOO,DIA}$, $mult_{k,G,ZOO,NOFIX,CYN}$, $mult_{k,G,ZOO,OPA}$, $mult_{k,G,ZOO,FIX,CYN}$ and $mult_{k,G,ZOO,DET,PART}$ are user entered model constants (with values between 0 and 1), whereas $FF_{ZOO,DIA}$, $FF_{ZOO,NOFIX,CYN}$, $FF_{ZOO,OPA}$, $FF_{ZOO,FIX,CYN}$, and $FF_{ZOO,DET,PART}$ are calculated internally by AQUABC given in Equations A.2.15 – A.2.19.

$$FF_{ZOO,DIA} = \frac{PREF_{ZOO,DIA} \cdot \left([DIA - C] - FOOD_{MIN,ZOO}\right)}{[DIA - C] + k_{HS,DIA,ZOO}}$$

(Equation A.2.15)

$$FF_{ZOO,NOFIX,CYN} = \frac{PREF_{ZOO,NOFIX,CYN} \cdot \left([CYN - C]_{NOFIX} - FOOD_{MIN,ZOO}\right)}{[CYN - C]_{NOFIX} + k_{HS,NOFIX,CYN,ZOO}}$$

(Equation A.2.16)

$$FF_{ZOO,OPA} = \frac{PREF_{ZOO,OPA} \cdot \left([OPA - C] - FOOD_{MIN,ZOO}\right)}{[OPA - C] + k_{HS,OPA,ZOO}}$$

(Equation A.2.17)

$$FF_{ZOO,FIX,CYN} = \frac{PREF_{ZOO,FIX,CYN} \cdot \left([CYN - C]_{FIX} - FOOD_{MIN,ZOO}\right)}{[CYN - C]_{FIX} + k_{HS,FIX,CYN,ZOO}}$$

(Equation A.2.18)

$$FF_{ZOO,DET,PART} = \frac{PREF_{ZOO,DET,PART} \cdot \left([POC]_{DET} - FOOD_{MIN,ZOO}\right)}{[POC]_{DET} + k_{HS,DET,PART,ZOO}}$$

(Equation A.2.19)

The notation of Equations A.2.15 – A.2.19 is given below:

$FOOD_{MIN,ZOO}$: Minimum detectable concentration of any food source by zooplankton ($gC \cdot m^{-3}$)

$PREF_{ZOO,DIA}$: Preference of zooplankton on diatoms as a food source (dimensionless)

$k_{HS,DIA,ZOO}$: Monod type half-saturation concentration of zooplankton to calculate the diatoms food factor ($gC \cdot m^{-3}$)

$PREF_{ZOO,NOFIX,CYN}$: Preference of zooplankton on non-nitrogen fixing cyanobacteria as a food source (dimensionless)

$k_{HS,NOFIX,CYN,ZOO}$: Monod type half-saturation concentration of zooplankton to calculate the non-nitrogen fixing cyanobacteria food factor ($gC \cdot m^{-3}$)

$PREF_{ZOO,OPA}$: Preference of zooplankton on other planktonic algae as a food source (dimensionless)

$k_{HS,OPA,ZOO}$: Monod type half-saturation concentration of zooplankton to calculate the other planktonic algae food factor ($gC \cdot m^{-3}$)

$PREF_{ZOO,FIX,CYN}$: Preference of zooplankton on nitrogen fixing cyanobacteria as a food source (dimensionless)

$k_{HS,FIX,CYN,ZOO}$: Monod type half-saturation concentration of zooplankton to calculate the nitrogen fixing cyanobacteria food factor ($gC \cdot m^{-3}$)

$PREF_{ZOO,DET,PART}$: Preference of zooplankton on particulate detritus as a food

source (dimensionless)

$k_{HS,DET,PART,ZOO}$: Monod type half-saturation concentration of zooplankton to calculate the particulate detritus food factor ($gC \cdot m^{-3}$)

A.2.2 Zooplankton Respiration Rate

The respiration rate of zooplankton is given in Equation A.2.20

$$R_{ZOO,TOT,RESP} = R_{ZOO,INT,RESP} + R_{ZOO,MET,RESP} \quad \text{(Equation A.2.20)}$$

The notation of Equation A.2.20 is given below:

$R_{ZOO,TOT,RESP}$: Total respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)
$R_{ZOO,INT,RESP}$: Internal respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)
$R_{ZOO,MET,RESP}$: Respiration rate of zooplankton due to metabolic activities ($gC \cdot m^{-3} \cdot day^{-1}$)

Internal respiration rate of nitrogen fixing cyanobacteria given in Equation A.2.21.

$$R_{ZOO,INT,RESP} = k_{R,ZOO,20} \cdot \theta_{k,R,ZOO}^{(TEMP-20)} \cdot [ZOO - C] \quad \text{(Equation A.2.21)}$$

The notation of Equation A.2.21 is given below:

$k_{R,ZOO,20}$: Internal respiration rate constant of zooplankton at 20˚C (day^{-1})

$\theta_{k,R,ZOO}$: Arrhenius-type temperature correction coefficient for internal respiration rate constant of zooplankton (dimensionless)

Respiration rate of nitrogen fixing cyanobacteria due to metabolic activities is given in Equation A.2.22.

$$R_{ZOO,MET,RESP} = (1 - frac_{ZOO,EXCR}) \cdot R_{ZOO,MET,WASTE} \quad \text{(Equation A.2.22)}$$

The notation of Equation A.2.22 is given below:

$R_{ZOO.MET,WASTE}$: Metabolic waste production rate zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$frac_{ZOO,EXCR}$: Fraction of metabolic waste excreted as DOC zooplankton (dimensionless)

Metabolic waste production rate of nitrogen fixing cyanobacteria is given in Equation A.2.23.

$$R_{ZOO,MET,WASTE} = R_{ZOO,GROWTH} \cdot (1 - eff_{ZOO,GROWTH}) \quad \text{(Equation A.2.23)}$$

The notation of Equation A.2.23 is given below:

$R_{ZOO,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)
$eff_{ZOO,GROWTH}$: Efficiency of nitrogen fixing cyanobacteria growth (dimensionless)

A.2.3 Zooplankton Excretion Rate

The excretion rate of zooplankton is given in Equation A2.24

$$R_{ZOO,MET,RESP} = frac_{ZOO,EXCR} \cdot R_{ZOO,MET,WASTE} \quad \text{(Equation A.2.24)}$$

The notation of Equation A.2.24 is given below:

$R_{ZOO,MET,WASTE}$: Metabolic waste production rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)
$frac_{ZOO,EXCR}$: Fraction of metabolic waste excreted as DOC (dimensionless)

A.2.4 Zooplankton Death Rate

The death rate of nitrogen fixing cyanobacteria is given in Equation A.2.25

$$R_{ZOO,DEATH} = k_{D,ZOO,20} \cdot \theta_{k,D,ZOO}^{(TEMP-20)} \cdot FAC_{HYPOX,ZOO,D} \cdot [ZOO - C] \quad \text{(Equation A.2.25)}$$

The notation of Equation A.2.25 is given below:

$R_{ZOO.DEATH}$: Death rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$k_{D,ZOO,20}$: Death rate constant of zooplankton 20˚C (day^{-1})

$\theta_{k,D,ZOO,20}$: Arrhenius-type temperature correction coefficient for death rate constant of zooplankton (dimensionless)

$FAC_{HYPOX,ZOO,D}$: Acceleration factor of hypoxia on zooplankton death (dimensionless)

Calculation details of the acceleration factor of hypoxia on zooplankton death is given in Section A.3 where all the common calculation procedures corresponding to all phytoplankton and the zooplankton.

A.3 COMMON SUB-MODELS FOR PLANKTON

This section is devoted to common sub-models that are used by AQUABC in kinetic equations of phytoplankton or zooplankton state variables. For the following sections, an index notation is used for different plankton as descrşbed below:

i : Index for plankton (i = DIA, NOFIX, CYN, OPA, CYN FIX and ZOO)

DIA	: Diatoms
NOFIX, CYN	: Non-nitrogen fixing cyanobacteria
OPA	: Other planktonic algae
FIX, CYN	: Fixing cyanobacteria
ZOO	: Zooplankton

A.3.1 Effect of Temperature on Plankton Growth

The effect of the water temperature on the growth rate is considered as a multiplier between 0 and 1. For each plankton in AQUABC and optimum range of temperature between a lower and upper temperature is defined, where it is assumed that the relevant plankton group is under optimum conditions in terms of temperature (so limitation factor 1 as multiplier). Otherwise, two different exponential functions (one for the temperatures below the lower optimum temperature and one for the temperatures above the upper optimum temperature).

Temperature limitation on plankton is given in Equation A.3.1.

$$lim_{i,TEMP} = \begin{cases} \text{if } \left(TEMP < TEMP_{LOWER,OPT,i}\right) \\ \quad \exp\left(-\kappa_{LOWER,i} \cdot \left|TEMP_{LOWER,OPT,i} - TEMP\right|\right) \\ \text{if } \left(TEMP_{LOWER,OPT,i} \le TEMP \le TEMP_{UPPER,OPT,i}\right) \\ \quad 1 \\ \text{if } \left(TEMP > TEMP_{UPPER,OPT,i}\right) \\ \quad \exp\left(-\kappa_{UPPER,i} \cdot \left|TEMP_{UPPER,OPT,i} - TEMP\right|\right) \end{cases} \quad \text{(Equation A.3.1)}$$

The notation of Equation A.3.1 is given below:

$TEMP_{LOWER,OPT,i}$: Lower limit of the optimum temperature for the growth of the plankton group i (°C)

$TEMP_{UPPER,OPT,i}$: Upper limit of the optimum temperature for the growth of the plankton group i (°C)

$\kappa_{LOWER,i}$: Exponent for the temperatures below the lower limit of the optimum temperature for the growth of the plankton group i (dimensionless).

$\kappa_{UPPER,i}$: Exponent for the temperatures above the upper limit of the optimum temperature for the growth of the plankton group i (dimensionless).

A.3.2 Effect of Hypoxia on Plankton Death

AQUABC considers all the plankton as aerobic organisms. Therefore, lack all dissolved oxygen causes stress and is assumed to increase the death rate constant, where $FAC_{HYPOX,i,DEATH}$ is the multiplication factor that increases the death rate constant. There are three stages related to dissolved oxygen levels:

- Stage 1: No hypoxia stress, death rate constant is not increased.
- Stage 2: Hypoxia stress, death rate constant is increased.
- Stage 3: Extreme hypoxia stress, half of the plankton biomass is assumed to die at each time step

These stages are given in Equation A.3.2

$$FAC_{HYPOX,i,DEATH} = \begin{cases} \text{Stage 1:} & 1 & , \quad [O_2] > [O_2]_{HYPOX\ STRESS,i} \\ \text{Stage 2:} & coeff_{HPOX,\ DEATH,\ i} \cdot \theta_{HPOX,\ DEATH,\ i}^{([O_2]_{HYPOXSTRESS,i} - [O_2])} & , \quad 0.1 < [O_2] < [O_2]_{HYPOX\ STRESS,i} \\ \text{Stage 3:} & \dfrac{0.5}{\Delta t \cdot k_{D,20,\ i} \cdot \theta_{KD,\ i}^{\ TEMP-20}} & , \quad [O_2] < 0.1 \end{cases}$$

(Equation A.3.2)

The notation of Equation A.3.2 is given below:

$[O_2]_{HYPOX\ STRESS,i}$: Threshold concentration of dissolved oxygen for hypoxia stress for plankton i ($gO_2 \cdot m^{-3}$)

$coeff_{HPOX,\ DEATH,\ i}$: Multiplier for $FAC_{HYPOX,i,DEATH}$

$\theta_{HPOX,\ DEATH,\ i}$: Exponent for $FAC_{HYPOX,i,DEATH}$

$k_{D,20,i}$: Death rate constant of plankton i (day^{-1})

$\theta_{KD,\ i}$: Arrhenius type temperature correction factor the death rate constant of plankton i

A.4 DETRITAL PARTICULATE ORGANIC MATTER KINETICS

Detrital particulate organic matter is handled using three state variables; namely detrital particulate organic carbon, detrital particulate organic nitrogen and detrital particulate organic phosphorus. The main kinetic derivatives for detrital particulate organic matter is given in Equations A.4.1 – A.4.3.

$$\frac{d[POC]_{DET}}{dt} = \underbrace{R_{DIA,DEATH}}_{\substack{Formation\ of\ particulate\\ detritus\ carbon\\ by\ the\ death\ of\ diatoms}} + \underbrace{R_{NON,FIX,CYN,DEATH}}_{\substack{Formation\ of\ particulate\\ detritus\ carbon\ by\ the\ death\\ of\ non-nitrogen\ fixing\ cyanobacteria}} + \underbrace{R_{FIX,CYN,DEATH}}_{\substack{Formation\ of\ detritus\ carbon\ by\ the\\ death\ of\ nitrogen\ fixing\ cyanobacteria}} + \underbrace{R_{OPA,DEATH}}_{\substack{Formation\ of\ particulate\\ detritus\ carbon\ by\ the\\ death\ of\ other\ plankton}} + \underbrace{R_{ZOOP,DEATH}}_{\substack{Formation\ of\ particulate\\ detritus\ carbon\ by\ the\\ zooplankton}} - \underbrace{R_{ZOOP,GRAZ,POC}}_{\substack{Conversion\ of\ particulate\\ detritus\ carbon\ to\ zooplankton\\ carbon\ by\ zooplankton\ grazing\ on\ detritus}} - \underbrace{R_{DISS,POC}}_{\substack{Dissolution\ of\ particulate\ detritus\ carbon\ to\\ dissolved\ organic\ carbon}}$$

(Equation A.4.1)

$$\frac{d[PON]_{DET}}{dt} = \underbrace{\left(R_{DIA,DEATH} \cdot N{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ particulate\\ detritus\ nitrogen\\ by\ the\ death\ of\ diatoms}} + \underbrace{\left(R_{NON,FIX,CYN,DEATH} \cdot N{:}\,C_{NON,FIX,CYN}\right)}_{\substack{Formation\ of\ particulate\\ detritus\ nitrogen\ by\ the\ death\ of\\ non-nitrogen\ fixing\ cyanobacteria}} + \underbrace{\left(R_{FIX,CYN,DEATH} \cdot N{:}\,C_{FIX,CYN}\right)}_{\substack{Formation\ of\ particulate\\ detritus\ nitrogen\ by\ the\ death\ of\\ nitrogen\ fixing\ cyanobacteria}} + \underbrace{\left(R_{OPA,DEATH} \cdot N{:}\,C_{OPA}\right)}_{\substack{Formation\ of\ particulate\\ detritus\ nitrogen\ by\ the\ death\ of\\ other\ planktonic\ algae}} + \underbrace{\left(R_{ZOOP,DEATH} \cdot N{:}\,C_{ZOOP}\right)}_{\substack{Formation\ of\ detritus\ nitrogen\ by\\ the\ death\ of\ zooplankon}} - \underbrace{\left(R_{ZOOP,GRAZ,POC} \cdot N{:}\,C_{POC}\right)}_{\substack{Conversion\ of\ detritus\ nitrogen\ to\ zooplankton\\ nitrogen\ by\ zooplankton\ grazing\ on\ detritus}} - \underbrace{R_{DISS,PON}}_{\substack{Dissolution\ of\ particulate\ detritus\ nitrogen\ to\\ dissolved\ organic\ nitrogen}}$$

(Equation A.4.2)

$$\frac{d[POP]_{DET}}{dt} = \underbrace{\left(R_{DIA,DEATH} \cdot P{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ particulate\ detritus\ phosphorus\ by\ the\ death\ of\ diatoms}} + \underbrace{\left(R_{NON,FIX,CYN,DEATH} \cdot P{:}\,C_{NON,FIX,CYN}\right)}_{\substack{Formation\ of\ particulate\ detritus\ phosphorus\ by\ the\ death\ of\ non-nitrogen\ fixing\ cyanobacteria}}$$
$$+ \underbrace{\left(R_{FIX,CYN,DEATH} \cdot P{:}\,C_{FIX,CYN}\right)}_{\substack{Formation\ of\ particulate\ detritus\ phosphorus\ by\ the\ death\ of\ nitrogen\ fixing\ cyanobacteria}} + \underbrace{\left(R_{OPA,DEATH} \cdot P{:}\,C_{OPA}\right)}_{\substack{Formation\ of\ particulate\ detritus\ phosphorus\ by\ the\ death\ of\ other\ planktonic\ algae}}$$
$$+ \underbrace{\left(R_{ZOOP,DEATH} \cdot P{:}\,C_{ZOOP}\right)}_{\substack{Formation\ of\ particulate\ detritus\ phosphorus\ by\ the\ death\ of\ zooplankon}} - \underbrace{\left(R_{ZOOP,GRAZ,POC} \cdot P{:}\,C_{POC}\right)}_{\substack{Conversion\ of\ detritus\ phosphorus\ to\ zooplankton\ nitrogen\ by\ zooplankton\ grazing\ on\ detritus}}$$
$$- \underbrace{R_{DISS,POP}}_{\substack{Dissolution\ of\ particulate\ detritus\ phosphorus\ to\ dissolved\ organic\ phosphorus}}$$

(Equation A.4.3)

The notation of Equation A.4.1 – A.4.3 is given below:

$R_{DIA,DEATH}$: Death rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NON,FIX,CYN,DEATH}$: Death rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,DEATH}$: Death rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,DEATH}$: Death rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,DEATH}$: Death rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$N{:}\,C_{DIA}$: Nitrogen to carbon ratio for diatoms (dimensionless)

$P{:}\,C_{DIA}$: Phosphorus to carbon ratio for diatoms (dimensionless)

$N{:}\,C_{NOFIX,CYN}$: Nitrogen to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{NOFIX,CYN}$: Phosphorus to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$N{:}\,C_{OPA}$: Nitrogen to carbon ratio for other planktonic algae (dimensionless)

$P{:}\,C_{OPA}$: Phosphorus to carbon ratio for other planktonic algae (dimensionless)

$N{:}\,C_{FIX,CYN}$: Nitrogen to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{FIX,CYN}$: Phosphorus to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$N:C_{ZOOP}$: Nitrogen to carbon ratio for zooplankton (dimensionless)

$P:C_{ZOOP}$: Phosphorus to carbon ratio for zooplankton (dimensionless)

$N:C_{POC}$: Nitrogen to carbon ratio for detrital particulate organic matter (dimensionless)

$P:C_{POC}$: Phosphorus to carbon ratio for detrital particulate organic matter (dimensionless)

$R_{DISS,POC}$: Dissolution rate of particulate detritus carbon to dissolved organic carbon ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DISS,PON}$: Dissolution rate of particulate detritus nitrogen to dissolved organic nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{DISS,POP}$: Dissolution rate of particulate detritus phosphorus to dissolved organic phosphorus ($gP \cdot m^{-3} \cdot day^{-1}$)

$N:C_{DIA}$, $P:C_{DIA}$, $N:C_{NOFIX,CYN}$, $P:C_{NOFIX,CYN}$, $N:C_{OPA}$, $P:C_{OPA}$, $N:C_{FIX,CYN}$, $P:C_{FIX,CYN}$ are user entered stoichiometric model constants, whereas $N:C_{ZOOP}$, $P:C_{ZOOP}$, $N:C_{POC}$, $P:C_{POC}$ are calculated internally by AQUABC given in Equation A.2.4 - Equation A.2.7 and will not be repeated here.

