The community-centered ~~aquatic~~ freshwater biogeochemistry model unified RIVE v1.0: a unified version for water column

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Abstract.

Research on mechanisms of organic matter degradation, bacterial activities, phytoplankton dynamics, and other processes has led to the development of numerous sophisticated water quality models~~since one of the first in~~ . The earliest model, dating back to 1925, ~~based on first order~~ was based on first-order kinetics for organic matter degradation. The community-centered ~~aquatic~~ freshwater biogeochemistry model RIVE was initially developed in 1994 and has ~~since~~ subsequently been integrated into several software programs such as Seneque-Riverstrahler, pyNuts-Riverstrahler, PROSE/PROSE-PA and Barman. After 30 years of research, the use of different programming languages including Qbasic, Visual Basic, Fortran, ANSI C and Python, as well as parallel evolution and the addition of new formalisms, raise questions about their comparability.

This paper presents a unified version of the RIVE model for the water column, including formalisms for bacterial communities (heterotrophic and nitrifying), primary producers, zooplankton, nutrients, inorganic carbon, and dissolved oxygen cycles. The unified RIVE model is open source and implemented in Python 3 to create pyRIVE 1.0, and in ANSI C to create C-RIVE 0.32. The organic matter degradation module is validated by simulating batch experiments. The comparability of the pyRIVE 1.0 and C-RIVE 0.32 softwares is verified by modeling a river stretch case study~~, which~~ . The case study considers the full biogeochemical cycles (microorganisms, nutrients, carbon, and oxygen) in the water column, as well as the effects of light and water temperature. The results show that the simulated concentrations of all state variables, including microorganisms and chemical species, are very similar for pyRIVE 1.0 and C-RIVE 0.32. This open-source project highly encourages contributions from the ~~aquatic~~ freshwater biogeochemistry community to further advance the project and achieve common objectives.

1 Introduction

Modeling of the water quality of ~~an aquatic~~ a freshwater system (river, lake ~~,~~ or reservoir) is critical to understand and manage its functioning~~which~~ . The functioning of a freshwater system is the results of complex interrelated biogeochemical processes. The first water quality model developed by Streeter and Phelps (1925) describes the degradation of organic matter (OM) in river. The organic matter, measured globally by biochemical oxygen demand in 5 days (BOD5), is considered to be degraded according to a first-order kinetics. Although dating back more than a century (the study was completed in 1915, but publication

was delayed to 1925 due to World War I (Hellweger, 2015)), this model is still widely used to represent the dynamics of organic matter in ~~aquatic environments~~ water quality modeling. (Hellweger, 2015).

While the role of microorganisms in the degradation of organic matter has been acknowledged since the end of the 19th century, there is an important limitation of this type of representation~~is that the~~. The microbiological nature of the organic matter degradation process and the bacterial population dynamics intrinsically involved are completely obscured~~, being~~. They are implicitly taken into account only through a biodegradability constant of ~~OM~~ organic matter and its dependence on temperature. Microbial biogeochemical work in the 1980s-1990s led to the elucidation of the detailed mechanisms of the organic matter degradation process and the associated heterotrophic bacterial activities (Fuhrman and Azam, 1982; Azam et al., 1983; Somville and Billen, 1983; Servais et al., 1985; Rego et al., 1985; Fontigny et al., 1987; Servais et al., 1987; Billen et al., 1988; Servais et al., 1989; Billen et al., 1990; Garnier et al., 1992a, b). This new corpus of knowledge led to the development and the formulation of the biogeochemical model RIVE (Billen et al., 1994; Garnier and Billen, 1994)~~,~~. It is capable of simulating the degradation of OM in ~~aquatic~~ freshwater systems and the associated oxygen consumption by bacterial activities, which is more realistic than the model of Streeter and Phelps (1925). In RIVE model, the **HSB** model (Billen and Servais, 1989; Billen, 1991) is used to represent the degradation of organic matter and heterotrophic bacterial activities. This model simulates the exoenzymatic hydrolysis of particulate and dissolved organic matter (split into biodegradable and refractory pools), including **H**igh weight polymers, into small monomeric **S**ubstrates~~, which~~. These substrates are subsequently assimilated by **B**acteria for their growth and respiration.

Apart from the degradation of organic matter, the ~~*Aquaphy*~~ AQUAPHY model (Lancelot et al., 1991) is been used for simulating the dynamics of phytoplankton in the RIVE model (Billen et al., 1994). The model simulates explicitly photosynthesis of phytoplankton, growth, mortality and respiration processes. ~~The~~ In addition to water temperature, the photosynthesis depends on the light intensity while the growth is controlled by nutrients availability and ~~the~~ small organic metabolites. The small organic metabolites are formed either directly by photosynthesis or by catabolysis of reserve products. This conceptualization allows for a growth of phytoplankton during dark periods. In addition, the model also introduces a limiting factor of nutrients in the growth of phytoplankton and considers the cycling of nutrients during the life cycle of phytoplankton.

Since its initial development by Billen et al. (1994), the RIVE model co-exists within several softwares (Tab. A1) developed for different aquatic compartments and supported by the PIREN-Seine program (https://www.piren-seine.fr/). The RIVE model was firstly applied in river systems using the Riverstrahler drainage network approach (Billen et al., 1994; Garnier et al., 1995). It was initially coded in Qbasic, and later on piloted by a GIS graphical interface Seneque-Riverstrahler (Visual Basic, (Ruelland et al., 2007)). And it is now fully integrated within the pyNuts-Riverstrahler (https://gitlab.in2p3.fr/rive/pynuts/~~) modeling environment to describe~~, Python framework (Thieu et al., 2017)). It can model the biogeochemical functioning of hydrographic networks at scales ranging from local to continental~~(Python framework, (Thieu et al., 2017))~~. RIVE model was also applied to lentic ~~aquatic~~ freshwater systems like regulated reservoirs (BarMan software (Garnier et al., 2000; Thieu et al., 2006; Yan et al., 2022a)~~) or~~, Tab. A1.) or simulating hydro-biodynamic functioning of highly human impacted river system (ProSe software – Even et al. (1998, 2004, 2007); Flipo et al. (2004); Vilmin et al. (2015b), and ProSe-PA software – Wang et al. (2019, 2023a), https://gitlab.com/prose-pa/prose-pa, developed in ANSI C coupled with a self developed lex and yacc

parser, Tab. A1.). The RIVE model is also coupled with the Soil & Water Assessment Tool (SWAT) to simulate the water quality of the Vienne basin, France (Manteaux et al., 2023, submitted) and incorporated into the QUAL-NET model (Minaudo et al., 2018) to simulate river eutrophication in the drainage network of the Middle Loire River Corridor, France. Moreover, the RIVE model is implemented into the VEMALA V3 model for simulating phosphorus and nitrogen loading in the Finnish watersheds (Korppoo et al., 2017).

Based on above implementations, different versions of the RIVE model code ~~has~~ have simulated successfully a large variety of ~~aquatic~~ freshwater systems (lake ~~,~~ or reservoirs, river systems) across the world~~with parameter values~~ . The parameter values were determined through laboratory experiments or calibrated with observation data (Garnier et al., 1992a; Servais and Garnier, 1993; Garnier and Billen, 1994; Billen et al., 1994; Garnier et al., 1995). These applications (Tab. A1) were carried out for different networks and scales as well as various degrees of anthropogenic impacts in a wide climatic gradient using either Riverstrahler (possibly with its Seneque or pyNuts environments) or PROSE/PROSE-PA, such as the Seine River (France) (Billen et al., 1994; Garnier et al., 1995; Even et al., 1998, 2004, 2007; Billen et al., 2007; Servais et al., 2007; Thieu et al., 2009, 2010; Vilmin et al., 2015b, a; Aissa-Grouz et al., 2016; Vilmin et al., 2016; Desmit et al., 2018; Vilmin et al., 2018; Romero et al., 2019; Marescaux et al., 2020; Wang et al., 2022), the Danube river (Romania and Bulgaria) (Garnier et al., 2002), the Red River (China and Vietnam) (Le et al., 2010; Phuong Quynh et al., 2014; Le et al., 2015; Nguyen et al., 2016) and its distributary Day-Nhue River (Luu et al., 2021), the Lule and Kalix rivers (Sweden) (Sferratore et al., 2008), the Scheldt river (Belgium and Netherlands) (Billen et al., 2005; Thieu et al., 2009), the Zenne River (Belgium) (Garnier et al., 2013), the Mosel River (Germany) (Garnier et al., 1999a), the Somme River (France) (Thieu et al., 2009, 2010), the Loire River (France) (Garnier et al., 2018a), the Lot River (France) (Garnier et al., 2018b) and the Orgeval watershed (France) (Flipo et al., 2004, 2007; Garnier et al., 2014). Moreover, the RIVE model has been applied to the stagnant systems ~~(~~also (e.g. sand-pit lake ~~, reservoirs) also (Garnier and Billen, 1994; Garnier et al., 2000; Yan et al., 2022a)~~(Lake Crétail - France, (Garnier and Billen, 1994)), reservoirs (Marne, Aube, Seine - France, (Garnier et al., 2000; Yan et al., 2022a))).

After 30 years of research, the parallel evolutions of these codes, the numerical adaptations inherent in programming languages (Qbasic, Visual Basic, Fortran, Python and ANSI C) and the addition of new formalisms, raise the question of their comparability~~and the~~ . The identification of a unified version of RIVE model is then necessary. A project aiming at unifying these RIVE implementations ~~to bring~~ was undertaken. The unified version brings together all recent developments, especially the ones achieved with Python ~~3~~ and ANSI C programming languages~~, was undertaken to~~ . This action will strengthen the collaboration of the research teams involved in the development of the model. This paper presents then a unified version of RIVE for water column (called unified RIVE v1.0) with a presentation of the formalisms for the ~~carbon cycle – that~~ biogeochemical cycles. That integrates the bacterial communities (heterotrophic and nitrifying), primary producers, zooplankton and fate of detritic organic matter either particulate or dissolved as well as biodegradable and refractory, and the associated nutrients and dissolved oxygen cycles. The most recent developments on the modeling of inorganic forms of carbon are also presented. The unified RIVE v1.0 included in pyRIVE 1.0 (tested with Python 3 versions up to 3.10 release) and C-RIVE 0.32 is open source and therefore available to the scientific community. A numerical experiment is then introduced to evaluate the comparability of the pyRIVE 1.0 and C-RIVE 0.32 through a systematic comparison of simulations produced under controlled condi-

tions. We thus establish a reference framework to evaluate different implementations (programming languages, performance - comparability) of the unified RIVE v1.0 formulation, that continues to evolve in several water quality models.

2 Model description

The unified RIVE v1.0 model simulates the cycling of carbon, nutrients and oxygen within an ~~aquatic~~ freshwater system (river, lake, reservoir). Biogeochemical cycles are simulated with a community-centered or agent-based model. That means ~~the aquatic~~ that the freshwater system functioning is explicitly modeled~~by microorganisms' activities (~~, taking into consideration the activities of microorganisms such as phytoplankton, zooplankton, heterotrophic bacteria, and nitrifying bacteria~~) and physical processes (oxygen reaeration , dilution) in relation with the macronutrients and their fractions – for instance for the~~ . Additionally, it accounts for physical processes like oxygen reaeration and dilution. This modeling approach is developed in relation to water temperature, macronutrients and organic matter, (particulate, dissolved, ~~biodegradable fractions are considered~~and biodegradable fractions). The organic matter degradation, nitrifying bacteria dynamics, primary producer dynamics, zooplankton dynamics, nutrients and inorganic carbon cycling are described subsequently. A high number of model parameters are used to characterize the microorganisms' properties and most of them have been determined through field or laboratory experiments under controlled conditions. This paper presents a focus on the conceptualization of the unified RIVE v1.0 model in water column exclusively. ~~However, the~~ While RIVE model does have applications for sediment dynamics and its interaction with the water column ~~will be explored~~ (Even et al., 2004; Thouvenot et al., 2007; Billen et al., 2015; Vilmin et al., 2015a, 2016; Yan et al., 2022b) , relevant community-centred efforts need to be made in future work, which is not the focus of this study.

2.1 Organic matter degradation

The mechanisms of organic matter degradation by the activity of heterotrophic bacteria are represented using **HSB** model (Billen and Servais, 1989; Billen, 1991). It contains three variables: **H**, **H**igh weight ~~polymer~~ polymers (large molecules) which form the majority of dissolved and particulate organic matter, but ~~which~~ must be exoenzymatically hydrolyzed to be accessible to heterotrophic bacteria; **S**, small monomeric **S**ubstrates (SMS), directly accessible to microbial uptake; **B**, heterotrophic **B**acteria that ~~uptakes~~ absorbs the substrates for their growth and respiration (Fig. 1). In diagrams of this paper (for instance HSB model, Fig. 1), the state variables are represented by circles and represent either concentrations or stocks entering and leaving the (biogeochemical) processes. The biogeochemical processes are represented by squares.

The high weight polymer (total organic carbon) is conceptually divided for each phase (Dissolved (HD) and Particulate (HP)), into three pools. Each pool is characterized by a specific biodegradability: (1) rapidly biodegradable in 5 days (HD_1 and HP_1); (2) slowly biodegradable in 45 days (HD_2 and HP_2); (3) refractory (HD_3 and HP_3).

2.1.1 Heterotrophic bacteria dynamics

The dynamic of heterotrophic bacteria is explicitly simulated: growth, mortality, respiration etc. The growth of heterotrophic bacteria depends on water temperature and the availability of small monomeric substrate (SMS)~~, which~~ . The dependence

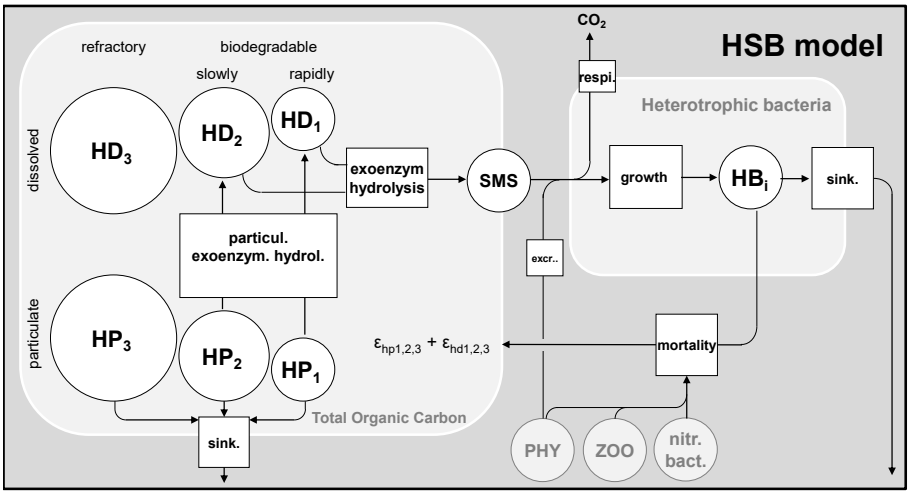

Figure 1. Flowchart of HSB model. HD: dissolved high weight polymer; HP: particulate high weight polymer; SMS: small monomeric substrate; HB: heterotrophic bacteria; PHY: phytoplankton; ZOO: zooplankton; nitr. bact.: Nitrifying bacteria; extr. excretion of phytoplankton; sink.: sinking. respi.: respiration; $\epsilon_{hp1,2,3}$ and $\epsilon_{hd1,2,3}$: Proportion to convert dead biomass to HP and HD

is represented by Monod equation (Monod, 1949). A ~~maximum rate of small monomeric substrate uptake ($b_{max,hb}$~~maximal substrate uptake rate at 20 °C ($b_{max20,hb}$) and a bacterial growth yield (Y_{hb}) are used to ~~represent the growth~~ calculate the growth rate of heterotrophic bacteria (μ_{hb_i}) (Eq. (3)). The fraction of uptake not used for growth ($1 - Y_{hb}$) is respired.

