How much do bacterial growth properties and biodegradable dissolved organic matter control water quality at low flow?

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Abstract. ~~Development~~ The development of accurate water quality modeling tools is necessary for integrated water quality management of river systems. ~~The existing~~ Even though some water quality models can simulate dissolved oxygen (DO) concentration ~~quite well~~ accurately during high flow periods and phytoplankton blooms in rivers~~; however, there are discrepancies during the summer low-flow season that are assumed to be due to the uncertainties related to the organic matter contribution~~

5 ~~of the model boundary conditions. Therefore, we~~ , significant discrepancies remain during low flow periods, when the dilution capacity of the rivers is reduced. We use the C-RIVE biogeochemical model to evaluate the influence of controlling parameters on DO simulations at low flow. ~~Three Sobol~~ Based on a coarse model pre-analysis, three sensitivity analyses (SA) are carried out ~~based on a coarse model pre-analysis whose aim is to develop SA scenarios providing a reduction in the number of model parameters and computation cost as well as hiding inter-parameter interactions~~ using the Sobol method. The parameters studied

10 are related to bacterial community (e.g., bacterial growth rate), organic matter (OM; ~~repartition~~ partitioning and degradation of OM into constituent fractions), and physical factors (e.g., reoxygenation of the river due to navigation and wind)~~, whose variation ranges are selected based on a detailed literature review~~. Bacterial growth and mortality rates are found to be by far the two most influential parameters, followed by bacterial growth yield. More refined SA results indicate that the biodegradable fraction of dissolved organic matter (BDOM) and the bacterial growth yield are the most influential parameters under

15 conditions of a high net bacterial growth rate (= growth rate – mortality rate), while bacterial growth yield is independently dominant in low net growth situations. Based on the results of this study, proposals are made for in situ measurement of BDOM under an urban area water quality monitoring network that provides high-frequency data. The results also indicate the need for bacterial community monitoring in order to detect potential bacterial community shifts after transient events such as combined sewer overflows and post-infrastructure improvement in treatment plants. Furthermore, we discuss the integration of BDOM

20 in data assimilation ~~software~~ framework for better estimation of BDOM contribution from boundary conditions~~, which would result in improved water quality modeling~~.

1 Introduction

Dissolved ~~oxgyen~~ oxygen (DO) has been considered the most important indicator of water quality in surface water resources ~~(Odum, 1956; Escoffier et al., 2018)~~ (Streeter and Phelps, 1925; Odum, 1956; Escoffier et al., 2018), because it integrates the

25 biological functioning of a system as well as the impact of anthropogenic forcing. It is the main variable used to evaluate river metabolism (Odum, 1956; Staehr et al., 2010; Demars et al., 2015) by comparing the gross primary production (GPP) with ecosystem respiration (ER) and defining whether an ecosystem is autotrophic or heterotrophic based on the net ecosystem production (NEP = GPP-ER) being positive or negative, respectively (Garnier et al., 2020). Maintaining a sufficient level of DO is necessary for the overall health of rivers, not only because of the life dependency of water species (Garvey et al., 2007),

30 but also for preventing smell and taste degradation (Bailey and Ahmadi, 2014).

The situation of rivers during low flow is of particular interest since studies have demonstrated that the river water quality during such flow periods is more vulnerable to degradation due to lower dilution rates. This is particularly the case if the river receives organic matter load from ~~wastewater~~ waste water treatment plants (WWTP) and combined ~~sewage~~ sewer overflows (CSO)~~, thereby leading~~. These OM loads lead to heterotrophic conditions ~~(Seidl et al., 1998a; Even et al., 2004; Vilmin et al., 2016; Garnie~~

35 in the river, where very low DO levels and high fish mortality can be observed (Seidl et al., 1998a; Even et al., 2004; Vilmin et al., 2016; Ga . Therefore, river water quality modeling has been one of the main research interests of water quality managers and researchers ever since the use of the very first water quality model (Streeter and Phelps, 1925) to more complex ones ~~(Even et al., 1998; Flipo, 2005; Wa~~ ~~, aiming~~ (Billen et al., 1994; Garnier et al., 1995; Even et al., 1998; Vanrolleghem et al., 2001; Flipo, 2005; Wang et al., 2013) . Its aim is to identify the main determinants of DO evolution and to forecast the response of aquatic systems to human-induced

40 pressure, in particular due to ~~releases of wastewater plants~~ waste water treatment plants (WWTPs) outflows.