$R_{DIA,DEATH}$, $R_{NON,FIX,CYN,DEATH}$, $R_{OPA,DEATH}$, $R_{FIX,CYN,DEATH}$ and $R_{ZOO,DEATH}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Dissolution rates of particulate detritus carbon, nitrogen and phosphorus are given in Equations A.4.4 – A.4.6

$$R_{DISS,POC} = \left(k_{DISS,DET,POC,20} + K_{PHYT,DISS,DET,POC}\right) \cdot \theta_{k,DISS,DET,POC}^{(TEMP-20)} \cdot [POC]_{DET}$$

(Equation A.4.4)

$$R_{DISS,PON} = \left(k_{DISS,DET,PON,20} + K_{PHYT,DISS,DET,PON}\right) \cdot \theta_{k,DISS,DET,PON}^{(TEMP-20)} \cdot [PON]_{DET}$$

(Equation A.4.5)

$$R_{DISS,POP} = \left(k_{DISS,DET,POP,20} + K_{PHYT,DISS,DET,POP}\right) \cdot \theta_{k,DISS,DET,POP}^{(TEMP-20)} \cdot [POP]_{DET}$$

(Equation A.4.6)

The notation of Equations A.4.4 – A.4.6 is given below:

$k_{DISS,DET,POC,20}$: Dissolution rate constant of detritus particulate organic carbon due to “abiotic processes” at 20˚C (day^{-1})

$K_{PHYT,DISS,DET,POC}$: Dissolution rate constant of detritus particulate organic carbon due to “phytoplankton mediated processes” at 20˚C (day^{-1})

$\theta_{k,DISS,DET,POC}$: Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic carbon (dimensionless)

$k_{DISS,DET,PON,20}$: Dissolution rate constant of detritus particulate organic nitrogen due to "abiotic processes" at 20˚C (day^{-1})

$K_{PHYT,DISS,DET,PON}$: Dissolution rate constant of detritus particulate organic nitrogen due to "phytoplankton mediated processes" at 20˚C (day^{-1})

$\theta_{k,DISS,DET,POP}$: Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic nitrogen (dimensionless)

$k_{DISS,DET,POP,20}$: Dissolution rate constant of detritus particulate organic phosphorus due to "abiotic processes" at 20˚C (day^{-1})

$K_{PHYT,DISS,DET,POP}$: Dissolution rate constant of detritus particulate organic phosphorus due to "phytoplankton mediated processes" at 20˚C (day^{-1})

$\theta_{k,DISS,DET,POP}$: Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic phosphorus (dimensionless)

Dissolution rate constant of detritus particulate organic carbon, nitrogen and phosphorus due to "phytoplankton mediated processes" at 20˚C are given in Equations A.4.7 – A.4.9.

$$K_{PHYT,DISS,DET,POC} = FAC_{PHYT,DET,POC} \cdot [PHYT - C] \quad \text{(Equation A.4.7)}$$

$$K_{PHYT,DISS,DET,PON} = FAC_{PHYT,DET,PON} \cdot [PHYT - C] \quad \text{(Equation A.4.8)}$$

$$K_{PHYT,DISS,DET,POP} = FAC_{PHYT,DET,POP} \cdot [PHYT - C] \quad \text{(Equation A.4.9)}$$

The notation of Equations A.4.4 – A.4.6 is given below:

$FAC_{PHYT,DET,POC}$: Multiplier for phytoplankton mediated particulate detritus carbon dissolution rate constant ($gC^{-1} \cdot m^3 \cdot day^{-1}$)

$FAC_{PHYT,DET,PON}$: Multiplier for phytoplankton mediated particulate detritus nitrogen dissolution rate constant ($gN^{-1} \cdot m^3 \cdot day^{-1}$)

$FAC_{PHYT,DET,POP}$: Multiplier for phytoplankton mediated particulate detritus phosphorus dissolution rate constant ($gP^{-1} \cdot m^3 \cdot day^{-1}$)

$[\mathrm{PHYT-C}]$: Total phytoplankton carbon ($gC \cdot m^{-3}$)

Total phytoplankton carbon is given in Equation A.4.7

$$[\mathrm{PHYT-C}] = [\mathrm{DIA-C}] + [\mathrm{CYN-C}]_{\mathrm{NOFIX}} + [\mathrm{OPA-C}] + [\mathrm{CYN-C}]_{\mathrm{FIX}}$$

(Equation A.4.7)

A.5 DISSOLVED ORGANIC MATTER KINETICS

Dissolved organic matter is handled using three state variables; namely dissolved organic carbon, dissolved organic nitrogen and dissolved organic phosphorus. The main kinetic derivatives for dissolved organic matter is given in Equations A.5.1 – A.5.3.

$$\frac{\mathrm{d[DOC]}}{\mathrm{dt}} = \underbrace{\mathrm{R_{DISS,POC}}}_{\substack{Dissolution\ of\ detritus\ carbon\ to \\ dissolved\ organic\ carbon}} + \underbrace{\mathrm{R_{ZOOP.EXCR}}}_{\substack{Relase\ of\ dissolved\ organic\ carbon \\ by\ zooplankton\ excretion}} + \underbrace{\mathrm{R_{DIA,EXCR}}}_{\substack{Relase\ of\ dissolved\ organic\ carbon \\ by\ diatom\ excretion}} + \underbrace{\mathrm{R_{NON,FIX,CYN,EXCR}}}_{\substack{Relase\ of\ dissolved\ organic\ carbon\ by \\ non-nitrogen\ fixing\ cyanobacteria\ excretion}} + \underbrace{\mathrm{R_{FIX,CYN,EXCR}}}_{\substack{Relase\ of\ dissolved\ organic\ carbon\ by \\ nitrogen\ fixing\ cyanobacteria\ excretion}} + \underbrace{\mathrm{R_{OPA,EXCR}}}_{\substack{Relase\ of\ dissolved\ organic\ carbon\ by \\ nitrogen\ fixing\ cyanobacteria\ excretion}} - \underbrace{\mathrm{R_{MIN,DOC}}}_{\substack{Mineralization\ of\ dissolved\ organic\ carbon}}$$

(Equation A.5.1)

$$\frac{\mathrm{d[DON]}}{\mathrm{dt}} = \underbrace{\mathrm{R_{DISS,PON}}}_{\substack{Dissolution\ of\ detritus\ nitrogen\ to \\ dissolved\ organic\ nitrogen}} + \underbrace{\mathrm{R_{ZOOP.EXCR,DON}}}_{\substack{Relaase\ of\ dissolved\ organic\ nitrogen \\ by\ zooplankton\ excretion}} + \underbrace{\left(\mathrm{R_{DIA,EXCR}} \cdot \mathrm{N{:}\,C_{DIA}}\right)}_{\substack{Relaase\ of\ dissolved\ organic \\ nitrogen\ by\ diatom\ excretion}} + \underbrace{\left(\mathrm{R_{NON,FIX,CYN,EXCR}} \cdot \mathrm{N{:}\,C_{NON,FIX,CYN}}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ nitrogen \\ by\ non-nitrogen\ fixing\ cyanobacteria\ excretion}} + \underbrace{\left(\mathrm{R_{FIX,CYN,EXCR}} \cdot \mathrm{N{:}\,C_{FIX,CYN}}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ nitrogen \\ by\ nitrogen\ fixing\ cyanobacteria\ excretion}} + \underbrace{\left(\mathrm{R_{OPA,EXCR}} \cdot \mathrm{N{:}\,C_{OPA}}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ nitrogen \\ by\ other\ planktonic\ alggae\ excretion}} - \underbrace{\mathrm{R_{MIN,DON}}}_{\substack{Mineralization\ of\ dissolved \\ organic\ nitrogen}}$$

(Equation A.5.2)

$$\frac{d[DOP]}{dt} = \underbrace{R_{DISS,POP}}_{\substack{Dissolution\ of\ detritus\ phosphorus\ to \\ dissolved\ organic\ phosphorus}} + \underbrace{R_{ZOOP.EXCR,DOP}}_{\substack{Relaase\ of\ dissolved\ organic\ phosphorus \\ by\ zooplankton\ excretion}}$$
$$+ \underbrace{\left(R_{DIA,EXCR} \cdot P{:}\,C_{DIA}\right)}_{\substack{Relaase\ of\ dissolved\ organic \\ phosphorus\ by\ diatom\ excretion}} + \underbrace{\left(R_{NON,FIX,CYN,EXCR} \cdot P{:}\,C_{NON,FIX,CYN}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ phosphorus \\ by\ non-nitrogen\ fixing\ cyanobacteria\ excretion}}$$
$$+ \underbrace{\left(R_{FIX,CYN,EXCR} \cdot P{:}\,C_{FIX,CYN}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ phosphorus \\ by\ nitrogen\ fixing\ cyanobacteria\ excretion}}$$
$$+ \underbrace{\left(R_{OPA,EXCR} \cdot P{:}\,C_{OPA}\right)}_{\substack{Relaase\ of\ dissolved\ organic\ phosphorus \\ by\ other\ planktonic\ alggae\ excretion}} - \underbrace{R_{MIN,DOP}}_{\substack{Mineralization\ of\ dissolved \\ organic\ phosphorus}}$$

(Equation A.5.3)

The notation of Equations A.5.1 – A.5.3 is given below:

$R_{DIA,EXCR}$: Death rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NON,FIX,CYN,EXCR}$: Non-nitrogen fixing cyanobacteria excretion rate ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,EXCR}$: Excretion rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,EXCR}$: Excretion rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,EXCR}$: Excretion rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$N{:}\,C_{DIA}$: Nitrogen to carbon ratio for diatoms (dimensionless)

$P{:}\,C_{DIA}$: Phosphorus to carbon ratio for diatoms (dimensionless)

$N{:}\,C_{NOFIX,CYN}$: Nitrogen to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{NOFIX,CYN}$: Phosphorus to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$N{:}\,C_{OPA}$: Nitrogen to carbon ratio for other planktonic algae (dimensionless)

$P{:}\,C_{OPA}$: Phosphorus to carbon ratio for other planktonic algae (dimensionless)

$N{:}\,C_{FIX,CYN}$: Nitrogen to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{FIX,CYN}$: Phosphorus to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$N{:}\,C_{ZOOP}$: Nitrogen to carbon ratio for zooplankton (dimensionless)

$P{:}\,C_{ZOOP}$: Phosphorus to carbon ratio for zooplankton (dimensionless)

$N{:}\,C_{POC}$: Nitrogen to carbon ratio for detrital particulate organic matter (dimensionless)

$P:C_{POC}$: Phosphorus to carbon ratio for detrital particulate organic matter

(dimensionless)

$R_{DISS,POC}$: Dissolution rate of particulate detritus carbon to dissolved organic carbon ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DISS,PON}$: Dissolution rate of particulate detritus nitrogen to dissolved organic nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{DISS,POP}$: Dissolution rate of particulate detritus phosphorus to dissolved organic phosphorus ($gP \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOC}$: Mineralization rate of particulate detritus carbon to dissolved inorganic carbon ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DON}$: Mineralization rate of particulate detritus nitrogen to ammonia nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOP}$: Mineralization rate of particulate detritus phosphorus to phosphate phosphorus ($gP \cdot m^{-3} \cdot day^{-1}$)

$N:C_{DIA}$, $P:C_{DIA}$, $N:C_{NOFIX,CYN}$, $P:C_{NOFIX,CYN}$, $N:C_{OPA}$, $P:C_{OPA}$, $N:C_{FIX,CYN}$, $P:C_{FIX,CYN}$ are user entered stoichiometric model constants, whereas $N:C_{ZOOP}$, $P:C_{ZOOP}$, $N:C_{POC}$, $P:C_{POC}$ are calculated internally by AQUABC given in Equation A.2.4 - Equation A.2.7 and will not be repeated here.

$R_{DIA,EXCR}$, $R_{NON,FIX,CYN,EXCR}$, $R_{OPA,EXCR}$, $R_{FIX,CYN,EXCR}$ and $R_{ZOO,EXCR}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Dissolution rates of particulate detritus carbon, nitrogen and phosphorus are given in Equations A.4.4 – A.4.6 in Section A.4 and will therefore not be repeated here.

Dissolved organic matter mineralization is conducted following a decoupled approach, where DOC, DON and DOP are allowed to mineralize using different rate constants. Mineralization rates of dissolved carbon, nitrogen and phosphorus are given in Equations A.5.4 – A.5.6:

$$R_{MIN,DOC} = R_{MIN,DOC,DOXY} + R_{MIN,DOC,NO3} \quad \text{(Equation A.5.4)}$$

$$R_{MIN,DON} = R_{MIN,DON,DOXY} + R_{MIN,DON,NO3} \quad \text{(Equation A.5.5)}$$

$$R_{MIN,DOP} = R_{MIN,DOP,DOXY} + R_{MIN,DOP,NO3} \quad \text{(Equation A.5.6)}$$

The notation of Equations A.5.4 – A.5.6 is given below:

$R_{MIN,DOC}$: Mineralization rate of dissolved organic carbon ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DON}$: Mineralization rate of dissolved organic nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOP}$: Mineralization rate of dissolved organic phosphorus ($gP \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOC,DOXY}$: Mineralization rate of dissolved organic carbon, where dissolved oxygen

is utilized as the final electron acceptor ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOC,NO3}$: Mineralization rate of dissolved organic carbon, where nitrate is utilized

as the final electron acceptor ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DON,DOXY}$: Mineralization rate of dissolved organic nitrogen, where dissolved oxygen is utilized as the final electron acceptor ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DON,NO3}$: Mineralization rate of dissolved organic nitrogen, where nitrate is utilized as the final electron acceptor ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOP,DOXY}$: Mineralization rate of dissolved organic phosphorus, where dissolved oxygen is utilized as the final electron acceptor ($gP \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOP,NO3}$: Mineralization rate of dissolved organic phosphorus, where nitrate is utilized as the final electron acceptor ($gP \cdot m^{-3} \cdot day^{-1}$)

Mineralization rates of dissolved organic carbon are given in Equations A.5.7 and A.5.8.

$$R_{MIN,DOC,DOXY} = \left(k_{MIN,DOC,DOXY,20} + K_{PHYT,MIN,DOC}\right) \cdot \theta_{MIN,DOC,DOX}^{(TEMP-20)} \cdot pHCorr_{DOC,MIN,DOXY} \cdot \frac{[O_2]}{k_{HS,DOXY,RED,LIM} + [O_2]} \cdot \frac{[DOC]}{k_{HS,DOC,MIN,DOXY} + [DOC]} \cdot [DOC]$$

(Equation A.5.7)

$$R_{MIN,DOC,NO3N} = k_{MIN,DOC,NO3,20} \cdot \theta_{MIN,DOC,NO3}^{(TEMP-20)} \cdot pHCorr_{DOC,MIN,NO3} \cdot \frac{k_{HS,DOXY,RED,INHIB}}{k_{HS,DOXY,RED,INHIB} + [O_2]} \cdot \frac{[NO_3 - N]}{k_{HS,NO3,RED,LIM} + [NO_3 - N]} \cdot \frac{[DOC]}{k_{HS,NO3,RED,LIM} + [DOC]} \cdot [DOC]$$

(Equation A.5.8)

The notation of Equations A.5.7 – A.5.8 is given below:

$k_{MIN,DOC,DOXY,20}$: Mineralization rate constant of dissolved organic carbon due to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$K_{PHYT,MIN,DOC}$: Mineralization rate constant of dissolved organic carbon due to "phytoplankton mediated processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$k_{MIN,DOC,NO3,20}$: Mineralization rate constant of dissolved organic carbon due to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor (day^{-1})

$\theta_{MIN,DOC,DOXY}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic carbon, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$\theta_{MIN,DOC,NO3}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic carbon, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DOC,MIN,DOXY}$: pH correction factor for mineralization rate of dissolved organic

carbon, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DOC,MIN,NO3}$: pH correction factor for mineralization rate of dissolved organic

carbon, where nitrate is utilized as final electron acceptor (dimensionless)

$k_{HS,DOXY,RED,LIM}$: Monod type half saturation concentration of dissolved oxygen for

dissolved organic carbon mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved oxygen as oxidizing agent ($gO_2 \cdot m^{-3}$)

$k_{HS,DOC,MIN,DOXY}$: Monod type half saturation concentration of dissolved organic carbon for dissolved organic carbon mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic carbon as substrate ($gC \cdot m^{-3}$)

$k_{HS,DOXY,RED,INHIB}$: Reversed Monod type half saturation concentration of dissolved

oxygen dissolved for organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the inhibiting effects of the lack of presence dissolved oxygen competing as an energetically more efficient oxidizing agent than nitrate ($gO_2 \cdot m^{-3}$)

$k_{HS,NO3,RED,LIM}$: Monod type half saturation concentration of nitrate nitrogen for

dissolved organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of nitrate as oxidizing agent ($gN \cdot m^{-3}$)

$k_{HS,DOC,MIN,NO3}$: Monod type half saturation concentration of dissolved organic carbon for dissolved organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic carbon as substrate ($gC \cdot m^{-3}$)

Mineralization rates of dissolved organic nitrogen and dissolved organic phosphorus are given in Equations A.5.9 - A.5.12

$$R_{MIN,DON,DOXY} = \left(k_{MIN,DON,DOXY,20} + K_{PHYT,MIN,DON}\right) \cdot \theta_{MIN,DON,DOXY}^{(TEMP-20)} \cdot pHCorr_{DON,MIN,DOXY} \cdot \frac{[O_2]}{k_{HS,DOXY,RED,LIM} + [O_2]} \cdot \frac{[DON]}{k_{HS,DON,MIN,DOXY} + [DON]} \cdot [DON]$$

(Equation A.5.9)

$$R_{MIN,DON,NO3N} = k_{MIN,DON,NO3,20} \cdot \theta_{MIN,DON,NO3}^{(TEMP-20)} \cdot pHCorr_{DON,MIN,NO3} \cdot \frac{k_{HS,DOXY,RED,INHIB}}{k_{HS,DOXY,RED,INHIB} + [O_2]} \cdot \frac{[NO_3 - N]}{k_{HS,NO3,RED,LIM} + [NO_3 - N]} \cdot$$

$$\frac{[DON]}{k_{HS,NO3,RED,LIM} + [DON]} \cdot [DON]$$

(Equation A.5.10)

$$R_{MIN,DOP,DOXY} = \left(k_{MIN,DOP,DOXY,20} + K_{PHYT,MIN,DON}\right) \cdot \theta_{MIN,DOP,DOXY}^{(TEMP-20)} \cdot pHCorr_{DOP,MIN,DOXY} \cdot \frac{[O_2]}{k_{HS,DOXY,RED,LIM} + [O_2]} \cdot \frac{[DOP]}{k_{HS,DOP,MIN,DOXY} + [DOP]} \cdot [DOP]$$

(Equation A.5.11)

$$R_{MIN,DOP,NO3N} = k_{MIN,DOP,NO3,20} \cdot \theta_{MIN,DOP,NO3}^{(TEMP-20)} \cdot pHCorr_{DOP,MIN,NO3} \cdot \frac{k_{HS,DOXY,RED,INHIB}}{k_{HS,DOXY,RED,INHIB} + [O_2]} \cdot \frac{[NO_3 - N]}{k_{HS,NO3,RED,LIM} + [NO_3 - N]} \cdot \frac{[DOP]}{k_{HS,NO3,RED,LIM} + [DOP]} \cdot [DOP]$$

(Equation A.5.12)

The notation of Equations A.5.9 – A.5.12 is given below:

$k_{MIN,DON,DOXY,20}$: Mineralization rate constant of dissolved organic nitrogen due to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$K_{PHYT,MIN,DON}$: Mineralization rate constant of dissolved organic nitrogen due to "phytoplankton mediated processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$k_{MIN,DON,NO3,20}$: Mineralization rate constant of dissolved organic nitrogen due to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor (day^{-1})

$\theta_{MIN,DON,DOXY}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic nitrogen, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$\theta_{MIN,DON,NO3}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic nitrogen, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DON,MIN,DOXY}$: pH correction factor for mineralization rate of dissolved organic

nitrogen, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DON,MIN,NO3}$: pH correction factor for mineralization rate of dissolved organic
nitrogen, where nitrate is utilized as final electron acceptor (dimensionless)

$k_{HS,DON,MIN,DOXY}$: Monod type half saturation concentration of dissolved organic nitrogen for dissolved organic nitrogen mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic nitrogen as substrate ($gN \cdot m^{-3}$)

$k_{HS,DON,MIN,NO3}$: Monod type half saturation concentration of dissolved organic nitrogen for dissolved organic nitrogen mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic nitrogen as substrate ($gN \cdot m^{-3}$)

$k_{MIN,DOP,DOXY,20}$: Mineralization rate constant of dissolved organic phosphorus due
to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$K_{PHYT,MIN,DOP}$: Mineralization rate constant of dissolved organic phosphorus due
to "phytoplankton mediated processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor (day^{-1})

