The community-centered aquatic 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 1925, based on first order kinetics for organic matter degradation. The community-centered aquatic biogeochemistry model RIVE was initially developed

5 in 1994 and has since 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 communi-

10 ties (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 considers the full biogeochemical cycles (microorganisms, nutrients, carbon, and oxygen) in the water column, as well as the effects of light and water tempera-

15 ture. 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 biogeochemistry community to further advance the project and achieve common objectives.

1 Introduction

Modeling of the water quality of an aquatic system (river, lake, reservoir) is critical to understand and manage its functioning

20 which 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 (Hellweger, 2015).

25   While the role of microorganisms in the degradation of organic matter has been acknowledged since the end of the 19th
century, an important limitation of this type of representation is that the microbiological nature of the organic matter degradation
process and the bacterial population dynamics intrinsically involved are completely obscured, being implicitly taken into
account only through a biodegradability constant of OM 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
30 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), capable of simulating the degradation of OM in aquatic systems and the
associated oxygen consumption by bacterial activities, which is more realistic than the model of Streeter and Phelps (1925). In
35 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 are
subsequently assimilated by **B**acteria for their growth and respiration.

    Apart from the degradation of organic matter, the *Aquaphy* model (Lancelot et al., 1991) is been used for simulating the
40 dynamics of phytoplankton in the RIVE model (Billen et al., 1994). The model simulates explicitly photosynthesis, growth,
mortality and respiration processes. The photosynthesis depends on the light intensity while the growth is controlled by nu-
trients availability and the small organic metabolites 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 intro-
duces a limiting factor of nutrients in the growth of phytoplankton and considers the cycling of nutrients during the life cycle
45 of phytoplankton.

    Since its initial development by Billen et al. (1994), the RIVE model co-exists within several softwares 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,
50 (Ruelland et al., 2007)). And it is now fully integrated within the pyNuts-Riverstrahler (https://gitlab.in2p3.fr/rive/pynuts/)
modeling environment to describe 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 systems like regulated
reservoirs (BarMan software (Garnier et al., 2000; Thieu et al., 2006; Yan et al., 2022a)) or hydro-biodynamic functioning
of highly human impacted river system (PROSE software – Even et al. (1998, 2004, 2007); Flipo et al. (2004); Vilmin et al.
55 (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). 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
60   and nitrogen loading in the Finnish watersheds (Korppoo et al., 2017).

Based on above implementations, different versions of the RIVE model code has simulated successfully a large variety of aquatic systems (lake, reservoirs, river systems) across the world with parameter values 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
65   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.,
70   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
75   model has been applied to the stagnant systems (sand-pit lake, reservoirs) also (Garnier and Billen, 1994; 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 identification of a unified version of RIVE model. A project aiming at unifying these RIVE imple-
80   mentations to bring together all recent developments, especially the ones achieved with Python 3 and ANSI C programming languages, was undertaken to strengthen the collaboration of the research teams involved in the development of the model. This paper presents a unified version of RIVE for water column (called unified RIVE v1.0) with a presentation of the formalisms for the carbon cycle – 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
85   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 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 conditions. We thus establish a reference framework to evaluate different implementations of the unified RIVE v1.0 formulation, that continues to evolve in several water
90   quality models.

2 Model description

The unified RIVE v1.0 model simulates the cycling of carbon, nutrients and oxygen within an aquatic system (river, lake, reservoir). Biogeochemical cycles are simulated with a community-centered or agent-based model. That means the aquatic system functioning is explicitly modeled by microorganisms' activities (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 organic matter, particulate, dissolved, biodegradable fractions are considered. 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 sediment dynamics and its interaction with the water column will be explored in future work.

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 (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 the substrates for their growth and respiration (Fig. 1).

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 the availability of small monomeric substrate (SMS), which is represented by Monod equation (Monod, 1949). A maximum rate of small monomeric substrate uptake ($b_{max,hb}$) and a bacterial growth yield (Y_{hb}) are used to represent the growth of heterotrophic bacteria (μ_{hb_i}) (Eq. (2)). The fraction of uptake not used for growth ($1 - Y_{hb}$) is respired.

$$b_{hb_i} = b_{max,hb_i} \frac{[SMS]}{[SMS] + K_{sms,hb_i}} \tag{1}$$

$$\mu_{hb_i} = Y_{hb_i} b_{hb_i} \tag{2}$$

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

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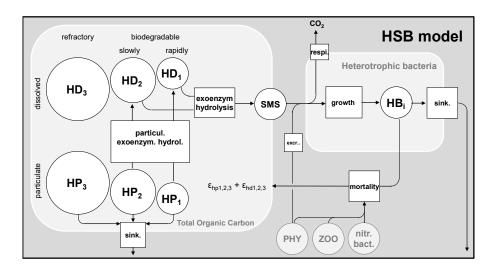
Figure 1. Flowchart of HSB model. HD: dissolved high weight polymer; HP: particulate high weight polymer; SMS: small monomeric substrate; HB: heterotrophic bacteria; PHY: phytoplankton; ZOO: zooplankton; nitr. bact.: Nitrifying bacteria; extr. excretion of phytoplankton; sink.: sinking. respi.: respiration;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

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

μ_{hb_i}: 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. (3)). 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).

$$\frac{d[HB_i]}{dt} = (\mu_{hb_i} - k_{d,hb_i} - k_{sink,hb_i})[HB_i] \tag{3}$$
$$k_{sink,hb_i} = \frac{vs_{hb_i}}{depth}$$

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

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

k_{sink,hb_i}: Sinking rate of the ith species of heterotrophic bacteria, [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. (4)) while a Michaelis-

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Menten function (Michaelis and Menten, 1913) is used to express the exoenzymatic hydrolysis of HD depending on its concentration and heterotrophic bacterial biomass (Eq. (5)).

$$\frac{d[HP_i]}{dt} = -k_{hp_i} * [HP_i] + (\sum_j k_{d,j}[LS]_j)\epsilon_{hp_i} - k_{sink,hp_i}[HP_i] \tag{4}$$

140   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}]

$k_{d,j}$: Mortality rate of the jth living species (such as phytoplankton, zooplankton, bacteria etc.), [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, $i \in \{1,2\}$, [-]

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

$$\frac{d[HD_i]}{dt} = -e_{max,hd_i}\frac{[HD_i]}{[HD_i] + K_{hd_i}}\sum_k [HB_k] + k_{hp_i} * [HP_i] + (\sum_j k_{d,j}[LS]_j))\epsilon_{hd_i} \tag{5}$$

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

e_{max,hd_i}: Maximum hydrolysis rate of HD_i, $i \in \{1,2\}$, [h^{-1}]

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

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

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

$[LS]_j$: Concentration of the jth 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

155   The unified RIVE v1.0 model includes the description of the nitrification microbial process, mediated by two types of nitrifying bacteria 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^+ and NO_2^- 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

160   functions (Eq. (6)).

$$\mu_{aob} = \mu_{aob,max}\left(\frac{[NH_4^+]}{[NH_4^+] + K_{nh_4,aob}}\right)\left(\frac{[O_2]}{[O_2] + K_{o_2,aob}}\right) \tag{6}$$

$$\mu_{nob} = \mu_{nob,max}\left(\frac{[NO_2^-]}{[NO_2^-] + K_{no_2,nob}}\right)\left(\frac{[O_2]}{[O_2] + K_{o_2,nob}}\right) \tag{7}$$
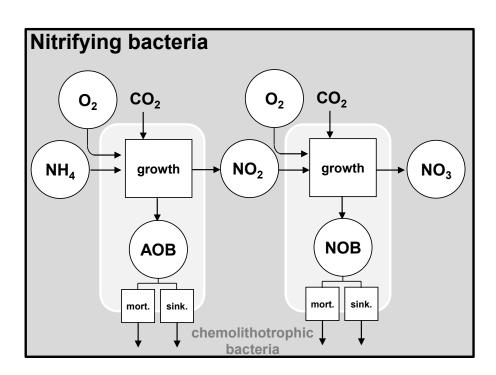
Figure 2. Nitrifying bacteria dynamics. AOB: ammonia-oxidizing bacteria; NOB: nitrite-oxidizing bacteria; mort.: mortality; sink.: sinking

With $\mu_{aob,max}$ and $\mu_{nob,max}$: Maximum growth rates of AOB and NOB, respectively, [h^{-1}]

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

165 $K_{o_2,aob}$ 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.

$$\frac{d[AOB]}{dt} = (\mu_{aob} - k_{d,aob} - k_{sink,aob})[AOB] \tag{8}$$

$$\frac{d[NOB]}{dt} = (\mu_{nob} - k_{d,nob} - k_{sink,nob})[NOB] \tag{9}$$

With $k_{d,aob}$ and $k_{d,nob}$: Mortality rate of AOB and NOB, [h^{-1}]

170 $k_{sink,aob}$ and $k_{sink,nob}$: Sinking rate of AOB and NOB, [h^{-1}]

$[AOB]$ 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):