$$b_{hb_i} = b_{max,hb_i} max20,hb_i f(T)_{hb_i} \frac{[SMS]}{[SMS] + K_{sms,hb_i}} \tag{1}$$

$$f(T)_{hb_i} = \frac{e^{-\frac{(T-T_{opt,hb_i})^2}{\sigma^2_{hb_i}}}}{e^{-\frac{(20-T_{opt,hb_i})^2}{\sigma^2_{hb_i}}}} \tag{2}$$

$$\mu_{hb_i} = Y_{hb_i} b_{hb_i} \tag{3}$$

With ~~b_{max,hb_i}: Maximum rate of substrate uptake by~~ b_{hb_i}: Effective substrate uptake rate of the ith species of heterotrophic bacteria, [h^{-1}]

b_{max20,hb_i}: Maximal substrate uptake rate of the ith species of heterotrophic bacteria at 20 °C, [h^{-1}]

$[SMS]$: ~~small~~ Small monomeric substrate concentration, [mgC L^{-1}]

K_{sms,hb_i}: Half-saturation constant for small monomeric substrate of the ith species of heterotrophic bacteria, [mgC L^{-1}]

$f(T)_{hb_i}$: Water temperature weight of the ith species of heterotrophic bacteria at T °C, [-]

T_{opt,hb_i}: Optimal temperature of the ith species of heterotrophic bacteria for its growth, [°C]

σ_{hb_i}: Range of temperature for the ith species of heterotrophic bacteria, [°C]

Y_{hb_i}: Bacterial growth yield of the ith species of heterotrophic bacteria, [-]

μ_{hb_i}: ~~Growth~~ Effective growth rate of the ith species of heterotrophic bacteria, [h^{-1}]

A sinking velocity (vs_{hb}) is associated to each particulate species to represent particulate sinking by gravity. The mortality of heterotrophic bacteria is simulated by a fist order kinetics (Eq. (4)). The dead biomass of living species is converted into varying types of organic matter content, including both dissolved and particulate forms, based on specified proportions (ϵ_{hd} and ϵ_{hp}, Fig. 1).

$$\frac{d[HB_i]}{dt} = (\mu_{hb_i} - k_{d,hb_i} d20,hb_i f(T)_{hb_i} - k_{sink,hb_i})[HB_i] \quad (4)$$

$$k_{sink,hb_i} = \frac{vs_{hb_i}}{depth}$$

With ~~k_{d,hb_i}: Mortality~~ μ_{hb_i}: Effective growth rate of the ith species of heterotrophic bacteria, [h^{-1}]

~~vs_{hb_i}: Sinking velocity~~ k_{d20,hb_i}: Mortality rate of the ith species of heterotrophic bacteria at 20 °C, [~~m~~ h^{-1}]

k_{sink,hb_i}: Sinking rate of the ith species of heterotrophic bacteria, [h^{-1}]

$[HB_i]$: Biomass concentration of the ith species of heterotrophic bacteria, [mgC L^{-1}]

$f(T)_{hb_i}$: Water temperature weight at T °C defined by equation (2), [-]

vs_{hb_i}: Sinking velocity of the ith species of heterotrophic bacteria, [m h^{-1}]

$depth$: Water depth, [m]

2.1.2 Hydrolysis of high weight polymer

The particulate biodegradable high weight polymer (HP_1 and HP_2) is firstly hydrolyzed to the dissolved biodegradable high weight polymer (HD_1 and HD_2). The dissolved biodegradable high weight polymer is then hydrolyzed exoenzymatically to small monomeric substrate (Fig. 1). The hydrolysis of HP is represented by a first order kinetics (Eq. (5)) while a Michaelis-Menten function (Michaelis and Menten, 1913) is used to express the exoenzymatic hydrolysis of HD ~~depending on its concentration and heterotrophic bacterial biomass~~ (Eq. (6)).

$$\frac{d[HP_i]}{dt} = -k_{hp_i} * [HP_i] + (\sum_j k_{d,j}[LS]_{d20,j} f(T)_j [LS]_j)\epsilon_{hp_i} - k_{sink,hp_i}[HP_i] \quad (5)$$

With $[HP_i]$: Concentration of particulate high weight polymer, $i \in \{1,2\}$, [mgC L^{-1}]

k_{hp_i}: Hydrolysis rate of HP_i, $i \in \{1,2\}$, [h^{-1}]

~~$k_{d,j}$~~ $f(T)_j$: Water temperature weight of the jth living species at T °C defined like the equation (2), [-]

$k_{d20,j}$: Mortality rate of the jth living species (such as phytoplankton, zooplankton, bacteria etc.) at 20 °C, [h^{-1}]

$[LS]_j$: Concentration of the jth living species, [mgC L^{-1}]

ϵ_{hp_i}: Proportion to convert the dead biomass to HP_i, $i \in \{1,2\}$, [-]

k_{sink,hp_i}: Sinking rate for HP_i, $i \in \{1,2\}$, [h^{-1}]

$$\frac{d[HD_i]}{dt} = -e_{max,hd_i}\frac{[HD_i]}{[HD_i]+K_{hd_i}}\sum_k HB_k(e_{max20,hd_i,hb_k} f(T)_k \frac{[HD_i]}{[HD_i]+K_{hd_i,hb_k}}[HB_k]) + k_{hp_i} * [HP_i] + (\sum_j k_{d,j}[LS]_{d20,j} f(T)_j [I \quad (6)$$

With $[HD_i]$: concentration of dissolved high weight polymer, $i \in \{1,2\}$, [mgC L^{-1}]

~~e_{max,hd_i}~~ e_{max20,hd_i,hb_k}: Maximum hydrolysis rate of HD_i at 20 °C related to HB_k, $i \in \{1,2\}$, [h^{-1}]

~~K_{hd_i}~~ $f(T)_k$: Water temperature weight of the k^{th} species of heterotrophic bacteria at T °C (Eq. (2)), [-]

K_{hd_i,hb_k}: Half-saturation constant for HD_i related to HB_k, $i \in \{1,2\}$, [mgC L^{-1}]

$[HB_k]$: Concentration of the k^{th} species of heterotrophic bacteria, [mgC L^{-1}]

~~$k_{d,j}$~~ $k_{d20,j}$: Mortality rate of the j^{th} living species (such as phytoplankton, zooplankton, bacteria etc.) at 20 °C, [h^{-1}]

$f(T)_j$: Water temperature weight of the j^{th} living species at T °C defined like the equation (2), [-]

$[LS]_j$: Concentration of the j^{th} living species, [mgC L^{-1}]

ϵ_{hd_i}: Proportion to convert the dead biomass to HD_i, $i \in \{1,2\}$, [-]

2.2 Nitrifying bacteria dynamics

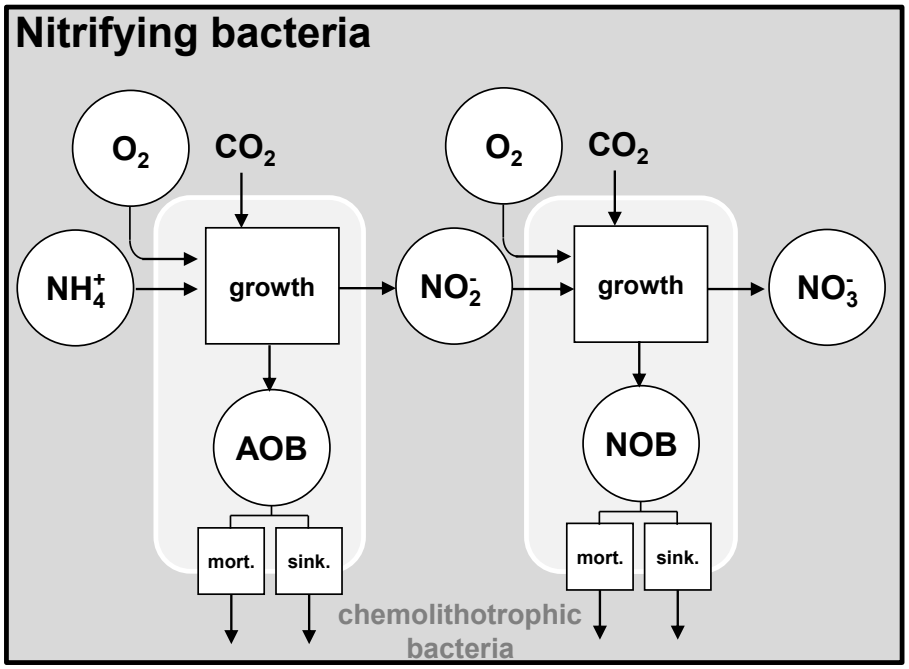

Figure 2. Nitrifying bacteria dynamics. AOB: ammonia-oxidizing bacteria; NOB: nitrite-oxidizing bacteria; mort.: mortality; sink.: sinking

The unified RIVE v1.0 model includes the description of the nitrification microbial process, mediated by two types of nitrifying bacteria. They are respectively responsible for the production of nitrite ($NH_4^+ + \frac{3}{2}O_2 \longrightarrow NO_2^- + 2H^+ + H_2O$) and nitrate ($NO_2^- + \frac{1}{2}O_2 \longrightarrow NO_3^-$). The nitrifying bacteria get energy by oxidizing NH_4^+ (ammonium) and NO_2^- (nitrite) for their growth. These two bacteria are named AOB (ammonia-oxidizing bacteria) and NOB (nitrite-oxidizing bacteria) respectively (Brion and Billen, 1998). The growth of nitrifying bacteria is limited by the availability of ammonium, nitrite and oxygen, which is represented with Monod functions (Eq. (7)). The effect of water temperature is taken into account also.

$$\mu_{aob} = \mu_{aob,max} max20_{,aob} f(T)_{aob} \left(\frac{[NH_4^+]}{[NH_4^+] + K_{nh_4,aob}}\right)\left(\frac{[O_2]}{[O_2] + K_{o_2,aob}}\right) \quad (7)$$

$$\mu_{nob} = \mu_{nob,max} max20_{,nob} f(T)_{nob} \left(\frac{[NO_2^-]}{[NO_2^-] + K_{no_2,nob}}\right)\left(\frac{[O_2]}{[O_2] + K_{o_2,nob}}\right) \quad (8)$$

With ~~$\mu_{aob,max}$ and $\mu_{nob,max}$: Maximum~~ μ_{aob} and μ_{nob}: Effective growth rate of AOB and NOB, [h^{-1}]

$\mu_{max20,aob}$ and $\mu_{max20,nob}$: Maximal growth rates of AOB and NOB at 20 °C, respectively, [h^{-1}]

$f(T)_{aob}$ and $f(T)_{nob}$: Water temperature weight at T °C defined like the equation (2), [-]

$K_{nh_4,aob}$ and $K_{no_2,nob}$: Half-saturation constants for NH_4^+ (AOB) and for NO_2^- (NOB), [mgN L^{-1}]

$K_{o_2,aob}$ and $K_{o_2,nob}$: Half-saturation constants for oxygen (AOB and NOB), [mgO_2 L^{-1}]

The mortality and sinking of nitrifying bacteria are simulated the same way than for other living species.

$$\frac{d[AOB]}{dt} = (\mu_{aob} - k_{d,aob} d20_{,aob} f(T)_{aob} - k_{sink,aob})[AOB] \quad (9)$$

$$\frac{d[NOB]}{dt} = (\mu_{nob} - k_{d,nob} d20_{,nob} f(T)_{nob} - k_{sink,nob})[NOB] \quad (10)$$

With ~~$k_{d,aob}$ and $k_{d,nob}$~~ μ_{aob} and μ_{nob}: Effective growth rate of AOB and NOB defined by (7) and (8), [h^{-1}]

$k_{d20,aob}$ and $k_{d20,nob}$: Mortality rate of AOB and NOB at 20 °C, [h^{-1}]

$k_{sink,aob}$ and $k_{sink,nob}$: Sinking rate of AOB and NOB, [h^{-1}]

$f(T)_{aob}$ and $f(T)_{nob}$: Water temperature weight at T °C defined like the equation (2), [-]

$[AOB]$ and $[NOB]$: Concentrations of AOB and NOB, [mgC L^{-1}]

2.3 Primary producer dynamics

The behavior of primary producers is represented using the AQUAPHY model (Lancelot et al., 1991). Biomass of a phytoplankton species is composed of three different cellular constituents (Fig. 3):

(a) The structural and functional macromolecules of the cell, **F**; mainly proteins, chlorophyll and structural lipids (such as membranes)

(b) Polysaccharides playing the role of reserve products, **R**;

(c) Monomeric (amino acids) and oligomeric precursors for macromolecular synthesis, **S**

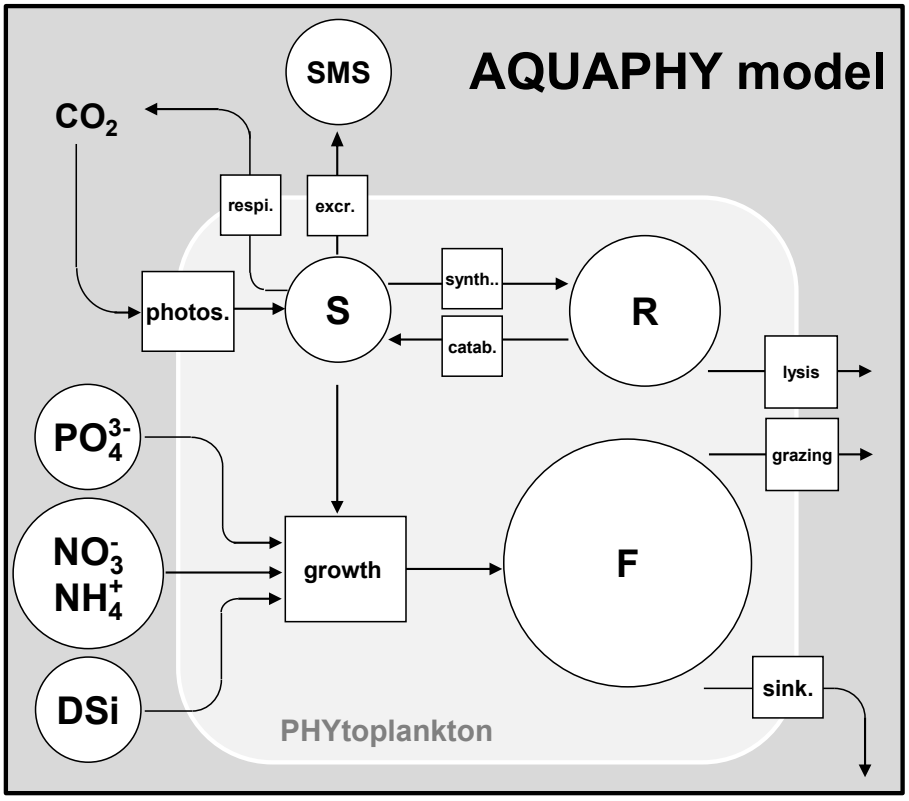

Figure 3. Description of ~~Aquaphy~~ AQUAPHY model. F: functional marcromolecules of the cell; R: reserve products; S: Monomeric (amino acids) and oligomeric precursors for macromolecular synthesis. Phytoplankton biomass equals to the sum of the three cellular constituents (F, R, S). SMS: small monomeric substrate. photos.: photosynthesis; respi.: respiration; excr.: excretion; synth.: synthesis; catab.: catabolysis; sink.: sinking

At any time, the biomass of the jth phytoplankton species (mgC L^{-1}), $[PHY]_j$, is equal to the sum of the three internal constituents (Eq. (11)), $[F]_j$, $[R]_j$, $[S]_j$:

$$[PHY]_j = [F]_j + [R]_j + [S]_j \tag{11}$$

The most common way of measuring phytoplankton biomass is ~~in~~ using the chlorophyll *a* concentration (μgchla L^{-1}). A carbon/chlorophyll *a* ratio of 35 mgC/μgchl*a* is therefore considered to convert experimental data into ~~a model state variable. The~~ phytoplankton biomass. The initial proportions of different constituents (F, R, S) are fixed (Lancelot et al., 1991). They are only used to determine the initial concentrations of the three cellular constituents and their concentrations in incoming water fluxes for each phytoplankton species. According to Lancelot et al. (1991), the structural and functional macromolecules of the cell ($[F]_j$) account for about 85% of the phytoplankton biomass ($[PHY]_j$), while the reserve products ($[R]_j$) account for about 10% of the biomass~~(Lancelot et al., 1991)~~. The remainder (5%) of the biomass constitutes the small precursors for macromolecules synthesis ($[S]_j$). Theses proportions of F, S, R are updated at each time step for each phytoplankton species.