$k_{MIN,DOP,NO3,20}$: Mineralization rate constant of dissolved organic phosphorus due
to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor (day^{-1})

$\theta_{MIN,DOP,DOXY}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$\theta_{MIN,DOP,NO3}$: Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DOP,MIN,DOXY}$: pH correction factor for mineralization rate of dissolved organic
phosphorus, where dissolved oxygen is utilized as final electron acceptor (dimensionless)

$pHCorr_{DOP,MIN,NO3}$: pH correction factor for mineralization rate of dissolved organic
phosphorus, where nitrate is utilized as final electron acceptor (dimensionless)

$k_{HS,DOP,MIN,DOXY}$: Monod type half saturation concentration of dissolved organic nitrogen for dissolved organic phosphorus mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic phosphorus as substrate ($gP \cdot m^{-3}$)

$k_{HS,DOP,MIN,NO3}$: Monod type half saturation concentration of dissolved organic nitrogen for dissolved organic phosphorus mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic phosphorus as substrate ($gP \cdot m^{-3}$)

$pHCorr_{DOC,MIN,NO3}$, $pHCorr_{DON,MIN,NO3}$ and $pHCorr_{DOP,MIN,NO3}$ are given in Equations A.5.13-A.5.18.

$$pHCorr_{DOC,MIN,DOXY} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DOC,MIN,DOXY}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DOC,MIN,DOXY}\right) \\ \text{if } \left(pH_{LOWER,OPT,DOC,MIN,DOXY} \le pH \le pH_{UPPER,OPT,DOC,MIN,DOXY}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DOC,MIN,DOXY}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DOC,MIN,DOXY} - pH\right) \end{cases}$$

(Equation A.5.13)

$$pHCorr_{DON,MIN,DOXY} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DON,MIN,DOXY}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DON,MIN,DOXY}\right) \\ \text{if } \left(pH_{LOWER,OPT,DON,MIN,DOXY} \le pH \le pH_{UPPER,OPT,DON,MIN,DOXY}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DON,MIN,DOXY}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DON,MIN,DOXY} - pH\right) \end{cases}$$

(Equation A.5.14)

$$pHCorr_{DOP,MIN,DOXY} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DOP,MIN,DOXY}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DOP,MIN,DOXY}\right) \\ \text{if } \left(pH_{LOWER,OPT,DOP,MIN,DOXY} \le pH \le pH_{UPPER,OPT,DOP,MIN,DOXY}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DOP,MIN,DOXY}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DOP,MIN,DOXY} - pH\right) \end{cases}$$

(Equation A.5.15)

$$pHCorr_{DOC,MIN,NO3} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DOC,MIN,NO3}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DOC,MIN,NO3}\right) \\ \text{if } \left(pH_{LOWER,OPT,DOC,MIN,NO3} \le pH \le pH_{UPPER,OPT,DOC,MIN,NO3}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DOC,MIN,NO3}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DOC,MIN,NO3} - pH\right) \end{cases}$$

(Equation A.5.16)

$$pHCorr_{DON,MIN,NO3} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DON,MIN,NO3}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DON,MIN,NO3}\right) \\ \text{if } \left(pH_{LOWER,OPT,DON,MIN,NO3} \le pH \le pH_{UPPER,OPT,DON,MIN,NO3}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DON,MIN,NO3}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DON,MIN,NO3} - pH\right) \end{cases}$$

(Equation A.5.17)

$$pHCorr_{DOP,MIN,NO3} = \begin{cases} \text{if } \left(pH < pH_{LOWER,OPT,DOP,MIN,NO3}\right) \\ \quad \exp\left(pH - pH_{LOWER,OPT,DOP,MIN,NO3}\right) \\ \text{if } \left(pH_{LOWER,OPT,DOP,MIN,NO3} \le pH \le pH_{UPPER,OPT,DOP,MIN,NO3}\right) \\ \quad 1 \\ \text{if } \left(pH > pH_{UPPER,OPT,DOP,MIN,NO3}\right) \\ \quad \exp\left(pH_{UPPER,OPT,DOP,MIN,NO3} - pH\right) \end{cases}$$

(Equation A.5.18)

The notation of Equations A.5.13 – A.5.18 is given below:

$pH_{LOWER,OPT,DOC,MIN,DOXY}$: Minimum value for optimum pH for dissolved ogranic carbon minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DOC,MIN,DOXY}$: Maximum value for optimum pH for dissolved ogranic carbon minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DON,MIN,DOXY}$: Minimum value for optimum pH for dissolved ogranic nitrogen minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DON,MIN,DOXY}$: Maximum value for optimum pH for dissolved ogranic nitrogen minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DOP,MIN,DOXY}$: Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DOP,MIN,DOXY}$: Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DOC,MIN,NO3}$: Minimum value for optimum pH for dissolved ogranic carbon minerlization with nitrate as the final electron acceptor

$pH_{LOWER,OPT,DOC,MIN,NO3}$: Maximum value for optimum pH for dissolved ogranic carbon minerlization with nitrate as the final electron acceptor

$pH_{LOWER,OPT,DON,MINNO3}$: Minimum value for optimum pH for dissolved ogranic nitrogen minerlization with nitrate as the final electron acceptor

$pH_{LOWER,OPT,DON,MIN,NO3}$: Maximum value for optimum pH for dissolved ogranic

nitrogen minerlization with nitrate as the final electron acceptor

$pH_{LOWER,OPT,DOP,MIN,NO3}$: Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor

$pH_{LOWER,OPT,DOP,MIN,NO3}$: Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor

A.6 INORGANIC NUTRIENT KINETICS

AQUABC considers inorganic nitrogen compunds, inorganic silicon compunds, phosphates, and inorganic carbon as inorganic nutrients.

A.6.1 Inorganic Nitrogen

Inorganic nitrogen is handled using two state variables; namely ammonia nitrogen and nitrate nitrogen. The main kinetic derivatives for ammonia nitrogen and nitrate nitrogen is given in Equations A.6.1.1 and Equations A.6.1.2.

$$\frac{d[NH4-N]}{dt} = \underbrace{\left(R_{DIA,TOT,RESP}\cdot N{:}\,C_{DIA}\right)}_{\substack{Release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ diatoms}} + \underbrace{\left(R_{NON,FIX,CYN,TOT,RESP}\cdot N{:}\,C_{NON,FIX,CYN}\right)}_{\substack{Release\ of\ ammonia\ nitrogen\ by\ total\ respiration\\ of\ non-nitrogen\ fixing\ cyanobacteria}}$$
$$+ \underbrace{\left(R_{FIX,CYN,TOT,RESP}\cdot N{:}\,C_{FIX,CYN}\right)}_{\substack{Release\ of\ ammonia\ nitrogen\ by\ total\\ respiration\ of\ nitrogen\ fixing\ cyanobacteria}} + \underbrace{\left(R_{OPA,TOT,RESP}\cdot N{:}\,C_{OPA}\right)}_{\substack{Release\ of\ ammonia\ nitrogen\ by\ total\\ respiration\ of\ other\ planktonic\ algae}}$$
$$+ \underbrace{\left(R_{ZOO,TOT,RESP}\cdot N{:}\,C_{ZOO}\right)}_{\substack{Release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ zooplankton}} - \underbrace{\left(R_{DIA,GROWTH}\cdot Pref_{NH4N,DIA}\cdot N{:}\,C_{DIA}\right)}_{Uptake\ of\ ammonia\ nitrogen\ by\ growth\ of\ diatoms}$$
$$- \underbrace{\left(R_{NON,FIX,CYN,GROWTH}\cdot Pref_{NH4N,DON,NON,FIX,CYN}\cdot N{:}\,C_{NON,FIX,CYN}\right)}_{Uptake\ of\ ammonia\ nitrogen\ by\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria}$$
$$- \underbrace{\left(R_{FIX,CYN,GROWTH}\cdot Pref_{NH4N,DON,FIX,CYN}\cdot N{:}\,C_{FIX,CYN}\right)}_{Uptake\ of\ ammonia\ nitrogen\ by\ growth\ of\ nitrogen\ fixing\ cyanobacteria}$$
$$- \underbrace{\left(R_{OPA,GROWTH}\cdot Pref_{NH4N,OPA}\cdot N{:}\,C_{OPA}\right)}_{\substack{Uptake\ of\ ammonia\ nitrogen\ by\\ growth\ of\ other\ planktonic\ algae}} + \underbrace{R_{NITRIFICATION}}_{\substack{Conversion\ of\\ ammonia\ nitrogen\ to\\ nitrate\ nitrogen}}$$
$$+ \underbrace{R_{MIN,DON}}_{\substack{Release\ of\ ammonia\\ nitrogen\ by\\ organic\ nitrogen\\ mineralization}} - \underbrace{R_{AMMONIA,VOLATIL}}_{\substack{Loss\ of\ ammonia\ nitrogen\\ by\ volatilizaton}}$$

(Equation A.6.1.1)

$$\frac{d[NO3-N]}{dt} = \underbrace{R_{NITRIFICATION}}_{\substack{Conversion\ of\ ammonia\ nitrogen\ to \\ nitrate\ nitrogen\ by\ nitrification}} - \underbrace{R_{DENITRIFICATION}}_{Loss\ of\ nitrate\ by\ denitrification}$$
$$- \underbrace{\left(R_{DIA,GROWTH} \cdot \left(1 - Pref_{NH4N,DIA}\right) \cdot N{:}\,C_{DIA}\right)}_{Uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ diatoms}$$
$$- \underbrace{\left(R_{NON,FIX,CYN,GROWTH} \cdot \left(1 - Pref_{NH4N,DON,NON,FIX,CYN}\right) \cdot N{:}\,C_{NON,FIX,CYN}\right)}_{Uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria}$$
$$- \underbrace{\left(R_{FIX,CYN,GROWTH} \cdot \left(1 - Pref_{NH4N,DON,FIX,CYN}\right) \cdot N{:}\,C_{FIX,CYN}\right)}_{Uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ nitrogen\ fixing\ cyanobacteria}$$
$$- \underbrace{\left(R_{OPA,GROWTH} \cdot \left(1 - Pref_{NH4N,OPA}\right) \cdot N{:}\,C_{OPA}\right)}_{Uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ other\ planktonic\ algae}$$

(Equation A.6.1.2)

The notation of Equation A.6.1.1 and Equation A.6.1.2 is given below:

$R_{DIA,TOT,RESP}$: Total respiration rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,TOT,RESP}$: Total respiration rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,TOT,RESP}$: Total respiration rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,TOT,RESP}$: Total respiration rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,TOT,RESP}$: Total respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,GROWTH}$: Growth rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,GROWTH}$: Growth rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,GROWTH}$: Growth rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$N{:}\,C_{DIA}$: Nitrogen to carbon ratio for diatoms (dimensionless)

$N{:}\,C_{NOFIX,CYN}$: Nitrogen to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$N{:}\,C_{OPA}$: Nitrogen to carbon ratio for other planktonic algae (dimensionless)

$N{:}\,C_{FIX,CYN}$: Nitrogen to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$N{:}\,C_{ZOOP}$: Nitrogen to carbon ratio for zooplankton (dimensionless)

$N{:}\,C_{POC}$: Nitrogen to carbon ratio for detrital particulate organic matter (dimensionless)

$Pref_{NH4N,DIA}$: Ammonia preference factor for nitrogen uptake by diatoms (dimensionless)

$Pref_{NH4N,DON,NON,FIX,CYN}$: Ammonia plus dissolved organic nitrogen preference factor for

nitrogen uptake by non-nitrogen fixing cyanobacteria (dimensionless)

$Pref_{NH4N,OPA}$: Ammonia preference factor for nitrogen uptake by other planktonic algae (dimensionless)

$Pref_{NH4N,DON,FIX,CYN}$: Ammonia plus dissolved organic nitrogen preference factor for nitrogen uptake by nitrogen fixing cyanobacteria (dimensionless)

$R_{MIN,DON}$: Mineralization rate of dissolved organic nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{NITRIFICATION}$: Nitrification rate of ammonia nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{DENITRIFICATION}$: Denitrification rate of nitrate nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$R_{AMMONIA,VOLATIL}$: Volatilization rate of ammonia nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$N:C_{DIA}$, $N:C_{NOFIX,CYN}$, , $N:C_{OPA}$ and $N:C_{FIX,CYN}$, are user entered stoichiometric model constants, whereas, $N:C_{ZOOP}$, $N:C_{POC}$, are calculated internally by AQUABC given in Equation A.2.4 - Equation A.2.7 and will not be repeated here.

$R_{DIA,TOT,RESP}$, $R_{NON,FIX,CYN,TOT,RESP}$, $R_{OPA,TOT,RESP}$, $R_{FIX,CYN,TOT,RESP}$ and $R_{ZOO,TOT,RESP}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Mineralization rate of dissolved organic matter is explained in detail in the previous section, so $R_{MIN,DON}$ will not be repeated here.

The nitrification rate is given in Equation A.6.1.3

$$R_{NITRIFICATION} = k_{NITR,20} \cdot \theta_{NITR}^{(TEMP-20)} \cdot pHCorr_{NITR} \cdot \frac{[O_2]}{k_{HS,NITR,DOXY} + [O_2]} \cdot \frac{[NH_4 - N]}{k_{HS,NITR} + [NH_4 - N]} \cdot [NH_4 - N]$$

(Equation A.6.1.3)

The notation of Equation A.6.1.3 is given below

$k_{NITR,20}$: Nitrification rate constant (day^{-1})

θ_{NITR} : Arrhenius type temperature correction coefficient for nitrification rate (dimensionless)

$pHCorr_{NITR}$: pH correction factor for nitrification rate (dimensionless)

$k_{HS,NITR,DOXY}$: Monod type half saturation concentration of dissolved oxygen for

nitrification simulating the effects of the lack of dissolved oxygen as the oxidizing agent ($gO_2 \cdot m^{-3}$)

$k_{HS,NITR}$: Monod type half saturation concentration of ammonia nitrogen for nitrification simulating the effects of the lack of dissolved oxygen substrate ($gN \cdot m^{-3}$)

The pH correction factor for nitrification rate is given in Equation A.6.1.4

$$pHCorr_{NITR} = \begin{cases} \text{if } (pH < pH_{LOWER,OPT,NITR}) \\ \quad \exp(pH - pH_{LOWER,OPT,NITR}) \\ \text{if } (pH_{LOWER,OPT,NITR} \le pH \le pH_{UPPER,OPT,NITR}) \\ \quad 1 \\ \text{if } (pH > pH_{UPPER,OPT,NITR}) \\ \quad \exp(pH_{UPPER,OPT,NITR} - pH) \end{cases} \quad \text{(Equation A.6.1.4)}$$

The notation of Equation A.6.1.4 is given below

$pH_{LOWER,OPT,NITR}$: Minimum value for optimum pH for nitrification
$pH_{UPPER,OPT,NITR}$: Maximum value for optimum pH for nitrification

AQUABC does not have a separate process called denitrification. Denitrification is the mineralization rate of dissolved organic carbon, where nitrate is utilized as the final electron acceptor and it is quantified in nitrate nitrogen mass consumed per unit volume and unit time. The chemical equation of the denitrification process is given below:

$$C H_2 O + \frac{4}{5} NO_3 - N \rightarrow \frac{1}{2} N_2 + CO_2$$

Recalculating the stoichiometry, there are 0.93 grams of nitrate nitrogen denitrified per gram organic carbon mineralized. Therefore, denitrification rate is given in Equation A.6.1.5

$$R_{DENITRIFICATION} = 0.93 \cdot R_{MIN,DOC,NO3} \quad \text{(Equation A.6.1.5)}$$

The notation of Equation A.6.1.5 is given below:

$R_{MIN,DOC,NO3}$: Mineralization rate of dissolved organic carbon, where nitrate is utilized as the final electron acceptor ($gC \cdot m^{-3} \cdot day^{-1}$)

Volatilization rate of ammonia nitrogen is given in Equation A.6.1.6

$$R_{AMMONIA,VOLATIL} = K_A \cdot \left(\frac{32}{17}\right)^{0.25} \cdot \left([NH_3 - N] - [NH_3 - N]_S \cdot \left(\frac{14}{17}\right)\right)$$

(Equation A.6.1.6)

The notation of Equation A.6.1.6 is given below:

K_A : Reaeration rate constant for dissolved oxygen (day^{-1})

$[NH_3 - N]$: Concentration of unionized ammonia ($gN \cdot m^{-3}$)

$[NH_3 - N]_S$: Saturation concentration of unionized ammonia in water ($gN \cdot m^{-3}$)

Reaeration rate constant for dissolved oxygen contains detailed information and will therefore be given in the section related to dissolved oxygen. AQUABC considers the saturation concentration of unionized ammonia in water zero assuming that the partial pressure of unionized ammonia in gas form in the atmosphere would be zero.

Concentration of unionized ammonia is given in Equation A.6.1.7.

$$[NH_3 - N] = \frac{[NH_4 - N]}{1 + 10^{0.09018 + \frac{2729.92}{Temp + 273.16} - pH}}$$

Ammonia preference factors for nitrogen uptake by diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae and nitrogen fixing algae are given in Equation A.6.1.8 to A.6.1.11.

$$Pref_{NH4N,DIA} = \frac{[NH4 - N] \cdot [NO3 - N]}{(k_{HS,DIN,DIA} + [NH4 - N]) \cdot (k_{HS,DIN,DIA} + [NO3 - N])} + \frac{k_{HS,DIN,DIA} \cdot [NH4 - N]}{([NH4 - N] + [NO3 - N]) \cdot (k_{HS,DIN,DIA} + [NO3 - N])}$$

(Equation A.6.1.8)

$$Pref_{NH4N,DON,NON,FIX,CYN} = \frac{([NH4 - N] + Frac_{AVAIL,DON} \cdot [DON]) \cdot [NO3 - N]}{(k_{HS,DIN,NON,FIX,CYN} + ([NH4 - N] + Frac_{AVAIL,DON} \cdot [DON])) \cdot (k_{HS,DIN,NON,FIX,CYN} + [NO3 - N])} + \frac{k_{HS,DIN,NON,FIX,CYN} \cdot ([NH4 - N] + Frac_{AVAIL,DON} \cdot [DON])}{([NH4 - N] + Frac_{AVAIL,DON} \cdot [DON] + [NO3 - N]) \cdot (k_{HS,DIN,NON,FIX,CYN} + [NO3 - N])}$$

(Equation A.6.1.9)

$$Pref_{NH4N,OPA} = \frac{[NH4 - N] \cdot [NO3 - N]}{(k_{HS,DIN,OPA} + [NH4 - N]) \cdot (k_{HS,DIN,OPA} + [NO3 - N])} + \frac{k_{HS,DIN,OPA} \cdot [NH4 - N]}{([NH4 - N] + [NO3 - N]) \cdot (k_{HS,DIN,OPA} + [NO3 - N])}$$

(Equation A.6.1.10)

$$Pref_{NH4N,DON,FIX,CYN} =$$

$$\frac{\left([\mathrm{NH4-N}]+\mathrm{Frac_{AVAIL,DON}}\cdot[\mathrm{DON}]\right)\cdot[\mathrm{NO3-N}]}{\left(\mathrm{k_{HS,DIN,FIX,CYN}}+[\mathrm{NH4-N}]+\mathrm{Frac_{AVAIL,DON}}\cdot[\mathrm{DON}]\right)\cdot\left(\mathrm{k_{HS,DIN,FIX,CYN}}+[\mathrm{NO3-N}]\right)}$$

+

$$\frac{\mathrm{k_{HS,DIN,FIX,CYN}}\cdot\left([\mathrm{NH4-N}]+\mathrm{Frac_{AVAIL,DON}}\cdot[\mathrm{DON}]\right)}{\left([\mathrm{NH4-N}]+\mathrm{Frac_{AVAIL,DON}}\cdot[\mathrm{DON}]+[\mathrm{NO3-N}]\right)\cdot\left(\mathrm{k_{HS,DIN,FIX,CYN}}+[\mathrm{NO3-N}]\right)}$$

(Equation A.6.1.11)

The notation of Equations A.6.1.8 to A.6.1.11 is given below:

$\mathrm{k_{HS,DIN,DIA}}$: Monod type half-saturation concentration of diatom growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$\mathrm{k_{HS,DIN,NON,FIX,CYN}}$: Monod type half-saturation concentration of non-nitrogen fixing cyanobacteria growth for dissolved nitrogen ($gN \cdot m^{-3}$)

$\mathrm{k_{HS,DIN,DIA}}$: Monod type half-saturation concentration of other planktonic algae growth for dissolved inorganic nitrogen ($gN \cdot m^{-3}$)

$\mathrm{k_{HS,DIN,FIX,CYN}}$: Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved nitrogen ($gN \cdot m^{-3}$)

$\mathrm{Frac_{AVAIL,DON}}$: Fraction of dissolved organic nitrogen available for cyanobacteria growth as dissolved nitrogen source (dimensionless)

A.6.2 Inorganic Phosphorus

Inorganic phosphorus is handled using one state variable; the phosphate phosphorus. The main kinetic derivative for phosphate phosphorus is given in Equation A.6.2.1.

$$\frac{d[PO4-P]}{dt} = \underbrace{\left(R_{DIA,TOT,RESP} \cdot P{:}\,C_{DIA}\right)}_{\substack{Release\ of\ phosphate\ phosphorus\ by\\ total\ respiration\ of\ diatoms}} + \underbrace{\left(R_{NON,FIX,CYN,TOT,RESP} \cdot P{:}\,C_{NON,FIX,CYN}\right)}_{Release\ of\ phosphate\ phosphorus\ by\ total\ respiration\ of\ non-nitrogen\ fixing\ cyanobacteria}$$
$$+ \underbrace{\left(R_{FIX,CYN,TOT,RESP} \cdot P{:}\,C_{FIX,CYN}\right)}_{\substack{Release\ of\ phosphate\ phosphorus\\ by\ total\ respiration\\ of\ nitrogen\ fixing\ cyanobacteria}} + \underbrace{\left(R_{OPA,TOT,RESP} \cdot P{:}\,C_{OPA}\right)}_{Release\ of\ phosphate\ phosphorus\ by\ total\ respiration\ of\ other\ planktonic\ algae}$$
$$+ \underbrace{\left(R_{ZOO,TOT,RESP} \cdot P{:}\,C_{ZOO}\right)}_{\substack{Release\ of\ phosphate\ phosphorus\ by\ total\\ respiration\ of\ zooplankton}} + \underbrace{R_{MIN,DOP}}_{\substack{Release\ of\ phosphate\ phosphorus\ by\\ organic\ phosphorus\ mineralization}}$$
$$- \underbrace{\left(R_{DIA,GROWTH} \cdot P{:}\,C_{DIA}\right)}_{\substack{Uptake\ of\ phosphate\ phosphorus\\ by\ growth\ of\ diatoms}} - \underbrace{\left(R_{NON,FIX,CYN,GROWTH} \cdot P{:}\,C_{NON,FIX,CYN}\right)}_{\substack{Uptake\ of\ phosphate\ phosphorus\ by\ growth\\ of\ non-nitrogen\ fixing\ cyanobacteria}}$$
$$- \underbrace{\left(R_{FIX,CYN,GROWTH} \cdot P{:}\,C_{FIX,CYN}\right)}_{\substack{Uptake\ of\ phosphate\ phosphorus\\ by\ growth\\ of\ nitrogen\ fixing\ cyanobacteria}} - \underbrace{\left(R_{OPA,GROWTH} \cdot P{:}\,C_{OPA}\right)}_{\substack{Uptake\ of\ phosphate\ phosphorus\\ by\ growth\\ of\ other\ planktonic\ algae}}$$

(Equation A.6.2.1)

The notation of Equation A.6.2.1 is given below:

$R_{DIA,TOT,RESP}$: Total respiration rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,TOT,RESP}$: Total respiration rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,TOT,RESP}$: Total respiration rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,TOT,RESP}$: Total respiration rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,TOT,RESP}$: Total respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,GROWTH}$: Growth rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,GROWTH}$: Growth rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,GROWTH}$: Growth rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$P{:}\,C_{DIA}$: Phosphorus to carbon ratio for diatoms (dimensionless)

$P{:}\,C_{NOFIX,CYN}$: Phosphorus to carbon ratio for non-nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{OPA}$: Phosphorus to carbon ratio for other planktonic algae (dimensionless)

$P{:}\,C_{FIX,CYN}$: Phosphorus to carbon ratio for nitrogen fixing cyanobacteria (dimensionless)

$P{:}\,C_{ZOOP}$: Phosphorus to carbon ratio for zooplankton (dimensionless)

$R_{MIN,DON}$: Mineralization rate of dissolved organic nitrogen ($gN \cdot m^{-3} \cdot day^{-1}$)

$P{:}\,C_{DIA}$, $P{:}\,C_{NOFIX,CYN}$, $P{:}\,C_{OPA}$,$P{:}\,C_{FIX,CYN}$ are user entered model constants, whereas, $P{:}\,C_{ZOOP}$, are calculated internally by AQUABC given in previous sections and will therefore not be repeated here.

$R_{DIA,TOT,RESP}$, $R_{NON,FIX,CYN,TOT,RESP}$, $R_{OPA,TOT,RESP}$, $R_{FIX,CYN,TOT,RESP}$ and $R_{ZOO,TOT,RESP}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Mineralization rate of dissolved organic matter is explained in detail in the previous section, so $R_{MIN,DOP}$ will not be repeated here.

A.6.3 Inorganic Silicon

Inorganic silicon is handled using two state variables; namely dissolved silicon and particulate silicon. The main kinetic derivatives for dissolved silicon and particulate silicon are given in Equation A.6.3.1 and Equation A.6.3.2.

$$\frac{d[Si(OH)_4 - Si]}{dt} = R_{DISS,Si} + \underbrace{\left(R_{DIA,TOT,RESP} \cdot Si{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ dissolved\ silicon \\ by\ total\ respiration\ of\ diatoms}} + \underbrace{\left(R_{DIA,EXCR} \cdot Si{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ dissolved\ silicon \\ by\ excretion\ of\ diatoms}} - \underbrace{\left(R_{DIA,GROWTH} \cdot Si{:}\,C_{DIA}\right)}_{\substack{Uptake\ of\ dissolved\ silicon \\ by\ growth\ of\ diatoms}}$$

(Equation A.6.3.1)

$$\frac{d[PSi]}{dt} = \underbrace{\left(R_{DIA,DEATH} \cdot Si{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ particulate\ silicon \\ by\ diatoms\ death}} + \underbrace{\left(R_{ZOO,FEEDING,DIA} \cdot Si{:}\,C_{DIA}\right)}_{\substack{Formation\ of\ particulate\ silicon\ by \\ zooplankton\ grazing\ on\ diatoms}} - \underbrace{R_{DISS,PSi}}_{\substack{Dissolution\ of\ particulate\ silicon \\ to\ dissolved\ silicon}}$$

(Equation A.6.3.2)

The notation of Equation A.6.3.1 and Equation A.6.3.2 are given below:

$R_{DIA,TOT,RESP}$	: Total respiration rate of diatoms ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{DIA,EXCR}$	: Excretion rate of diatoms ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{DIA,GROWTH}$	: Growth rate of diatoms ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{DIA,DEATH}$	: Death rate of diatoms ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{ZOOP,DIA,DEATH}$	: Death rate of diatoms due to grazing by zooplankton ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{ZOO,FEEDING,DIA}$	: Feeding rate of zooplankton on diatoms ($gC{\cdot}m^{-3}{\cdot}day^{-1}$)
$R_{DISS,Si}$	: Dissolution rate of particulate silicon ($gSi{\cdot}m^{-3}{\cdot}day^{-1}$)
$Si{:}\,C_{DIA}$	: Silicon to carbon ratio for diatoms (dimensionless)

$Si{:}\,C_{DIA}$, $Si{:}\,C_{NOFIX,CYN}$, $Si{:}\,C_{OPA}$ and $Si{:}\,C_{FIX,CYN}$ are user entered stoichiometric model constants. $R_{DIA,TOT,RESP}$, $R_{DIA,EXCR}$, $R_{DIA,GROWTH}$ and $R_{DIA,DEATH}$ are given before and will not be

repeated here. See the subsections related to diatoms. $R_{ZOO,FEEDING,DIA}$ is given in section A.2 and will not be repeated here. The dissolution rate of particulate silicon is given in Equation A.6.3.3

$$R_{DISS,POC} = k_{DISS,PSi,20} \cdot \theta_{k,DISS,PSi}^{(TEMP-20)} \cdot [PSi] \quad \text{(Equation A.6.3.3)}$$

The notation of Equation A.6.3.3 is given below

$k_{DISS,PSi,20}$: Dissolution rate constant of particulate silicon at 20˚C (day^{-1})

$\theta_{k,DISS,PSi}$: Arrhenius type temperature correction factor for dissolution rate constant of particulate silicon (dimensionless)

A.6.4 Inorganic Carbon

The main kinetic derivative for inorganic carbon is given in Equation A.6.4.1.

$$\frac{d[DIC]}{dt} = \underbrace{R_{AERATION,DIC}}_{\substack{Exchange\ of\ dissolved\ inorganic\ carbon\ with\ the\ atmosphere\ by\ rearation}} + \underbrace{R_{DIA,TOT,RESP}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ diatom\ respiration}} + \underbrace{R_{CYN,TOT,RESP}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ non-nitrogen\ fixing\ cyanobacteria\ respiration}} +$$

$$\underbrace{R_{FIX,CYN,TOT,RESP}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ nitrogen\ fixing\ cyanobacteria\ respiration}} + \underbrace{R_{OPA,TOT,RESP}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ other\ planktonic\ algae\ respiration}} + \underbrace{R_{ZOO,TOT,RESP}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ zooplankton\ respiration}} +$$

$$\underbrace{R_{DOC,MIN}}_{\substack{Release\ of\ dissolved\ inorganic\ carbon\ by\ dissolved\ organic\ carbon\ mineralization}} - \underbrace{R_{DIA,GROWTH}}_{\substack{Uptake\ of\ dissolved\ inorganic\ carbon\ by\ diatom\ growth}} - \underbrace{R_{CYN,GROWTH}}_{\substack{Uptake\ of\ dissolved\ inorganic\ carbon\ by\ non-nitrogen\ fixing\ cyanobacteria\ growth}} -$$

$$\underbrace{R_{FIX,CYN,GROWTH}}_{\substack{Uptake\ of\ dissolved\ inorganic\ carbon\ by\ nitrogen\ fixing\ cyanobacteria\ growth}} - \underbrace{R_{OPA,GROWTH}}_{\substack{Uptake\ of\ dissolved\ inorganic\ carbon\ by\ other\ planktonic\ algae\ growth}}$$

(Equation A.6.4.1)

The notation of Equation A.6.4.1 is given below:

$R_{DIA,TOT,RESP}$: Total respiration rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,TOT,RESP}$: Total respiration rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,TOT,RESP}$: Total respiration rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,TOT,RESP}$: Total respiration rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{ZOO,TOT,RESP}$: Total respiration rate of zooplankton ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,GROWTH}$: Growth rate of diatoms ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{NOFIX,CYN,GROWTH}$: Growth rate of non-nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{OPA,GROWTH}$: Growth rate of other planktonic algae ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{FIX,CYN,GROWTH}$: Growth rate of nitrogen fixing cyanobacteria ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{MIN,DOC}$: Mineralization rate of dissolved organic carbon ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{AERATION,DIC}$: Exchange rate of dissolved inorganic carbon with atmosphere ($gC \cdot m^{-3} \cdot day^{-1}$)

$R_{DIA,TOT,RESP}$, $R_{NON,FIX,CYN,TOT,RESP}$, $R_{OPA,TOT,RESP}$, $R_{FIX,CYN,TOT,RESP}$, $R_{DIA,GROWTH}$, $R_{NON,FIX,CYN,GROWTH}$, $R_{OPA,GROWTH}$, $R_{FIX,CYN,GROWTH}$ and $R_{ZOO,TOT,RESP}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Mineralization rate of dissolved organic matter is explained in detail in the previous section, so $R_{MIN,DOC}$ will not be repeated here.

Exchange rate of dissolved inorganic carbon with atmosphere is given in Equation A.6.5.2

$$R_{AERATION,DIC} = K_A \cdot 0.923 \cdot ([CO_2]_{SAT} - [H_2CO_3])$$

(Equation A.6.5.2)

The notation of Equation A.6.5.2 is given below:

K_A : Reaeration rate constant for dissolved oxygen (day^{-1})

$[CO_2]_{SAT}$: Saturation concentration of carbon dioxide in water ($moles \cdot L^{-1}$)

$[H_2CO_3]$: Concentration of un dissociated dissolved inorganic carbon ($moles \cdot L^{-1}$)

Reaeration rate constant for dissolved oxygen contains detailed information and will therefore be given in the section related to dissolved oxygen.

Saturation concentration of carbon dioxide in water is calculated based on the Henry formula as given in Equation A.6.5.3.

$$[CO_2]_{SAT} = 10^{\frac{2385.73}{Temp+273.16} - (0.0152642 \cdot (Temp+273.16)) + 14.0184} . 10^{-3.416}$$

(Equation A.6.5.3)

where the first term is the Henry constant for carbon dioxide and the second term is the partial pressure of carbon dioxide in the atmosphere.

Concentration of un dissociated dissolved inorganic carbon is calculated by CO2SYS, which is integrated into AQUABC as a Fortran module.

A.7 ALKALINITY KINETICS

AQUABC considers non-conservative alkalinity where each process that creates positive ions or destroy negative ions would increase the alkalinity. The main kinetic derivative for alkalinity is given in Equation A.7.1

$$\frac{d[Akalinity]}{dt} = \underbrace{R_{ALKALINITY,NH4,GEN}}_{Gain\ of\ alkalinity\ by\ ammonium\ generation} + \underbrace{R_{ALKALINITY,NO3,CONS}}_{Gain\ of\ alkalinity\ by\ nitrate\ consumption} + \underbrace{R_{ALKALINITY,PO4,CONS}}_{Gain\ of\ alkalinity\ by\ phosphate\ consumption}$$
$$- \underbrace{R_{ALKALINITY,N4H,CONS}}_{Loss\ of\ alkalinity\ by\ ammonium\ consumption} - \underbrace{R_{ALKALINITY,PO4,GEN}}_{Loss\ of\ alkalinity\ by\ phosphate\ generation}$$

(Equation A.7.1)

The notation of Equation A.7.1 is given below:

$R_{ALKALINITY,NH4,GEN}$: Gain of alkalinity by ammonium generation (moles·L^{-1}·day^{-1})
$R_{ALKALINITY,NO3,CONS}$: Gain of alkalinity by nitrate consumption (moles·L^{-1}·day^{-1})
$R_{ALKALINITY,PO4,CONS}$: Gain of alkalinity by phosphate consumption (moles·L^{-1}·day^{-1})
$R_{ALKALINITY,N4H,CONS}$: Loss of alkalinity by ammonium consumption (moles·L^{-1}·day^{-1})
$R_{ALKALINITY,PO4,GEN}$: Loss of alkalinity by phosphate generation (moles·L^{-1}·day^{-1})

The process rates in Equation A.7.1 are given in Equations A.7.2-A.7.6:

$$R_{ALKALINITY,NH4,GEN} = \underbrace{\frac{R_{DIA,TOT,RESP} \cdot N{:}\,C_{DIA}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\ generation\\ due\ to\ the\ release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ diatoms}}$$
$$+ \underbrace{\frac{R_{NON,FIX,CYN,TOT,RESP} \cdot N{:}\,C_{NON,FIX,CYN}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\ generation\\ due\ to\ the\ release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ non-nitrogen\ fixing\ cyanobacteria}}$$
$$+ \underbrace{\frac{R_{FIX,CYN,TOT,RESP} \cdot N{:}\,C_{FIX,CYN}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\ generation\\ due\ to\ the\ release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ o\ nitrogen\ fixing\ cyanobacteria}}$$
$$+ \underbrace{\frac{R_{OPA,TOT,RESP} \cdot N{:}\,C_{OPA}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\ generation\\ due\ to\ the\ release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ other\ planktonic\ algae}}$$
$$+ \underbrace{\frac{R_{ZOO,TOT,RESP} \cdot N{:}\,C_{ZOO}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\ generation\\ due\ to\ the\ release\ of\ ammonia\ nitrogen\ by\\ total\ respiration\ of\ zooplankton}} + \underbrace{\frac{R_{MIN,DON}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ gain\ by\ ammonium\\ generation\ due\ to\ the\ release\\ of\ ammonia\ nitrogen\ by\\ dissolved\ organic\ nitrogen\\ mineralization}}$$

(Equation A.7.2)

$$R_{ALKALINITY,NO3,CONS} = \underbrace{\frac{R_{DENITRIFICATION}}{14007}}_{\substack{Alkalinity\ gain\ by\ nitrate\ consumption\ due\ to\ the\ denitrification}} + \underbrace{\frac{R_{DIA,GROWTH} \cdot \left(1 - Pref_{NH4N,DIA}\right) \cdot N{:}\,C_{DIA}}{14007}}_{\substack{Alkalinity\ gain\ by\ nitrate\ consumption\ due\ to\ the\ uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ diatoms}}$$

$$+ \underbrace{\frac{R_{NON,FIX,CYN,GROWTH} \cdot \left(1 - Pref_{NH4N,NON,FIX,CYN}\right) \cdot N{:}\,C_{NON,FIX,CYN}}{14007}}_{Alkalinity\ gain\ by\ nitrate\ consumption\ due\ to\ the\ uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria}$$

$$+ \underbrace{\frac{R_{FIX,CYN,GROWTH} \cdot \left(1 - Pref_{NH4N,FIX,CYN}\right) \cdot N{:}\,C_{FIX,CYN}}{14007}}_{Alkalinity\ gain\ by\ nitrate\ consumption\ due\ to\ the\ uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ nitrogen\ fixing\ cyanobacteria}$$

$$+ \underbrace{\frac{R_{OPA,GROWTH} \cdot \left(1 - Pref_{NH4N,OPA}\right) \cdot N{:}\,C_{OPA}}{14007}}_{Alkalinity\ gain\ bynitrate\ consumption\ due\ to\ the\ uptake\ of\ nitrate\ nitrogen\ by\ growth\ of\ other\ planktonic\ algae}$$

(Equation A.7.3)

$$R_{ALKALINITY,PO4,CONS} = \underbrace{\frac{R_{DIA,GROWTH} \cdot P{:}\,C_{DIA}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Alkalinity\ gain\ by\ phosphate\ consumption\ due\ to\ the\ uptake\ of\ phosphate\ phosphorus\ by\ growth\ of\ diatoms}}$$

$$+ \underbrace{\frac{R_{NON,FIX,CYN,GROWTH} \cdot P{:}\,C_{NON,FIX,CYN}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Alkalinity\ gain\ by\ phosphate\ consumption\ due\ to\ the\ uptake\ of\ phosphate\ phosphorus\ by\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria}}$$

$$+ \underbrace{\frac{R_{FIX,CYN,GROWTH} \cdot P{:}\,C_{FIX,CYN}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Alkalinity\ gain\ by\ phosphate\ consumption\ due\ to\ the\ uptake\ of\ phosphate\ phosphorus\ by\ growth\ of\ nitrogen\ fixing\ cyanobacteria}}$$

$$+ \underbrace{\frac{R_{OPA,GROWTH} \cdot P{:}\,C_{OPA}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Alkalinity\ gain\ by\ phosphate\ consumption\ due\ to\ the\ uptake\ of\ phosphate\ phosphorus\ by\ growth\ of\ other\ planktonic\ algae}}$$