175 (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**
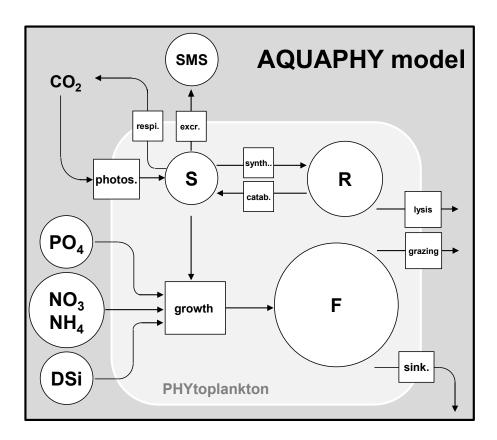

Figure 3. Description of Aquaphy model. F: functional marcromolecules of the cell; R: reserve products; S: Monomeric (amino acids) and oligomeric precursors for macromolecular synthesis. Phytoplankton biomass equals to the sum of the three cellular constituents (F, R, S). SMS: small monomeric substrate. 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
180   constituents (Eq. (10)), $[F]_j$, $[R]_j$, $[S]_j$:

$$[PHY]_j = [F]_j + [R]_j + [S]_j \qquad (10)$$

The most common way of measuring phytoplankton biomass is in chlorophyll *a* concentration (μgchla). A carbon/chlorophyll
a ratio of 35 mgC/μgchl*a* is therefore considered to convert experimental data into a model state variable. The structural and
functional macromolecules of the cell ($[F]_j$) account for about 85% of the phytoplankton biomass ($[PHY]_j$), while the reserve
185   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. (11)) and the active irradiance ($I(z)$, μE m^{-2} s^{-1}).

$$P(z)_{phy_j} = P_{max,phy_j}(1 - e^{-\frac{\alpha_{phy_j} I(z)}{P_{max,phy_j}}})e^{-\frac{\beta_{phy_j} I(z)}{P_{max,phy_j}}} \qquad (11)$$

with P_{max,phy_j}: Maximum rate of photosynthesis of the jth phytoplankton species, [h^{-1}]

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 $P(z)$.

$$p_{phy_j} = \frac{\int_0^{depth} P(z)_{phy_j}\,\mathrm{d}z}{depth} \qquad (12)$$

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. (13)). 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}).

$$I(z) = I_0 e^{-\eta z} \qquad (13)$$

$$\eta = \eta_{base} + \eta_{chla}[chla] + \eta_{ss}[SS]$$

with 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}]

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, [μgchl$a$ L^{-1}]

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

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

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2.3.2 Growth

215 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, Si) from the environment (Fig. 3). The nutrients can potentially control phytoplankton growth by limiting it if they are not present in sufficient quantities. The limitation of nutrients is represented using multiple Monod functions (Eq. (14)). 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).

220
$$\mu_{F_j} = \mu_{max,F_j} \left(\frac{\frac{[S_j]}{[F_j]}}{\frac{[S_j]}{[F_j]} + K_{S,phy_j}} \right) Nut\_lim \tag{14}$$

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

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

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

225 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 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

230 The respiration rate of phytoplankton (r_{phy}) is divided into two components (Eq. (15)): one ($R_{m,phy}$) ensuring the survival of the cell (maintenance process), the other ($R_{\mu,phy}$) corresponding to energetic cost of growth.

$$r_{phy_j} = R_{m,phy_j} + \mu_{F_j} R_{\mu,phy_j} \tag{15}$$

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

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

235 μ_{F_j}: Effective growth rate of the jth phytoplankton species (Eq. (14)), [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).

240
$$e_{phy_j} = E_{cst,phy_j} + p_{phy_j} E_{phot,phy_j} \tag{16}$$

With 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. (12)), [h^{-1}]

The variation of small monomeric substrate (SMS) can then be established (Eq. (17)).

$$\frac{d[SMS]}{dt} = hydr - \sum_i b_{hb_i}[HB_i] + \sum_j e_{phy_j}[F_j] \tag{17}$$

With $hydr$: Hydrolysis of the dissolved high weight polymer HD$_1$ and HD$_2$ (Eq. (5)), [mgC L^{-1} h^{-1}]

b_{hb_i}: Effective rate of substrate uptake by the ith heterotrophic bacteria species (Eq. (2)), [h^{-1}]

e_{phy_j}: Effective excretion rate of the jth phytoplankton species (Eq. (16)), [h^{-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. (18)).

$$s_{R,phy_j} = s_{R,max,phy_j} \frac{\frac{[S_j]}{[F_j]}}{\frac{[S_j]}{[F_j]} + K_{S,phy_j}} \tag{18}$$

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

Three ways of phytoplankton disappearance 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 ($k_{d,phy}$, h^{-1}). For ease of presentation, all three processes are assumed in an overall disappearance rate d_{phy} (h^{-1}).

$$d_{phy_j} = k_{d,phy_j} + k_{sink,phy_j} + \sum_i \frac{b_{zoo_i}[ZOO_i]}{\sum_{k=1}^{NS}[PHY_k]} \tag{19}$$

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

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

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

b_{zoo_i}: Grazing rate of the ith zooplankton species (Eq. (24), 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}]

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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.

$$\frac{d[S_j]}{dt} = (p_{phy_j} - r_{phy_j} - \mu_{F_j} - s_{R,phy_j})[F_j] + c_{R,phy_j}[R_j] - e_{phy_j}[F_j] - d_{phy_j}[S_j] \tag{20}$$

$$\frac{d[R_j]}{dt} = s_{R,phy_j}[F_j] - c_{R,phy_j}[R_j] - d_{phy_j}[R_j] \tag{21}$$

$$\frac{d[F_j]}{dt} = (\mu_{F_j} - d_{phy_j})[F_j] \tag{22}$$

$$\frac{d[PHY_j]}{dt} = (p_{phy_j} - r_{phy_j} - e_{phy_j})[F_j] - d_{phy_j}[PHY_j] \tag{23}$$

With: p_{phy_j}: Photosynthesis rate of the jth phytoplankton species (Eq. (12)), [h^{-1}]

r_{phy_j}: Respiration rate of the jth phytoplankton species (Eq. (15)), [h^{-1}]

μ_{F_j}: Growth rate of the jth phytoplankton species (Eq. (14)), [h^{-1}]

s_{R,phy_j}: Synthesis rate of reserve products of the jth phytoplankton species (Eq. (18)), [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. (16)), [h^{-1}]

d_{phy_j}: Disappearance rate of the jth phytoplankton species(Eq. (19)), [h^{-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 ($b_{max,zoo}$ limited by the phytoplankton biomass based on a Monod function (Eq. (24)). 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. (19)). The growth rate of zooplankton is considered proportional to grazing rate using a growth yield factor (Eq. (25)).

$$b_{zoo_i} = b_{max,zoo_i} \frac{(\sum_j^{NS}[PHY_j] - [PHY_0]_{zoo_i})}{(\sum_j^{NS}[PHY_j] - [PHY_0]_{zoo_i}) + K_{phy,zoo_i}} \tag{24}$$

$$\mu_{zoo_i} = Y_{zoo_i} b_{zoo_i} \tag{25}$$

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

$\sum_j^{NS}[PHY_j]$: 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}]

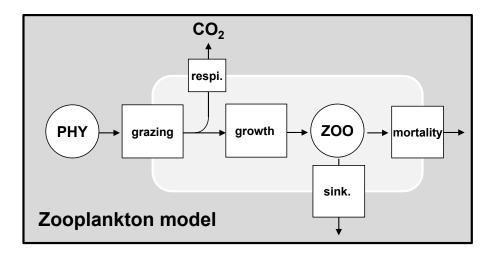300 Y_{zoo_i}: Growth yield of the ith zooplankton species, [-]

Figure 4. 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 ($k_{d,zoo}$).

$$r_{zoo_i} = (1 - Y_{zoo_i}) \times b_{zoo_i} \qquad (26)$$

305   $$\frac{d[ZOO_i]}{dt} = (Y_{zoo_i} b_{zoo_i} - k_{d,zoo_i} - k_{sink,zoo_i})[ZOO_i] \qquad (27)$$

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, [h^{-1}]

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

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

2.5   Nutrients 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) 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.

$$\frac{d[uptN]}{dt} = \sum_i \frac{(\mu_{F_i} + e_{phy_i})[F_i]}{C/N} \tag{28}$$

$$uptNH_4^+ = min\left([NH_4^+], uptN(\frac{[NH_4^+]}{[NH_4^+] + [NO_3^-]})^{0.025}\right) \tag{29}$$

$$uptNO_3^- = uptN - uptNH_4^+ \tag{30}$$

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

$$\frac{d[uptSi]}{dt} = \frac{\mu_{F,dia}[F_{dia}]}{C/Si} \tag{32}$$

With μ_{F_i}: Growth rate of the ith phytoplankton species (Eq. (14)), [h^{-1}]

e_{phy_i}: Excretion rate of the ith phytoplankton species (Eq. (16)), [h^{-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}]