~~The proportions proposed by Lancelot et al. (1991) are only used to determine the initial concentrations of the three cellular constituents and the concentrations of the three cellular constituents in external inflows for each phytoplankton species.~~

2.3.1 Photosynthesis

The photosynthesis process forms small precursors (**S**) by fixing carbon dioxide. Its rate is determined by the photosynthesis-irradiance relationship (Platt et al., 1980) including three parameters (Eq. (12)) and the active irradiance ($I(z)$, μE m^{-2} s^{-1}).

~~$P(z)_{phy_j} = P_{max,phy_j}(1 - e^{-\frac{\alpha_{phy_j} I(z)}{P_{max,phy_j}}})e^{-\frac{\beta_{phy_j} I(z)}{P_{max,phy_j}}}$~~

$$P(z)_{phy_j} = P_{max20,phy_j} f(T)_{phy_j}(1 - e^{-\frac{\alpha_{phy_j} I(z)}{P_{max20,phy_j} f(T)}})e^{-\frac{\beta_{phy_j} I(z)}{P_{max20,phy_j} f(T)}} \quad (12)$$

(13)

with ~~P_{max,phy_j}: Maximum rate of photosynthesis~~ $P(z)_{phy_j}$: Photosynthesis rate of of the jth phytoplankton species at water depth z m, [h^{-1}]

P_{max20,phy_j}: Maximal photosynthesis rate of the jth phytoplankton species at 20 °C, [h^{-1}]

$f(T)_{phy_j}$: Water temperature weight of the jth phytoplankton species at T °C defined like the equation (2), [-]

α_{phy_j}: Photosynthetic efficiency of the jth phytoplankton species, [h^{-1} (μE m^{-2} s^{-1})$^{-1}$]

β_{phy_j}: Photoinhibition capacity of the jth phytoplankton species, [h^{-1} (μE m^{-2} s^{-1})$^{-1}$]

$I(z)$: Photosynthetically Active Radiation (PAR) or active irradiance in water column at depth z m, [μE m^{-2} s^{-1}] or [W m^{-2}]

The averaged photosynthesis rate of the jth phytoplankton species over water column is obtained by integrating $P(z)$.

$$p_{phy_j} = \frac{\int_0^{depth} P(z)_{phy_j}\,\mathrm{d}z}{depth} \quad (14)$$

where $depth$ is the water height (m) and p_{phy_j} is the averaged photosynthesis rate over water column (h^{-1}).

The active irradiance at water depth z m ($I(z)$) follows the Beer–Lambert law (Eq. (15)). The decrease of active irradiance from water surface to water bottom is represented by light extinction coefficient (η). The extinction coefficient is composed of three parts: pure water (η_{base}), suspended solid (η_{ss}) and algal self-shading (η_{chla}).

$$I(z) = I_0 e^{-\eta z} \quad (15)$$
$$\eta = \eta_{base} + \eta_{chla}[chla] + \eta_{ss}[SS]$$

with $I(z)$: Active irradiance at water depth z m, [μE m^{-2} s^{-1}] or [W m^{-2}]

I_0: Photosynthetically Active Radiation (PAR), or active irradiance at water surface, measured by the Photosynthetic Photon[1] Flux Density (PPFD) [μE m^{-2} s^{-1}] or [W m^{-2}]

[1]Photons within the range of visible light between 400 and 700 nm

η: Light extinction coefficient, [m^{-1}]

η_{base}: Light extinction coefficient related to pure water, [m^{-1}]

η_{chla}: Linear algal self-shading light extinction coefficient, [m^{-1} (μgchl$a$ L^{-1})$^{-1}$]

η_{ss}: Light extinction coefficient related to suspended solid, [m^{-1} (mg L^{-1})$^{-1}$]

$[chla]$: Total chlorophyll a concentration, [$\mu gchla$ L^{-1}]

$[SS]$: Suspended solid concentration, [mg L^{-1}]

2.3.2 Growth

The growth of phytoplankton involves the transformation of small precursors (**S**) into structural and functional macromolecules (**F**), which also requires the uptake of ~~nutrients (N, P,~~ dissolved inorganic nutrients (nitrogen - N, phosphorus - P, silicon - Si) from the environment (Fig. 3). The nutrients can potentially ~~control phytoplankton growth by limiting it if they are not present in sufficient quantities~~ limit phytoplankton growth if their quantities are insufficient. The limitation of nutrients is represented using multiple Monod functions (Eq. (16)). The maximum growth rate (μ_{max,F_j}) is itself weighted by a limitation based on the availability of small precursors (**S**). The limitation by dissolved silica (DSi) is applied only for diatoms (DIA).

$$\mu_{F_j} = \mu_{max,F_j} max20,F_j f(T)_{phy_j} \left(\frac{\frac{[S_j]}{[F_j]}}{\frac{[S_j]}{[F_j]} + K_{S,phy_j}}\right) Nut\_lim \quad (16)$$

$$Nut\_lim = min\left(\frac{[N]}{[N]+K_{N,phy_j}} \frac{[DIN]}{[DIN]+K_{N,phy_j}}, \frac{[P]}{[P]+K_{P,phy_j}} \frac{[DIP]}{[DIP]+K_{P,phy_j}}, \frac{[Si]}{[Si]+K_{Si,phy_j}} \frac{[DSi]}{[DSi]+K_{Si,phy_j}}\right) \quad (17)$$

$$\text{or } Nut\_lim = min\left(\frac{[N]}{[N]+K_{N,phy_j}} \frac{[DIN]}{[DIN]+K_{N,phy_j}}, \frac{[P]}{[P]+K_{P,phy_j}} \frac{[DIP]}{[DIP]+K_{P,phy_j}}\right)$$

With ~~μ_{max,F_j}: Maximum~~ μ_{F_j}: Effective growth rate of functional macromolecules for the jth phytoplankton species, [h^{-1}]

~~$[N]$, $[P]$ and $[Si]$~~ μ_{max20,F_j}: Maximal growth rate of functional macromolecules for the jth phytoplankton species at 20 °C, [h^{-1}]

$f(T)_{phy_j}$: Water temperature weight of the jth phytoplankton species at T °C defined like the equation (2), [-]

$[S_j]$ and $[F_j]$: Concentrations of small precursors and functional macromolecules for the jth phytoplankton species, [mgC L^{-1}]

K_{S,phy_j}: Half-saturation constant for small precursors of the jth phytoplankton species, [-]

Nut_lim: Nutrients limiting factor, [-]

$[DIN]$, $[DIP]$ and $[DSi]$: Concentrations of ~~nitrogen ($[N] = [NO_3^-] + [NH_4^+]$~~ dissolved inorganic nitrogen ($[DIN] = [NO_3^-] + [NH_4^+]$, mgN L^{-1}), ~~phosphorus ($[P] = [PO_4^{3-}]$~~ dissolved inorganic phosphorus ($[DIP] = [PO_4^{3-}]$, mgP L^{-1}) and dissolved silica (DSi, mgSi L^{-1})

~~K_{S,phy_j}: Half-saturation constant for small precursors of the jth phytoplankton species,~~ K_{N,phy_j} and K_{P,phy_j}: Half-saturation constant for dissolved inorganic nitrogen and phosphorus of the jth phytoplankton species, [mgN L^{-1}] and [mgP L^{-1}]

K_{Si,phy_j}: Half-saturation constant for dissolved silica in case of diatoms, [mgSi L^{-1}]

2.3.3 Respiration

The respiration rate of phytoplankton (r_{phy}) is divided into two components (Eq. (18)): one ($R_{m,phy}$) ensuring the survival of the cell (maintenance process), the other ($R_{\mu,phy}$) corresponding to energetic cost of growth.

$$r_{phy_j} = R_{m,phy_j\, m20,phy_j\, f(T)_{phy_j}} + \mu_{F_j} R_{\mu,phy_j} \tag{18}$$

with ~~R_{m,phy_j}~~ r_{phy_j}: Respiration rate of the jth phytoplankton species, [h^{-1}]

R_{m20,phy_j}: Maintenance respiration rate of the jth phytoplankton species at 20 °C, [h^{-1}]

$f(T)_{phy_j}$: Water temperature weight of the jth phytoplankton species at T °C defined like the equation (2), [-]

R_{μ,phy_j}: Respiration for energetic cost of the jth phytoplankton species, [-]

μ_{F_j}: Effective growth rate of the jth phytoplankton species (Eq. (16)), [h^{-1}]

2.3.4 Excretion

Included later by Garnier et al. (1998), the phytoplankton excretion (e_{phy}) includes two terms: a constant excretion rate ($E_{cst,phy}$) and another that depends on the photosynthesis rate ($E_{phot,phy}$). The product of excretion is the small monomeric substrate (SMS), assimilated directly by heterotrophic bacteria for their growth and respiration (Fig. 1).

$$e_{phy_j} = E_{cst,phy_j} + p_{phy_j} E_{phot,phy_j} \tag{19}$$

With e_{phy_j}: Excretion rate of the jth phytoplankton species, [h^{-1}]

E_{cst,phy_j}: Basic excretion rate of the jth phytoplankton species, [h^{-1}]

E_{phot,phy_j}: Excretion of the jth phytoplankton species related to photosynthesis, [-]

p_{phy_j}: Photosynthesis rate of the jth phytoplankton species (Eq. (14)), [h^{-1}]

The variation of small monomeric substrate (SMS) can then be established (Eq. (20)).

$$\frac{d[SMS]}{dt} = hydr - \sum_i b_{hb_i}[HB_i] + \sum_j e_{phy_j}[F_j] \tag{20}$$

With $hydr$: Hydrolysis of the dissolved high weight polymer HD_1 and HD_2 (Eq. (6)), [mgC L^{-1} h^{-1}]

b_{hb_i}: Effective rate of substrate uptake by the ith heterotrophic bacteria species (Eq. (3)), [h^{-1}]

$[HB_i]$: Biomass concentration of the ith species of heterotrophic bacteria, [mgC L^{-1}]

e_{phy_j}: Effective excretion rate of the jth phytoplankton species (Eq. (19)), [h^{-1}]

$[F_j]$: Concentration of functional macromolecules for the jth phytoplankton species, [mgC L^{-1}]

2.3.5 Synthesis and catabolysis of reserve products

The carbon fixed in the cell by photosynthesis forms small precursors (**S**) that can be transformed, either into functional macromolecules (**F**), or into reserve products (**R**). The synthesis of reserve products is limited by the $\frac{[S]}{[F]}$ ratio based on a

Michaelis-Menten like function (Eq. (21)).

$$s_{R,phy_j} = s_{R,max,phy_j} \, R,max20,phy_j \, f(T)_{phy_j} \frac{\frac{[S_j]}{[F_j]}}{\frac{[S_j]}{[F_j]} + K_{S,phy_j}} \quad (21)$$

With ~~s_{R,max,phy_j}: Maximum~~ s_{R,phy_j}: Synthesis rate of reserve products of jth phytoplankton species, [h^{-1}]

$s_{R,max20,phy_j}$: Maximal synthesis rate of reserve products of jth phytoplankton species at 20 °C, [h^{-1}]

$f(T)_{phy_j}$: Water temperature weight of jth phytoplankton species at T °C defined like the equation (2), [-]

$[S_j]$ and $[F_j]$: Concentrations of small precursors and functional macromolecules for the jth phytoplankton species, [mgC L^{-1}]

K_{S,phy_j}: Half-saturation constant for small precursors of the jth phytoplankton species, [-]

Reserve products (**R**) are likely to be catabolized to produce small precursors (**S**). A first order kinetic ($c_{R,phy}$, h^{-1}) is used to represent catabolysis of reserve product.

2.3.6 ~~Disappearance~~ Extinction of phytoplankton

Three ways of phytoplankton ~~disappearance~~ extinction are implemented in the unified RIVE v1.0: lysis, sinking and grazing by zooplankton (Sct. 2.4.1). The phytoplankton lysis is represented by a first order kinetics using a mortality rate (~~$k_{d,phy}$~~ $k_{d20,phy}$, h^{-1}). For ease of presentation, all three processes are assumed in an overall ~~disappearance~~ extinction rate d_{phy} (h^{-1}).

$$d_{phy_j} = k_{d,phy_j} \, d20,phy_j \, f(T)_{phy_j} + k_{sink,phy_j} + \sum_i \frac{b_{zoo_i}[ZOO_i]}{\sum_{k=1}^{NS}[PHY_k]} \quad (22)$$

With d_{phy_j}: ~~Disappearance~~ Extinction rate of the jth phytoplankton species, [h^{-1}]

~~k_{d,phy_j}~~ k_{d20,phy_j}: Mortality rate of the jth phytoplankton species at 20 °C, [h^{-1}]

$f(T)_{phy_j}$: Water temperature weight of jth phytoplankton species at T °C defined like the equation (2), [-]

k_{sink,phy_j}: Sinking rate of the jth phytoplankton species, [h^{-1}]

b_{zoo_i}: Grazing rate of the ith zooplankton species (Eq. (27), section 2.4.1), [h^{-1}]

$[ZOO_i]$: Zooplankton concentration of the ith zooplankton species, [mgC L^{-1}]

$\sum_{k=1}^{NS}[PHY_k]$: Total phytoplankton concentration (with NS the Number of phytoplankton species grazed by zooplankton), [mgC L^{-1}]

2.3.7 Phytoplankton budgets

According to the processes related to phytoplankton (photosynthesis, growth, mortality etc.), the different budgets can be established for the jth phytoplankton species as follows.

$$\frac{d[S_j]}{dt} = (p_{phy_j} - r_{phy_j} - \mu_{F_j} - s_{R,phy_j})[F_j] + c_{R,phy_j}[R_j] - e_{phy_j}[F_j] - d_{phy_j}[S_j] \quad (23)$$

$$\frac{d[R_j]}{dt} = s_{R,phy_j}[F_j] - c_{R,phy_j}[R_j] - d_{phy_j}[R_j] \quad (24)$$

$$\frac{d[F_j]}{dt} = (\mu_{F_j} - d_{phy_j})[F_j] \quad (25)$$

$$\frac{d[PHY_j]}{dt} = (p_{phy_j} - r_{phy_j} - e_{phy_j})[F_j] - d_{phy_j}[PHY_j] \quad (26)$$

With: p_{phy_j}: Photosynthesis rate of the jth phytoplankton species (Eq. (14)), [h^{-1}]

r_{phy_j}: Respiration rate of the jth phytoplankton species (Eq. (18)), [h^{-1}]

μ_{F_j}: Growth rate of the jth phytoplankton species (Eq. (16)), [h^{-1}]

s_{R,phy_j}: Synthesis rate of reserve products of the jth phytoplankton species (Eq. (21)), [h^{-1}]

c_{R,phy_j}: Catabolysis rate of reserve products of the jth phytoplankton species, [h^{-1}]

e_{phy_j}: Excretion rate of the jth phytoplankton species (Eq. (19)), [h^{-1}]

d_{phy_j}: ~~Disappearance~~ Extinction rate of the jth phytoplankton species(Eq. (22)), [h^{-1}]

$[S_j]$, $[F_j]$ and $[R_j]$: Concentrations of $[S_j]$, $[F_j]$ and $[R_j]$ for the jth phytoplankton species, [mgC L^{-1}]

$[PHY_j]$: Biomass concentration of the jth phytoplankton species, [mgC L^{-1}]

2.4 Zooplankton dynamics

The zooplankton dynamics include the grazing on phytoplankton, the growth, the respiration, the mortality and the sinking (Fig. 4).