(Equation A.7.4)

$$
\begin{aligned}
&R_{ALKALINITY,N4H,CONS} \\
&= \underbrace{\frac{2 \cdot R_{NITRIFICATION}}{14007} \cdot frac_{NH4N} + \frac{R_{NITRIFICATION}}{14007} \cdot frac_{NH3N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ and\ nitrate \\ generation\ due\ to\ the\ nitrification\ of\ ammonia\ nitrogen \\ to\ nitrate\ nitrogen}} \\
&+ \underbrace{\frac{R_{DIA,GROWTH} \cdot Pref_{NH4N,DIA} \cdot N{:}C_{DIA}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ due\ to\ the\ uptake\ of\ ammonia\ nitrogen \\ by\ growth\ of\ diatoms}} \\
&+ \underbrace{\frac{R_{DIA,GROWTH} \cdot Pref_{NH4N,DIA} \cdot N{:}C_{DIA}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ due\ to\ the\ uptake\ of\ ammonia\ nitrogen \\ by\ growth\ of\ diatoms}} \\
&+ \underbrace{\frac{R_{NON,FIX,CYN,GROWTH} \cdot Pref_{NH4N,NON,FIX,CYN} \cdot N{:}C_{NON,FIX,CYN}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ due\ to\ the\ uptake\ of\ ammonia\ nitrogen\ by \\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria}} \\
&+ \underbrace{\frac{R_{FIX,CYN,GROWTH} \cdot Pref_{NH4N,FIX,CYN} \cdot N{:}C_{FIX,CYN}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ due\ to\ the\ uptake\ of\ ammonia\ nitrogen\ by \\ growth\ of\ nitrogen\ fixing\ cyanobacteria}} \\
&+ \underbrace{\frac{R_{OPA,GROWTH} \cdot Pref_{NH4N,OPA} \cdot N{:}C_{OPA}}{14007} \cdot frac_{NH4N}}_{\substack{Alkalinity\ loss\ by\ ammonium\ consumption\ due\ to\ the\ uptake\ of\ ammonia\ nitrogen\ by \\ growth\ of\ other\ planktonic\ algae}}
\end{aligned}
$$

(Equation A.7.5)

$$
\begin{aligned}
&R_{ALKALINITY,PO4,GEN} \\
&= \underbrace{\frac{R_{MIN,DOP}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Alkalinity\ loss\ by\ phosphate\ generation\ due\ to\ the\ release\ of\ phosphate\ phosphorus \\ by\ organic\ phosphorus\ mineralization}} + \underbrace{\frac{R_{DIA,TOT,RESP} \cdot P{:}C_{DIA}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Release\ of\ phosphate\ phosphorus\ by \\ total\ respiration\ of\ diatoms}} \\
&+ \underbrace{\frac{R_{NON,FIX,CYN,TOT,RESP} \cdot P{:}C_{NON,FIX,CYN}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Release\ of\ phosphate\ phosphorus\ by\ total\ respiration \\ of\ non-nitrogen\ fixing\ cyanobacteria}} \\
&+ \underbrace{\frac{R_{FIX,CYN,TOT,RESP} \cdot P{:}C_{FIX,CYN}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Release\ of\ phosphate\ phosphorus \\ by\ total\ respiration \\ of\ nitrogen\ fixing\ cyanobacteria}} \\
&+ \underbrace{\frac{R_{OPA,TOT,RESP} \cdot P{:}C_{OPA}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Release\ of\ phosphate\ phosphorus\ by\ total \\ respiration\ of\ other\ planktonic\ algae}} \\
&+ \underbrace{\frac{R_{ZOO,TOT,RESP} \cdot P{:}C_{ZOO}}{30974} \cdot PO4_{EQ,CONST}}_{\substack{Release\ of\ phosphate\ phosphorus\ by\ total \\ respiration\ of\ zooplankton}}
\end{aligned}
$$

(Equation A.7.6)

$R_{DIA,TOT,RESP}$, $R_{NON,FIX,CYN,TOT,RESP}$, $R_{OPA,TOT,RESP}$, $R_{FIX,CYN,TOT,RESP}$, $R_{DIA,GROWTH}$, $R_{NON,FIX,CYN,GROWTH}$, $R_{OPA,GROWTH}$, $R_{FIX,CYN,GROWTH}$ and $R_{ZOO,TOT,RESP}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Mineralization rate of dissolved organic matter is explained in detail in the previous section, so $R_{MIN,DOC}$ will not be repeated here.

The notation of Equations A.7.2 - A.7.6 is given below:

$frac_{NH3N}$: Fraction of unionized ammonia nitrogen in total ammonia nitrogen (dimensionless)

$frac_{NH4N}$: Fraction of ionized ammonia nitrogen in total ammonia nitrogen (dimensionless)

$PO4_{EQ,CONST}$: Phosphate equivalent anion constant (dimensionless)

Unionized and ionized ammonia load fractions are given in Equation A.7.7 and Equation A.7.8 respectively.

$$frac_{NH3} = \frac{1}{1 + 10^{0.09018 + \frac{2729.92}{Temp + 273.16} - pH}}$$

(Equation A.7.7)

$$frac_{NH4N} = 1 - frac_{NH3}$$

(Equation A.7.8)

Phosphate equivalent anion constant is calculated the dissociations of phosphoric acid (a three-prothic weak acid) considering the following three equilibrium reactions below:

$$H_3PO_4 \leftrightarrow H_2PO_4^- + H^+$$

$$H_2PO_4^- \leftrightarrow HPO_4^{2-} + H^+$$

$$HPO_4^{2-} \leftrightarrow PO_4^{3-} + H^+$$

where,

$$K_{1,PO4} = \frac{[H_2PO_4^-] \cdot [H^+]}{[H_3PO_4]}$$

(Equation A.7.9)

$$K_{2,PO4} = \frac{[H_2PO_4^-] \cdot [H^+]}{[H_2PO_4^-]}$$

(Equation A.7.10)

$$K_{3,PO4} = \frac{[H_2PO_4^-] \cdot [H^+]}{[H_2PO_4^-]}$$

(Equation A.7.11)

Phosphate equivalent anion constant is given in Equations A.7.12 to A.7.15

$$PO4_{EQ,CONST} = \alpha_{H2PO4} + 2 \cdot \alpha_{HPO4} + 3 \cdot \alpha_{PO4}$$

(Equation A.7.12)

$$\alpha_{H2PO4} = \frac{[H_2PO_4^-]}{[H_3PO_4] + [H_2PO_4^-] + [HPO_4^{2-}] + [PO_4^{3-}]}$$

(Equation A.7.13)

$$\alpha_{HPO4} = \frac{[HPO_4^{2-}]}{[H_3PO_4] + [H_2PO_4^-] + [HPO_4^{2-}] + [PO_4^{3-}]}$$

(Equation A.7.14)

$$\alpha_{PO4} = \frac{[PO_4^{3-}]}{[H_3PO_4] + [H_2PO_4^-] + [HPO_4^{2-}] + [PO_4^{3-}]}$$

(Equation A.7.15)

Combining equations A.7.9 to A.7.11 and A.7.13 to A.7.15, it is possible to derive Equations A.7.16 to A.7.18, which are used together with Equation A.7.12 to yield $PO4_{EQ,CONST}$.

$$\alpha_{H2PO4} = \frac{K_{1,PO4} \cdot [H^+]^2}{[H^+]^3 + K_{1,PO4} \cdot [H^+]^2 + K_{1,PO4} \cdot K_{2,PO4} \cdot [H^+] + K_{1,PO4} \cdot K_{2,PO4} \cdot K_{3,PO4}}$$

(Equation A.7.167)

$$\alpha_{HPO4} = \frac{K_{1,PO4} \cdot K_{2,PO4} \cdot [H^+]}{[H^+]^3 + K_{1,PO4} \cdot [H^+]^2 + K_{1,PO4} \cdot K_{2,PO4} \cdot [H^+] + K_{1,PO4} \cdot K_{2,PO4} \cdot K_{3,PO4}}$$

(Equation A.7.1)

$$\alpha_{PO4} = \frac{K_{1,PO4} \cdot K_{2,PO4} \cdot K_{3,PO4}}{[H^+]^3 + K_{1,PO4} \cdot [H^+]^2 + K_{1,PO4} \cdot K_{2,PO4} \cdot [H^+] + K_{1,PO4} \cdot K_{2,PO4} \cdot K_{3,PO4}}$$

(Equation A.7.18)

The dissociation constants $K_{1,PO4}$ $K_{2,PO4}$ and $K_{3,PO4}$ are calculated by CO2SYS which is integrated into AQUABC.

A.8 DISSOLVED OXYGEN KINETICS

Dissolved oxygen is related to many processes and has therefore a relatively large main equation (Equation A.8.1).

$$\frac{d[O_2]}{dt} = \underbrace{R_{AERATION}}_{\substack{Exchange\ of\ oxygen\ with\ the \\ atmosphere\ by\ reaeretion}} - \underbrace{(4.57 \cdot R_{NITRIFICATION})}_{\substack{Uptake\ of\ dissolved\ oxygen \\ by\ nitrification}} + \underbrace{\left(R_{DIA,GROWTH} \cdot \left(O_2{:}\,C_{DIA} + \frac{48}{14} \cdot \frac{14}{12} \cdot (1 - Pref_{NH4N,DIA})\right)\right)}_{Release\ of\ dissolved\ oxygen\ by\ growth\ of\ diatoms} + \underbrace{\left(R_{NON,FIX,CYN,GROWTH} \cdot \left(O_2{:}\,C_{NON,FIX,CYN} + \frac{48}{14} \cdot \frac{14}{12} \cdot (1 - Pref_{NH4N,NON,FIX,CYN})\right)\right)}_{Release\ of\ dissolved\ oxygen\ by\ growth\ of\ non-nitrogen\ fixing\ cyanobacteria} + \underbrace{\left(R_{FIX,CYN,GROWTH} \cdot \left(O_2{:}\,C_{FIX,CYN} + \frac{48}{14} \cdot \frac{14}{12} \cdot (1 - Pref_{NH4N,FIX,CYN})\right)\right)}_{Release\ of\ dissolved\ oxygen\ by\ growth\ of\ nitrogen\ fixing\ cyanobacteria} + \underbrace{\left(R_{OPA,GROWTH} \cdot \left(O_2{:}\,C_{OPA} + \frac{48}{14} \cdot \frac{14}{12} \cdot (1 - Pref_{NH4N,OPA})\right)\right)}_{Release\ of\ dissolved\ oxygen\ by\ growth\ of\ other\ planktonic\ algae} - \underbrace{(R_{DIA,TOT,RESP} \cdot O_2{:}\,C_{DIA})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by\ total \\ respiration\ of\ diatoms}} - \underbrace{(R_{NON,FIX,CYN,TOT,RESP} \cdot O_2{:}\,C_{NON,FIX,CYN})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by\ total\ respiration \\ of\ non-nitrogen\ fixing\ cyanobacteria}} - \underbrace{(R_{FIX,CYN,TOT,RESP} \cdot O_2{:}\,C_{FIX,CYN})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by\ total\ respiration \\ of\ nitrogen\ fixing\ cyanobacteria}} - \underbrace{(R_{OPA,TOT,RESP} \cdot O_2{:}\,C_{OPA})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by\ total \\ respiration\ of\ other\ planktonic\ algae}} - \underbrace{(R_{ZOO,TOT,RESP} \cdot O_2{:}\,C_{ZOO})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by\ total \\ respiration\ of\ zooplankton}} - \underbrace{(R_{MIN} \cdot O_2{:}\,C_{DOC})}_{\substack{Uptake\ of\ dissolved\ oxygen\ by \\ organic\ matter\ mineralization}}$$

(Equation A.8.1)

$R_{DIA,GROWTH}$, $R_{NON,FIX,CYN,GROWTH}$, $R_{OPA,GROWTH}$ and $R_{FIX,CYN,GROWTH}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, and nitrogen fixing cyanobacteria.

$R_{DIA,TOT,RESP}$, $R_{NON,FIX,CYN,TOT,RESP}$, $R_{OPA,TOT,RESP}$, $R_{FIX,CYN,TOT,RESP}$ and $R_{ZOO,TOT,RESP}$ are given before and will not be repeated here. See the subsections related to diatoms, non-nitrogen fixing cyanobacteria, other planktonic algae, nitrogen fixing cyanobacteria and zooplankton.

Mineralization rate of dissolved organic matter is explained in detail in the previous section, so $R_{MIN,DOC}$ will not be repeated here.

$R_{NITRIFICATION}$, which is the nitrification rate is given before and will not be repeated here.

The notation of Equation A.8.1 is given below:

$O_2 : C_{DIA}$: Stochiometric ratio of oxygen to carbon for diatoms (dimensionless)

$O_2 : C_{NON,FIX,CYN}$: Stochiometric ratio of oxygen to carbon for non-nitrogen fixing Cyanobacteria (dimensionless)

$O_2 : C_{FIX,CYN}$: Stochiometric ratio of oxygen to carbon for nitrogen fixing Cyanobacteria (dimensionless)

$O_2 : C_{OPA}$: Stochiometric ratio of oxygen to carbon for other planktonic algae (dimensionless)

$O_2 : C_{ZOO}$: Stochiometric ratio of oxygen to carbon for zooplankton (dimensionless)

$O_2 : C_{DOC}$: Stochiometric ratio of oxygen to carbon for dissolved organic Matter (dimensionless)

$R_{AERATION}$: Reaeration rate ($gO_2 \cdot m^{-3} \cdot day^{-1}$)

The reaeration rate is calculated using Equation A.8.2

$$R_{AERATION} = K_A \cdot ([O_2]_{SAT} - [O_2])$$

The notation of Equation A.8.2 is given below:

$[O_2]_{SAT}$: Saturation concentration of dissolved oxygen ($gO_2 \cdot m^{-3}$)
K_A : The reaeration rate constant (day^{-1})

The saturation concentration of dissolved oxygen is calculated using Equation A.8.3

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

The notation of Equation A.8.3 is given below:

o_{sf} : Saturation concentration of dissolved oxygen in saline water at sea level ($gO_2 \cdot m^{-3}$)
P : Atmospheric pressure (atm)
P_w : Partial pressure of water vapour (atm)
θ : Temperature dependent parameter

Temperature dependent parameter is calculated using Equation A.8.4

$$\theta = 0.000975 - 1.426 \cdot 10^{-5} \mathrm{Temp} + 6.436 \cdot 10^{-8} \mathrm{Temp}^2 \quad \text{(Equation A.8.4)}$$

Partial pressure of water vapour is calculated using Equation A.8.5.

$$P_w = \exp\left(11.8571 - \frac{3840.7}{\mathrm{Temp} + 273.16} - \frac{216961}{(\mathrm{Temp} + 273.16)^2}\right) \quad \text{(Equation A.8.5)}$$

The air pressure is calculated using Equation A.8.6.

$$P = 1 - 0.0875 \cdot H \quad \text{(Equation A.8.6)}$$

The notation of Equation A.8.6 is given below:

H : Elevation of the water surface above the mean sea level (m)

The saturation concentration of dissolved oxygen in saline water at sea level is calculated using Equation A.8.7

$$\ln(o_{ss}) = \ln(o_{sf}) - S \cdot \left(1.7674 \cdot 10^{-2} - \frac{10.7540}{T + 273.16} + \frac{2140.7\ 10^3}{(T + 273.16)^2}\right) \quad \text{(Equation A.8.7)}$$

The notation of Equation A.8.6 is given below:

S : Salinity (ppt)
T : Water temperature (°C)
o_{sf} : Saturation concentration of dissolved oxygen in fresh water at sea level ($gO_2 \cdot m^{-3}$)

Saturation concentration of dissolved oxygen in fresh water at sea level is calculated using Equation A.8.8

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

(Equation A.8.8)

The reaeration rate constant is either entered by the user as a model constant or internally calculated by AQUABC. In case of internal calculation, tge reaeration rate constant (day^{-1}) is calculated as a function of wind speed, air and water temperature, and depth using one of three formulas given in Equations A.8.9, A.8.10 and A.8.11.

$$K_A = \frac{86400}{100 \cdot D_j} \cdot \left(\frac{D_{OW}}{\nu_W}\right)^{2/3} \cdot \left(\frac{\rho_a}{\rho_W}\right)^{1/2} \frac{\kappa^{1/3}}{\Gamma} \cdot \sqrt{C_d}\,(100 \cdot W) \quad \text{(Equation A.8.9)}$$

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

(Equation A.8.10)

$$K_A = \frac{86400}{100 \cdot D_j} \cdot \left(\frac{D_{OW} \cdot \rho_a \cdot v_a \cdot \sqrt{C_d}}{\kappa \cdot z_0 \cdot \rho_W \cdot v_W} \right)^{1/2} \cdot \sqrt{100 \cdot W}$$ (Equation A.8.11)

The notation of equations A.8.9, A.8.10 and A.8.11 is given below:

w wind speed at 10 cm above surface ($m \cdot s^{-1}$)

T_a air temperature (°C)

ρ_a density of air, a function of T_a ($g \cdot cm^{-3}$)

ρ_w density of water assumed as 1.0 ($g \cdot cm^{-3}$)

v_a viscosity of air as a function of T_a ($cm^2 \cdot s^{-1}$)

v_W viscosity of water, a function of T ($cm^2 \cdot s^{-1}$)

D_{OW} diffusivity of oxygen in water as a function of T ($cm^2 \cdot s^{-1}$)

κ von Karman's coefficient (0.4)

v_t transitional shear velocity, set to 9, 10, and 10 for small, medium, and large scales ($cm^2 \cdot s^{-1}$)

v_c critical shear velocity, set to 22, 11, and 11 for small, medium, and large scales ($cm^2 \cdot s^{-1}$)

z_e equivalent roughness, set to 0.25, 0.35, and 0.35 for small, medium, and large scales (cm)

z_0 effective roughness as a function of z_e, Γ, C_d, v_t, v_a, and W (cm)

λ inverse of Reynolds number, set to 10, 3, and 3 for small, medium, and large scales

Γ non dimensional coefficient, set to 10, 6.5, and 5 for small, medium, and large scales

Γ_u non dimensional coefficient, a function of Γ, v_c, C_d, and W

C_d drag coefficient as a function of z_e, Γ, v_a, κ, v_t, and W

Equation A.8.9 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 A.8.10 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 A.8.10 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 B : MODEL CONSTANTS AND THEIR VALUES AFTER PRELIMINARY CALIBRATION

B.1 Model Constants Related to Diatoms

Symbol	Description	Unit	Calibrated value
$k_{G,DIA,MAX}$	Growth rate constant for diatoms at optimum conditions	day^{-1}	1.80
$eff_{DIA,GROWTH}$	Efficiency of diatom growth	dimensionless	0.95[a]
$TEMP_{LOWER,\ OPT,\ DIA}$	Lower limit of the optimum temperature for the growth of the diatoms	C°	3.00
$TEMP_{UPPER,\ OPT,\ DIA}$	Upper limit of the optimum temperature for the growth of the diatoms	C°	24.00
$\kappa_{LOWER,\ DIA}$	Exponent for the temperatures below the lower limit of the optimum temperature for the growth of diatoms	dimensionless	0.04
$\kappa_{UPPER,\ DIA}$	Exponent for the temperatures above the upper limit of the optimum temperature for the growth of diatoms	dimensionless	0.06
$k_{R,DIA,20}$	Dark respiration rate constant of diatoms at 20°C	day^{-1}	0.025[a]
$\theta_{k,R,DIA}$	Arrhenius-type temperature correction coefficient for dark respiration rate constant of diatoms	dimensionless	1.04
$k_{D,DIA,20}$	Death rate constant of diatoms at 20°C	day^{-1}	0.03[a]
$\theta_{k,D,DIA}$	Arrhenius-type temperature correction coefficient for death rate constant of diatoms	dimensionless	1.02
$k_{HS,DIN,DIA}$	Monod type half-saturation concentration of diatom growth for dissolved inorganic nitrogen	$gN \cdot m^{-3}$	0.03
$k_{HS,DIP,DIA}$	Monod type half-saturation concentration of diatom growth for dissolved inorganic phosphorus	$gP \cdot m^{-3}$	0.01
$k_{HS,DSi,DIA}$	Monod type half-saturation concentration of diatom growth for dissolved inorganic silicon	$gSi \cdot m^{-3}$	0.150
$k_{HS,O2,DIA}$	Monod type half-saturation concentration of diatom growth for dissolved oxygen	$gO_2 \cdot m^{-3}$	0.6
$frac_{DIA,EXCR}$	Fraction of metabolic waste excreted as DOC	dimensionless	0.3
$I_{S,DIA}$	Light saturation constant for diatoms	langleys	200
$[O_2]_{HYPOX,\ STRESS,\ DIA}$	Threshold concentration of dissolved oxygen for hypoxia stress for diatoms	$gO_2 \cdot m^{-3}$	0.7
$coeff_{HYPOX,\ DEATH,\ DIA}$	Multiplier at the exponent to calculate the dissolved oxygen lack stress related death acceleration factor for diatoms	dimensionless	1.2
$\theta_{\ HYPOX,\ DEATH,\ DIA}$	Exponent base to calculate the dissolved oxygen lack stress related death acceleration factor for diatoms	dimensionless	1.04
$N: C_{DIA}$	Nitrogen to carbon ratio for diatoms	dimensionless	0.18[a]
$P: C_{DIA}$	Phosphorus to carbon ratio for diatoms	dimensionless	0.024
$Si: C_{DIA}$	Silicon to carbon ratio for diatoms	dimensionless	0.25
$O_2: C_{DIA}$	Oxygen to carbon ratio for diatoms	dimensionless	2.66
$C: CHLA_{DIA}$	Carbon to Chlorophyll-A value for diatoms	dimensionless	30

[a] Calibrated value.