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

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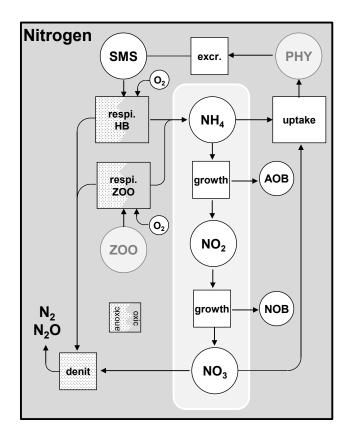
Figure 5. Cycling of nitrogen. PHY: phytoplankton species; HB: heterotrophic bacteria; ZOO: zooplankton species; AOB: ammonia-oxidizing bacteria; NOB: Nitrite-oxidizing bacteria; respi.: respiration; excr.: excretion; denit: denitrification

for growth of heterotrophic bacteria and zooplankton.

$$respHB = \sum_i (1 - Y_{hb_i}) b_{hb_i} [HB_i] \tag{33}$$

$$respZOO = \sum_j (1 - Y_{zoo_j}) b_{zoo_j} [ZOO_j] \tag{34}$$

$$relN = \frac{respHB}{C/N} + \frac{respZOO}{C/N} \tag{35}$$

$$relP = \frac{respHB}{C/P} + \frac{respZOO}{C/P} \tag{36}$$

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

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

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

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

15

$relP$: 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-
350   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. (37) and (38)). The denitrification occurs when dissolved oxygen is not present
in sufficient quantity (Fig. 5).

$$nitr_{aob} = \sum_i \frac{\mu_{aob_i}}{Y_{aob_i}}[AOB_i] \tag{37}$$

$$nitr_{nob} = \sum_j \frac{\mu_{nob_j}}{Y_{nob_j}}[NOB_j] \tag{38}$$

355   With μ_{aob_i} and μ_{nob_j}: Growth rates of the ith AOB species and the jth NOB species, [h^{-1}]

Y_{aob_i} and Y_{nob_j}: Growth yields of the ith AOB species and the jth 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}]

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

360   $$\frac{d[NO_3^-]}{dt} = -denit + nitr_{nob} - \frac{uptNO_3^-}{dt} \tag{39}$$

$$\frac{d[NH_4^+]}{dt} = relN - nitr_{aob} - \frac{uptNH_4^+}{dt} \tag{40}$$

$$\frac{d[NO_2^-]}{dt} = nitr_{aob} - nitr_{nob} \tag{41}$$

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

$nitr_{nob}$: Nitrification by NOB, [mgN L^{-1} h^{-1}]

365   $nitr_{aob}$: Nitrification by AOB, [mgN L^{-1} h^{-1}]

$\frac{uptNO_3^-}{dt}$: Uptake of NO_3^- by phytoplankton growth (Eq. (30)), [mgN L^{-1} h^{-1}]

$relN$: Release of nitrogen by respiration of heterotrophic bacteria and zooplankton (Eq. (35)), [mgN L^{-1} h^{-1}]

$\frac{uptNH_4^+}{dt}$: Uptake of NH_4^+ by phytoplankton growth (Eq. (29)), [mgN L^{-1} h^{-1}]

2.5.4 Phosphate adsorption desorption

370   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
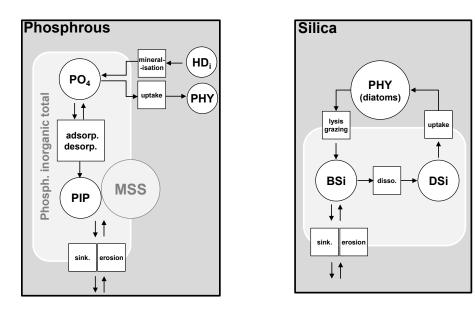suspended solids (MSS) to form PIP (particulate inorganic phosphorus).

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

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

$$\frac{PIP}{MSS} = P_{ac} \times \frac{PO_4}{PO_4 + K_{ps}} \tag{42}$$

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

P_{ac}: Maximum adsorption capacity of MSS, [mgP mgMSS^{-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$_4$ and TIP (total inorganic phosphorus):

380   $$TIP = PO_4 + PIP \tag{43}$$

This relationship can be written:

$$PO4 = \frac{(TIP - P_{ac} \times MSS - K_{ps}) + \sqrt{(-TIP + P_{ac} \times MSS + K_{ps})^2 + 4 * TIP * K_{ps}}}{2} \tag{44}$$

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

385   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):

$$BSi_{disso.} = Kb_{Si} * BSi \tag{45}$$

$$Kb_{Si} = Kb_{Si20} * ftp_{Si}(T) \tag{46}$$

390 $$ftp_{Si}(T) = exp(\frac{60000}{8.314} \times (\frac{1}{275} - \frac{1}{273 + T})) \tag{47}$$

With Kb_{Si20}: Dissolution rate of biogenic silica at 20 °C, [h^{-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
395 sediment oxygen demand (not shown here) are also included in unified RIVE v1.0 model. An oxygen budget can then be
established (Eq. (48)).

$$\frac{d[O_2]}{dt} = rea + \frac{32}{12}(\sum_i (p_{phy_i} - r_{phy_i})[F_i] - respHB - \sum_j r_{zoo_j}[ZOO_j]) - \frac{32}{14}(\frac{3}{2}nitr_{aob} + \frac{1}{2}nitr_{nob}) \tag{48}$$

$$rea = \frac{k_{rea}}{depth}([O_2]_{sat} - [O_2]) \tag{49}$$

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

400 $depth$: 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 ith phytoplankton species (Eq. (12)), [h^{-1}]

405 r_{phy_i}: Respiration rate of the ith phytoplankton species (Eq. (15)), [h^{-1}]

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

$respHB$: Respiration of all heterotrophic bacteria species (Eq. (33)), [mgC L^{-1} h^{-1}]

r_{zoo_j}: Respiration rate of the jth zooplankton species (Eq. (26)), [h^{-1}]

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

410 $\frac{32}{14}$: Molar mass ratio between dissolved oxygen and nitrogen, [mgO$_2$/mgN]

$nitr_{aob}$: Nitrification to produce nitrite by oxidizing NH$_4^+$ (Eq. (37), with $\frac{3}{2}$ the stoichiometric coefficient), [mgN L^{-1} h^{-1}]

$nitr_{nob}$: Nitrification to produce nitrate by oxidizing NO$_2^-$ (Eq. (38), 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
415 (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:

420

$$[\text{DIC}] = [\text{H}_2\text{CO}_3] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}] \tag{50}$$

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).

$$[\text{CO}_2(\text{aq})] = \frac{[\text{DIC}]\frac{[\text{H}^+]}{\text{K}_1}}{\left(1 + \frac{[\text{H}^+]}{\text{K}_1} + \frac{\text{K}_2}{[\text{H}^+]}\right)} \tag{51}$$

With K_1, K_2: Equilibrium constants of carbonate equilibrium reactions (Stumm and Morgan, 1996), [mol L^{-1}]

425 $[H^+]$: 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}).

$$F_{CO_2} = k_{co2}([CO_2(sat)] - [CO_2(aq)]) \tag{52}$$

430 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.

435 (1987) and Wanninkhof (1992), the gas transfer velocity of CO_2 (k_{co2}) at water temperature T (°C) can be calculated as:

$$k_{co2} = k_{600}\sqrt{\frac{600}{Sc_{CO_2}(T)}} \tag{53}$$

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,

$$Sc_{CO_2}(T) = 1911.1 - 118.11T + 3.4527T^2 - 0.04132T^3 \tag{54}$$

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.

$$\frac{dTA}{dt} = [(\frac{14}{106} \times \frac{(respPHY + respHB + respZOO)}{12}) + \frac{(denit - 2 \cdot nitr_{aob})}{14} \tag{55}$$

$$+(\frac{17}{106} \times \frac{uptNO_3^-}{uptN} - \frac{15}{106} \times \frac{uptNH_4^+}{uptN}) \times \frac{\sum(\mu_{F_i} + e_{phy_i})[F_i]}{12}] \times 1000 + TA_{Net\_Input} \tag{56}$$

$$\frac{dDIC}{dt} = (respPHY + respHB + respZoo) + denit \times \frac{12}{14} \times \frac{5}{4} \tag{57}$$

$$-\sum p_{phy_i}[F_i] + \frac{F_{CO_2}}{depth} + DIC_{Net\_Input} \tag{58}$$

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 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. Their definitions and reference values are provided in appendix.

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 and PIP are derived from it according to Eq. (43) and Eq.(44). TIP is subject to release by heterotrophic bacteria and zooplankton respiration (Eq.

470 (36)), uptake by phytoplankton and settling of PIP together with MSS. However, the PO_4 is treated as a state variable and released by respiration (Eq. (36)) in C-RIVE 0.32 and only PIP (particulate inorganic phosphorus) is derived from the equation (42).