2.4.1 Grazing and Growth

The grazing on phytoplankton by zooplankton and the growth of zooplankton are expressed based on a ~~maximum grazing rate ($b_{max,zoo}$~~ maximal grazing rate at 20 °C ($b_{max20,zoo}$) limited by the phytoplankton biomass based on a Monod function (Eq. (27)). The grazing of zooplankton takes place only when the total phytoplankton biomass exceeds a certain threshold ($[PHY_0]$). No specific preference for grazing on particular phytoplankton species is considered among zooplankton species. Instead, the phytoplankton biomass grazed by the ith species of zooplankton is divided proportionally among each species of phytoplankton (Eq. (22)). The growth rate of zooplankton is considered proportional to grazing rate using a growth yield factor

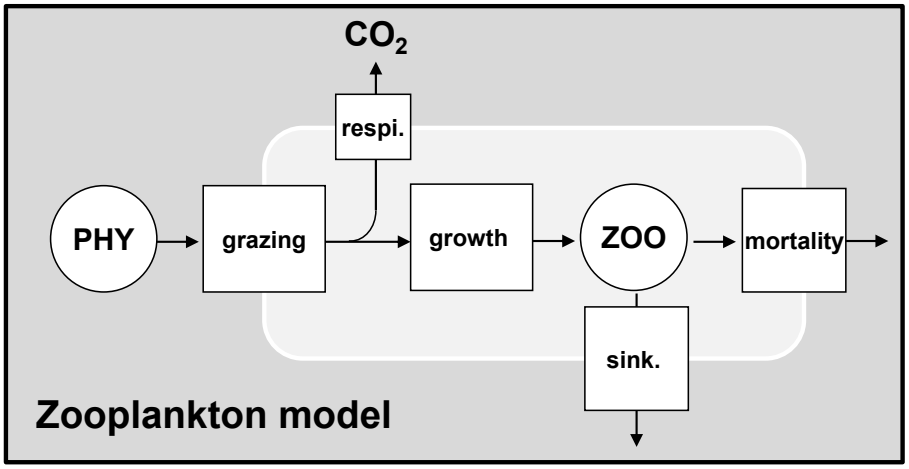

Figure 4. Dynamics of zooplankton. PHY: phytoplankton species; ZOO: zooplankton species; respi.: respiration; sink.: sinking

(Eq. (28)).

$$b_{zoo_i} = b_{max,zoo_i} max20,zoo_i f(T)_{zoo_i} \frac{(\sum_j^{NS}[PHY_j] - [PHY_0]_{zoo_i})}{(\sum_j^{NS}[PHY_j] - [PHY_0]_{zoo_i}) + K_{phy,zoo_i}} \quad (27)$$

$$\mu_{zoo_i} = Y_{zoo_i} b_{zoo_i} \quad (28)$$

With ~~b_{max,zoo_i}: Maximum~~ b_{zoo_i}: Effective grazing rate of the ith zooplankton species, [h^{-1}]

b_{max20,zoo_i}: Maximal grazing rate of the ith zooplankton species at 20 °C, [h^{-1}]

$f(T)_{zoo_i}$: Water temperature weight of the ith zooplankton species at T °C defined like the equation (2), [-]

$\sum_j^{NS}[PHY_j]$: Total phytoplankton biomass with NS the number of phytoplankton species grazed by zooplankton, [mgC L^{-1}]

$[PHY_0]_{zoo_i}$: Phytoplankton biomass threshold above which grazing takes place for the ith zooplankton species, [mgC L^{-1}]

K_{phy,zoo_i}: Half-saturation constant for phytoplankton biomass of the ith zooplankton species, [mgC L^{-1}]

μ_{zoo_i}: Growth rate of the ith zooplankton species, [h^{-1}]

Y_{zoo_i}: Growth yield of the ith zooplankton species, [-]

~~Dynamics of zooplankton. PHY: phytoplankton species; ZOO: zooplankton species; respi.: respiration; sink.: sinking~~

2.4.2 Respiration and Mortality

Grazed phytoplankton not used for zooplankton growth is respired (Fig. 4). The rate of respiration is then obtained by $(1 - Y_{zoo}) \times b_{zoo}$. The mortality of zooplankton is simulated by a first order kinetics (~~$k_{d,zoo}$).~~ $k_{d20,zoo}$).

$$r_{zoo_i} = (1 - Y_{zoo_i}) \times b_{zoo_i} \quad (29)$$

$$\frac{d[ZOO_i]}{dt} = (Y_{zoo_i} b_{zoo_i} - k_{d,zoo_i} d20,zoo_i f(T)_{zoo_i} - k_{sink,zoo_i})[ZOO_i] \quad (30)$$

With r_{zoo_i}: Respiration rate of the ith zooplankton species, [h^{-1}]

Y_{zoo_i}: Growth yield of the ith zooplankton species, [-]

b_{zoo_i}: Effective grazing rate of the ith zooplankton species (Eq. (27)), [h^{-1}]

~~k_{d,zoo_i}~~ k_{d20,zoo_i}: Mortality rate of the ith zooplankton species at 20 °C, [h^{-1}]

$f(T)_{zoo_i}$: Water temperature weight of the ith zooplankton species at T °C defined like the equation (2), [-]

k_{sink,zoo_i}: Sinking rate of the ith zooplankton species, [h^{-1}]

$[ZOO_i]$: Biomass concentration of the ith zooplankton species, [mgC L^{-1}]

2.5 ~~Nutrients~~ Nutrient cycling

As shown above, several processes related to nutrients are taken into account: uptake by phytoplankton, mineralization, nitrification, denitrification (Fig. 5, and Fig. 6).

2.5.1 Uptake of nutrients (N, P, Si) by phytoplankton

The ~~Redfield stoichiometry (Redfield et al., 1963)~~ Redfield-Conley stoichiometry (C:N:P:Si = 106:16:1:42, (Redfield et al., 1963; Conley e is used to determine the composition of carbon, nitrogen, and phosphorus in organic matter. Constant C/N, C/P and C/Si mass ratios are considered to calculate the uptake of nutrient associated to phytoplankton growth.

$$\frac{d[uptN]}{dt} = \sum_i \frac{(\mu_{F_i} + e_{phy_i})[F_i]}{C/N} \tag{31}$$

$$uptNH_4^+ = min\left([NH_4^+], uptN(\frac{[NH_4^+]}{[NH_4^+] + [NO_3^-]})^{0.025}\right) \tag{32}$$

$$uptNO_3^- = uptN - uptNH_4^+ \tag{33}$$

$$\frac{d[uptP]}{dt} = \sum_i \frac{(\mu_{F_i} + e_{phy_i})[F_i]}{C/P} \tag{34}$$

$$\frac{d[uptSi]}{dt} = \frac{\mu_{F,dia}[F_{dia}]}{C/Si} \tag{35}$$

With μ_{F_i}: ~~Growth~~ Effective growth rate of the ith phytoplankton species (Eq. (16)), [h^{-1}]

e_{phy_i}: Excretion rate of the ith phytoplankton species (Eq. (19)), [h^{-1}]

$[F_i]$: Functional macromolecules concentration of the ith phytoplankton species, [mgC L^{-1}]

$[NH_4^+]$ and $[NO_3^-]$: Concentrations of ammonium and nitrate, [mgN L^{-1}]

$uptN$: Uptake of nitrogen for phytoplankton growth, [mgN L^{-1}]

$uptNH_4^+$: Uptake of NH_4^+ for phytoplankton growth, [mgN L^{-1}]

$uptNO_3^-$: Uptake of NO_3^- for phytoplankton growth, [mgN L^{-1}]

$uptP$: Uptake of phosphorus for phytoplankton growth, [mgP L^{-1}]

C/N: Carbon to nitrogen mass ratio, [mgC/mgN]

C/P: Carbon to phosphorus mass ratio, [mgC/mgP]

C/Si: Carbon to silica mass ratio, [mgC/mgSi]

$uptSi$: Uptake of silica for diatoms growth, [mgSi L^{-1}]

$\mu_{F,dia}$: Effective growth rate of Diatoms, [h^{-1}]

$[F_{dia}]$: Functional macromolecules (**F**) concentration of Diatoms, [mgC L^{-1}]

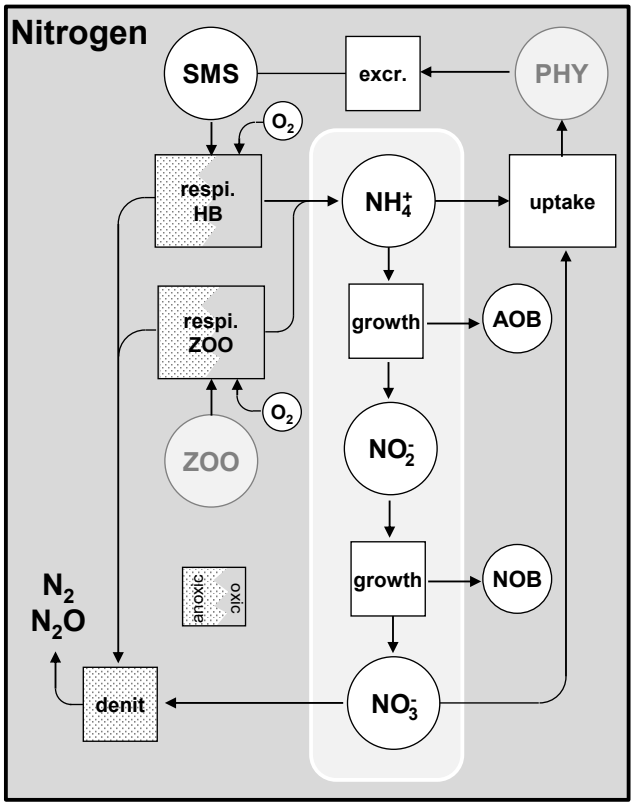

Figure 5. Cycling of nitrogen. PHY: phytoplankton species; HB: heterotrophic bacteria; ZOO: zooplankton species; AOB: ammonia-oxidizing bacteria; NOB: Nitrite-oxidizing bacteria; respi.: respiration; excr.: excretion; denit: denitrification

2.5.2 Release of nutrients by mineralization

The mineralization of organic matter by heterotrophic bacteria and zooplankton is achieved by its oxidation through respiration (Fig. 5). The process consumes organic matter and releases nitrogen and phosphorus from the fraction that is not assimilated

for growth of heterotrophic bacteria and zooplankton.

$$respHB = \sum_i (1 - Y_{hb_i}) b_{hb_i} [HB_i] \tag{36}$$

$$respZOO = \sum_j (1 - Y_{zoo_j}) b_{zoo_j} [ZOO_j] \tag{37}$$

$$relN = \frac{respHB}{C/N} + \frac{respZOO}{C/N} \tag{38}$$

$$relP = \frac{respHB}{C/P} + \frac{respZOO}{C/P} \tag{39}$$

With $respHB$: Respiration of heterotrophic bacteria species, [mgC L^{-1} h^{-1}]

Y_{hb_i}: Growth yield of the i^{th} heterotrohpic bacteria species, [-]

b_{hb_i}: Effective rate of substrate uptake by the i^{th} heterotrophic bacteria species (Eq. (1)), [h^{-1}]

$[HB_i]$: Concentration of the i^{th} heterotrohpic bacteria species, [mgC L^{-1}]

$respZOO$: Respiration of zooplankton species, [mgC L^{-1} h^{-1}]

Y_{zoo_j}: Growth yield of the j^{th} zooplankton species, [-]

b_{zoo_j}: Effective grazing rate of the j^{th} zooplankton species (Eq. (27)), [h^{-1}]

$[ZOO_j]$: Concentration of the j^{th} zooplankton species, [mgC L^{-1}]

$relN$: Release of nitrogen, [mgN L^{-1} h^{-1}]

C/N: Carbon to nitrogen mass ratio, [mgC/mgN]

$relP$: Release of phosphorus, [mgP L^{-1} h^{-1}]

C/P: Carbon to phosphorus mass ratio, [mgC/mgP]

2.5.3 Nitrification and denitrification

As mentioned in the section 2.2, the nitrification process (Fig. 2 and Fig. 5) is related to the growth of AOB (ammonia-oxidizing bacteria) and NOB (nitrite-oxidizing bacteria). Growth yields (Y_{aob_i} and Y_{nob_j}) are used to describe the amount of nitrogen consumed by nitrifying bacteria (Eq. (40) and (41)). The denitrification occurs when dissolved oxygen is not present in sufficient quantity (Fig. 5).

$$nitr_{aob} = \sum_i \frac{\mu_{aob_i}}{Y_{aob_i}} [AOB_i] \tag{40}$$

$$nitr_{nob} = \sum_j \frac{\mu_{nob_j}}{Y_{nob_j}} [NOB_j] \tag{41}$$

With μ_{aob_i} and μ_{nob_j}: ~~Growth~~ Effective growth rates of the i^{th} AOB species (Eq. (7)) and the j^{th} NOB species (Eq. (8)), [h^{-1}]

Y_{aob_i} and Y_{nob_j}: Growth yields of the i^{th} AOB species and the j^{th} NOB species, [mgC/mgN]

$nitr_{aob}$: Nitrification $NH_4^+ + \frac{3}{2}O_2 \longrightarrow NO_2^- + H_2O + 2H^+$, [mgN L^{-1} h^{-1}]

$nitr_{nob}$: Nitrification $NO_2^- + \frac{1}{2}O_2 \longrightarrow NO_3^-$, [mgN L^{-1} h^{-1}]

$[AOB_i]$ and $[NOB_j]$: Biomass concentrations of the i^{th} AOB species and the j^{th} NOB species, [mgC L^{-1}]

The budgets of NO_3^-, NH_4^+ and NO_2^- can then be established.

$$\frac{d[NO_3^-]}{dt} = -denit + nitr_{nob} - \frac{uptNO_3^-}{dt} \tag{42}$$

$$\frac{d[NH_4^+]}{dt} = relN - nitr_{aob} - \frac{uptNH_4^+}{dt} \tag{43}$$

$$\frac{d[NO_2^-]}{dt} = nitr_{aob} - nitr_{nob} \tag{44}$$

With $denit$: Denitrification, [mgN L^{-1} h^{-1}]

$nitr_{nob}$: Nitrification by NOB (Eq. (41)), [mgN L^{-1} h^{-1}]

$nitr_{aob}$: Nitrification by AOB (Eq. (40)), [mgN L^{-1} h^{-1}]

$\frac{uptNO_3^-}{dt}$: Uptake of NO_3^- by phytoplankton growth (Eq. (33)), [mgN L^{-1} h^{-1}]

$relN$: Release of nitrogen by respiration of heterotrophic bacteria and zooplankton (Eq. (38)), [mgN L^{-1} h^{-1}]

$\frac{uptNH_4^+}{dt}$: Uptake of NH_4^+ by phytoplankton growth (Eq. (32)), [mgN L^{-1} h^{-1}]

2.5.4 Phosphate adsorption desorption

Orthophosphate (PO_4^{3-}) is released by mineralization and uptaken by phytoplankton exactly as inorganic nitrogen (Fig. 6). Once released in the water column, however, orthophosphates are subject to a process of adsorption-desorption on mineral suspended solids (MSS) to form PIP (particulate inorganic phosphorus). In addition, the impact of sediment dynamics on P fluxes should be considered in the future work in unified RIVE. Vilmin et al. (2015a) showed that P fluxes are mainly driven by hydrological conditions and sediment-related processes in Seine river system.