Large discrepancies exist between DO simulations and observations during low-flow periods ~~and most models are not able to simulate the evolution of DO accurately. In water quality modeling studies at low flow,~~ in water quality models. These mismatches were found in the QUESTOR model ~~was~~ applied on the Thames (UK) ~~, which demonstrated discrepancies between observed and simulated DO at low flow (Hutchins et al., 2020)and uncertainties related to benthic respiration were~~

45 ~~revealed to be the main reason for the mismatch. The Riverstrahler model was applied at low flow~~ (Hutchins et al., 2020), in the Riverstrahler model applied on the Mosel river (Germany) (Garnier et al., 1999), the Scheldt river (Belgium) (Thieu et al., 2009), and the Seine river (France) (Garnier et al., 2020)~~where discrepancies were noticed between the modeled and observed DO. Yang et al. (2010) used~~. Yang et al. (2010) found the same results in the WASP model ~~to estimate DO in low-flow streams~~ and noted that the uncertainty of the model lies in ~~the difficulty to characterize accurately the~~ characterization

50 of OM degradation and nitrification rates. ~~The~~ Bailey and Ahmadi (2014) found similar results in the QUAL2E-OTIS water quality model~~shows similar discrepancies, which led Bailey and Ahmadi (2014) to conduct a sensitivity analysis to identify the governing parameters on DO~~. The ProSe model ~~, which will be used in this study,~~ also has mismatches at low flow ~~(Vilmin et al., 2018; Garnier et al., 2020; Wang et al., 2022). Moreover, Cox (2003) compares the existing water quality models on lowland rivers (flowing slowly with low DO content) and emphasizes that the existing models lack one or more of the~~

55 ~~required criteria, in particular the inability to account for the expected uncertainties. On the other hand, Wang et al. (2019b, 2022)~~ (Even et al., 2004, 2007; Vilmin et al., 2018; Garnier et al., 2020; Wang et al., 2022). Among the parameters that control DO concentration in water (Cox, 2003), Wang et al. (2022) assume that the uncertainties related to ~~parameterization of (i)~~ the parameterization of OM degradation kinetics and ~~(ii) repartition of OM input from~~ OM biodegradability at system's boundaries (tributary rivers, WWTPs, and CSOs~~among dissolved and particulate pools play a~~) play a major role in the discrepancies

60 ~~during non-bloom low-flow periods, without explicitly quantifying their relative influences. However, in this paper, parameters representing OM kinetics and OM repartition are included with the ones of Wang et al. (2018) to quantify their impact on DO variation.~~ observed during low flow periods.

~~Therefore~~In order to objectively evaluate the controlling parameters of DO during such periods, a sensitivity analysis (SA) is ~~necessary to study the role of the organic matter contributed by the model boundary conditions on the evolution of DO and river~~

65 ~~metabolism during low-flow periods via a parameterization of the organic matter repartition into biodegradable fractions and its degradation by bacterial decomposition~~conducted. Several applications of SA methods can be found for water quality modeling ~~as in Nossent et al. (2011) and for DO and NO_3 modeling as in Bailey and Ahmadi (2014). Wang et al. (2018) summarized a list of~~ (Nossent et al., 2011; Bailey and Ahmadi, 2014; Cho et al., 2017; Wang et al., 2018). Moreover, SA applications in hydrological and water quality modeling ~~and applied SA in contrasting hydrological and trophic contexts, where bacterial~~

70 ~~parameters were identified as the most influential in a 80-h non-bloom low-flow period. However, the sensitivity of water quality models has not been investigated for long-term (= 45 days to be consistent with the batch test for biodegradable fractions of OM (Servais et al., 1995)) low-flow periods against new parameters accounting for boundary condition uncertainties (OM repartition and degradation) as well as against bacterial and physical parameters~~are summarized by (Reusser et al., 2011; Wang et al., 2018). In this study, the Sobol method (Sobol, 1993) is chosen in order to understand the inter-parameter interactions.