B.2 Model Constants Related to Non-Nitrogen Fixing Cyanobacteria

Symbol	Description	Unit	Calibrated value
$k_{G,NOFIX,CYN,MAX}$	Growth rate constant for non-nitrogen fixing cyanobacteria at optimum conditions	day^{-1}	4.5[a]
$eff_{NOFIX,CYN,GROWTH}$	Efficiency of non-nitrogen fixing cyanobacteria growth	dimensionless	0.90
$TEMP_{LOWER,\ OPT,NONFIX,\ CYN}$	Lower limit of the optimum temperature for the growth of the non-nitrogen fixing cyanobacteria	C°	16.00
$TEMP_{UPPER,\ OPT,\ NONFIX,\ CYN}$	Upper limit of the optimum temperature for the growth of the non-nitrogen fixing cyanobacteria	C°	26.00
$\kappa_{LOWER,\ NONFIX,\ CYN}$	Exponent for the temperatures below the lower limit of the optimum temperature for the growth of non-nitrogen fixing cyanobacteria	dimensionless	0.10[a]
$\kappa_{UPPER,\ NONFIX,\ CYN}$	Exponent for the temperatures above the upper limit of the optimum temperature for the growth of non-nitrogen fixing cyanobacteria	dimensionless	0.10[a]
$k_{R,NOFIX,CYN,20}$	Dark respiration rate constant of non-nitrogen fixing cyanobacteria at 20˚C	day^{-1}	0.06
$\theta_{k,R,NOFIX,CYN}$	Arrhenius-type temperature correction coefficient for dark respiration rate constant of non-nitrogen fixing cyanobacteria	dimensionless	1.04
$k_{D,NOFIX,CYN,20}$	Death rate constant of non-nitrogen fixing cyanobacteria at 20˚C	day^{-1}	0.05[a]
$\theta_{k,D,NOFIX,CYN}$	Arrhenius-type temperature correction coefficient for death rate constant of non-nitrogen fixing cyanobacteria	dimensionless	1.05
$k_{HS,DIN,NOFIX,CYN}$	Monod type half-saturation concentration of non-nitrogen fixing growth for dissolved inorganic nitrogen	$gN \cdot m^{-3}$	0.03[a]
$k_{HS,DIP,NOFIX,CYN}$	Monod type half-saturation concentration of non-nitrogen fixing growth for dissolved inorganic phosphorus	$gP \cdot m^{-3}$	0.001[a]
$k_{HS,O2,NOFIX,CYN}$	Monod type half-saturation concentration of non-nitrogen fixing growth for dissolved oxygen	$gO_2 \cdot m^{-3}$	0.6
$frac_{NOFIX,CYN,EXCR}$	Fraction of metabolic waste excreted as DOC	dimensionless	0.3
$I_{S,NOFIX,CYN}$	Light saturation constant for non-nitrogen fixing cyanobacteria	langleys	200.0
$[O_2]_{HYPOX\ STRESS,\ NONFIX,\ CYN}$	Threshold concentration of dissolved oxygen for hypoxia stress for non-nitrogen fixing cyanobacteria	$gO_2 \cdot m^{-3}$	0.7
$coeff_{HYPOX,\ DEATH,\ NONFIX,\ CYN}$	Multiplier to calculate the dissolved oxygen lack stress related death acceleration factor for non-nitrogen fixing cyanobacteria	dimensionless	1.5
$\theta_{HYPOX,\ DEATH,\ NONFIX,\ CYN}$	Multiplier at the exponent base to calculate the dissolved oxygen lack stress related death acceleration factor for non-nitrogen fixing cyanobacteria	dimensionless	1.1
$N: C_{NOFIX,CYN}$	Nitrogen to carbon ratio for non-nitrogen fixing cyanobacteria	dimensionless	0.18[a]
$P: C_{NOFIX,CYN}$	Phosphorus to carbon ratio for non-nitrogen fixing cyanobacteria	dimensionless	0.024
$O_2: C_{NOFIX,CYN}$	Oxygen to carbon ratio for non-nitrogen fixing cyanobacteria	dimensionless	2.66
$C: CHLA_{NOFIX,CYN}$	Carbon to Chlorophyll-A value for non-nitrogen fixing cyanobacteria	dimensionless	40

[a] Calibrated value.

B.3 Model Constants Related to Nitrogen Fixing Cyanobacteria

Symbol	Description	Unit	Calibrated value
$k_{G,FIX,CYN,MAX}$	Growth rate constant for nitrogen fixing cyanobacteria at optimum conditions	day^{-1}	3[a]
$eff_{FIX,CYN,GROWTH}$	Efficiency of nitrogen fixing cyanobacteria growth	dimensionless	0.95[a]
$TEMP_{LOWER,\ OPT,\ FIX,\ CYN}$	Lower limit of the optimum temperature for the growth of the nitrogen fixing cyanobacteria	C˚	20.00[a]
$TEMP_{UPPER,\ OPT,\ FIX,\ CYN}$	Upper limit of the optimum temperature for the growth of the nitrogen fixing cyanobacteria	C˚	26.00
$\kappa_{LOWER,\ FIX,\ CYN}$	Exponent for the temperatures below the lower limit of the optimum temperature for the growth of nitrogen fixing cyanobacteria	dimensionless	0.10[a]
$\kappa_{UPPER,\ FIX,\ CYN}$	Exponent for the temperatures above the upper limit of the optimum temperature for the growth of nitrogen fixing cyanobacteria	dimensionless	0.10[a]
$k_{R,FIX,CYN,20}$	Dark respiration rate constant of nitrogen fixing cyanobacteria at 20˚C	day^{-1}	0.06
$\theta_{k,R,FIX,CYN}$	Arrhenius-type temperature correction coefficient for dark respiration rate constant of nitrogen fixing cyanobacteria	dimensionless	1.04
$k_{D,FIX,CYN,20}$	Death rate constant of nitrogen fixing cyanobacteria at 20˚C	day^{-1}	0.12
$\theta_{k,D,FIX,CYN}$	Arrhenius-type temperature correction coefficient for death rate constant of nitrogen fixing cyanobacteria	dimensionless	1.05
$k_{HS,DIN,FIX,CYN}$	Monod type half-saturation concentration of nitrogen fixing growth for dissolved inorganic nitrogen	$gN \cdot m^{-3}$	0.03[a]
$k_{HS,DIP,FIX,CYN}$	Monod type half-saturation concentration of nitrogen fixing growth for dissolved inorganic phosphorus	$gP \cdot m^{-3}$	0.000025
$k_{HS,O2,FIX,CYN}$	Monod type half-saturation concentration of nitrogen fixing growth for dissolved oxygen	$gO_2 \cdot m^{-3}$	0.6
$I_{S,FIX,CYN}$	Light saturation constant for nitrogen fixing cyanobacteria	langleys	0.3
$[O_2]_{HYPOX\ STRESS,\ FIX,\ CYN}$	Threshold concentration of dissolved oxygen for hypoxia stress for nitrogen fixing cyanobacteria	$gO_2 \cdot m^{-3}$	200.0
$coeff_{HYPOX,\ DEATH,\ FIX,\ CYN}$	Multiplier at the exponent to calculate the dissolved oxygen lack stress related death acceleration factor for nitrogen fixing cyanobacteria	dimensionless	0.7
$\theta_{HYPOX,\ DEATH,\ FIX,\ CYN}$	Exponent base to calculate the dissolved oxygen lack stress related death acceleration factor for nitrogen fixing cyanobacteria	dimensionless	1.5
$I_{S,FIX,CYN}$	Light saturation constant for nitrogen fixing cyanobacteria	langleys	1.1
$N: C_{FIX,CYN}$	Nitrogen to carbon ratio for nitrogen fixing cyanobacteria	dimensionless	0.18[a]
$P: C_{FIX,CYN}$	Phosphorus to carbon ratio for nitrogen fixing cyanobacteria	dimensionless	0.047[a]
$O_2: C_{FIX,CYN}$	Oxygen to carbon ratio for nitrogen fixing cyanobacteria	dimensionless	2.66
$C: CHLA_{FIX,CYN}$	Carbon to Chlorophyll-A value for nitrogen fixing cyanobacteria	dimensionless	40
r_{FIX}	Effectivity parameter when cyanobacteria switch to nitrogen fixing state	dimensionless	1.0[a]
$k_{HS,NFIX}$	Monod type half-saturation concentration of nitrogen fixing cyanobacteria growth for dissolved inorganic nitrogen to continuously switch off the nitrogen fixation process. This constant is used in a reversed way compared to standard Monod model. In this approach, increase of available nitrogen concentration for uptake will diminish nitrogen fixation	$gN \cdot m^{-3}$	0.008

[a] Calibrated value.

B.4 Model Constants Related to Other Planktonic Algae

Symbol	Description	Unit	Calibrated value
$k_{G,OPA,MAX}$	Growth rate constant for other planktonic algae at optimum conditions	day^{-1}	2
$eff_{OPA,GROWTH}$	Efficiency of other planktonic algae growth	dimensionless	0.90[a]
$TEMP_{LOWER,\ OPT,\ OPA}$	Lower limit of the optimum temperature for the growth of the other planktonic algae	C°	12.00
$TEMP_{UPPER,\ OPT,\ OPA}$	Upper limit of the optimum temperature for the growth of the other planktonic algae	C°	20.00
$\kappa_{LOWER,\ OPA}$	Exponent for the temperatures below the lower limit of the optimum temperature for the growth of other planktonic algae	dimensionless	0.05
$\kappa_{UPPER,\ OPA}$	Exponent for the temperatures above the upper limit of the optimum temperature for the growth other planktonic algae	dimensionless	0.10
$k_{R,OPA,20}$	Dark respiration rate constant of other planktonic algae at 20˚C	day^{-1}	0.03[a]
$\theta_{k,R,OPA}$	Arrhenius-type temperature correction coefficient for dark respiration rate constant of other planktonic algae	dimensionless	1.02
$k_{D,OPA20}$	Death rate constant of other planktonic algae at 20˚C	day^{-1}	0.03
$\theta_{k,D,OPA}$	Arrhenius-type temperature correction coefficient for death rate constant of other planktonic algae	dimensionless	1.02
$k_{HS,DIN,OPA}$	Monod type half-saturation concentration of other planktonic algae growth for dissolved inorganic nitrogen	$gN \cdot m^{-3}$	0.03[a]
$k_{HS,DIP,OPA}$	Monod type half-saturation concentration of other planktonic algae growth for dissolved inorganic phosphorus	$gP \cdot m^{-3}$	0.015
$k_{HS,O2,OPA}$	Monod type half-saturation concentration of other planktonic algae growth for dissolved oxygen	$gO_2 \cdot m^{-3}$	0.6
$frac_{OPA,EXCR}$	Fraction of metabolic waste excreted as DOC	dimensionless	0.3
$I_{S,OPA}$	Light saturation constant for other planktonic algae	langleys	300.0
$[O_2]_{HYPOX\ STRESS,\ OPA}$	Threshold concentration of dissolved oxygen for hypoxia stress for other planktonic algae	$gO_2 \cdot m^{-3}$	0.70
$coeff_{HYPOX,\ DEATH,\ OPA}$	Multiplier at the exponent to calculate the dissolved oxygen lack stress related death acceleration factor for other planktonic algae	dimensionless	1.20
$\theta_{HYPOX,\ DEATH,\ OPA}$	Exponent base to calculate the dissolved oxygen lack stress related death acceleration factor for other planktonic algae	dimensionless	1.04
$N:C_{OPA}$	Nitrogen to carbon ratio for other planktonic algae	dimensionless	0.180[a]
$P:C_{OPA}$	Phosphorus to carbon ratio for other planktonic algae	dimensionless	0.024
$O_2:C_{OPA}$	Oxygen to carbon ratio for other planktonic algae	dimensionless	2.66
$C:CHLA_{OPA}$	Carbon to Chlorophyll-A value for other planktonic algae	dimensionless	30.00

[a] Calibrated value.

B.5 Model Constants Related to Zooplankton

Symbol	Description	Unit	Calibrated value
$k_{G,ZOO,MAX}$	Growth rate constant for zooplankton at optimum conditions	day^{-1}	0.8[a]
$eff_{ZOO,GROWTH}$	Efficiency of zooplankton growth	dimensionless	0.80
$TEMP_{LOWER,\ OPT,\ ZOO}$	Lower limit of the optimum temperature for the growth of the zooplankton	C°	8.00[a]
$TEMP_{UPPER,\ OPT,\ ZOO}$	Upper limit of the optimum temperature for the growth of the zooplankton	C°	15.00[a]
$\kappa_{LOWER,\ ZOO}$	Exponent for the temperatures below the lower limit of the optimum temperature for the growth of zooplankton	dimensionless	0.02[a]
$\kappa_{UPPER,\ ZOO}$	Exponent for the temperatures above the upper limit of the optimum temperature for the growth zooplankton	dimensionless	0.04[a]
$mult_{k,G,ZOO,DIA}$	Zooplankton growth rate constant multiplier for diatoms as food source	dimensionless	1.00
$mult_{k,G,ZOO,NOFIX,CYN}$	Zooplankton growth rate constant multiplier for non-nitrogen fixing cyanobacteria as food source	dimensionless	1.00
$mult_{k,G,ZOO,OPA}$	Zooplankton growth rate constant multiplier for other planktonic as food source	dimensionless	1.00
$mult_{k,G,ZOO,FIX,CYN}$	Zooplankton growth rate constant multiplier for nitrogen fixing cyanobacteria as food source	dimensionless	1.00
$mult_{k,G,ZOO,DET,PART}$	Zooplankton growth rate constant multiplier for particulate detrital carbon as food source	dimensionless	0.3[a]
$PREF_{ZOO,DIA}$	Preference of zooplankton on diatoms as a food source	$gC{\cdot}m^{-3}$	0.06[a]
$PREF_{ZOO,NOFIX,CYN}$	Preference of zooplankton on non-nitrogen fixing cyanobacteria as a food source	$gC{\cdot}m^{-3}$	0.05[a]
$PREF_{ZOO,FIX,CYN}$	Preference of zooplankton on nitrogen fixing cyanobacteria as a food source	$gC{\cdot}m^{-3}$	0.07
$PREF_{ZOO,OPA}$	Preference of zooplankton on other planktonic algae as a food source	$gC{\cdot}m^{-3}$	0.05[a]
$PREF_{ZOO,DET,PART}$	Preference of zooplankton on other particulate detritus as a food source	$gC{\cdot}m^{-3}$	0.77
$k_{HS,DIA,ZOO}$	Zooplankton half saturation growth for diatoms	$gC{\cdot}m^{-3}$	0.10
$k_{HS,NOFIX,CYN,ZOO}$	Zooplankton half saturation growth for non-fixing cyanobacteria	$gC{\cdot}m^{-3}$	0.07
$k_{HS,FIX,CYN,ZOO}$	Zooplankton half saturation growth for fixing Cyanobacteria	$gC{\cdot}m^{-3}$	0.07
$k_{HS,OPA,ZOO}$	Zooplankton half saturation growth for other planktonic algae	$gC{\cdot}m^{-3}$	0.15
$k_{HS,DET,PART,ZOO}$	Zooplankton half saturation growth for particulate organic carbon	$gC{\cdot}m^{-3}$	0.5
$FOOD_{MIN,ZOO}$	Zooplankton minimum food concentration for feeding	$gC{\cdot}m^{-3}$	0.02
$k_{R,ZOO,20}$	Dark respiration rate constant of zooplankton at 20˚C	day^{-1}	0.1[a]
$\theta_{k,R,ZOO}$	Arrhenius-type temperature correction coefficient for dark respiration rate constant of zooplankton	dimensionless	1.08[a]
$k_{D,ZOO20}$	Death rate constant of zooplankton at 20˚C	day^{-1}	0.25[a]
$\theta_{k,D,ZOO}$	Arrhenius-type temperature correction coefficient for death rate constant of zooplankton	dimensionless	1.08[a]
$k_{HS,O2,ZOO}$	Monod type half-saturation concentration of zooplankton growth for dissolved oxygen	$gO_2{\cdot}m^{-3}$	1.20
$frac_{ZOO,EXCR}$	Fraction of metabolic waste excreted as DOC	dimensionless	0.30
$[O_2]_{HYPOX\ STRESS,\ ZOO}$	Threshold concentration of dissolved oxygen for hypoxia stress for zooplankton	$gO_2{\cdot}m^{-3}$	2.00
$coeff_{HYPOX,\ DEATH,\ ZOO}$	Multiplier at the exponent to calculate the dissolved oxygen lack stress related death acceleration factor for zooplankton	dimensionless	1.06
$\theta_{HYPOX,\ DEATH,\ ZOO}$	Exponent base to calculate the dissolved oxygen lack stress related death acceleration factor for zooplankton	dimensionless	1.20
$O_2:C_{ZOO}$	Oxygen to carbon ratio for zooplankton	dimensionless	2.66

[a] Calibrated value.

B.6 Model Constants Related to Detrital Particulate Organic Matter

Symbol	Description	Unit	Calibrated value
$k_{DISS,DET,POC,20}$	Dissolution rate constant of detritus particulate organic carbon due to "abiotic processes" at 20˚C	day^{-1}	0.001[a]
$FAC_{PHYT,DET,POC}$	Multiplier for phytoplankton mediated particulate detritus carbon dissolution rate constant	$gC^{-1}\cdot m^3\cdot day^{-1}$	0.01
$\theta_{k,DISS,DET,POC}$	Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic carbon	dimensionless	1.00[a]
$k_{DISS,DET,PON,20}$	PON dissolution rate not dependent on phytoplankton	$gN\cdot m^{-3}\cdot day^{-1}$	0.06[a]
$FAC_{PHYT,DET,PON}$	Multiplier for phytoplankton mediated particulate detritus nitrogen dissolution rate constant	$gN^{-1}\cdot m^3\cdot day^{-1}$	0.01[a]
$\theta_{k,DISS,DET,PON}$	Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic nitrogen	dimensionless	1.09[a]
$k_{HS,DISS,DIN}$	Reversed Monod-Type half saturation concentration for dissolved inorganic nitrogen to slow down phytoplankton mediated detrital particulate nitrogen dissolution if dissolved inorganic nitrogen is abundant	$gN\cdot m^{-3}$	0.15[a]
$k_{DISS,DET,POP,20}$	POP phosphorus dissolution rate not dependent on phytoplankton	$gP\cdot m^{-3}\cdot day^{-1}$	0.15[a]
$FAC_{PHYT,DET,POP}$	Multiplier for phytoplankton mediated particulate detritus phosphorus dissolution rate constant	$gP^{-1}\cdot m^3\cdot day^{-1}$	0.03[a]
$\theta_{k,DISS,DET,POP}$	Arrhenius type temperature correction factor for dissolution rate constant of detritus particulate organic phosphorus	dimensionless	1.09[a]
$k_{HS,DISS,DIP}$	Reversed Monod-Type half saturation concentration for dissolved inorganic phosphorus to slow down phytoplankton mediated detrital particulate phosphorus dissolution if dissolved inorganic phosphorus is abundant	$gP\cdot m^{-3}$	0.020[a]
$k_{DISS,PSi,20}$	Dissolution rate constant of particulate silicon at 20˚C	day^{-1}	0.001
$\theta_{k,DISS,PSi}$	Arrhenius type temperature correction factor for dissolution rate constant of particulate silicon	dimensionless	1.04
$FAC_{PHYT,MIN,DOC}$	DOC phytoplankton linear factor for mineralisation rate	$gC\cdot m^{-3}\cdot day^{-1}$	0.05[a]
$k_{HS,MIN,DIN}$	Reversed Monod-Type half saturation concentration for dissolved inorganic nitrogen to slow down phytoplankton mediated dissolved organic nitrogen mineralization if dissolved inorganic nitrogen is abundant	$gN\cdot m^{-3}$	0.05
$FAC_{PHYT,MIN,DON}$	DON phytoplankton linear factor for mineralisation rate	$gN\cdot m^{-3}\cdot day^{-1}$	0.005[a]
$k_{HS,MIN,DIP}$	Reversed Monod-Type half saturation concentration for dissolved inorganic nitrogen to slow down phytoplankton mediated dissolved organic phosphorus mineralization if dissolved inorganic phosphorus is abundant	$gP\cdot m^{-3}$	0.025
$FAC_{PHYT,MIN,DOP}$	DOP phytoplankton linear factor for mineralisation rate	$gP\cdot m^{-3}\cdot day^{-1}$	0.01[a]

[a] Calibrated value.