The process is represented according to an instantaneous hyperbolic equilibrium relationship of the form:

$$\frac{PIP}{MSS}\frac{[PIP]}{[MSS]} = P_{ac} \times \frac{PO_4}{PO_4 + K_{ps}} \frac{[PO_4^{3-}]}{[PO_4^{3-}] + K_{ps}} \tag{45}$$

With $\frac{PIP}{MSS}\frac{[PIP]}{[MSS]}$: Inorganic P content of MSS, [mgP mgMSS^{-1}]

$[PIP]$ and $[MSS]$: Concentrations of PIP and MSS, [mgP L^{-1}] and [mgMSS^{-1}]

P_{ac}: Maximum adsorption capacity of MSS, [mgP mgMSS^{-1}]

$[PO_4^{3-}]$: Concentration of orthophosphate, [mgP L^{-1}]

K_{ps}: Half saturation adsorption constant, [mgP L^{-1}]

Considering this equilibrium instantaneously reached implies that a relationship exists between the variables PIP, MSS, PO_4^{3-} and TIP (total inorganic phosphorus):

$$[TIP] = [PO_4^{3-}] + [PIP] \tag{46}$$

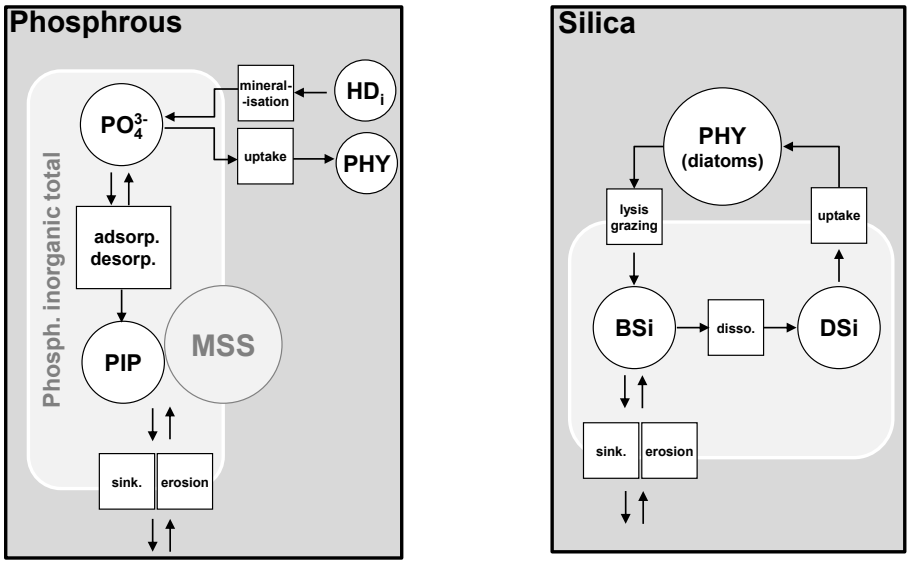

Figure 6. Phosphorus and silica dynamics. HD: dissolved high weight polymer; PHY: phytoplankton; PIP: particulate inorganic phosphorus; MSS: mineral suspended solids; BSi: biogenic silica; DSi: dissolved silica; adsorp.: adsorption; desorp.: desorption; sink.: sinking; disso. dissolution

This equilibrium relationship can be written:

$$PO4[PO_4^{3-}] = \frac{(TIP - P_{ac} \times MSS - K_{ps}) + \sqrt{(-TIP + P_{ac} \times MSS + K_{ps})^2 + 4 * TIP * K_{ps}}}{2} \quad ([TIP] - P_{ac} \times [MSS] - K_{ps}) + \quad (47)$$

With $[PO_4^{3-}]$: Concentration of orthophosphate, [mgP L^{-1}]
$[TIP]$ and $[MSS]$: Concentrations of TIP and MSS, [mgP L^{-1}] and [mgMSS^{-1}]
P_{ac}: Maximal adsorption capacity of MSS, [mgP mgMSS^{-1}]
K_{ps}: Half saturation adsorption constant, [mgP L^{-1}]

2.5.5 Silica dynamics

Dissolved silica (DSi) is produced by the dissolution of dead frustules of diatoms (designated as biogenic silica, BSi). The rock wheathering contributes also dissolved silica while it is considered as null in unified RIVE v1.0. DSi is uptaken by the growth of diatoms (Fig. 6). Biogenic silica is produced by the lysis and grazing of diatoms, settles down and dissolves according to a

first order kinetics, dependent on water temperature (Rickert et al., 2002):

$$BSi_{disso.} = Kb_{Si} * [BSi] \quad (48)$$

$$Kb_{Si} = Kb_{Si20} * ftp_{Si}(T) \quad (49)$$

$$ftp_{Si}(T) = exp(\frac{60000}{8.314} \times (\frac{1}{275} - \frac{1}{273+T})) \quad (50)$$

With Kb_{Si20}: Dissolution rate of biogenic silica at 20 °C, [h^{-1}]

$[BSi]$: Concentration of biogenic silica, [mgSi L^{-1}]

T: Water temperature, [°C]

2.6 Dissolved oxygen

Dissolved oxygen is especially influenced by photosynthesis and respiration. The reaeration at the water-air interface ~~and sediment~~ is also included in unified RIVE v1.0 model. The sediment dynamics are important for sediement oxygen demand (not shown here)~~are also included in unified RIVE v1.0 model~~. Vilmin et al. (2016) showed that benthic respiration accounts for one third of the total Seine river respiration. Relevant efforts about sediment dynamics need to be made in future work, which is not the focus of this study. An oxygen budget can then be established (Eq. (51)).

$$\frac{d[O_2]}{dt} = rea + \frac{32}{12}(\sum_i (p_{phy_i} - r_{phy_i})[F_i] - respHB - \sum_j r_{zoo_j}[ZOO_j]) - \frac{32}{14}(\frac{3}{2} nitr_{aob} + \frac{1}{2} nitr_{nob}) \quad (51)$$

$$rea = \frac{k_{rea}}{depth}([O_2]_{sat} - [O_2]) \quad (52)$$

With, k_{rea}: Reaeration coefficient, [m h^{-1}]

$depth$: Water height, [m]

$[O_2]_{sat}$: Saturated concentration of dissolved oxygen in water, [mgO_2 L^{-1}]

$[O_2]$: Concentration of dissolved oxygen in water, [mgO_2 L^{-1}]

$\frac{32}{12}$: Molar mass ratio between dissolved oxygen and carbon, [mgO_2/mgC]

p_{phy_i}: Photosynthesis rate of the i^{th} phytoplankton species (Eq. (14)), [h^{-1}]

r_{phy_i}: Respiration rate of the i^{th} phytoplankton species (Eq. (18)), [h^{-1}]

$[F_i]$: Functional biomass concentration of the i^{th} phytoplankton species, [mgC L^{-1}]

$respHB$: Respiration of all heterotrophic bacteria species (Eq. (36)), [mgC L^{-1} h^{-1}]

r_{zoo_j}: Respiration rate of the j^{th} zooplankton species (Eq. (29)), [h^{-1}]

$[ZOO_j]$: Biomass concentration of the j^{th} zooplankton species, [mgC L^{-1}]

$\frac{32}{14}$: Molar mass ratio between dissolved oxygen and nitrogen, [mgO_2/mgN]

$nitr_{aob}$: Nitrification to produce nitrite by oxidizing NH_4^+ (Eq. (40), with $\frac{3}{2}$ the stoichiometric coefficient), [mgN L^{-1} h^{-1}]

$nitr_{nob}$: Nitrification to produce nitrate by oxidizing NO_2^- (Eq. (41), with $\frac{1}{2}$ the stoichiometric coefficient), [mgN L^{-1} h^{-1}]

2.7 Inorganic carbon

An inorganic carbon module is implemented in unified RIVE v1.0. The carbonate system is described by a set of equations (named the CO_2 module) based on a previous representation provided by Gypens et al. (2004) and adapted for freshwater environments (Marescaux et al., 2020). In this module, four state variables are defined: dissolved inorganic carbon (DIC), total alkalinity (TA), acidity (pH) and aqueous carbon dioxide (CO_2(aq)).

2.7.1 CO_2 flux at air-water interface

The DIC is defined as the sum of three dissolved carbonate species:

$$[\mathrm{DIC}] = [\mathrm{H_2CO_3}] + [\mathrm{HCO_3}^-] + [\mathrm{CO_3}^{2-}] \tag{53}$$

The calculation of pH is derived from Culberson (1980) using TA and DIC. Then the aqueous carbon dioxide (CO_2 (aq)) is derived from the carbonate chemical equilibrium using DIC and pH (Marescaux et al., 2020; Yan et al., 2022a).

$$[\mathrm{CO_2(aq)}] = \frac{[\mathrm{DIC}]\frac{[\mathrm{H^+}]}{\mathrm{K_1}}}{(1 + \frac{[\mathrm{H^+}]}{\mathrm{K_1}} + \frac{\mathrm{K_2}}{[\mathrm{H^+}]})} \tag{54}$$

With K_1, K_2: Equilibrium constants of carbonate equilibrium reactions (Stumm and Morgan, 1996), [mol L^{-1}]
$[H^+]$: Concentration of hydrogen ions with pH $= -\log([H^+])$, [mol L^{-1}]
$[DIC]$: Concentration of dissolved inorganic carbon, [mgC L^{-1}]

The flux of CO_2 at water-air interface (F_{CO_2}, gC m^{-2} h^{-1}) is calculated based on Fick's first law (Fick, 1855) with a gas transfer velocity of CO_2 (k_{co2}).

$$F_{CO_2} = k_{co2}([CO_2(sat)] - [CO_2(aq)]) \tag{55}$$

With k_{co2}: Gas transfer velocity of CO_2, [m h^{-1}]
$[CO_2(sat)]$: Solubility of CO_2 in water, calculated based on Henry's law (Weiss, 1974), [mgC L^{-1}]
$[CO_2(aq)]$: Aqueous carbon dioxide concentration, [mgC L^{-1}]

The gas transfer velocity of CO_2 (k_{co2}) depends on water temperature and k_{600} (gas transfer velocity of CO_2 for a Schmidt number of 600, corresponding to a temperature of 20 °C in freshwater). According to Wilke and Chang (1955), Jähne et al. (1987) and Wanninkhof (1992), the gas transfer velocity of CO_2 (k_{co2}) at water temperature T (°C) can be calculated as:

$$k_{co2} = k_{600}\sqrt{\frac{600}{Sc_{CO_2}(T)}} \tag{56}$$

where k_{600} (m h^{-1}) is the gas transfer velocity of CO_2 for a Schmidt number of 600, and $Sc_{CO_2}(T)$ is the Schmidt number (dimensionless) calculated with the water temperature in Celsius degree (°C). The $Sc_{CO_2}(T)$ can be determined as,

$$Sc_{CO_2}(T) = 1911.1 - 118.11T + 3.4527T^2 - 0.04132T^3 \tag{57}$$

2.7.2 Budgets of TA and DIC

The processes such as respiration, photosynthesis, nitrification, denitrification and input flows affect TA and DIC. The unified RIVE v1.0 considers these processes explicitly.

$$\frac{dTA}{dt} = [(\frac{14}{106} \times \frac{(respPHY + respHB + respZOO)}{12}) + \frac{(denit - 2 \cdot nitr_{aob})}{14} + (\frac{17}{106} \times \frac{uptNO_3^-}{uptN} - \frac{15}{106} \times \frac{uptNH_4^+}{uptN}) \times \frac{\sum(\mu_{F_i} + e_{phy_i})[F_i]}{12}] \times 1000 + TA_{Net\_Input} \quad (58)$$

$$\frac{dDIC}{dt} = (respPHY + respHB + respZoo) + denit \times \frac{12}{14} \times \frac{5}{4} - \sum p_{phy_i}[F_i] + \frac{F_{CO_2}}{depth} + DIC_{Net\_Input} \quad (59)$$

where TA_{Net_input} (μmol L^{-1} h^{-1}) and DIC_{Net_input} (mgC L^{-1} h^{-1}) are the net input fluxes. The respiration of all phytoplankton, bacteria, zooplankton species ($respPHY$, $respHB$, $respZOO$, mgC L^{-1} h^{-1}) transform organic carbon to CO_2 by full oxidization. The denitrification ($denit$, mgN L^{-1} h^{-1}) is considered also in the calculation of TA and DIC. F_{CO_2} (gC m^{-2} h^{-1}) is the CO_2 flux at air-water interface. $depth$ is the water depth (m). $\frac{14}{106}$, $\frac{17}{106}$, $\frac{15}{106}$, $\frac{5}{4}$ are the stoichiometry coefficients of biogeochemical processes (Marescaux et al., 2020).

2.8 Kinetic parameters in unified RIVE model

~~116~~ 120 parameters are used to describe the aforementioned processes considering three phytoplankton species and two heterotrophic bacteria species. Some of them depend on water temperature and are calculated with a water temperature function (Eq. (2)). Their definitions and reference values are provided in appendix ~~.~~B.

3 Results

3.1 Digital implementation with Python 3 (pyRIVE 1.0) or ANSI C (C-RIVE 0.32)

The above unified governing equations are implemented in Python 3 to create pyRIVE 1.0 (https://doi.org/10.48579/PRO/Z9ACP1; Thieu et al. (2023)) and in ANSI C to create C-RIVE 0.32 (https://doi.org/10.5281/zenodo.7849609; Wang et al. (2023b)), respectively. A Jupyter Notebook is used for pedagogical exercises with pyRIVE 1.0, while C-RIVE 0.32 needs to be compiled with gcc under a Linux or a MAC OS operating system. In addition, the user interface of C-RIVE 0.32 uses its own parser based on flex and bison, which allows the software to read ASCII files.

In practice, the number of living species is predefined in pyRIVE 1.0 while we have the ability to define as many species as desired in C-RIVE 0.32 (Tab. 1). For instance, three communities of phytoplankton (DIA: Diatoms; GRA: Green algae; CYA: Cyanobacteria), two populations of heterotrophic bacteria distinct by their growth rate and size (small one SHB and large one LHB; Garnier et al. (1992a)) and two zooplankton communities (ZOR: Rotifer and ZOC: MicroCrustaceans; Billen et al. (1994); Garnier et al. (1995, 2000)) are predefined in pyRIVE 1.0.

In addition, the TIP (total inorganic phosphorus) is considered as a state variable in pyRIVE 1.0. PO_4^{3-} and PIP are derived from it according to Eq. (46) and Eq.(47). TIP is subject to release by heterotrophic bacteria and zooplankton respiration (Eq. (39)), uptake by phytoplankton and settling of PIP together with MSS. However, the PO_4^{3-} is treated as a state variable and released by respiration (Eq. (39)) in C-RIVE 0.32 and only PIP (particulate inorganic phosphorus) is derived from the equation (45).

Table 1. Number of living species defined in pyRIVE 1.0 and C-RIVE 0.32 which implement the unified RIVE v1.0

Species	PHY	HB	AOB	NOB	ZOO
pyRIVE 1.0	3	2	1	1	2
C-RIVE 0.32	User-defined	User-defined	User-defined	User-defined	User-defined

3.2 Modeling of the organic matter degradation by unified RIVE v1.0 (HSB model)

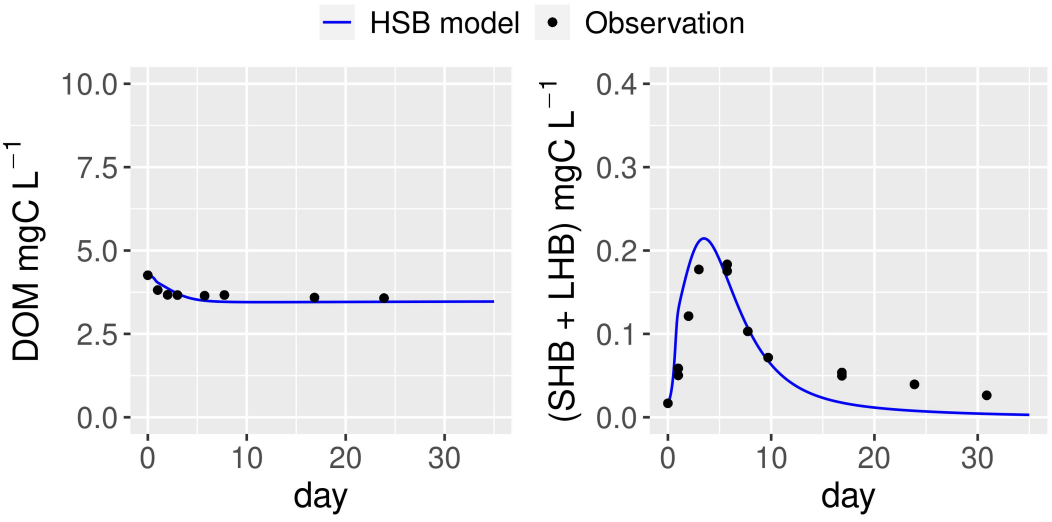

Figure 7. Simulation of the dynamics of heterotrophic bacteria in a filtered and reinoculated sample of the drainage pond water (Seine basin, France) in February 2021 (Garnier et al., 2021) by HSB model (unified RIVE v1.0). DOM: Dissolved organic matter; SHB: Small heterotrophic bacteria.

The ability of the HSB model (Fig. 1) to simulate organic matter degradation has been verified by modelling two batch experiments conducted by Garnier et al. (2021). Two water samples ~~, one~~ were used in the study. One sample was obtained from a drainage pond ~~(located in France) and the other~~ in the Seine basin, France, in February 2021 (Fig. 7). The other sample was collected from an urban sewage collector ~~(at~~ in Rosny-sur-Seine, France~~),~~ , in February 2021 (Fig. 8). These samples

were incubated in the dark at a temperature of 21°C for a period of 45 days, during which aerobic bacteria consumed organic matter (Servais et al., 1995). Only DOM and bacterial biomass are measured during batch experiments and then used to show validation. The HSB model is able to effectively reproduce the concentrations of dissolved organic matter and bacterial biomass with a trial-error adjustment of its parameter values (Fig. ~~?? and ??~~7 and 8). The parameter values are kept the same for both water samples.