75 ~~This paper investigates not only the influence of bacterial properties on DO evolution at low flow, but also, for~~For the first time, the ~~role~~ influence of bacterial properties and that of the quantity and different fractions of OM sources are investigated on DO evolution at low flow using C-RIVE model (Vilmin et al., 2012; Wang et al., 2018). It is conducted for better understanding of the short-term (5 days) and mid-term (45 days) effects of the rapidly and slowly biodegradable OM, respectively. To further understand ~~its functioning , the intra-parameter interactions are considered to evaluate the hiding effect of one parameter on the~~

80 ~~others. Moreover, a long period simulation (45 days) is conducted that leads to a better understanding of the mid-term effect of slowly biodegradable OM~~the functioning of the Sobol' SA, the inter-parameter interactions are calculated to address how one parameter hides the influence of other parameters. On the basis of the SA results, suggestions are made for water quality monitoring in urban areas. Finally, proposals are made for a better integration of the influential parameters in data assimilation.

Based on the above discussion, ~~the following~~ we address three research questions~~are proposed to be answered in this study~~

85 :

1. What are the influential parameters controlling DO during a post-bloom summer low flow period where discrepancies are observed in different water quality models? Is a model that includes bacteria physiological parameters (growth and yield rates) only sufficient to describe DO variation?

2. To what extent is the knowledge of the quantity of OM share, especially that of the biodegradable fraction of dissolved
90   organic matter (BDOM), influential for water quality modeling?

3. What is the hierarchy (importance ranking) among the influential parameters ?

~~In this article, the sensitivity of C-RIVE (Vilmin et al., 2012; Wang et al., 2018), the biogeochemical module of ProSe-PA (Wang et al., 2019b), is investigated against the background of the aforementioned parameters based on 45- and 5-day DO~~

simulations. After incorporation of new parameters to account for repartition and degradation of OM, SA is conducted on a synthetic river system mimicking the Seine. Finally, the parameters influencing the evolution of DO and those governing the degradation and repartition of OM are selected. On the basis of the results, proposals are made for a better integration of the influential parameters in data assimilation where the model is coupled with observation data to make an optimal estimate of the temporal evolution of the parameters as well as to produce better simulation results (Cho et al., 2020). Finally, some suggestions are made for water quality monitoring in urban areas in order to fulfill the modeling and monitoring requirements.

2   Material and methods

This section describes the forward model, the new parameterization and the bibliographically reviewed variation ranges, the SA strategy, and the simulations settings of the study. Since the main goal is to use a SA method to determine the controlling parameters that influence DO evolution during a summer low-flow period, we consider Here we represent the C-RIVE model (section 2.1) as the forward model of the study and identify the parameters that need to be included in the study. Then, two new sets of parameters are added to the study to account for the uncertainties related to the parameterization of OM degradation kinetics and its repartition partitioning into different constituent fractions(section ??). This is followed by the determination of the variation ranges of the introduced parameters (section 2.1.2).

Three different SAs are carried out on the basis of a specific SA strategy Then, the strategy for conducting different SAs is detailed in section 2.3 based on which 260K - 360K simulations are run with the forward model on a case study resembling a non-bloom low flow (section 2.2). Depending on the output of these simulations that are DO time series, the Sobol SA method (section ??) is implemented to determine the influential parameters. The Sobol indices are calculated up to the second order so as to observe the inter-parameter interactions in addition to their direct and total effects.