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

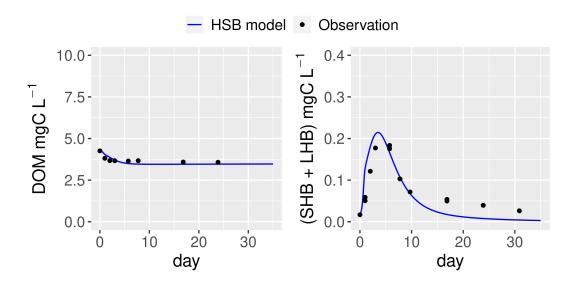## 3.2 Modeling of the organic matter degradation by unified RIVE v1.0 (HSB model)

Figure 7. Simulation of the dynamics of heterotrophic bacteria in a filtered and reinoculated sample of the drainage pond water (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

475 experiments conducted by Garnier et al. (2021). Two water samples, one obtained from a drainage pond (located in France) and the other collected from an urban sewage collector (at Rosny-sur-Seine, France), 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). 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. 7 and 8). The parameter values are kept the same for both water samples.
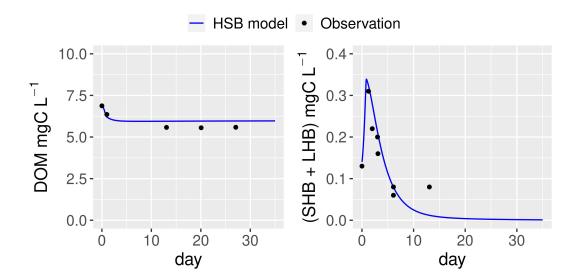

Figure 8. Simulation of the dynamics of heterotrophic bacteria in a filtered and reinoculated sample of the urban sewage water (Garnier et al., 2021) by HSB model (unified RIVE v1.0). DOM: Dissolved organic matter; SHB: Small heterotrophic bacteria; LHB: Large heterotrophic bacteria

480 ## 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.

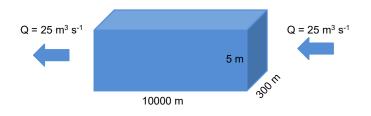### 3.3.1 River stretch morphology and hydraulic conditions

Figure 9. Geometric and hydraulic description of a river stretch

485   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 m³ s⁻¹ which corresponds to a residence time of 7 days. The water height is fixed at 5
meters.

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	[mgO₂ 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	[-]

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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
490 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
495 are to 0, the more similar are the concentrations simulated by the two softwares (pyRIVE 1.0 and C-RIVE 0.32).

$$PBIAS = 100 \frac{\sum_{i=1}^{i=N}(C_i - Py_i)}{\sum_{i=1}^{i=N}} \tag{59}$$

$$MAD = \frac{\sum_{i=1}^{i=N}|C_i - Py_i|}{N} \tag{60}$$

$$MaAD = max(|C_i - Py_i|) \tag{61}$$

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
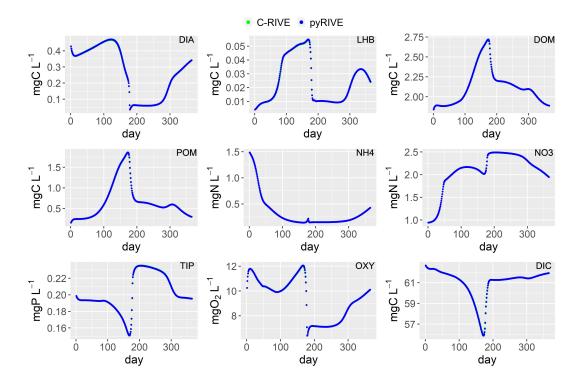500 Python 3). N is the number of values.

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

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	$2.24 \cdot 10^{-3}$	$1.65 \cdot 10^{-2}$

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}, relatively low, is obtained for dissolved oxygen concentration while the mean absolute difference (MAD) for dissolved oxygen concentration is 0.00678 mgO$_2$ L^{-1}

505 (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

510 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 by pyRIVE 1.0 and C-RIVE 0.32. 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%.

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4   Discussion

515   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 4.2) and its benefits for scientific community (Section 4.3).

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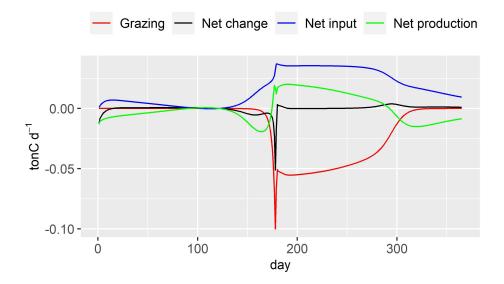

Figure 11. Budget fluxes of DIA (tonC d^{-1}). Grazing: Zooplankton grazing fluxes; Net production: Eq. (23); Net input: input flux - output flux; Net change: daily variation of DIA in the river stretch

520   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

525   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

530   net production, leading to a simulated increase in DIA biomass. This trend continues until day 130 when the maximum DIA
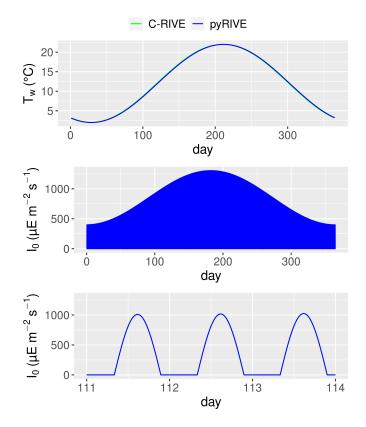
Figure 12. Simulated water temperature, active irradiance and zoom of active irradiance for days 111-114

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

535   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. (24)). 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

540   until day 260 (Fig. 10), which means that the net production and net input in DIA biomass are balanced by the grazing of 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.
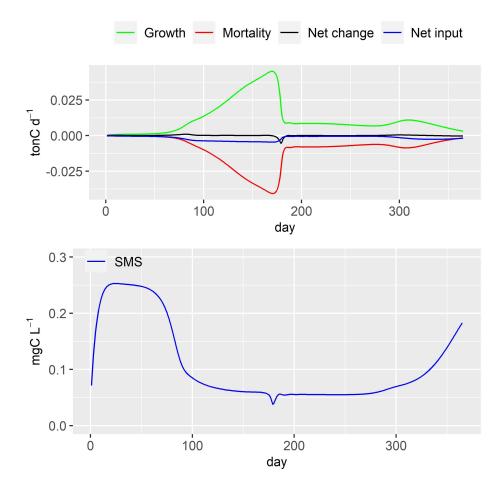
Figure 13. Large heterotrophic bacteria (LHB) dynamics and simulated concentrations of small monomeric substrate (SMS). Net change: daily variation of LHB in river stretch; Net input: input flux - output flux

The growth rate of large heterotrophic bacteria (LHB) increases (Fig. 13) with the increase of water temperature, causing

545   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 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 it increases in conjunction with the rise in SMS concentration, which is synchronized with the increase in phytoplankton biomass.

550   **4.2   Model limitations and future developments of unified RIVE**

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.

4.3   Benefit of unified RIVE model

The unified RIVE provides a set of governing equations of aquatic 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 the location in the network (Garnier et al., 2020), which is of great interest to the different research teams involved in aquatic research such as 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 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 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 simu-

585 lations of the two digital implementations (Python 3 for pyRIVE 1.0 and ANSI C for C-RIVE 0.32), which estimate 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. 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 sil-

590 ica 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 biogeochemistry community are strongly

595 encouraged to achieve a better understanding of aquatic system 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.

600 (2023).

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

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

Aquatic 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 parameter values necessary for running unified RIVE v1.0 are provided hereafter.