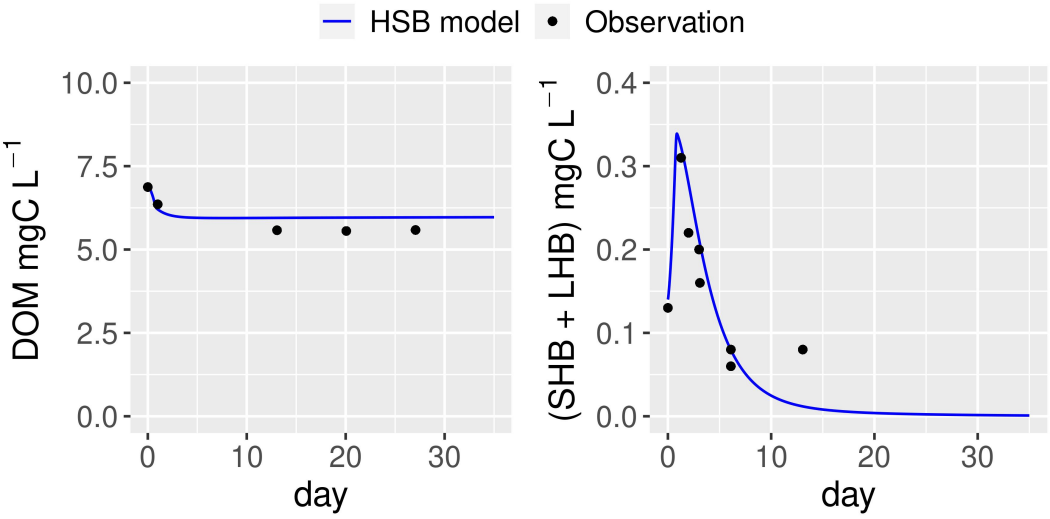

Figure 8. Simulation of the dynamics of heterotrophic bacteria in a filtered and reinoculated sample of the urban sewage water (Rosny-sur-Seine, France) in February 2021 (Garnier et al., 2021) by HSB model (unified RIVE v1.0). DOM: Dissolved organic matter; SHB: Small heterotrophic bacteria; LHB: Large heterotrophic bacteria

3.3 A river stretch simulated with unified RIVE v1.0: pyRIVE 1.0 *vs.* C-RIVE 0.32

A river stretch with a Strahler order of 8 (Fig. 9) is designed to compare the results simulated by two versions of unified RIVE v1.0 implemented in pyRIVE 1.0 and C-RIVE 0.32. The case study allows us to compare the two versions of unified RIVE v1.0 under transient contrasting conditions i) between species communities, and ii) temporally for each species community.

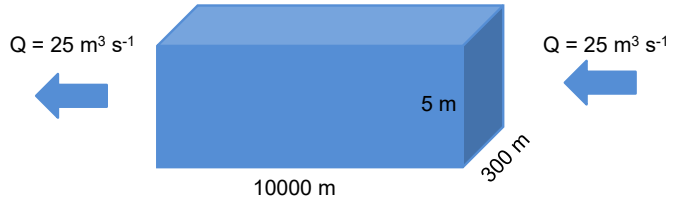

Figure 9. Geometric and hydraulic description of a river stretch

3.3.1 River stretch morphology and hydraulic conditions

~~Geometric and hydraulic description of a river stretch~~

The stretch measures 10000 meters long and 300 meters width. To simplify the boundary conditions, the upstream inflow and downstream outflow are fixed at 25 $m^3\ s^{-1}$ which corresponds to a residence time of 7 days. The water height is fixed at 5 meters.

3.3.2 Simulation settings and evaluation strategy

The concentrations of all water quality variables of inflow are defined as their initial concentrations in the stretch and remain constant during the simulation (Tab. 2). Since this paper focuses on the conceptualization of the unified RIVE v1.0 in water column, no exchange between benthic layer and water column are considered. The time step of the simulation is 6 min and a simulation period of 365 days is considered. To compare the results of the two digital implementations of unified RIVE v1.0, daily concentrations at 00:00 are plotted. Three statistical criteria (PBIAS: Percent Bias (%); MAD: Mean Absolute Difference; MaAD: Maximum Absolute Difference) are calculated to evaluate the similarity of the two set of results. The closer the criteria are to 0, the more similar are the concentrations simulated by the two softwares (pyRIVE 1.0 and C-RIVE 0.32).

$$PBIAS = 100\frac{\sum_{i=1}^{i=N}(C_i - Py_i)}{\sum_{i=1}^{i=N}} \tag{60}$$

$$MAD = \frac{\sum_{i=1}^{i=N}|C_i - Py_i|}{N} \tag{61}$$

$$MaAD = max(|C_i - Py_i|) \tag{62}$$

Where C_i represent the concentrations simulated by C-RIVE 0.32 (in ANSI C) and Py_i those simulated by pyRIVE 1.0 (in Python 3). N is the number of values.

3.3.3 Simulated concentrations of water quality variables

The concentrations simulated by pyRIVE 1.0 and C-RIVE 0.32 are very similar (and superimposed) for all water quality variables (Fig. 10). A maximum absolute difference (MaAD) of 0.0307 $mgO_2\ L^{-1}$, which is relatively low, is obtained for dissolved oxygen concentration~~while the~~. The mean absolute difference (MAD) for dissolved oxygen concentration is 0.00678 $mgO_2\ L^{-1}$ (Tab. 3) and the corresponding percent bias (PBIAS) is 0%. The MaAD of 0.0307 $mgO_2\ L^{-1}$ for dissolved oxygen is cause of the depletion of CYA S (small precursors S of cyanobacteria, Fig. 3) at the beginning of the simulation (not shown here). To correct this depletion of CYA S, the growth of functional macromolecules (CYA F) is reduced according to the availability of CYA S in C-RIVE 0.32. That's why the simulated concentrations of CYA (cyanobacteria) depict a MaAD of 0.0321 $mgC\ L^{-1}$ between pyRIVE 1.0 and C-RIVE 0.32. Due to this auto-correction in C-RIVE 0.32, the simulated concentrations of CYA by C-RIVE 0.32 are slightly smaller than those simulated by pyRIVE 1.0 (PBIAS $= -1.2\%$). The values of PBIAS indicate also the similarity between the ~~simulated concentrations~~ concentrations simulated by pyRIVE 1.0 and C-RIVE 0.32.

Table 2. Initial concentrations and boundary conditions

Species	Description	C_{init}	$C_{boundary}$	Unit
SHB	Small heterotrophic bacteria	0.005	0.005	[mgC L^{-1}]
LHB	Large heterotrophic bacteria	0.004	0.004	[mgC L^{-1}]
AOB	Ammonia-oxidizing bacteria	0.001	0.001	[mgC L^{-1}]
NOB	Nitrite-oxidizing bacteria	0.0002	0.0002	[mgC L^{-1}]
DIA	Diatoms	0.447	0.447	[mgC L^{-1}]
GRA	Green algae	0.539	0.539	[mgC L^{-1}]
CYA	Cyanobacteria	0.662	0.662	[mgC L^{-1}]
ZOR	Rotifer	$9.33{\cdot}10^{-5}$	$9.33{\cdot}10^{-5}$	[mgC L^{-1}]
ZOC	MicroCrustaceans	$9.33{\cdot}10^{-6}$	$9.33{\cdot}10^{-6}$	[mgC L^{-1}]
SMS	Small monomeric substrate	0.036	0.036	[mgC L^{-1}]
DOM_1	Rapidly biodegradable dissolved organic matter	0.022	0.022	[mgC L^{-1}]
DOM_2	Slowly biodegradable dissolved organic matter	0.174	0.174	[mgC L^{-1}]
DOM_3	Dissolved refractory organic matter	1.625	1.625	[mgC L^{-1}]
POM_1	Rapidly biodegradable particulate organic matter	0.005	0.005	[mgC L^{-1}]
POM_2	Slowly biodegradable particulate organic matter	0.021	0.021	[mgC L^{-1}]
POM_3	Particulate refractory organic matter	0.107	0.107	[mgC L^{-1}]
NH4	Ammonium	1.5	1.5	[mgN L^{-1}]
NO2	Nitrite	0.016	0.016	[mgN L^{-1}]
NO3	Nitrate	0.941	0.941	[mgN L^{-1}]
TIP	Total inorganic phosphorus	0.2	0.2	[mgP L^{-1}]
DSi	Dissolved silica	3.090	3.090	[mgSi L^{-1}]
MSS	Mineral suspended solids	2.611	2.611	[mg L^{-1}]
OXY	Dissolved oxygen	9.446	9.446	[mgO_2 L^{-1}]
TA	Total alkalinity	5291	5291	[μmol L^{-1}]
DIC	Dissolved inorganic carbon	62.728	62.728	[mgC L^{-1}]
CO2(aq)	Aqueous carbon dioxide	0.343	0.343	[mgC L^{-1}]
pH	Acidity	8.659	8.695	[-]

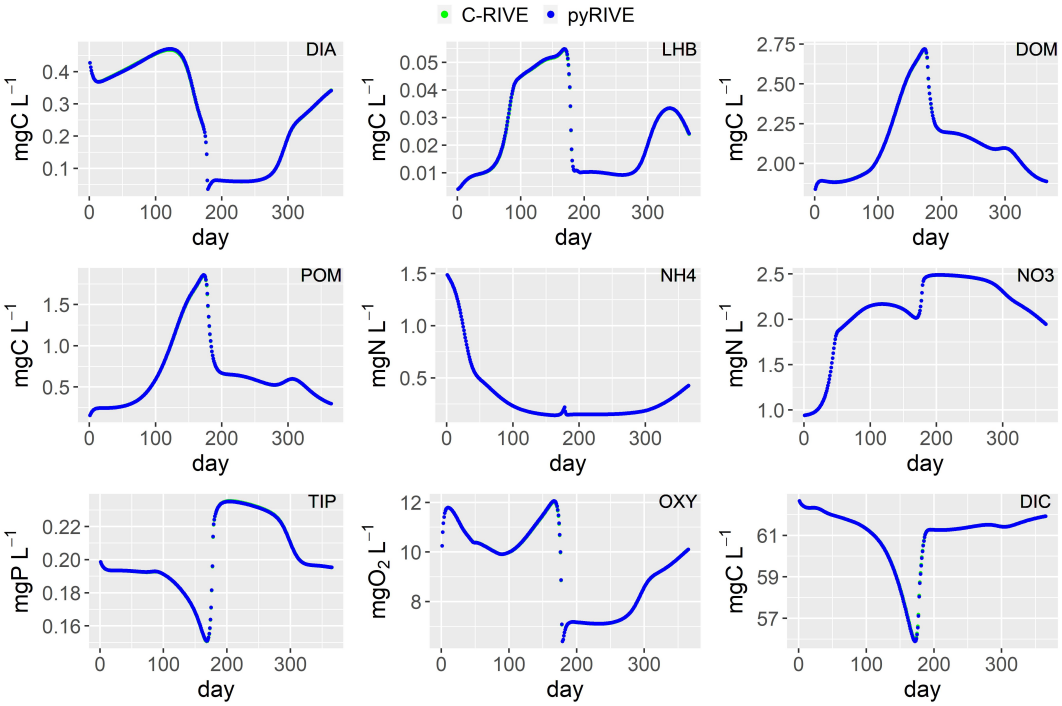

Figure 10. Simulated concentrations of main species by pyRIVE 1.0 and C-RIVE 0.32. See table 2 for their definitions

Except for CYA, the discrepancies of other variables are extremely low compared to their concentrations (PBIAS $\leq 0.6\%$). More than half of simulated variables have a PBIAS of 0%.

4 Discussion

The results show the ability of the unified RIVE v1.0 to simulate correctly the organic mater degradation and the similarity of its two digital implementations (pyRIVE 1.0 and C-RIVE 0.32). Here, we discuss the biogeochemical cycling simulated by unified RIVE v1.0 in water column (Section 4.1), the model limitations, the future developments (Section 4.3) and its benefits for scientific community (Section 4.4).

4.1 Biogeochemical cycling in water column simulated by unified RIVE v1.0

The unified RIVE v1.0 simulates the dynamics of microorganisms involving biogeochemical cycling, although the boundary conditions are defined as constant for modeling a river stretch (Fig. 9). Here we interpret the dynamics of diatoms (DIA) and large heterotrophic bacteria (LHB). For this purpose, the budget fluxes of DIA and LHB are calculated.

The decreasing of DIA biomass from day 1 to day 15 is related to the low water temperature and low active irradiance which limit its photosynthesis (Fig. 10, Fig. 12). The optimal temperature for the growth of DIA is 21 °C while the water

Table 3. Statistical criteria for comparing the simulated variables by pyRIVE 1.0 and C-RIVE 0.32 which implement the unified RIVE v1.0. PBIAS: Percent Bias [%]; MAD: Mean Absolute Difference; MaAD: Maximum Absolute Difference. The units of MAD and MaAD are either [mgC L^{-1}] or [mgN L^{-1}] or [mgP L^{-1}] or [mgSi L^{-1}] or [μmol L^{-1}].

Species	PBIAS	MAD	MaAD	Species	PBIAS	MAD	MaAD
SHB	-0.4	$2.07 \cdot 10^{-5}$	$1.40 \cdot 10^{-4}$	LHB	-0.4	$1.10 \cdot 10^{-4}$	$4.27 \cdot 10^{-4}$
AOB	0	$1.78 \cdot 10^{-5}$	$6.95 \cdot 10^{-5}$	NOB	0	$4.85 \cdot 10^{-6}$	$1.98 \cdot 10^{-5}$
DIA	-0.1	$1.07 \cdot 10^{-3}$	$3.63 \cdot 10^{-3}$	GRA	-0.1	$4.98 \cdot 10^{-4}$	$1.87 \cdot 10^{-3}$
CYA	-1.2	$7.26 \cdot 10^{-3}$	$3.15 \cdot 10^{-2}$	ZOR	-0.2	$2.26 \cdot 10^{-4}$	$2.89 \cdot 10^{-3}$
ZOC	0	$5.25 \cdot 10^{-9}$	$1.69 \cdot 10^{-7}$	SMS	-0.6	$6.65 \cdot 10^{-4}$	$4.31 \cdot 10^{-3}$
DOM_1	0.1	$6.54 \cdot 10^{-5}$	$3.61 \cdot 10^{-4}$	DOM_2	-0.1	$3.94 \cdot 10^{-4}$	$1.34 \cdot 10^{-3}$
DOM_3	0	$4.06 \cdot 10^{-4}$	$2.06 \cdot 10^{-3}$	OXY	0	$6.78 \cdot 10^{-3}$	$3.07 \cdot 10^{-2}$
POM_1	-0.3	$4.68 \cdot 10^{-4}$	$2.27 \cdot 10^{-3}$	POM_2	-0.3	$7.80 \cdot 10^{-4}$	$3.97 \cdot 10^{-3}$
POM_3	-0.2	$4.06 \cdot 10^{-4}$	$2.06 \cdot 10^{-3}$	NH4	0	$4.66 \cdot 10^{-5}$	$5.28 \cdot 10^{-4}$
NO2	0	$2.13 \cdot 10^{-5}$	$3.42 \cdot 10^{-4}$	NO3	0	$4.04 \cdot 10^{-4}$	$1.90 \cdot 10^{-3}$
TIP	0	$1.45 \cdot 10^{-4}$	$3.62 \cdot 10^{-4}$	DSi	0	$1.81 \cdot 10^{-3}$	$8.46 \cdot 10^{-3}$
TA	0	$4.39 \cdot 10^{-2}$	$2.65 \cdot 10^{-1}$	pH	0	$1.14 \cdot 10^{-3}$	$7.22 \cdot 10^{-3}$
DIC	0	$8.49 \cdot 10^{-3}$	$6.54 \cdot 10^{-2}$	CO2(aq)	0	$2.24 \cdot 10^{-3}$	$1.65 \cdot 10^{-2}$

temperature is lower than 3 °C (Fig. 12). The low photosynthesis rate leads to a negative net production (Fig. 11, green line), which is the difference between the fluxes of photosynthesis and the combined fluxes of respiration, mortality, and excretion. During this period, while the input factors play a positive role, the net change of DIA is still negative (Fig. 11, black line). Over the following days, as the water temperature and active irradiance increase (Fig. 12), the net production shows an increase. However, it still remains negative. The net change of DIA shifts to a positive direction due to a combination of net input and net production, leading to a simulated increase in DIA biomass. This trend continues until day 130 when the maximum DIA biomass is reached (Fig. 10). The decline in DIA biomass simulated from day 130 onwards is due to a combination of factors. Firstly, the input factor could be contributing to the decrease when the DIA biomass exceeds the concentration of DIA in input flow (0.447 mgC L^{-1}, Tab. 2, Fig. 10). Additionally, the net production rate is also playing a role (Fig. 11). Although photosynthesis rate is increasing with water temperature and active irradiance until day 179 (not shown here), it is not enough to compensate for the other processes occurring in the diatom population (days 150 - 170), resulting in an overall decrease in biomass. Despite the positive contributions of net input and net production on DIA biomass around day 175, a significant decrease in biomass occurred due to zooplankton grazing (Fig. 11, red line). Two factors impact the zooplankton dynamics: water temperature and half-saturation constant of grazing (Eq. (27)). The optimal temperature for zooplankton is 25 °C and the half-saturation constant of grazing for zooplankton is set to 0.4 mgC L^{-1}. Then, a equilibrium of DIA biomass is simulated until day 260 (Fig. 10), which means that the net production and net input in DIA biomass are balanced by the grazing of