2.1   ProSe-PA

ProSe-PA results from the coupling of the ProSe hydro-biogeochemical model with a particle filter (Wang et al., 2019b, 2022). It was developed to assimilate high-frequency observation data for a better estimation of the model parameters and an improvement in ProSe simulation results. The ProSe model has been developed to simulate the hydro-biogeochemical evolution of the Seine from upstream of Paris until Poses (close to the estuary) and has been applied and validated numerous times (Even et al., 1998, 2007; Flipo et al., 2004, 2007; Polus et al., 2011; Raimonet et al., 2015; Vilmin et al., 2015b, a; Wang et al., 2022). In this model, the river is divided into longitudinal cells of specific length, where three sets of equations corresponding to the three modules of ProSe-PA are solved (hydrodynamics, transport, and biogeochemical). First, the hydrodynamic equations are used to determine the discharge, velocity, and depth at each cell and at each time step, followed by the transport equations for advection, dispersion, and diffusion, and finally the biogeochemical RIVE model equations for the concentrations of all the dissolved and particulate matter.

2.0.1 ~~C-RIVE Biogeochemical model~~

2.1 C-RIVE Biogeochemical model

C-RIVE is a C ANSI library that implements RIVE ~~(Billen et al., 1994) concepts . It is the biogeochemical module of ProSe-PA (Wang et al., 2019b), which~~ concepts (Billen et al., 1994; Garnier et al., 1995). It simulates the cycles of carbon, ~~O_2~~oxygen, and other nutrients both in the water ~~and sediment columns of the river . The exchange of dissolved and particulate material between the two layers occurs through diffusion (Boudreau, 1997) and sedimentation-resuspension (due to shear flow and river navigation) (Martin, 2001; Even et al., 2004; Vilmin et al., 2015b), respectively. Numerous applications of RIVE exist for the ProSe and RIVERSTRAHLER softwares (See for instance Garnier et al. (1995, 2005); Even et al. (1998); Flipo et al. (2004, 2007); Thieu).~~

~~RIVE simulates the macro-nutrients cycles (C,N,P,O_2) based on the physiology of~~ column and sediments of river systems (Fig. 1). The model is community centered and explicitly describes micro-organisms~~living in water and/or sediments (heterotrophic bacteria, nitrifying bacteria, and phytoplankton), the kinetics of underlying physical-chemical processes, and carbon and nutrient inputs. Model parameters (a hundred to a few hundreds depending on the number of mico-organisms' species simulated) are mostly determined through experiments~~' communities, such as phytoplankton and heterotrophic bacteria. The physiological parameters of those communities were determined through multiple lab experiments. Both the RIVE model and its parameters were coupled in two river water quality models : RIVERSTRAHLER (Billen et al., 1994) and ProSe (Even et al., 1998). These two models are calibrated and validated on real case applications in different river basins over the world such as in the Danube river (Romania and Bulgaria) (Garnier et al., 2002), in the Day-Nhue river (Vietnam) (Luu et al., 2021), in the Grand Morin river (France) (Flipo et al., 2004, 2007), in the Lule and Kalix rivers (Sweden) (Sferratore et al., 2008), in the Mosel river (Germany) (Garnier et al., 1999), in the Red river system (Vietnam and China) (Quynh et al., 2014), in the Scheldt river (Belgium and Netherlands) (Billen et al., 2005; Thieu et al., 2009), in the Seine river (France) (Even et al., 2004, 2007; Raimonet et al., 201 , in the Somme river (France) (Thieu et al., 2009, 2010), and in the Zenne river (Belgium) (Garnier et al., 2013). ~~Wang et al. (2018) summarized the list of physical, bacterial, and phytoplanktonic parameters related to the carbon cycle with their variation ranges. We examine the equations for DO and OM evolution to understand the role of the different parameters and to select the appropriate parameters for inclusion in the SA.~~

2.1.1 ~~Dissolved oxygen evolution equations~~

~~DO in the water column (Fig. 1) depends on physical, bacterial, and phytoplanktonic processes:~~

$$\frac{d[O_2]}{dt} = \frac{d[O_2]}{dt}_{physical} + \frac{d[O_2]}{dt}_{phytoplanktonic} + \frac{d[O_2]}{dt}_{bacterial}$$