Table B1. Heterotrophic and nitrifying Bacteria related parameters

Parameter	Description	Value	Unit
$^*b_{max,lhb}$	Maximal substrate (SMS) uptake rate of LHB	0.6	$[h^{-1}]$
$^*b_{max,shb}$	Maximal substrate (SMS) uptake rate of SHB	0.16	$[h^{-1}]$
$^*Y_{lhb}$	Growth yield of LHB	0.25	[-]
$^*Y_{shb}$	Growth yield of SHB	0.25	[-]
$^*k_{d20,lhb}$	Mortality rate of LHB	0.05	$[h^{-1}]$
$^*k_{d20,shb}$	Mortality rate of SHB	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	°C
$^*\mu_{max,aob}$	Maximal growth rate of AOB	0.07	$[h^{-1}]$
$^*\mu_{max,nob}$	Maximal growth rate of NOB	0.05	$[h^{-1}]$
$K_{o2,aob}$	Half-saturation constant of AOB for O_2	0.64	$[mgO_2\ L^{-1}]$
$K_{o2,nob}$	Half-saturation constant of NOB for O_2	1.088	$[mgO_2\ L^{-1}]$
$K_{nh4,aob}$	Half-saturation constant of AOB for NH_4^+	0.75	$[mgN\ L^{-1}]$
$K_{no2,nob}$	Half-saturation constant of NOB for NO_2^-	0.05	$[mgN\ L^{-1}]$
$K_{sms,lhb}$	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	$[mgC\ L^{-1}]$
$^*Y_{aob}$	Growth yield of AOB	0.07	[mgC/mgN]
$^*Y_{nob}$	Growth yield of AOB	0.02	[mgC/mgN]
$^*k_{d,aob}$	Mortality rate of AOB	0.005	$[h^{-1}]$
$^*k_{d,nob}$	Mortality rate of NOB	0.005	$[h^{-1}]$
vs_{aob}	Sinking velocity of AOB	0.005	$[m\ h^{-1}]$
vs_{nob}	Sinking velocity of NOB	0.005	$[m\ h^{-1}]$
$T_{opt,aob}$	Optimal temperature of AOB	23	[°C]
σ_{aob}	Range of temperature for AOB	18	[°C]
$T_{opt,nob}$	Optimal temperature of NOB	23	[°C]
σ_{nob}	Range of temperature for NOB	18	[°C]

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

Table B2. Primary producer dynamics related parameters

Parameter	Description	Value	Unit
$^*P_{dia,max}$	Maximum rate of photosynthesis for diatoms	0.2	$[\text{h}^{-1}]$
$^*P_{gra,max}$	Maximum rate of photosynthesis for green algae	0.25	$[\text{h}^{-1}]$
$^*P_{cya,max}$	Maximum rate of photosynthesis for cyanobacteria	0.1	$[\text{h}^{-1}]$
α_{dia}	Photosynthetic efficiency of diatoms	0.0012	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
α_{gra}	Photosynthetic efficiency of green algae	0.0012	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
α_{cya}	Photosynthetic efficiency of cyanobacteria	0.0012	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
β_{dia}	Photoinhibition capacity of diatoms	0.0	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
β_{gra}	Photoinhibition capacity of green algae	0.0	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
β_{cya}	Photoinhibition capacity of cyanobacteria	0.0	$[\text{h}^{-1}\,(\mu\text{E m}^{-2}\,\text{s}^{-1})^{-1}]$
η_{base}	Light extinction related coefficient for pure water	0.2	$[\text{m}^{-1}]$
η_{chla}	Light algal self-shading light extinction coefficient	0.02	$[\text{m}^{-1}\,(\mu\text{gchl}a\,\text{L}^{-1})^{-1}]$
η_{ss}	Light extinction coefficient related to suspended solid	0.042	$[\text{m}^{-1}\,(\text{mg L}^{-1})^{-1}]$
$^*\mu_{dia,max}$	Maximal growth rate of diatoms	0.05	$[\text{h}^{-1}]$
$^*\mu_{gra,max}$	Maximal growth rate of green algae	0.05	$[\text{h}^{-1}]$
$^*\mu_{cya,max}$	Maximal growth rate of cyanobacteria	0.025	$[\text{h}^{-1}]$
$K_{S,dia}$	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	$[\text{mgN L}^{-1}]$
$K_{N,gra}$	Half-saturation constant for nitrogen of green algae	0.014	$[\text{mgN L}^{-1}]$
$K_{N,cya}$	Half-saturation constant for nitrogen of cyanobacteria	0.014	$[\text{mgN L}^{-1}]$
$K_{P,dia}$	Half-saturation constant for phosphorus of diatoms	0.0155	$[\text{mgP L}^{-1}]$
$K_{P,gra}$	Half-saturation constant for phosphorus of green algae	0.062	$[\text{mgP L}^{-1}]$
$K_{P,cya}$	Half-saturation constant for phosphorus of cyanobacteria	0.062	$[\text{mgP L}^{-1}]$
$K_{Si,dia}$	Half-saturation constant for silica of diatoms	0.196	$[\text{mgSi L}^{-1}]$
$^*R_{m,dia}$	Maintenance respiration coefficient of diatoms	0.002	$[\text{h}^{-1}]$
$^*R_{m,gra}$	Maintenance respiration coefficient of green algae	0.002	$[\text{h}^{-1}]$
$^*R_{m,cya}$	Maintenance respiration coefficient of cyanobacteria	0.002	$[\text{h}^{-1}]$
$R_{\mu,dia}$	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 $f(T) = \dfrac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B3. Primary producer dynamics related parameters (continue)

Parameter	Description	Value	Unit
$E_{cst,dia}$	Basic excretion rate of diatoms	0.006	$[\text{h}^{-1}]$
$E_{cst,gra}$	Basic excretion rate of green algae	0.006	$[\text{h}^{-1}]$
$E_{cst,cya}$	Basic excretion rate of cyanobacteria	0.006	$[\text{h}^{-1}]$
$E_{phot,dia}$	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	[-]
$^*S_{R,max,dia}$	Maximal rate of reserve products synthesis for diatoms	0.15	$[\text{h}^{-1}]$
$^*S_{R,max,gra}$	Maximal rate of reserve products synthesis for green algae	0.2	$[\text{h}^{-1}]$
$^*S_{R,max,cya}$	Maximal rate of reserve products synthesis for cyanobacteria	0.075	$[\text{h}^{-1}]$
$^*C_{R,max,dia}$	Maximal rate of reserve products catabolism for diatoms	0.2	$[\text{h}^{-1}]$
$^*C_{R,max,gra}$	Maximal rate of reserve products catabolism for green algae	0.2	$[\text{h}^{-1}]$
$^*C_{R,max,cya}$	Maximal rate of reserve products catabolism for cyanobacteria	0.2	$[\text{h}^{-1}]$
$^*k_{d,dia}$	Rate of diatoms mortality	0.025	$[\text{h}^{-1}]$
$^*k_{d,gra}$	Rate of green algae mortality	0.035	$[\text{h}^{-1}]$
$^*k_{d,cya}$	Rate of cyanobacteria mortality	0.006	$[\text{h}^{-1}]$
vs_{dia}	Sinking velocity of diatoms	0.006	$[\text{m}\,\text{h}^{-1}]$
vs_{gra}	Sinking velocity of green algae	0.001	$[\text{m}\,\text{h}^{-1}]$
vs_{cya}	Sinking velocity of cyanobacteria	0.006	$[\text{m}\,\text{h}^{-1}]$
$T_{opt,dia}$	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 $f(T) = \dfrac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ where T is water temperature in °C.

Table B4. Organic matter dynamics parameters

Parameter	Description	Value	Unit
$^*e_{max,dom_1}$	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}	DOM_1 fraction in lysis products	0.2	$[-]$
ϵ_{dom_2}	DOM_2 fraction in lysis products	0.2	$[-]$
ϵ_{dom_3}	DOM_3 fraction in lysis products	0.1	$[-]$
ϵ_{pom_1}	POM_1 fraction in lysis products	0.2	$[-]$
ϵ_{pom_2}	POM_2 fraction in lysis products	0.2	$[-]$
ϵ_{pom_3}	POM_3 fraction in lysis products	0.1	$[-]$
$^*k_{pom_1}$	POM_1 hydrolysis rate constant	0.005	$[h^{-1}]$
k_{pom_2}	POM_2 hydrolysis rate constant	0.00025	$[h^{-1}]$
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	$[mgC\,L^{-1}]$

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

Table B5. Zooplankton parameters

Parameter	Description	Value	Unit
$^{*}\mu_{max,zor}$	Maximal growth rate of ZOR	0.025	[h^{-1}]
$^{*}\mu_{max,zoc}$	Maximal growth rate of ZOC	0.015	[h^{-1}]
$^{*}B_{max,zor}$	Maximal grazing rate of ZOR	0.1	[h^{-1}]
$^{*}B_{max,zoc}$	Maximal grazing rate of ZOC	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}]
$^{*}k_{d,zor}$	Mortality rate of ZOR	0.007	[h^{-1}]
$^{*}k_{d,zoc}$	Mortality rate of ZOC	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 $f(T) = \dfrac{e^{-\frac{(T-T_{opt})^2}{\sigma^2}}}{e^{-\frac{(20-T_{opt})^2}{\sigma^2}}}$ 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 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}]

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References

Aissa-Grouz, N., Garnier, J., and Billen, G.: Long trend reduction of phosphorus wastewater loading in the Seine: determination of phosphorus speciation and sorption for modeling algal growth, Environmental Science and Pollution Research, https://doi.org/10.1007/s11356-016-7555-7, 2016.

620

Alexander, R. B., Elliott, A. H., Shankar, U., and McBride, G. B.: Estimating the sources and transport of nutrients in the Waikato River Basin, New Zealand, Water Resources Research, 38, 4–1–4–23, https://doi.org/10.1029/2001WR000878, 2002.

Azam, F., Fenchel, T., Gray, J., Meyer, L., and Thingstad, F.: The Ecological Role of Water-Column Microbes in the Sea, Marine Ecology Progress Series, 10, 257–263, 1983.