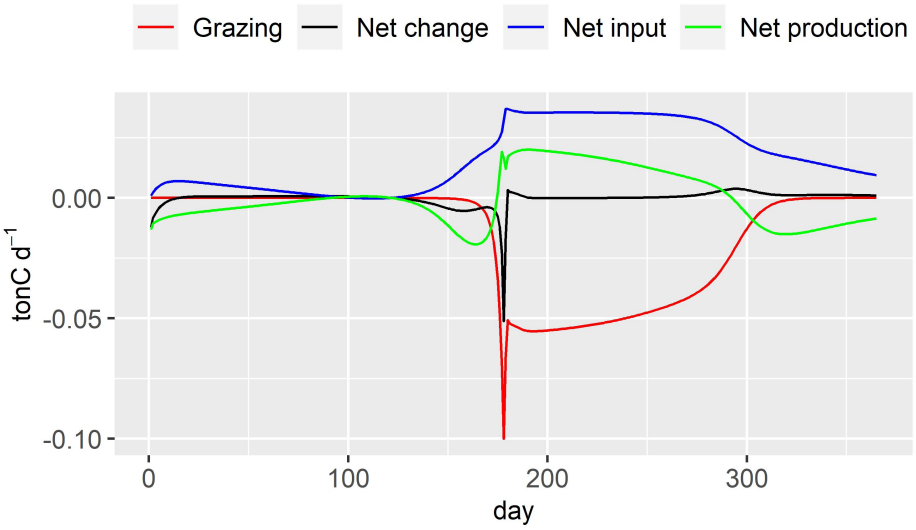

Figure 11. Budget fluxes of DIA (tonC d^{-1}). Grazing: Zooplankton grazing fluxes; Net production: Eq. (26); Net input: input flux - output flux; Net change: daily variation of DIA in the river stretch

zooplankton. The input in DIA biomass primarily contributes to the increase in DIA biomass from day 260 (Fig. 11). As the water temperature and active irradiance decrease during this time, the net production of DIA decreases and changes to negative by day 292.

~~Large heterotrophic bacteria (LHB) dynamics and simulated concentrations of small monomeric substrate (SMS). Net change: daily variation of LHB in river stretch; Net input: input flux - output flux~~

The growth rate of large heterotrophic bacteria (LHB) increases (Fig. 13) with the increase of water temperature, causing a rise in LHB biomass until day 170 (Fig. 10). The fast decrease of small monomeric substrate (SMS) around day 175, synchronized with the grazing of zooplankton (Fig. 11), causes a decrease in growth rate of LHB~~while its~~ . Its mortality rate is not impacted (not shown here). Consequently, this leads to a significant reduction in LHB biomass around day 175 (Fig. 10). The biomass of LHB remains stable until day ~~260, after which~~ 260. After that, it increases in conjunction with the rise in SMS concentration, which is synchronized with the increase in phytoplankton biomass.

4.2 Complexity and strengths of the RIVE model

Complexity can be understood in terms of the large number of variables represented and interacting with each other. The RIVE model is a multi-element, multi-form model and the kinetics it represents inevitably incorporate a large number of parameters. This is especially true as the RIVE model has opted for an explicit representation of the living communities (bacteria, phytoplankton, zooplankton, etc.) involved in the carbon and nutrient cycles. The model has thus become more

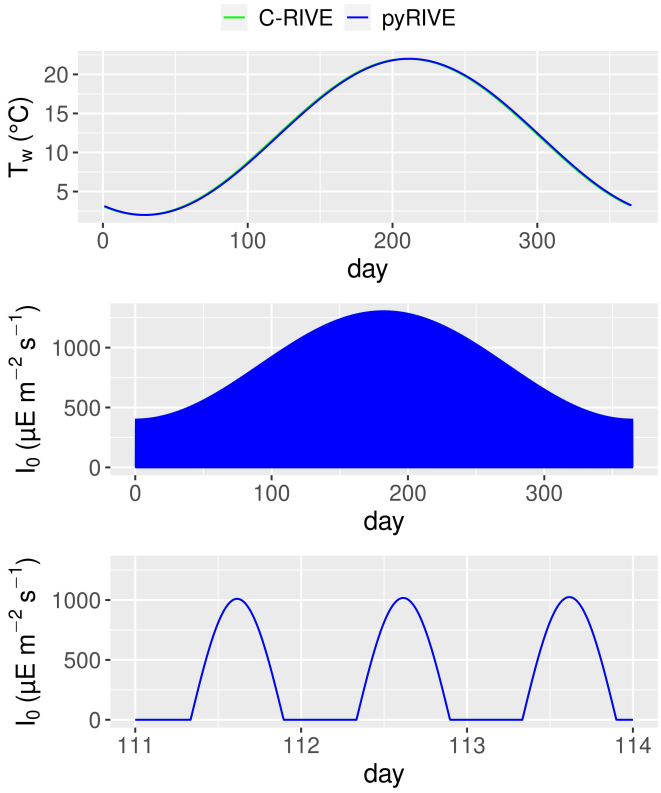

Figure 12. Simulated water temperature, active irradiance and zoom of active irradiance for days 111-114

complex over time and the addition of new processes (and therefore new parameters) has, as far as possible, been systematically based on experimental work in the laboratory or in the field to reduce the ranges of uncertainty around the kinetic parameters.

The RIVE model is designed as a tool for generating knowledge about the functioning of freshwater ecosystems and therefore it documents a large number of the biogeochemical processes, whether they are expressed weakly or strongly in a given freshwater ecosystem. The underlying hypothesis is that environmental factors control the intensity with which the various processes involved in the overall functioning of a hydrosystem are expressed.

Nevertheless, some work has specifically focused on analyzing the influence of RIVE parameters, particularly those controlling oxygen levels (Wang et al., 2018). This work identified key physical and physiological parameters. Based on the result of sensitivity analysis, a continuous oxygen data assimilation scheme has been developed (Prose-PA, (Wang et al., 2019, 2022)). The data assimilation allows to determine the physiological properties of microorganisms by integrating the associated uncertainties over time. The recent work of Hasanyar et al. (2023) has also helped to better quantify the sensitivity of oxygen to bacterial kinetics parameters as well as those relating to the composition of organic matter with the aims of parsimonious simplification of the number of parameters.

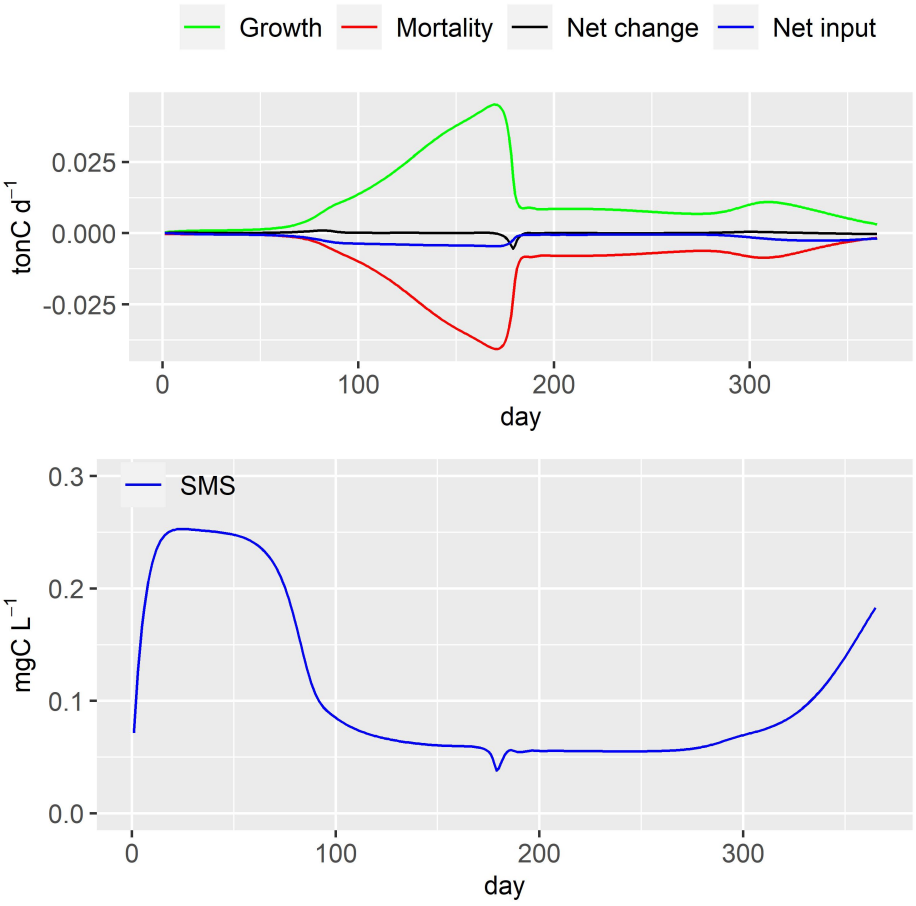

Figure 13. Large heterotrophic bacteria (LHB) dynamics and simulated concentrations of small monomeric substrate (SMS). Net change: daily variation of LHB in river stretch; Net input: input flux - output flux

In these two examples, RIVE (C-RIVE) biogeochemical modelling is implemented in much more complex modelling platforms (particle filter, data assimilation, etc.) and the various analyses (sensitivity, uncertainties, etc.) are also supported by an overall assessment of the performance of the model applied to the Seine River.

4.3 Model limitations and future developments of unified RIVE

665 Currently, the unified RIVE v1.0 presented in this paper describes only the biogeochemical processes in water column. Comparison of benthic processes and simulations have not been investigated yet. Previous studies showed that sediment plays an important role on the metabolism of river (Vilmin et al., 2016) and lakes (Yan et al., 2022b). A unified sediment module should be further elaborated, based on existing modules (Even et al., 2004; Flipo et al., 2004; Thouvenot et al., 2007; Billen et al.,

2015; Vilmin et al., 2015b) and implemented into unified RIVE. This sediment module will have to take into account not only the dissolved exchanges between the water column and the sediment but also the resuspension of particulates.

In addition, the unified RIVE v1.0 simulates phytoplankton dynamics, but periphyton or macrophyte development is not implemented in current versions. Flipo et al. (2004) showed that periphyton plays a major role in carbon cycling (primary productivity) in small rivers, not only in the carbon stock fixed at the bottom of the river but also in the carbon enrichment downstream of the river. These limitations should be considered in the future developments.

4.4 Benefit of unified RIVE model

The unified RIVE provides a set of governing equations of ~~aquatic~~ freshwater biogeochemical processes across different software platforms, such as pyNuts-Riverstrahler (Billen et al., 1994; Garnier et al., 1995; Thieu et al., 2017), PROSE-PA (Wang et al., 2019, 2023a), SWAT-RIVE (Manteaux et al., 2023, submitted), QUAL-NET (Minaudo et al., 2018), VEMALA V3 (Korppoo et al., 2017), Barman (Garnier et al., 2000; Thieu et al., 2006; Yan et al., 2022b), while incorporating the latest developments. The unicity of the kinetics is important for facilitating and reinforcing the collaboration nationally or internationally within different research teams. Thanks to the unicity property formerly pointed out by the river continuum concept Vannote et al. (1980), the softwares based on unified RIVE can leverage on the already identified parameter values~~whatever~~ , regardless of the location in the network (Garnier et al., 2020)~~, which~~ . This feature is of great interest to the different research teams involved in ~~aquatic research such as~~ freshwater quality research for instance river metabolism (Odum, 1956; Garnier and Billen, 2007; Escoffier et al., 2018; Gurung et al., 2019; Rodríguez-Castillo et al., 2019; Garnier et al., 2020; Segatto et al., 2020; Battin et al., 2023) or nutrient cycling (Garnier et al., 1999b; Alexander et al., 2002; Garnier et al., 2002; Billen et al., 2007; Lauerwald et al., 2013; Lindenschmidt et al., 2019; Maavara et al., 2020; Marescaux et al., 2020; Yan et al., 2022a).

Open science has become increasingly popular and even indispensable in scientific community as it allows for easier accessibility and the reproduction of the scientific results. The unified RIVE project, as an open-source project, allows for the dissemination and wider use of the RIVE biogeochemical model by creating a public repository with different programming languages.

5 Conclusions

This paper presents a conceptual ~~aquatic~~ freshwater biogeochemistry model: unified RIVE v1.0, programmed in Python 3 and ANSI C. The degradation of organic matter by heterotrophic bacteria, the dynamics of primary producer (phytoplankton) and zooplankton including carbon cycling and ~~nutrients~~ nutrient cycling are described exhaustively. In unified RIVE v1.0, the organic matter is degraded via bacteria activity, which is simulated by a HSB model. According to the results, the HSB model is able to model the organic matter degradation and bacterial dynamics in batch experiments. A case study is designed to compare the simulations of the two digital implementations (Python 3 for pyRIVE 1.0 and ANSI C for C-RIVE 0.32)~~, which estimate~~ . These implementations simulate similar concentrations of all state variables including microorganisms, organic carbon, nutrients, and inorganic carbon.

The river stretch case study allows us to compare the two implementations of unified RIVE V1.0 under transient contrasting conditions involving complex biogeochemical cycles. The specific dynamics of each simulated species depend on different ~~limitations~~limiting factors. The calculation of photosynthesis of phytoplankton (diatoms, chlorophyceae, cyanobacteria) takes into account the light that naturally presents a day/night variation. The development of diatoms specifically takes into account the dissolved silica in the simulated ~~aquatic~~ environment. The growth of microorganisms depend on the quantity of nutrients (primary producer, nitrifying bacteria) and the small monomeric substrate (heterotrophic bacteria). In addition, the effect of water temperature is also taken into account for the physiology of the simulated microorganisms' communities (photosynthesis, growth, respiration, mortality).

Finally, unified RIVE being an open-source project, contributions from the ~~aquatic~~ freshwater biogeochemistry community are strongly encouraged to achieve a better understanding of ~~aquatic system~~ freshwater ecosystem functioning and investigate further the future of river systems in a changing world.

Code availability. The C-RIVE 0.32 implements the unified RIVE v1.0 in ANSI C. It is available under Eclipse Public License 2.0 in the following Zenodo repository: https://doi.org/10.5281/zenodo.7849609; Wang et al. (2023b). pyRIVE 1.0 implements the unified RIVE v1.0 in Python 3 and is available under the Eclipse Public License 2.0 in InDoRES repository: https://doi.org/10.48579/PRO/Z9ACP1; Thieu et al. (2023).