The physical process depends on reaeration due to dams, wind, navigation, the oxygen holding capacity of water, and the diffusion of oxygen between the water-sediment interface as follows:

$$\frac{d[O_2]}{dt}\Big|_{physical} = \frac{K_{rea}}{h}([O_2]_{sat}(T) - [O_2]) - \frac{D_s}{h}([O_2]_{water} - [O_2]_{sed}) + \frac{d[O_2]}{dt}\Big|_{dams}$$

where, h: water depth m $[O_2]_{sat}(T)$: the saturated oxygen concentration at temperature T mgO_2/L D_s: the coefficient of diffusion between water and sediment layer m/s K_{rea}: the reoxygenation coefficient calculated from the empirical formula of Thibodeaux et al. (1994) as follows:

$$K_{rea} = \sqrt{\frac{D_m V_{wat}}{h}} + (K_{wind} V_{wind}^{2.23}(D_m * 10^4)^{2/3} + K_{navig})$$

where, K_{wind}: reoxygenation coefficient due to wind m/s V_{wind}: wind speed m/s V_{wat}: river flow velocity m/s K_{navig}: reoxygenation coefficient due to navigation m/s (Vilmin, 2014) D_m: molecular diffusivity of DO m^2/s The phytoplanktonic process depends on phytoplankton respiration ($R_{O_2,pp}$) and photosynthesis ($P_{O_2,pp}$) as follows:

$$\frac{d[O_2]}{dt}\Big|_{phytoplanktonic} = P_{O_2,pp} - R_{O_2,pp}$$

And the bacterial process that is the main source of oxygen consumption depends on the heterotrophic bacterial kinetics and the availability of substrate matter (S, considered to be the rapidly biodegradable dissolved organic matter, DOM_1, in this model) as follows:

$$\frac{d[O_2]}{dt}\Big|_{bacterial} = -\tau_{HB}(1 - Y_{HB})\, uptake$$

$$uptake = \frac{\mu_{max,HB} e^{\frac{-(T-T_{opt,HB})^2}{\sigma_{HB}^2}} \frac{[S]}{[S]+K_S}[HB]}{Y_{HB}}$$

where, HB: the concentration of heterotrophic bacteria (hereafter, called bacteria) $mgCL^{-1}$ τ_{HB}: 1.0 $molO_2/molC$ for full oxidation of OM in the respiration process Y_{HB}: the growth yield of heterotrophic bacteria $uptake$: the uptake of substrate (here S = DOM_1) for bacteria growth $mgCL^{-1}h^{-1}$ $T_{opt,HB}$: optimum temperature for the growth of bacteria $°C$ $\mu_{max,HB}$: the maximum growth rate of bacteria at $T_{opt,HB}$ $/h$ σ_{HB}: standard deviation of bacteria temperature function $°C$ K_s: Monod half-saturation constant for bacterial growth (uptake constant) $mgCL^{-1}$

2.1.1 Organic matter degradation equations

The OM in the Seine originates from (i) point releases from WWTP and CSO, (ii) diffuse sources due to soil leaching and surface degradation through tributary rivers , and (iii) mortality of bacteria and phytoplankton (Billen et al., 2001). illustrates

the OM related process of C-RIVE in the water column where the total organic matter (TOC) is initially divided into dissolved (DOM) and particulate (POM) forms. DOM is composed of three different biodegradable fractions of (i) DOM_1 as the limiting substrate (rapidly biodegradable DOM in 5 days) , (ii) DOM_2 (slowly biodegradable DOM in 45 days), and (iii) DOM_3 (refractory DOM) . Similarly, POM is composed of (i) POM_1 (rapidly biodegradable POM) , (ii) POM_2 (slowly biodegradable POM) In the C-RIVE model, DO in the water column depends on physical, bacterial, and phytoplanktonic processes (iii) POM_3 (refractory POM) . The benthic processes are not presented in Fig. 1 Fig. 1). The physical and phytoplanktonic processes tend to provide DO while bacterial processes consume DO. The bacterial respiration, that is the main source of oxygen consumption, depends on the heterotrophic bacterial kinetics and the availability of substrate matter. These equations are accessible in previous publications (Billen et al., 1988; Servais, 1989; Billen, 1991; Wang et al., 2018). For the readability of the paper, they are developed in the supplementary material sections A1 and A2 only.