625

Battin, T. J., Lauerwald, R., Bernhardt, E. S., Bertuzzo, E., Gener, L. G., Hall, R. O., Hotchkiss, E. R., Maavara, T., Pavelsky, T. M., Ran, L., Raymond, P., Rosentreter, J. A., and Regnier, P.: River Ecosystem Metabolism and Carbon Biogeochemistry in a Changing World, Nature, 613, 449–459, https://doi.org/10.1038/s41586-022-05500-8, 2023.

Billen, G.: Protein degradation in Aquatic Environments, in: Microbial Enzyme in Aquatic Environments, edited by Chrost, R., Springer Verlag, Berlin, 1991.

630

Billen, G. and Servais, P.: Modélisation des processus de dégradation bactérienne de la matière organique en milieu aquatique, in: Micro-organismes dans les écosystèmes océaniques, edited by et al., B., pp. 219–245, Masson Paris, 1989.

Billen, G., Servais, P., and Fontigny, A.: Growth and mortality in bacterial populations dynamics of aquatic environments, Arch. Hydrobiol. Beih. Ergebn. Limnol, 31, 173–183, 1988.

Billen, G., Servais, P., and Becquevort, S.: Dynamics of bacterioplankton in oligotrophic and eutrophic aquatic environments: bottom-up or

635

top-down control?, in: Fluxes Between Trophic Levels and Through the Water-Sediments Interface, edited by Bonin, D. and Golterman, H., pp. 37–42, Kluwer Academic Publishers, 1990.

Billen, G., Garnier, J., and Hanset, P.: Modelling phytoplankton development in whole drainage networks: the RIVERSTRAHLER Model applied to the Seine river system, Hydrobiologia, 289, 119–137, 1994.

Billen, G., Garnier, J., and Rousseau, V.: Nutrient fluxes and water quality in the drainage network of the Scheldt basin over the last 50 year,

640

Hydrobiologia, 540, 47–67, 2005.

Billen, G., Garnier, J., Mouchel, J.-M., and Silvestre, M.: The Seine system: Introduction to a multidisciplinary approach of the functioning of a regional river system, Sciences of Total Environment, 375, 1–12, 2007.

Billen, G., Garnier, J., and Silvestre, M.: A simplified algorithm for calculating benthic nutrient fluxes in river systems, Ann. Limnol. - Int. J. Lim., 51, 37–47, https://doi.org/10.1051/limn/2014030, 2015.

645

Brion, N. and Billen, G.: Une réévaluation de la méthode de mesure de l'activité nitrifiante autotrophe par la méthode d'incorporation de bicarbonate marqué $H^{14}CO_3^-$ et son application pour estimer des biomasses de bactéries nitrifiantes, Revue des Sciences de l'Eau, 11, 283–302, 1998.

Culberson, C. H.: Calculation of the in situ pH of seawater1, Limnology and Oceanography, 25, 150–152, https://doi.org/10.4319/lo.1980.25.1.0150, 1980.

650

Desmit, X., Thieu, V., Billen, G., Campuzano, F., Dulière, V., Garnier, J., Lassaletta, L., Ménesguen, A., Neves, R., Pinto, L., Silvestre, M., Sobrinho, J., and Lacroix, G.: Reducing marine eutrophication may require a paradigmatic change, Science of the Total Environment, 635, 1444–1466, https://doi.org/10.1016/j.scitotenv.2018.04.181, 2018.

Escoffier, N., Bensoussan, N., Vilmin, L., Flipo, N., Rocher, V., David, A., Métivier, F., and Groleau, A.: Estimating ecosystem metabolism from continuous multi-sensor measurements in the Seine River, Environmental Science and Pollution Research, 25, 23 451–23 467, https://doi.org/10.1007/s11356-016-7096-0, 2018.

Even, S., Poulin, M., Garnier, J., Billen, G., Servais, P., Chesterikoff, A., and Coste, M.: River ecosystem modelling: Application of the PROSE model to the Seine river (France), Hydrobiologia, 373, 27–45, https://doi.org/10.1023/A:1017045522336, 1998.

Even, S., Poulin, M., Mouchel, J. M., Seidl, M., and Servais, P.: Modelling oxygen deficits in the Seine river downstream of combined sewer overflows, Ecol. Model., 173, 177–196, 2004.

Even, S., Mouchel, J. M., Servais, P., Flipo, N., Poulin, M., Blanc, S., Chabanel, M., and Paffoni, C.: Modeling the impacts of Combined Sewer Overflows on the river Seine water quality, Sciences of Total Environment, 375, 140–151, https://doi.org/10.1016/j.scitotenv.2006.12.007, 2007.

Fick, A.: Ueber diffusion, Annalen der Physik und Chemie, J.A. Barth, 1855.

Flipo, N., Even, S., Poulin, M., Tusseau-Vuillemin, M. H., Améziane, T., and Dauta, A.: Biogeochemical Modelling at the River Scale: Plankton and Periphyton Dynamics - Grand Morin case study, France, Ecol. Model., 176, 333–347, 2004.

Flipo, N., Rabouille, C., Poulin, M., Even, S., Tusseau-Vuillemin, M. H., and Lalande, M.: Primary production in headwater streams of the Seine basin: the Grand Morin case study, Sciences of Total Environment, 375, 98–109, https://doi.org/10.1016/j.scitotenv.2006.12.015, 2007.

Fontigny, A., Billen, G., and Vives-Rego, J.: Some kinetic characteristics of exoproteolytic activity in coastal seawater, Estuarine Coastal and Shelf Science, 25, 127–133, https://doi.org/10.1016/0272-7714(87)90030-8, 1987.

Fuhrman, J. and Azam, F.: Thymidine Incorporation as a Measure of Heterotrophic Bacterioplankton Production in Marine Surface Waters: Evaluation and Field Results, Marine Biology, 66, 109–120, 1982.

Garnier, G., Weidenfeld, L., Billen, G., Martinez, A., Mercier, B., Rocher, V., Tabuchi, J.-P., and Azimi, S.: La matière organique dans le continuum terrestre-aquatique du bassin de la Seine, Rapport annuel PIREN-Seine, PIREN-Seine, https://doi.org/10.26047/PIREN.rapp.ann.2021.vol21, 2021.

Garnier, J. and Billen, G.: Ecological interactions in a shallow sand-pit lake (Lake Créteil, Parisian Basin, France): a modelling approach, Hydrobiologia, 275/276, 97–114, 1994.

Garnier, J. and Billen, G.: Production vs. Respiration in river systems: An indicator of an "ecological status", Science of the Total Environment, 375, 110–124, https://doi.org/10.1016/j.scitotenv.2006.12.006, 2007.

Garnier, J., Billen, G., and Servais, P.: Physiological characteristics and ecological role of small- and large-sized bacteria in a polluted river (Seine River, France), Arch. Hydrobiol. Beih., 37, 83–94, 1992a.

Garnier, J., Servais, P., and Billen, G.: Bacterioplankton in the Seine river (France): impact of the Parisian urban effluent, Can. J. Microbiol., 38, 56–64, 1992b.

Garnier, J., Billen, G., and Coste, M.: Seasonal succession of diatoms and chlorophycae in the drainage network of the river Seine: Observations and modelling, Limnol. Oceanogr., 40, 750–765, 1995.

Garnier, J., Billen, G., Hanset, P., Testard, P., and Coste, M.: Développement algal et eutrophisation dans le réseau hydrographique de la Seine, in: La Seine en son bassin-Fonctionnement écologique d'un système fluvial anthropisé, edited by Meybeck, M., de Marsily, G., and Fustec, E., pp. 593–626, Elsevier, 1998.

Garnier, J., Billen, G., and Palfner, L.: Understanding the Oxygen Budget and Related Ecological Processes in the River Mosel: The RIVER-
690   STRAHLER Approach, in: Man and River Systems, edited by Garnier, J. and Mouchel, J.-M., pp. 151–166, Springer Netherlands, Dor-
       drecht, https://doi.org/10.1007/978-94-017-2163-9_17, 1999a.

Garnier, J., Leporcq, B., Sanchez, N., and Philippon, X.: Biogeochemical mass-balances (C, N, P, Si) in three large reservoirs of the Seine
       Basin (France), Biogeochemistry, 47, 119–146, https://doi.org/10.1023/A:1006101318417, 1999b.

Garnier, J., Billen, G., Sanchez, N., and Leporcq, B.: Ecological functioning of the Marne Reservoir (upper Seine basin, France), Regul.
695   Rivers: Res. Mgmt., 16, 51–71, 2000.

Garnier, J., Billen, G., Hannon, E., Fonbonne, S., Videnina, Y., and Soulie, M.: Modeling transfer and retention of nutrients in the drainage
       network of the Danube River, Estuar. Coast. Shelf, 54, 285–308, 2002.

Garnier, J., Brion, N., Callens, J., Passy, P., Deligne, C., Billen, G., Servais, P., and Billen, C.: Modeling historical changes in nutrient
       delivery and water quality of the Zenne River (1790s–2010): The role of land use, waterscape and urban wastewater management, Journal
700   of Marine Systems, 128, 62–76, https://doi.org/10.1016/j.jmarsys.2012.04.001, 2013.