Appendix A: Various implementations of the RIVE model and its applications in different ~~aquatic~~ freshwater systems

Table A1. Various implementations of the RIVE model and its applications in different ~~aquatic~~ freshwater systems

~~Aquatic~~ Freshwater systems	Climates	Software platforms	References
Danube River (Romania and Bulgaria)	Continental	Riverstrahler	Garnier et al. (2002)
Day-Nhue River (Vietnam)	Tropical	Seneque-Riverstrahler	Luu et al. (2021)
Grand Morin River (France)	Temperate	PROSE	Flipo et al. (2004, 2007)
Loire River (France)	Temperate	Grafs-Seneque/Riverstrahler	Garnier et al. (2018a)
Lot River (France)	Temperate	Grafs-Seneque/Riverstrahler	Garnier et al. (2018b)
Lule and Kalix rivers (Sweden)	Subarctic	Riverstrahler	Sferratore et al. (2008)
Mosel River (Germany)	Temperate	Riverstrahler	Garnier et al. (1999a)
Orgeval watershed (France)	Temperate	Seneque-Riverstrahler	Garnier et al. (2014)
Red River (China and Vietnam)	Tropical	Seneque-Riverstrahler	Le et al. (2010); Phuong Quynh et al. (2014); Le et al. (2015); Nguyen et al. (2016)
Scheldt River (Belgium and Netherlands)	Temperate	Seneque-Riverstrahler	Billen et al. (2005); Thieu et al. (2009)
Somme River (France)	Temperate	Seneque-Riverstrahler	Thieu et al. (2009, 2010)
Seine River (France)	Temperate	Seneque-Riverstrahler	Billen et al. (2007); Thieu et al. (2009, 2010); Romero et al. (2019)
Seine River (France)	Temperate	pyNuts-Riverstrahler	Thieu et al. (2017); Desmit et al. (2018); Raimonet et al. (2018); Marescaux et al. (2020)
Seine River (France)	Temperate	PROSE/PROSE-PA	Even et al. (1998, 2004, 2007); Raimonet et al. (2015); Vilmin et al. (2015b, a, 2016, 2018); Wang (2019); Wang et al. (2022)
Zenne River (Belgium)	Temperate	Seneque-Riverstrahler	Garnier et al. (2013)
Sand-pit lake, reservoirs (France)	Temperate	Barman	Garnier and Billen (1994); Garnier et al. (2000); Thieu et al. (2006); Yan et al. (2022a)

Appendix B: Parameter values for unified RIVE v1.0

The ~~116~~ 120 parameter values necessary for running unified RIVE v1.0 are provided hereafter.

Table B1. Heterotrophic ~~and nitrifying Bacteria~~ bacteria related parameters

Parameter	Description	Value	Unit
~~$^{*}b_{max,lhb}$~~ $^{*}e_{max20,dom_1,lhb}$	Maximal hydrolysis rate of DOM_1 at 20 °C related to LHB	0.75	[h^{-1}]
$^{*}e_{max20,dom_1,shb}$	Maximal hydrolysis rate of DOM_1 at 20 °C related to SHB	0.75	[h^{-1}]
$^{*}e_{max20,dom_2,lhb}$	Maximal hydrolysis rate of DOM_2 at 20 °C related to LHB	0.25	[h^{-1}]
$^{*}e_{max20,dom_2,shb}$	Maximal hydrolysis rate of DOM_2 at 20 °C related to SHB	0.25	[h^{-1}]
$^{*}b_{max20,lhb}$	Maximal substrate (SMS) uptake rate of LHB at 20 °C	0.6	[h^{-1}]
~~$^{*}b_{max,shb}$~~ $^{*}b_{max20,shb}$	Maximal substrate (SMS) uptake rate of SHB at 20 °C	0.16	[h^{-1}]
~~$^{*}Y_{lhb}$~~ Y_{lhb}	Growth yield of LHB	0.25	[-]
~~$^{*}Y_{shb}$~~ Y_{shb}	Growth yield of SHB	0.25	[-]
$^{*}k_{d20,lhb}$	Mortality rate of LHB at 20 °C	0.05	[h^{-1}]
$^{*}k_{d20,shb}$	Mortality rate of SHB at 20 °C	0.02	[h^{-1}]
vs_{shb}	Sinking velocity of LHB	0.0	[m h^{-1}]
vs_{lhb}	Sinking velocity of LHB	0.02	[m h^{-1}]
$T_{opt,shb}$	Optimal temperature of SHB	20	°C
$T_{opt,lhb}$	Optimal temperature of LHB	22	°C
σ_{shb}	Range of temperature for SHB	17	°C
σ_{lhb}	Range of temperature for LHB	~~212~~ 12	°C
~~$^{*}\mu_{max,aob}$~~ $K_{sms,lhb}$	Half-saturation constant of LHB for small monomeric substrate	0.1	[mgC L^{-1}]
$K_{sms,shb}$	Half-saturation constant of SHB for small monomeric substrate	0.1	[mgC L^{-1}]
$K_{dom1,shb}$	Half-saturation constant for DOM_1 hydrolysis related to SHB	0.25	[mgC L^{-1}]
$K_{dom1,lhb}$	Half-saturation constant for DOM_1 hydrolysis related to LHB	0.25	[mgC L^{-1}]
$K_{dom2,shb}$	Half-saturation constant for DOM_2 hydrolysis related to SHB	2.5	[mgC L^{-1}]
$K_{dom2,lhb}$	Half-saturation constant for DOM_2 hydrolysis related to LHB	2.5	[mgC L^{-1}]

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B2. Nitrifying bacteria related parameters

Parameter
$^{*}\mu_{max20,aob}$
~~$^{*}\mu_{max,nob}$~~ $^{*}\mu_{max20,nob}$
$K_{o_2,aob}$
$K_{o_2,nob}$
$K_{nh_4,aob}$
$K_{no_2,nob}$
~~$K_{sms,lhb}$ Half-saturation constant of LHB for small monomeric substrate0.1 mgC L^{-1} $K_{sms,shb}$ Half-saturation constant of SHB for small monomeric~~
~~$^{*}Y_{nob}$~~ Y_{nob}
~~$^{*}k_{d,aob}$~~ $^{*}k_{d20,aob}$
~~$^{*}k_{d,nob}$~~ $^{*}k_{d20,nob}$
vs_{aob}
vs_{nob}
$T_{opt,aob}$
σ_{aob}
$T_{opt,nob}$
σ_{nob}

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B3. Primary producer dynamics related parameters

Parameter	Description	Value	Un
~~$^{*}P_{dia,max}$~~ $^{*}P_{max20,dia}$	~~Maximum rate of photosynthesis for diatoms~~ Maximal photosynthesis rate of diatoms at 20 °C	0.2	[h
~~$^{*}P_{gra,max}$~~ $^{*}P_{max20,gra}$	~~Maximum rate of photosynthesis for green algae~~ Maximal photosynthesis rate of green algae at 20 °C	0.25	[h
~~$^{*}P_{cya,max}$~~ $^{*}P_{max20,cya}$	~~Maximum rate of photosynthesis for cyanobacteria~~ Maximal photosynthesis rate of cyanobacteria at 20 °C	0.1	[h
α_{dia}	Photosynthetic efficiency of diatoms	0.0012	[h
α_{gra}	Photosynthetic efficiency of green algae	0.0012	[h
α_{cya}	Photosynthetic efficiency of cyanobacteria	0.0012	[h
β_{dia}	Photoinhibition capacity of diatoms	0.0	[h
β_{gra}	Photoinhibition capacity of green algae	0.0	[h
β_{cya}	Photoinhibition capacity of cyanobacteria	0.0	[h
η_{base}	Light extinction related coefficient for pure water	0.2	[m
η_{chla}	Light algal self-shading light extinction coefficient	0.02	[m
η_{ss}	Light extinction coefficient related to suspended solid	0.042	[m
~~$^{*}\mu_{dia,max}$~~ $^{*}\mu_{max20,dia}$	Maximal growth rate of diatoms at 20 °C	0.05	[h
~~$^{*}\mu_{gra,max}$~~ $^{*}\mu_{max20,gra}$	Maximal growth rate of green algae at 20 °C	0.05	[h
~~$^{*}\mu_{cya,max}$~~ $^{*}\mu_{max20,cya}$	Maximal growth rate of cyanobacteria at 20 °C	0.025	[h
$K_{S,dia}$	Half-saturation constant for small precursors of diatoms	0.06	[-
$K_{S,gra}$	Half-saturation constant for small precursors of green algae	0.06	[-
$K_{S,cya}$	Half-saturation constant for small precursors of cyanobacteria	0.06	[-
$K_{N,dia}$	Half-saturation constant for nitrogen of diatoms	0.014	[m
$K_{N,gra}$	Half-saturation constant for nitrogen of green algae	0.014	[m
$K_{N,cya}$	Half-saturation constant for nitrogen of cyanobacteria	0.014	[m
$K_{P,dia}$	Half-saturation constant for phosphorus of diatoms	0.0155	[m
$K_{P,gra}$	Half-saturation constant for phosphorus of green algae	0.062	[m
$K_{P,cya}$	Half-saturation constant for phosphorus of cyanobacteria	0.062	[m
$K_{Si,dia}$	Half-saturation constant for silica of diatoms	0.196	[m
~~$^{*}R_{m,dia}$~~ $^{*}R_{m20,dia}$	Maintenance respiration coefficient of diatoms at 20 °C	0.002	[h
~~$^{*}R_{m,gra}$~~ $^{*}R_{m20,gra}$	Maintenance respiration coefficient of green algae at 20 °C	0.002	[h
~~$^{*}R_{m,cya}$~~ $^{*}R_{m20,cya}$	Maintenance respiration coefficient of cyanobacteria at 20 °C	0.002	[h
$R_{\mu,dia}$	Energetic cost of growth of diatoms	0.5	[-
$R_{\mu,gra}$	Energetic cost of growth of green algae	0.5	[-
$R_{\mu,cya}$	Energetic cost of growth of cyanobacteria	0.5	[-

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

~~Primary producer dynamics related parameters (continue)~~

Table B3. Primary producer dynamics related parameters (continued)

Parameter	Description	Value	Unit
$E_{cst,dia}$	Basic excretion rate of diatoms	0.006	[h^{-1}]
$E_{cst,gra}$	Basic excretion rate of green algae	0.006	[h^{-1}]
$E_{cst,cya}$	Basic excretion rate of cyanobacteria	0.006	[h^{-1}]
$E_{phot,dia}$	Excretion constant of diatoms related to photosynthesis	0.001	[-]
$E_{phot,gra}$	Excretion constant of green algae related to photosynthesis	0.001	[-]
$E_{phot,cya}$	Excretion constant of cyanobacteria related to photosynthesis	0.001	[-]
~~$^*S_{R,max,dia}$~~ $^*S_{R,max20,dia}$	Maximal rate of reserve products synthesis for diatoms at 20 °C	0.15	[h^{-1}]
~~$^*S_{R,max,gra}$~~ $^*S_{R,max20,gra}$	Maximal rate of reserve products synthesis for green algae at 20 °C	0.2	[h^{-1}]
~~$^*S_{R,max,cya}$~~ $^*S_{R,max20,cya}$	Maximal rate of reserve products synthesis for cyanobacteria at 20 °C	0.075	[h^{-1}]
~~$^*C_{R,max,dia}$~~ $^*C_{R,max20,dia}$	Maximal rate of reserve products catabolism for diatoms at 20 °C	0.2	[h^{-1}]
~~$^*C_{R,max,gra}$~~ $^*C_{R,max20,gra}$	Maximal rate of reserve products catabolism for green algae at 20 °C	0.2	[h^{-1}]
~~$^*C_{R,max,cya}$~~ $^*C_{R,max20,cya}$	Maximal rate of reserve products catabolism for cyanobacteria at 20 °C	0.2	[h^{-1}]
~~$^*k_{d,dia}$~~ $^*k_{d20,dia}$	Rate of diatoms mortality at 20 °C	0.025	[h^{-1}]
~~$^*k_{d,gra}$~~ $^*k_{d20,gra}$	Rate of green algae mortality at 20 °C	0.025	[h^{-1}]
~~$^*k_{d,cya}$~~ $^*k_{d20,cya}$	Rate of cyanobacteria mortality at 20 °C	0.015	[h^{-1}]
vs_{dia}	Sinking velocity of diatoms	0.006	[m h^{-1}]
vs_{gra}	Sinking velocity of green algae	0.001	[m h^{-1}]
vs_{cya}	Sinking velocity of cyanobacteria	0.006	[m h^{-1}]
$T_{opt,dia}$	Optimal temperature of diatoms	21	[°C]
$T_{opt,gra}$	Optimal temperature of green algae	37	[°C]
$T_{opt,cya}$	Optimal temperature of cyanobacteria	37	[°C]
σ_{dia}	Range of temperature for diatoms	13	[°C]
σ_{gra}	Range of temperature for green algae	15	[°C]
σ_{cya}	Range of temperature for cyanobacteria	12	[°C]

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B4. Organic matter dynamics parameters

Parameter	Des
~~$^{*}e_{max,dom_1}$ Maximal rate of DOM$_1$ hydrolysis 0.75 h^{-1}~~	~~$^{*}e_{max,dom_2}$ Maximal rate of DOM$_2$ hydrolysis 0.25 h^{-1}~~ ϵ_{dom_1}	DO
ϵ_{dom_2}	DO
ϵ_{dom_3}	DO
ϵ_{pom_1}	PO
ϵ_{pom_2}	PO
ϵ_{pom_3}	PO
~~$^{*}k_{pom_1}$~~ $^{*}k_{pom_1,20}$	PO
k_{pom_2}	PO
~~K_{dom1} Half-saturation constant for DOM$_1$ hydrolysis 0.25 mgC L^{-1}~~ ~~K_{dom2} Half-saturation constant for DOM$_2$ hydrolysis 2.5 mgC L^{-1}~~	height

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B5. Zooplankton parameters

Parameter	Description	Value	Unit
~~$^{*}\mu_{max,zor}$~~ $^{*}\mu_{max20,zor}$	Maximal growth rate of ZOR at 20 °C	0.025	[h^{-1}]
~~$^{*}\mu_{max,zoc}$~~ $^{*}\mu_{max20,zoc}$	Maximal growth rate of ZOC at 20 °C	0.015	[h^{-1}]
~~$^{*}B_{max,zor}$~~ $^{*}b_{max20,zor}$	Maximal grazing rate of ZOR at 20 °C	0.1	[h^{-1}]
~~$^{*}B_{max,zoc}$~~ $^{*}b_{max20,zoc}$	Maximal grazing rate of ZOC at 20 °C	0.05	[h^{-1}]
$K_{phy,zor}$	Half-saturation constant for grazing phytplankton of ZOR	0.1	[mgC L^{-1}]
$K_{phy,zoc}$	Half-saturation constant for grazing phytplankton of ZOC	0.1	[mgC L^{-1}]
$PHY_{0,zor}$	Threshold phytoplankton concentration for grazing of ZOR	0.1	[mgC L^{-1}]
$PHY_{0,zoc}$	Threshold phytoplankton concentration for grazing of ZOC	0.1	[mgC L^{-1}]
~~$^{*}k_{d,zor}$~~ $^{*}k_{d20,zor}$	Mortality rate of ZOR at 20 °C	0.007	[h^{-1}]
~~$^{*}k_{d,zoc}$~~ $^{*}k_{d20,zoc}$	Mortality rate of ZOC at 20 °C	0.007	[h^{-1}]
$T_{opt,zor}$	Optimal temperature of ZOR	25	[°C]
$T_{opt,zoc}$	Optimal temperature of ZOC	25	[°C]
σ_{zor}	Range of temperature for ZOR	10	[°C]
σ_{zoc}	Range of temperature for ZOC	10	[°C]
vs_{zor}	Sinking velocity of ZOR	0.02	[m h^{-1}]
vs_{zoc}	Sinking velocity of ZOC	0.02	[m h^{-1}]

*: Parameters depend on water temperature and are multiplied by $f(T) = \frac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B6. Phosphate and Silica related parameters

Parameter	Description	Value	Unit
	Phosphate adsorption desorption		
P_{ac}	~~Maximum adorption~~ Maximal adsorption capacity of mineral suspended solids (MSS)	0.00558	[mgP/mgMSS]
K_{ps}	Half saturation adsorption constant	0.682	[mgP L^{-1}]
	Silica dynamiques		
Kb_{Si20}	Biogenic silica dissolution rate at 20 °C	0.0001	[h^{-1}]

Author contributions. **Shuaitao Wang:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Visualization, Writing – original draft. **Vincent Thieu:** Conceptualization, Methodology, Software, Formal analysis, Writing - Review & Editing, Supervision. **Gilles Billen:** Conceptualization, Methodology, Data curation, Formal analysis, Writing - Review & Editing. **Josette Garnier:** Conceptualization, Data curation, Formal analysis, Writing - Review & Editing. **Marie Silvestre:** Software, Writing - Review & Editing.

Audrey Marescaux: Conceptualization, Software. **Xingcheng Yan:** Software. **Nicolas Flipo:** Conceptualization, Methodology, Formal analysis, Software, Writing - Review & Editing, Supervision, Funding acquisition.

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