B.7 Model Constants Related to Dissolved Organic Carbon

Symbol	Description	Unit	Calibrated value
$k_{MIN,DOC,DOXY,20}$	Mineralization rate constant of dissolved organic carbon due to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor	day^{-1}	0.125[a]
$k_{MIN,DOC,NO3,20}$	Mineralization rate constant of dissolved organic carbon due to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor	day^{-1}	0.025
$\theta_{MIN,DOC,DOXY}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic carbon, where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.00[a]
$\theta_{MIN,DOC,NO3}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic carbon, where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.04
$k_{HS,DOC,MIN,DOXY}$	Monod type half saturation concentration of dissolved organic carbon for dissolved organic carbon mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic carbon as substrate	$gC \cdot m^{-3}$	0.00
$k_{HS,DOC,MIN,NO3}$	Monod type half saturation concentration of dissolved organic carbon for dissolved organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic carbon as substrate	$gC \cdot m^{-3}$	1.00
$k_{HS,DOXY,RED,LIM}$	Monod type half saturation concentration of dissolved oxygen for dissolved organic carbon mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved oxygen as oxidizing agent	$gO_2 \cdot m^{-3}$	1.00
$k_{HS,NO3,RED,LIM}$	Monod type half saturation concentration of nitrate nitrogen for dissolved organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of nitrate as oxidizing agent	$gN \cdot m^{-3}$	1.00
$k_{HS,DOXY,RED,INHIB}$	Reversed Monod type half saturation concentration of dissolved oxygen dissolved for organic carbon mineralization, where nitrate is utilized as final electron acceptor simulating the inhibiting effects of the lack of presence dissolved oxygen competing as an energetically more efficient oxidizing agent than nitrate ($gO_2 \cdot m^{-3}$)	$gO_2 \cdot m^{-3}$	0.10
$pH_{LOWER,OPT,DOC,MIN,DOXY}$	Minimum value for optimum pH for dissolved ogranic carbon minerlization with dissolved oxygen as the final electron acceptor		6.00
$pH_{UPPER,OPT,DOC,MIN,DOXY}$	Maximum value for optimum pH for dissolved ogranic carbon minerlization with dissolved oxygen as the final electron acceptor		9.00
$pH_{LOWER,OPT,DOC,MIN,NO3}$	Minimum value for optimum pH for dissolved ogranic carbon minerlization with nitrate as the final electron acceptor		6.00
$pH_{UPPER,OPT,DOC,MIN,NO3}$	Maximum value for optimum pH for dissolved ogranic carbon minerlization with nitrate as the final electron acceptor		9.00

[a] Calibrated value.

B.8 Model Constants Related to Dissolved Organic Nitrogen

Symbol	Description	Unit	Calibrated value
$k_{MIN,DON,DOXY,20}$	Mineralization rate constant of dissolved organic phosphorus due to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor	day^{-1}	0.010[a]
$k_{MIN,DON,NO3,20}$	Mineralization rate constant of dissolved organic phosphorus due to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor	day^{-1}	0.0012
$\theta_{MIN,DON,DOXY}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus , where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.08
$\theta_{MIN,DON,NO3}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus , where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.08
$k_{HS,DON,MIN,DOXY}$	Monod type half saturation concentration of dissolved organic phosphorus for dissolved organic phosphorus mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic carbon as substrate	$gP \cdot m^{-3}$	0.00
$k_{HS,DON,MIN,NO3}$	Monod type half saturation concentration of dissolved organic phosphorus or dissolved organic phosphorus mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic phosphorus as substrate	$gP \cdot m^{-3}$	0.05
$pH_{LOWER,OPT,DON,MIN,DOXY}$	Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor		6.00
$pH_{UPPER,OPT,DON,MIN,DOXY}$	Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor		6.00
$pH_{LOWER,OPT,DON,MIN,NO3}$	Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with nitrate as the final electron acceptor		9.00
$pH_{UPPER,OPT,DON,MIN,NO3}$	Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with nitrate as the final electron acceptor		9.00

[a] Calibrated value.

B.9 Model Constants Related to Dissolved Organic Phosphorus

Symbol	Description	Unit	Calibrated value
$k_{MIN,DOP,DOXY,20}$	Mineralization rate constant of dissolved organic phosphorus due to "bacterial and abiotic processes" at 20˚C, where dissolved oxygen is utilized as final electron acceptor	day^{-1}	0.010
$k_{MIN,DOP,NO3,20}$	Mineralization rate constant of dissolved organic phosphorus due to "bacterial and abiotic processes" at 20˚C, where nitrate is utilized as final electron acceptor	day^{-1}	0.0012
$\theta_{MIN,DOP,DOXY}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus , where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.08
$\theta_{MIN,DOP,NO3}$	Arrhenius type temperature correction coefficient for the mineralization rate of dissolved organic phosphorus , where dissolved oxygen is utilized as final electron acceptor (dimensionless)	dimensionless	1.08
$k_{HS,DOP,MIN,DOXY}$	Monod type half saturation concentration of dissolved organic phosphorus for dissolved organic phosphorus mineralization, where dissolved oxygen is utilized as final electron acceptor simulating the effects of the lack of dissolved organic phosphorus as substrate	$gP \cdot m^{-3}$	0.00
$k_{HS,DOP,MIN,NO3}$	Monod type half saturation concentration of dissolved organic phosphorus for dissolved organic phosphorus mineralization, where nitrate is utilized as final electron acceptor simulating the effects of the lack of dissolved organic phosphorus as substrate	$gP \cdot m^{-3}$	0.05
$pH_{LOWER,OPT,DOP,MIN,DOXY}$	Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor		6.00
$pH_{UPPER,OPT,DOP,MIN,DOXY}$	Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with dissolved oxygen as the final electron acceptor		6.00
$pH_{LOWER,OPT,DOP,MIN,NO3}$	Minimum value for optimum pH for dissolved ogranic phosphorus minerlization with nitrate as the final electron acceptor		9.00
$pH_{UPPER,OPT,DOP,MIN,NO3}$	Maximum value for optimum pH for dissolved ogranic phosphorus minerlization with nitrate as the final electron acceptor		9.00

B.10 Model Constants Related to Inorganic Nutrients

Symbol	Description	Unit	Calibrated value
$k_{NITR,20}$	Nitrification rate constant	day^{-1}	0.60
θ_{NITR}	Arrhenius type temperature correction coefficient for nitrification rate	dimensionless	1.045
$k_{HS,NITR,DOXY}$	Monod type half saturation concentration of dissolved oxygen for nitrification simulating the effects of the lack of dissolved oxygen as the oxidizing agent	$gO_2 \cdot m^{-3}$	2.00
$k_{HS,NITR,NH4N}$	Monod type half saturation concentration of ammonia nitrogen for nitrification simulating the effects of the lack of dissolved oxygen substrate	$gN \cdot m^{-3}$	0.03
$pH_{LOWER,OPT,NITR}$	Minimum value of optimum pH for nitrification		6.9
$pH_{UPPER,OPT,NITR}$	Maximum value of optimum pH for nitrification		8.2
$k_{DISS,PSi,20}$	Dissolution rate constant of particulate silicon	day^{-1}	0.001
$\theta_{k,DISS,PSi}$	Arrhenius type temperature correction factor for dissolution rate constant of particulate silicon	dimensionless	1.04

APPENDIX C.