Garnier, J., Billen, G., Vilain, G., Benoit, M., Passy, P., Tallec, G., Tournebize, J., Anglade, J., Billy, C., Mercier, B., Ansart,
       P., Azougui, A., Sebilo, M., and Kao, C.: Curative vs. preventive management of nitrogen transfers in rural areas: Lessons
       from the case of the Orgeval watershed (Seine River basin, France), Journal of Environmental Management, 144, 125–134,
       https://doi.org/10.1016/j.jenvman.2014.04.030, 2014.

705 Garnier, J., Ramarson, A., Billen, G., Théry, S., Thiéry, D., Thieu, V., Minaudo, C., and Moatar, F.: Nutrient inputs and hydrology together
       determine biogeochemical status of the Loire River (France): Current situation and possible future scenarios, Science of The Total Envi-
       ronment, 637-638, 609–624, https://doi.org/10.1016/j.scitotenv.2018.05.045, 2018a.

Garnier, J., Ramarson, A., Thieu, V., Némery, J., Théry, S., Billen, G., and Coynel, A.: How can water quality be improved when the urban
       waste water directive has been fulfilled? A case study of the Lot river (France), Environmental Science and Pollution Research, 25,
710   11 924–11 939, https://doi.org/10.1007/s11356-018-1428-1, 2018b.

Garnier, J., Marescaux, A., Guillon, S., Vilmin, L., Rocher, V., Billen, G., Thieu, V., Silvestre, M., Passy, P., Raimonet, M., Groleau, A.,
       Théry, S., Tallec, G., and Flipo, N.: The Handbook of Environmental Chemistry, chap. Ecological Functioning of the Seine River: From
       Long-Term Modelling Approaches to High-Frequency Data Analysis, pp. 1–28, Handbook of Environmental Chemistry, Springer, Berlin,
       Heidelberg, https://doi.org/10.1007/698_2019_379, 2020.

715 Gurung, A., Iwata, T., Nakano, D., and Urabe, J.: River Metabolism along a Latitudinal Gradient across Japan and in a global scale, Scientific
       Reports, 9, https://doi.org/10.1038/s41598-019-41427-3, 2019.

Gypens, N., Lancelot, C., and Borges, A. V.: Carbon dynamics and CO_2 air-sea exchanges in the eutrophied coastal waters of the Southern
       Bight of the North Sea: a modelling study, Biogeosciences, 1, 147–157, https://doi.org/10.5194/bg-1-147-2004, 2004.

Hellweger, F. L.: 100 Years since Streeter and Phelps: It Is Time To Update the Biology in Our Water Quality Models, Environmental Science
720   & Technology, 49, 6372–6373, https://doi.org/10.1021/acs.est.5b02130, 2015.

Jähne, B., Heinz, G., and Dietrich, W.: Measurement of the diffusion coefficients of sparingly soluble gases in water, Journal of Geophysical
       Research: Oceans, 92, 10 767–10 776, https://doi.org/10.1029/JC092iC10p10767, 1987.

Korppoo, M., Huttunen, M., Huttunen, I., Piirainen, V., and Vehviläinen, B.: Simulation of bioavailable phosphorus and ni-
       trogen loading in an agricultural river basin in Finland using VEMALA v.3, Journal of Hydrology, 549, 363–373,
725   https://doi.org/10.1016/j.jhydrol.2017.03.050, 2017.

Lancelot, C., Veth, C., and Mathot, S.: Modelling ice-edge phytoplankton bloom in the Scotia-Weddell sea sector of the southern ocean during spring 1998, J. Mar. System, 2, 333–346, 1991.

Lauerwald, R., Hartmann, J., Moosdorf, N., Dürr, H. H., and Kempe, S.: Retention of dissolved silica within the fluvial system of the conterminous USA, Biogeochemistry, 112, 637–659, 2013.

730   Le, T. P. Q., Billen, G., Garnier, J., Théry, S., Ruelland, D., Anh, N. X., and Van, M. C.: Nutrient (N, P, Si) transfers in the subtropical Red River system (China and Vietnam): Modelling and budget of nutrient sources and sinks, Journal of Asian Earth Sciences, 37, 259 – 274, https://doi.org/10.1016/j.jseaes.2009.08.010, 2010.

Le, T. P. Q., Billen, G., Garnier, J., and Chau, V.: Long-term biogeochemical functioning of the Red River (Vietnam): past and present situations, Reg. Environ. Change, 15, 329–339, https://doi.org/10.1007/s10113-014-0646-4, 2015.

735   Lindenschmidt, K.-E., Carr, M. K., Sadeghian, A., and Morales-Marin, L.: CE-QUAL-W2 model of dam outflow elevation impact on temperature, dissolved oxygen and nutrients in a reservoir, Scientific Data, 6, 312, https://doi.org/10.1038/s41597-019-0316-y, 2019.

Luu, M. T., Dinh, T. D., Trinh, D. A., and Doc, N. T.: Water Quality in an Urbanized River Basin Impacted by Multi-Pollution Sources: From Comprehensive Surveys to Modelling, ScienceAsia, 47, 86, https://doi.org/10.2306/scienceasia1513-1874.2021.014, 2021.

Maavara, T., Chen, Q., Van Meter, K., Brown, L. E., Zhang, J., Ni, J., and Zarfl, C.: River dam impacts on biogeochemical cycling, Nature
740   Reviews Earth & Environment, 1, 103–116, https://doi.org/10.1038/s43017-019-0019-0, 2020.

Manteaux, S., Sauvage, S., Samie, R., Monteil, C., Garnier, J., Thieu, V., Cakir, R., and Sánchez-Pérez, J.-M.: Modeling in-stream biogeochemical processes at catchment scale coupling SWAT and RIVE models, submitted to Environmental Modelling and Software, 2023.

Marescaux, A., Thieu, V., Gypens, N., Silvestre, M., and Garnier, J.: Modeling inorganic carbon dynamics in the Seine River continuum in France, Hydrology and Earth System Sciences, 24, 2379–2398, https://doi.org/10.5194/hess-24-2379-2020, 2020.

745   Michaelis, L. and Menten, M. L.: Die kinetik der invertinwirkung - The kinetics of invertin action, Biochemische Zeitschrift, 49, 333–369, 1913.

Minaudo, C., Curie, F., Jullian, Y., Gassama, N., and Moatar, F.: QUAL-NET, a high temporal-resolution eutrophication model for large hydrographic networks, Biogeosciences, 15, 2251–2269, https://doi.org/10.5194/bg-15-2251-2018, 2018.

Monod,   J.:   The   growth   of   bacterial   cultures,   Annual   Review   of   Microbiology,   3,   371–394,
750   https://doi.org/10.1146/annurev.mi.03.100149.002103, 1949.

Nguyen, H. T. M., Billen, G., Garnier, J., Rochelle-Newall, E., Ribolzi, O., Servais, P., and Le, T. P. Q.: Modelling of faecal indicator bacteria (FIB) in the Red River basin (Vietnam), Environmental Monitoring and Assessment, https://doi.org/10.1007/s10661-016-5528-4, 2016.

Odum, H. T.: Primary production in Flowing waters, Limnol. Oceanogr., 1, 795–801, 1956.

Phuong Quynh, T. L., Garnier, J., Billen, G., Lam Ngoc, T., and Chau Van, M.: Preminary results of riverstrahler model application to the
755   red river system (Vietnam), Vietnam Journal of Chemistry, 47, 110, https://doi.org/10.15625/4550, 2014.

Platt, T., Gallegos, C., and Harrison, W.: Photoinhibition of photosynthesis in natural assemblages of marine phytoplankton, J. Mar. Res., 38, 687–701, 1980.

Raimonet, M., Vilmin, L., Flipo, N., Rocher, V., and Laverman, A.: Modelling the fate of nitrite in an urbanized river using experimentally obtained nitrifier growth parameters, Water Research, 73, 373–387, https://doi.org/10.1016/j.watres.2015.01.026, 2015.

760   Raimonet, M., Thieu, V., Silvestre, M., Oudin, L., Rabouille, C., Vautard, R., and Garnier, J.: Landward perspective of coastal eutrophication potential under future climate change: The Seine River case (France), Frontiers in Marine Science, 5, 136, https://doi.org/10.3389/fmars.2018.00136, 2018.

Redfield, A., Ketchum, B., and Richards, F.: The Sea. Ideas and Observations on Progress in the Study of the Seas. The Composition of the Sea-Water Comparative and Descriptive Oceanography, vol. 2, chap. The influence of organisms on the composition of sea-water, pp. 26–77, Interscience Publishers, 1963.

765

Rego, J. V., Billen, G., Fontigny, A., and Somville, M.: Free and Attached proteolytic activity in water environments, Marine Ecology Progress Series, 21, 245–249, 1985.

Rickert, D., Schlüter, M., and Wallmann, K.: Dissolution kinetics of biogenic silica from the water column to the sediments, Geochimica et Cosmochimica Acta, 66, 439–455, https://doi.org/10.1016/S0016-7037(01)00757-8, 2002.

770

Rodríguez-Castillo, T., Estévez, E., González-Ferreras, A., and Barquín, J.: Estimating Ecosystem Metabolism to Entire River Networks, Ecosystems, 22, 892–911, https://doi.org/10.1007/s10021-018-0311-8, 2019.

Romero, E., Garnier, J., Billen, G., Ramarson, A., Riou, P., and Le Gendre, R.: Modeling the biogeochemical functioning of the Seine estuary and its coastal zone: Export, retention, and transformations, Limnology and Oceanography, 64, 895–912, https://doi.org/10.1002/lno.11082, 2019.

775

Ruelland, D., Billen, G., Brunstein, D., and Garnier, J.: SENEQUE: a multi-scaling GIS interface to the Riverstrahler model of the biogeochemical functioning of river systems., The Science of the total environment, 375, 257–73, https://doi.org/10.1016/j.scitotenv.2006.12.014, 2007.

Segatto, P., Battin, T., and Bertuzzo, E.: Modeling the coupled dynamics of stream metabolism and microbial biomass, Limnology and Oceanography, 65, 1573–1593, https://doi.org/10.1002/lno.11407, 2020.

780

Servais, P. and Garnier, J.: Contribution of Heterotrophic Bacterial Production to the Carbon Budget of the River Seine (France), Microb. Ecol., 25, 19–33, 1993.

Servais, P., Billen, G., and Vives-Rego, J.: Rate of Bacterial Mortality in Aquatic Environments, Appl. envir. Microbiol., 49, 1448–1454, 1985.

Servais, P., Billen, G., and Hascoët, M.-C.: Determination of the biodegradable fraction of dissolved organic matter in waters, Water Research,

785

21, 445–450, 1987.

Servais, P., Billen, G., Martinez, J., and Vives-Rego, J.: Estimating bacterial mortality by the disappearance of 3H-labeled intracellular DNA, FEMS Microbiology Letters, 62, 119–125, https://doi.org/10.1016/0378-1097(89)90021-9, 1989.

Servais, P., Barillier, A., and Garnier, J.: Determination of the biodegradable fraction of dissolved and particulate organic carbon in waters, Ann. Limnol. - Int. J. Lim., 31, 75–80, https://doi.org/10.1051/limn/1995005, 1995.

790

Servais, P., Billen, G., Goncalves, A., and Garcia-Armisen, T.: Modelling microbiological water quality in the Seine river drainage network: past, present and future situations, Hydrology and Earth System Sciences, 11, 1581–1592, https://doi.org/10.5194/hess-11-1581-2007, 2007.

Sferratore, A., Billen, G., Garnier, J., Smedberg, E., Humborg, C., and Rahm, L.: Modelling nutrient fluxes from sub-arctic basins: Comparison of pristine vs. dammed rivers, Journal of Marine Systems, 73, 236–249, https://doi.org/10.1016/j.jmarsys.2007.10.012, 2008.

795

Somville, M. and Billen, G.: A method for determining exoproteolytic activity in natural water, Limnol. Oceanogr., 28, 190–193, 1983.

Streeter, H. and Phelps, E. B.: A study of the pollution and natural purification of the Ohio River, Tech. Rep. 146, U.S. Public Health Service, Treasury Department, Washington DC, 1925.

Stumm, W. and Morgan, J.: Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, A Wiley-interscience publication, Wiley, 1996.

Thieu, V., Guillon, T., Billen, G., Josette, G., and Thouvenot, M.: Applicatif BARMAN - Notice d'utilisation., Rapport annuel PIREN-Seine, PIREN-Seine, https://doi.org/10.26047/PIREN.rapp.ann.2006.vol07, 2006.

Thieu, V., Billen, G., and Garnier, J.: Nutrient transfer in three contrasting NW European watersheds: The Seine, Somme, and Scheldt Rivers. A comparative application of the Seneque/Riverstrahler model, Water Research, 43, 1740–1754, https://doi.org/10.1016/j.watres.2009.01.014, 2009.

Thieu, V., Mayorga, E., Billen, G., and Garnier, J.: Subregional and downscaled global scenarios of nutrient transfer in river basins: Seine-Somme-Scheldt case study, Global Biogeochemical Cycles, 24, https://doi.org/10.1029/2009GB003561, 2010.

Thieu, V., Silvestre, M., Garnier, J., and Billen, G.: Introducing the biogeochemical pynuts-riverstrahler model to assess prospective scenario impact along the aquatic continuum in western eu-rivers, in: Proceedings of ASLO Aquatic Sciences Meeting: "Moutains to the Sea", Honolulu, USA, 2017.

Thieu, V., Silvestre, M., Wang, S., Marescaux, A., Yan, X., Garnier, J., and Billen, G.: pyRIVE, https://doi.org/10.48579/PRO/Z9ACP1, 2023.

Thouvenot, M., Billen, G., and Garnier, J.: Modelling nutrient exchange at the sediment-water interface of river systems, Journal of Hydrology, 341, 55–78, 2007.

Vannote, R., Minshall, G. W., Cummins, K., Sedell, J., and Cushing, C.: The River Continuum Concept, Can. J. Fish. Aquat. Sci., 37, 130–137, https://doi.org/10.1139/f80-017, 1980.

Vilmin, L., Aissa-Grouz, N., Garnier, J., Billen, G., Mouchel, J. M., Poulin, M., and Flipo, N.: Impact of hydro-sedimentary processes on the dynamics of soluble reactive phosphorus in the Seine River, Biogeochemistry, 122, 229–251, https://doi.org/10.1007/s10533-014-0038-3, 2015a.

Vilmin, L., Flipo, N., de Fouquet, C., and Poulin, M.: Pluri-annual sediment budget in a navigated river system: The Seine River (France), Sciences of Total Environment, 502, 48–59, https://doi.org/10.1016/j.scitotenv.2014.08.110, 2015b.

Vilmin, L., Flipo, N., Escoffier, N., Rocher, V., and Groleau, A.: Carbon fate in a large temperate human-impacted river system: Focus on benthic dynamics, Global Biogeochem. Cycles, 30, 1086–1104, https://doi.org/10.1002/2015GB005271, 2016.

Vilmin, L., Flipo, N., Escoffier, N., and Groleau, A.: Estimation of the water quality of a large urbanized river as defined by the European WFD: what is the optimal sampling frequency?, Environmental Science and Pollution Research, 25, 23 485–23 501, https://doi.org/10.1007/s11356-016-7109-z, 2018.

Wang, S.: Simulation du métabolisme de la Seine par assimilation de données en continu, Theses, Mines Paris – PSL, https://pastel.archives-ouvertes.fr/tel-02388690, 2019.

Wang, S., Flipo, N., and Romary, T.: Oxygen data assimilation for estimating micro-organism communities' parameters in river systems, Water Research, 165, 115 021, https://doi.org/10.1016/j.watres.2019.115021, 2019.

Wang, S., Flipo, N., Romary, T., and Hasanyar, M.: Particle filter for high frequency oxygen data assimilation in river systems, Environmental Modelling & Software, p. 105382, https://doi.org/10.1016/j.envsoft.2022.105382, 2022.

Wang, S., Flipo, N., and Romary, T.: Which filter for data assimilation in water quality models? Focus on oxygen reaeration and heterotrophic bacteria activity, Journal of Hydrology, 620, 129 423, https://doi.org/10.1016/j.jhydrol.2023.129423, 2023a.

Wang, S., Vilmin, L., Hasanyar, M., and Flipo, N.: C-RIVE, https://doi.org/10.5281/zenodo.7849609, 2023b.

Wanninkhof, R.: Relationship between wind speed and gas exchange over the ocean, Journal of Geophysical Research: Oceans, 97, 7373–7382, https://doi.org/10.1029/92JC00188, 1992.

Weiss, R.: Carbon dioxide in water and seawater: the solubility of a non-ideal gas, Marine Chemistry, 2, 203–215, https://doi.org/doi.org/10.1016/0304-4203(74)90015-2, 1974.

Wilke, C. R. and Chang, P.: Correlation of diffusion coefficients in dilute solutions, AIChE Journal, 1, 264–270, 840 https://doi.org/10.1002/aic.690010222, 1955.

Yan, X., Garnier, J., Billen, G., Wang, S., and Thieu, V.: Unravelling nutrient fate and CO2 concentrations in the reservoirs of the Seine Basin using a modelling approach, Water Research, 225, 119 135, https://doi.org/10.1016/j.watres.2022.119135, 2022a.

Yan, X., Thieu, V., Wu, S., and Garnier, J.: Reservoirs change pCO2 and water quality of downstream rivers: Evidence from three reservoirs in the Seine Basin, Water Research, 213, 118 158, https://doi.org/10.1016/j.watres.2022.118158, 2022b.