R script for ESTAS-AQUABC model calibration.

```
### GUI for AQUABC ver 0.4
require(gWidgets2)
## Select the RGtk2 toolkit
guikit = "RGtk2"
## Alternatively the tcltk toolkit could be selected
# guikit = "tcltk"
#library(gWidgetstcltk)
## cairoDevice allows plotting in GTK ggraphics widgets
library(cairoDevice)
options(guiToolkit = guikit )
###
###  set all directories to the scripts
SETUP = FALSE
###  set working directory to the scripts to load include files
if (.Platform$OS.type == "unix")
{
  setwd("~/Dropbox/AQUABC/scripts")
```

```
} else

{

  #gmessage("It is windows")

  setwd(file.path(Sys.getenv("USERPROFILE"), "Dropbox/AQUABC/scripts"))


}

###

source('setup.R')

###

source('readoutputs.R')

## Source code file contains  ReadPelagicProcNames, ReadPelagicBox and
ReadPelagicProcBox functions

###

source('readinputs.R')

##  Source code file contains ReadWCONST  WriteWCONST ReadOutSetup ReadInputFile
functions

###

source('plotoutputs.R')

##  Source code file contains ggplot_limiting_factors
ggplot_cum_limiting_factors  functions

###

source('names.R')

##  Source code file contains ReadSTVNames() and  ReadPelagicProcNames()

#

source('run_sims.R')

##  Source code file contains ReadScnFile(ScnFileName) and RunSimulations(scen)

### Read critical shear stress values for boxes

critical <- ReadSHStress()

source('dialogs.R')

###  Calibration scenario data structure  - outdated

setwd(inputs_path)

WCONST <- ReadWCONST("WCONST_01.txt")

constant_names <- as.character(WCONST[,5])

cur_scen <- data.frame("Constant" = 26,  "No steps" = 2, "Interval" = 0.05,"Exit
code" = 0, "Midpoint" = WCONST[26,3])

##  Source code file contains model_params

TESTING = FALSE
```

```
###  selection of phytoplancton groups 1 - diatoms, 2 - fixin , 3 - other, 4 -
non fixing
gr = 1 # diatoms default
## loaded data arrays
pel_box = NULL
pel_proc_box = NULL
flx_box = NULL
scen_box = NULL
###
box_no = 14
stv_selected = 1
disp_mode <- "stv"
### variable for the second axis in  graphs
sec_var = 1  # 1 - no second axis, 2 - temperature, 3 - shear stress
### Load air temperature and shear stress data from INPUTS
ss <- ReadSStress()
atmp <- ReadAirTemp()
### logical loaded or not variables
stv_ld  = FALSE
prc_ld = FALSE
flx_ld = FALSE
scen_ld = FALSE
scenbox_ld = FALSE
###
if (TESTING)   ## preload some data
{
  setwd("C:/AQUABC/OUTPUTS/")
  pel_proc_box <- ReadPelagicProcBox(proc_binbox_file_name, TRUE)
  pel_box = ReadPelagicBox(stv_binbox_file_name, TRUE)
  stv_ld  = TRUE
  prc_ld = TRUE
}
### Setup variables whether the results to display are loaded
#### Read the state variable names
stvnames = ReadSTVNames()
### Read the pelagic processes names
```

```
valid_proc_names <- rep(30,30)  ### global variable
procnames = ReadPelagicProcNames("PelagicProcesses_Final.xlsx")
### Read the measured data
measured_data <- ReadMeasured2()
meas.zoo <- ReadMeasured2(stat=TRUE)
### below is temporary
n2fix.zoo <-  readRDS(file.path(inputs_path, "n2fixzoo.rdata")) / 29.76190476
colnames(measured_data) <- stvnames[1:30, 1]
measured <- measured_data
# selected state variable
stv_selected = 1
# selected process
proc_selected = 1
### start with the main window

### Calibration scenario data structure
a <- c(0.1,0.2,0.3)
b <- c(1.1,1.2,1.3,1.4,1.5)
values <- list(a,b)
consts_s <- c(23,14)
cur_sim  <- CreateSim(consts_s, values)
###
####   filters to read bin file name
flt = list(
  "Process rates bin files" = list(patterns = c("*RATES.bin")),
  "State variables bin files" = list(patterns = c("*.bin")),
  "Mass balance bin files" = list(patterns = c("*BALANCES.bin"))
)
flt2 = list(
  "Constant values file" = list(patterns = c("WCONST*")),
  "Input file" = list(patterns = c("INPUT*")),
  "Output file" = list(patterns = c("PELAGIC_OUTPUT*"))
)
### Read INPUT.txt file fron exe directory
setwd(exe_path)
INPUT <- ReadInputFile("INPUT.txt")
```

```
### Read default input configuration files from default locations

#setwd(inputs_path)

#WCONST <- ReadWCONST("WCONST_01.txt")

## Need tronslate this from factor !!!


#OUTPUT_SETUP <- ReadInputFile("PELAGIC_OUTPUT_INFORMATION_FILE.txt")

OUTPUT_SETUP <-
read_table2("C:/AQUABC/INPUTS/PELAGIC_OUTPUT_INFORMATION_FILE.txt",

                            col_names = FALSE, col_types = cols(X1 =
col_integer(),

                                                                X2 =
col_logical(), X3 = col_logical(),

                                                                X4 =
col_logical()), skip = 1)

colnames(OUTPUT_SETUP) <- c("PELAGIC BOX
NO","PRODUCE_PEL_STATE_VAR_OUTPUTS","PRODUCE_PEL_PROCESS_RATE_OUTPUTS",
"PRODUCE_PEL_MASS_BALANCE_OUTPUTS")

#WCONST <- ReadWCONST(gfile(gettext("Select WCONST"), type="open", filter =
flt2,initial.dir = "C:/AQUABC/INPUTS/"))

#INPUT  <- ReadInputFile(gfile(gettext("Select INPUT"), type="open", filter =
flt2,initial.dir = "C:/AQUABC/INPUTS/"))

#PELAGIC_OUTPUT_INFORMATION_FILE.txt

#OUTPUT_SETUP <- ReadInputFile(gfile(gettext("Select OUTPUT Setup file"), type =
"open", filter = flt2,initial.dir = "C:/AQUABC/INPUTS/"))

input_files <- list(WCONST,INPUT,OUTPUT_SETUP)


## start with main window construction, so far invisible

win <- gwindow("AQUABC GUI", visible = TRUE)

### Functions for the menu item handling

###  Creat a stub for menu entries

#stub = function(...) galert("stub", parent = win)

stub  <- function(h,...) function(...)

{

  group <- ggroup(horizontal = FALSE, cont = gwindow())

  innergroup <- ggroup(container = group)

  gtext("Text area", container = group)

  gbutton("button 1", container = innergroup)

  gbutton("button 2", container = innergroup)

}
```

```
###

### function feed constant selected in combobox to  gdf
gproc2df <- function(h,...)
{

  print(svalue(h$obj))
  scen$Constant <<- match(svalue(h$obj), constant_names)
  message(sprintf(" Out Constant changed to: %i",scen$Constant))
  svalue(h$action) <- scen$Constant

}  ## end gproc2df

#### Load pelagic variables box dialog
load_pelbox <- function(h,...) {
  stv_binbox_file_name <<- gfile(gettext("Filename to load"), type = "open",
                                 initial.dir = outputs_path,
                                 filter = list("STV bin files" = list(patterns =
c("*00??.bin"))))
  gmessage(sprintf("Reading pelagic box from %s\n", stv_binbox_file_name))
  pel_box <<- ReadPelagicBox(stv_binbox_file_name,TRUE)
  assign("stv_ld", TRUE, envir = .GlobalEnv)
  #stv_ld <<- TRUE
  # enabled(sl) <<- TRUE
  # enabled(gc) <<- TRUE
  enabled(small_group) <<- TRUE
  svalue(sb) <<- "STV box loaded"
}
#### Load pelagic processes box dialog
load_pel_proc_box <- function(h,...) {
  proc_binbox_file_name <<- gfile(gettext("Filename to load"), type = "open",
                                  initial.dir = outputs_path,
                                  filter = list("Process rates bin files" =
list(patterns = c("*RATES.bin"))))
  #msgBox <- gmessage(sprintf("Reading pelagic processes box from %s\n PLease
wait...", proc_binbox_file_name), icon = "warning")
```

```
  #msgBox <- galert(sprintf("Reading pelagic processes box from %s\n PLease
wait...", proc_binbox_file_name),

  #       title = "message", delay = 30)

  pel_proc_box <<- ReadPelagicProcBox(proc_binbox_file_name,TRUE)

  assign("prc_ld", TRUE, envir = .GlobalEnv)

  prc_ld <<- TRUE

  enabled(small_group2) <<- TRUE

  svalue(sb) <<- "process box loaded"

  #dispose(msgBox)

  gmessage("Pelagic process box loaded")

  # svalue(sb) <<- proc_binbox_file_name

}

#### load fluxes box dialog

load_flux_box <- function(flx_ld,...){

  flx_binbox_file_name <<- gfile(gettext("Filename to load"),

                                 type = "open", initial.dir = outputs_path,

                                 filter = list("Fluxes bin files" =
list(patterns = c("NCES.bin"))))

  gmessage(sprintf("Reading pelagic fluxes box from %s\n",
flx_binbox_file_name))

  # pel_box <<- ReadPelagicBox(stv_binbox_file_name,TRUE)

  assign("scen_ld", TRUE, envir = .GlobalEnv)

  scen_ld <<- TRUE

  # svalue(sb) <<- flx_binbox_file_name

}

#### load sensitivity run dialog

load_run <- function(h,...){

  scen_file_name <<- gfile(gettext("Scenario to load"),

                           type = "open", initial.dir = outputs_path,

                           filter = list("Scenario files" = list(patterns =
c("*.scn"))))

  gmessage(sprintf("Reading from %s\n", scen_file_name))

  cur_scen <<- ReadScnFile(scen_file_name)

  assign("scenbox_ld", TRUE, envir = .GlobalEnv)

  scen_box <<- read_sen_run(box_no,cur_scen$Constant,cur_scen$No.steps*2+1) #
box_no, var_no, no_runs

  message("Sensitivity runs box loaded")

  scen_ld <<- TRUE
```

```
print(ggplot_sel_cal_var(scen_box,stv_selected,cur_scen$Constant,(cur_scen$No.steps*2+1),
                         cur_scen$Interval,
measured_data[,stv_selected],RSQ[stv_selected,]))   # (box,v1,c1,no_rn,interv, measured data, RSQ)
  scenbox_ld <<- TRUE
  disp_mode <<- "scn"
  assign("scen_ld", TRUE, envir = .GlobalEnv)
  enabled(small_group) <<- TRUE
  svalue(sb) <<- sprintf("Sensitivity run of constant %i loaded",cur_scen$Constant)
}
#### load scenario dialog
load_scen <- function(h,...){
  scen_file_name <<- gfile(gettext("Scenario to load"),
                           type = "open", initial.dir = outputs_path,
                           filter = list("Scenario files" = list(patterns = c("*.scn"))))
  gmessage(sprintf("Reading from %s", scen_file_name))
  ReadScnFile(scen_file_name)
  assign("scen_ld", TRUE, envir = .GlobalEnv)
  scen_ld <<- TRUE
  # svalue(sb) <<- flx_binbox_file_name
}

#### Display pelagic box dialog
display_pel_box <- function(h,...)
{
  if (stv_ld)
  {
    disp_mode <<- "stv"
    print(ggplot_selected_vars(pel_box,stv_selected,measured_data))
  }

  else
    gmessage("Pelagic box data not loaded")
}
```

```
#### Display processes box dialog
display_proc_box <- function(h,...)
{
  if (prc_ld)
  {
    disp_mode <<- "prc"
    print(ggplot_selected_process(pel_proc_box, stv_selected, proc_selected))
  }

  else
    gmessage("Pelagic processes box data not loaded")

}
#### Display fluxes box dialog
display_flux_box <- function(h,...)
{
  if (flx_ld)
  {
    disp_mode <<- "flx"
    gmessage("Pelagic fluxes box data loaded, but not displayed")
    print(ggplot_selected_process(pel_proc_box, stv_selected,proc_selected))
  }
  else
    gmessage("Pelagic fluxes box data not loaded")
}
#### Display limitation dialog
display_cum_lim <- function(h,...)
{
  if (prc_ld)
  {
    disp_mode <<- "lim"
    # gmessage("Pelagic fluxes box data loaded, but not displayed")
    print(ggplot_limiting_factors(pel_proc_box, 1))
  }
  else
    gmessage("Pelagic fluxes box data not loaded")
```

```
}
#### Display sensitivity run results
display_scen_box <- function(h,...)
{
  if (scenbox_ld)
  {
    disp_mode <<- "scn"

print(ggplot_sel_cal_var(scen_box,stv_selected,cur_scen$Constan,(cur_scen$No.ste
ps*2+1),cur_scen$Interval,measured_data[,current_var], RSQ[stv_selected,]))
  }
  else
    gmessage("Sensitivity analysis data not loaded")
}
###  load WCONST file
rdWCONST = function(h,...) {
  fname <- gfile(gettext("Filename to load"), type = "open", filter =
flt2,initial.dir = "C:/AQUABC/INPUTS/")
  gmessage(fname)
  WCONST = ReadWCONST(fname)
  constant_names <- as.character(WCONST[,5])
  svalue(sb) <- fname
}
###  load INPUT file
rdINPUT = function(h,...) {
  fname <- gfile(gettext("Filename to load"), type = "open", filter =
flt2,initial.dir = "C:/AQUABC/INPUTS/")
  gmessage(fname)
  INPUT <- ReadInputFile(fname)
  svalue(sb) <- fname
}
###   Edit sim using gdf function
edit_sim = function(h,...)
{
  values_list <- cur_sim$Values
  n.obs <- sapply(values_list , length)
  seq.max <- seq_len(max(n.obs))
```

```
  values.frm <- data.frame(sapply(values_list, "[", i = seq.max))
  dfname <- deparse(substitute( cur_sim$Values))
  w <- gbasicdialog(h,..,handler=function(h,...) {
      changed_list <- as.list(data.frame(values.frm))
      message(changed_list)
      #assign(dfname, df[,], .GlobalEnv)
      assign(cur_sim$Values,changed_list, .GlobalEnv)
    })
  g <- ggroup(cont=w, horizontal=FALSE)
  glabel("Edit a data frame", cont=g)
  df <-  gdf(values.frm, cont=g, expand=TRUE)
  size(w) <- c(400, 400)
  out <- visible(w)
  return(as.list(data.frame(values.frm)))  # retur back values list
}
####

###  Run simulation
run_sim = function(h,...)
  {

    #gbasicdialog(title = "Run simulations")
    # gmessage(cur_scen)
    run_simu <- function(DF, ...) {
    dfname <- deparse(substitute(DF))
    message(dfname)
    w <- gbasicdialog(..., handler=function(h,...) {

      insert(df, sprintf("Running %i simulations", cur_scen$No.steps*2+1),
font.attr=list(weight="bold"))
      RunSimulations(cur_scen)
      dispose(w)
    })

    g <- ggroup(cont=w, horizontal=FALSE)
    glabel("Sensitivity run parameters", cont=g)
```

```
    df <- gtext(sprintf("Running %i simulations", cur_scen$No.steps*2+1),
cont=g)

    size(w) <- c(400, 400)

    out <- visible(w)

  }

  run_simu(cur_scen)

  }

####  Menu list

l <- list(

  Model = list(INPUT = gaction("Model parameters", handler =model_params ,
parent = win),

                   WCONST = gaction("Load WCONST file", handler = rdWCONST,
parent = win),

                   INPUT = gaction("Load INPUT file", handler = rdINPUT, parent =
win)),

                   ## end of Options

  Simulations = list(Open = gaction("Load scenario", handler = load_scen, parent
= win),

                    SensSingle = gaction("Sensitivity run 1 constant", handler =
sens , parent = win),

                    SensMultiple = gaction("Sensitivity run multiple constants",
handler = stub, parent = win),

                    Stress = gaction("Change critical shear stress", handler =
shear_stress, parent = win),

                    Run = gaction("Run simulations", handler = run_sim, parent =
win)),## end of Run

  Load  = list(loadstv = gaction("Open STV outputs", icon = "open",

                                 handler = load_pelbox, parent = win),

               loadproc = gaction("Open process outputs", icon = "open",

                                  handler = load_pel_proc_box, parent = win),

               loadrun  = gaction("Load sensitivity run results ", icon =
"open",

                                   handler = load_run, parent = win),

               loadfluxes = gaction("Open fluxes outputs", icon = "open",

                                    handler = load_flux_box, parent = win)), #
end of Load

  Display = list(displaystv = gaction("Display Variables", handler =
display_pel_box,parent = win),

                  displaysbox = gaction("Display Sensitivity run results",
handler = display_scen_box,parent = win),
```

```
                displayproc = gaction("Display Procersses", handler =
display_proc_box,parent = win),

                displayspec1 = gaction("Display Diatom limiting",handler =
display_lim1,parent = win),

                displayspec2 = gaction("Display n-fixing cyano
limiting",handler = display_lim2,parent = win),

                displayspec3 = gaction("Display Non N-fixing cyano
limiting",handler = display_lim3,parent = win),

                displayspec4 = gaction("Display Other phytoplankton
limiting",handler = display_lim4,parent = win),

                displayspec4 = gaction("Display Nitrogen fixation",handler =
display_Nfix,parent = win),

                displayspec5 = gaction("Display cumulative limiting",handler =
display_cum_lim,parent = win)), # end of Display

  Options = list(quit = gaction("Graph options", handler = display_options,
parent = win)),

  Quit = list(quit = gaction("Quit", handler = function(...) dispose(win),
parent = win))

)

# end of menu list

### Windows system


sb <- gstatusbar("Nothing is loaded", cont = win)

# BigGroup <- ggroup(cont = win)

# ###

# distribution = glabel("Label",horizontal = FALSE)

# BigGroup = ggroup(cont = win)

# vgroup = ggroup(horizontal = FALSE, cont = BigGroup,visible = TRUE)

# tmp = gframe("Distribution", cont = vgroup)

# add(tmp, distribution)

# add(BigGroup, ggraphics(visible = TRUE))

###

### Create a menu

mb <- gmenu(l, cont = win)

group <- ggroup(horizontal = FALSE, cont = win)

g.d <- ggraphics(container = group, visible = TRUE, width = 1000, height = 600)

##  Two windows to place sliders and combo boxes to select state variables and
processes

### State variables
```

```
small_group <- gframe(text = "State variables",horizontal = FALSE,  pos = 0,
cont = group)

sl <- gslider(from = 1, to = 30, by = 1, value = 0, cont = small_group, expand =
TRUE, fill = "both")

gc <- gcombobox(stvnames[1:30,1], label = "", cont = small_group)

enabled(small_group) <- FALSE

###  Processes

no_cur_processes =   sum(procnames[,1,stv_selected] != "")

cur_procnames = procnames[1:no_cur_processes,1, stv_selected]

##

small_group2 <- gframe(text = "Processes",horizontal = FALSE,  pos = 0, cont =
group)

slproc <- gslider(from = 1, to = no_cur_processes, by = 1, value = 0, cont =
small_group2, expand = TRUE, fill = "both")

gproc <- gcombobox(procnames[1:no_cur_processes,1,stv_selected], label = "",
cont = small_group2)

enabled(small_group2) <- FALSE


## radio <- gradio(label = "Fix STV", cont = group)

## addHandlerChanged function to connect stv and processes selection via
comboboxes and sliders

## slproc2gproc based on the selection in procees gslider changes the value in
the process combobox

## and if process box is loaded  displays graph

slproc2gproc <- function(h, ...)

{

  # get value from a slider

  message("get value and number of stops from a slider")

  print(svalue(h$obj))

  print(h$obj[])

  if  (is.null(svalue(h$obj)))  { message("Exitting"); return()}

  svalue(h$action) <- procnames[svalue(h$obj),1, stv_selected]


  proc_selected <<- as.integer(svalue(h$obj))

  message(sprintf("feeding process %i selected by slider to a combo",
proc_selected))

  if (prc_ld)

  {

    visible(g.d) <- TRUE
```

```
    if (disp_mode == "prc") print(ggplot_selected_process(pel_proc_box,
stv_selected, proc_selected))


  }


  else
    message("No pelagic process box data loaded")


}


### function feeds stv delected in slider to combobox
sl2gc <- function(h, ...)
{
  svalue(h$action) <- stvnames[svalue(h$obj),1]
  # print(svalue(h$obj))
  stv_selected <<- as.integer(svalue(h$obj))
  no_cur_processes =   sum(procnames[,1,stv_selected] != "")
  cur_procnames = procnames[1:no_cur_processes,1, stv_selected]
  if (TRUE)
  {
    visible(g.d) <- TRUE
    if (disp_mode == "stv") print(ggplot_selected_vars(pel_box,stv_selected,
measured_data))
     # if (disp_mode == "prc") print(ggplot_selected_process(pel_proc_box,
stv_selected, proc_selected))
    if (disp_mode == "scn")
print(ggplot_sel_cal_var(scen_box,stv_selected,cur_scen$Constant,

(cur_scen$No.steps*2+1),cur_scen$Interval,measured_data[,stv_selected],
RSQ[stv_selected,]))
    #message("plotting slider to combo")
  }


  else
    message("No pelagic box data loaded")


}
### function feeds  processes relevant to selected state variable into combobox
```

```
gc2gproc <- function(h, ...)

{

  #stv_selected<<- match(svalue(h$obj), stvnames[,1])

  stv_selected <<- svalue(h$obj, index = TRUE)

  # message(sprintf("gc2gproc: feeding processes for variable %i selected in
combo to a combo", stv_selected))

  no_cur_processes =   sum(procnames[,1,stv_selected] != "")

  cur_procnames = procnames[1:no_cur_processes,1, stv_selected]

  h$action[] <-  cur_procnames  ## procnames[stv_selected,1,]

  # Select first process for a varaible

  svalue(h$action, index = TRUE) <- 1

  # print(svalue(h$action, index = TRUE))


}

### function feeds  processes into combobox only relevant to state variable
selected in slider

sl2gproc <- function(h, ...)

{

  stv_selected <<- svalue(h$obj)

  no_cur_processes =   sum(procnames[,1,stv_selected] != "")

  # message(sprintf("sl2gproc: feeding %i processes for variable %i selected in
slider to a combo\n",  no_cur_processes, stv_selected))

  cur_procnames = procnames[1:no_cur_processes,1, stv_selected]

  # Fill the combobox woth values of process names

  h$action[] <- cur_procnames

  # Select the first one

  svalue(h$action, index = TRUE) <- 1

  # message( h$action[])

  # print(svalue(h$obj))

}

### function feeds stv delected in combobox  to slider

gc2sl <- function(h, ...)

{


  print(svalue(h$obj))

  #stv_selected <<- match(svalue(h$obj), stvnames[,1])

  stv_selected <<- svalue(h$obj, index = TRUE)
```

```
  no_cur_processes =   sum(procnames[,1,stv_selected] != "")
  cur_procnames = procnames[1:no_cur_processes,1, stv_selected]
  svalue(h$action) <- stv_selected
  # sl[] <- seq(0, 2*pi, length=100)
  #stv_selected <<- as.integer(svalue(h$obj))
  if (disp_mode == "stv")
  {
    if (stv_ld)
    {
      visible(g.d) <- TRUE
      message("plotting  combo to slider")
      print(ggplot_selected_vars(pel_box,stv_selected, measured_data))

    }

    else
      message("No pelagic box data loaded")
  }

  if (disp_mode == "prc")
    {
    if (prc_ld) {
      visible(g.d) <- TRUE
      print(ggplot_selected_process(pel_proc_box, stv_selected,proc_selected))
    }

  }

  if (disp_mode == "scn")
print(ggplot_sel_cal_var(scen_box,stv_selected,cur_scen$Constant,

(cur_scen$No.steps*2+1),cur_scen$Interval,measured_data[,stv_selected],
RSQ[stv_selected,]))
  message("plotting slider to combo")

}  ## end gc2sl
sl2slproc <- function(h, ...)
```

```
{
  #message("svalue(h$obj) sl2slproc")
  #message(svalue(h$obj))
  stv_selected <<- svalue(h$obj)
  no_cur_processes =   sum(procnames[,1,stv_selected] != "")
  cur_procnames = procnames[1:no_cur_processes,1, stv_selected]
  #message(sprintf("sl2sproc: changes the slider to  %i processes for variable
%i selected in stv slider",  no_cur_processes, stv_selected))
  h$action[] <- seq(from = 1,  to = no_cur_processes, by = 1)
  svalue(h$action) <- 1
  #message("h$action[]")
  #message(h$action[])
  #print(cur_procnames)
}
gproc2slproc <- function(h, ...)
{

  message(svalue(h$obj))
  # proc_selected <<- match(svalue(h$obj), procnames[,1,stv_selected])
  proc_selected <<- svalue(h$obj, index = TRUE)
  # cur_procnames = procnames[1:no_cur_processes,1, stv_selected]
  message("h$action[] :")
  message(h$action[])
  message(sprintf("Fixin slider on  %i proccess rate selected in  combobox",
proc_selected))
  ## h$action[] <- seq(from = 1,  to = no_cur_processes, length = 1 )
  svalue(h$action) <- proc_selected
  if (prc_ld)
  {
    visible(g.d) <- TRUE
    if (disp_mode == "prc") print(ggplot_selected_process(pel_proc_box,
stv_selected, proc_selected))
  }
}

addHandlerChanged(sl, sl2gc, action = gc)   # Change stv from stv slider to stv
combo
```

```
addHandlerChanged(gc, gc2sl, action = sl)   # Change stv from stv combo to stv
slider

addHandlerChanged(gc, gc2gproc, action = gproc)   # Change prc from stv combo to
prc combo

addHandlerChanged(sl, sl2gproc, action = gproc)   # Change prc from stv slider
to prc combo

addHandlerChanged(sl,sl2slproc, action = slproc)        # Change prc from stv
slider to prc slider

addHandlerChanged(gproc, gproc2slproc, action = slproc)   # Change prc from prc
combo to prc slider

addHandlerChanged(slproc, slproc2gproc, action = gproc) #  Change prc from prc
slider to prc combo


visible(win) <- TRUE

## Create the device in it

d <- dev.cur()

# Set the handler to plot

stop()

obj <- gbutton("Plot", container = group,

               handler = function(h, ...) {

                 if (prc_ld)

                 {

                   visible(g.d) <- TRUE

                   print(ggplot_limiting_factors(pel_proc_box, 1))

                 }


               })

updatePlot <- function(h,...) {

  if (stv_ld)

  {

    visible(g.d) <- TRUE

    gmessage(sprintf("Updating from %s\n", stv_binbox_file_name))

    pel_box <- ReadPelagicBox(stv_binbox_file_name, TRUE)

  }

  #sb <- gstatusbar(current.bin, cont = win)

}


stop()
```

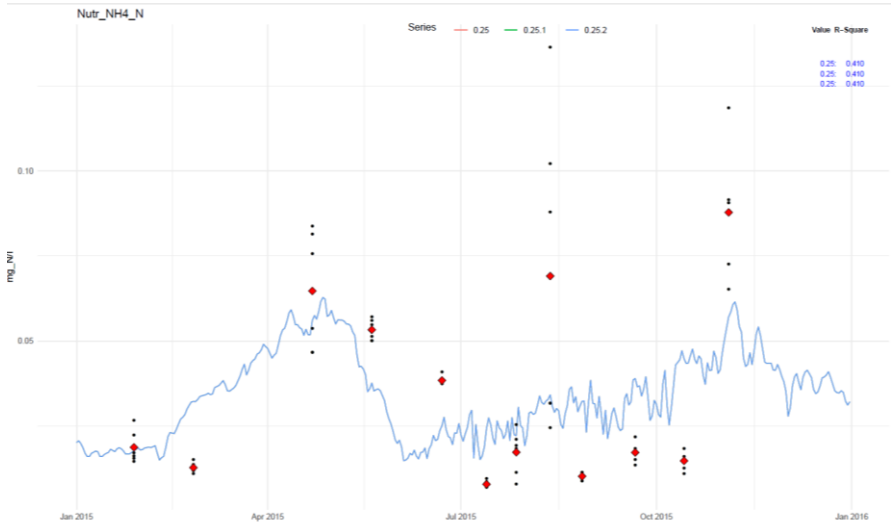

Figure 20. Calibration of NH_4-N concentration
20 pav. NH4-N koncentracijos kalibravimo rezultatas

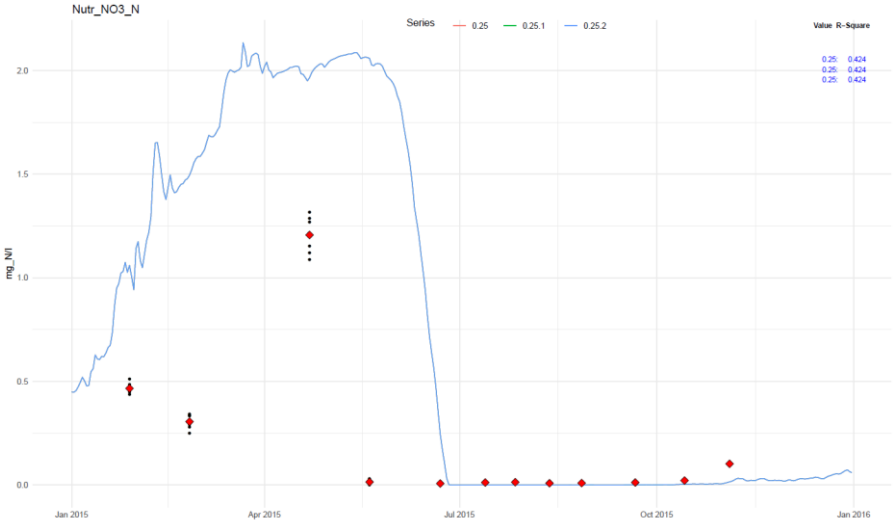

Figure 21. Calibration of NO_3-N concentration
21 pav. NO_3-N koncentracijos kalibravimo rezultatas

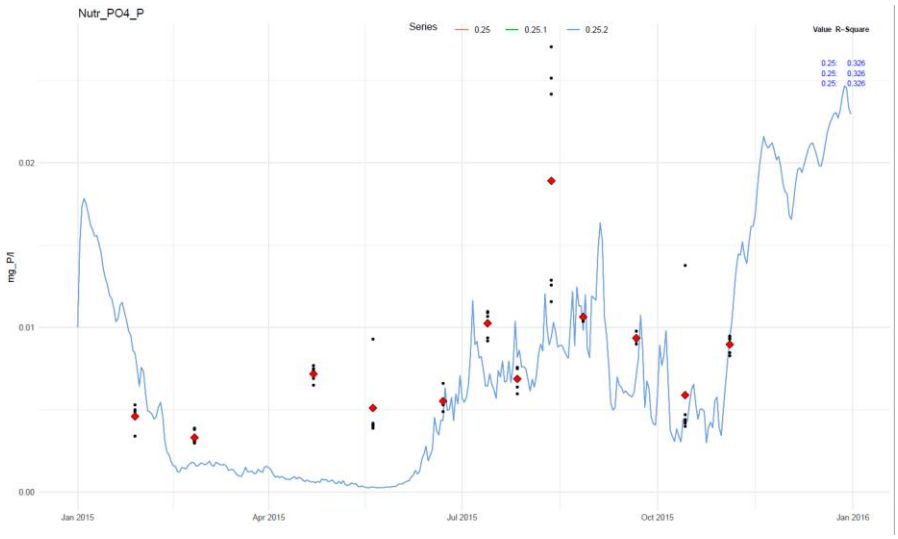

Figure 22. Calibration of PO_4-P concentration
22 pav. PO_4-P koncentracijos kalibravimo rezultatas