The degradation of OM happens through the uptake of small monomeric organic substrates (S, here $S = DOM_1$) by heterotrophic bacteria on the basis of the HSB model(Billen et al., 1988; Servais, 1989; Billen, 1991) and presented by Eq. and . These substrates are either the direct input (P_S) of DOM_1 from OM sources or produced from the exoenzymatic hydrolysis of the macromolecular fractions of both dissolved (DOM_2) and particulate (POM_1, POM_2) organic matter (Billen, 1991) or they originate from the phytoplankton excretion, which produces more easily utilizable OM (DOM_1) and microorganism lysis products that are macromolecular matter (Fig. 1) (Larsson and Hagstrom, 1979; Garnier and Benest, 1990; Billen, 1991).

$$\frac{d[S = DOM_1]}{dt} = hyd_{DOM_2} + hyd_{POM_{1,2}} - uptake_{HB} + P_S + P_E + P_L$$

where, P_S, P_E, P_L: represent DOM_1 from the direct input of OM sources, phytoplankton excretion, and microorganism lysis, respectively $mgCL^{-1}h^{-1}$ hyd_{DOM_2}: hydrolysis of DOM_2 into DOM_1 based on the exoenzymatic hydrolysis equation of Michaelis-Menten $mgCL^{-1}h^{-1}$ $hyd_{POM_{1,2}}$: hydrolysis of POM_1 and POM_2 into DOM_1 and DOM_2, respectively, by first-order kinetics $mgCL^{-1}h^{-1}$

$$hyd_{DOM_2} = k_{hyd,max} \frac{[DOM_2]}{[DOM_2] + K_{DOM2}} [HB]$$

$$uptake_{HB} = \mu_{max,HB} \frac{[DOM_1]}{[DOM_1] + K_s} [HB]$$

where, $uptake_{HB}$: uptake or consumption of DOM_1 by heterotrophic bacteria $mgCL^{-1}h^{-1}$ $k_{hyd,max}$: coefficient for hydrolysis of DOM_2 into DOM_1 /h K_{DOM2}: constant of semi-saturation for the hydrolysis of DOM_2 $mgCL^{-1}$

2.2 Parameterization of organic matter share (repartition) and degradation

In order to account for the uncertainties related to the parameterization of OM degradation kinetics and its repartition into different constituent fractions, the following two sets of parameters are introduced:

Figure 1. Schematic description of the OM-related processes accounted for by C-RIVE in the water column where OM is partitioned into six fractions of dissolved and particulate matter using the five partitioning parameters, namely, t, b_1, s_1, b_2, s_2; POM: particulate organic matter; DOM: dissolved organic matter; BDOM:biodegradable DOM, BPOM:biodegradable POM (subscripts 1, 2, and 3 refer to rapidly degradable, slowly degradable, and non-biodegradable fractions of OM, respectively); Blue dashed-double dotted lines: OM input from sources and partitioning between POM and DOM; Solid black lines: partitioning of DOM and POM into biodegradability pools ; Dotted black lines: Hydrolysis; Remaining solid lines: Biogeochemical processes. Resp.:Respiration; Photo,:Photosynthesis; PP: primary producers; HB: heterotrophic bacteria; WWTP: waste water treatment plant; CSO: combined sewer overflow

2.1.1 ~~OM degradation parameters~~

205 ~~The parameters related to OM degradation are K_s (represents uptake of DOM_1 by bacteria), K_{DOM2} and $k_{hyd,max}$ (represent hydrolysis of DOM_2 to DOM_1), which have been defined in section **??** and that already exist in C-RIVE. Hydrolysis parameters of POM are not considered in this study because the rate of hydrolysis of $POM_{1,2}$ is slower than that of DOM_2 by an order of magnitude of 100 to 1000 (Billen et al., 1994).~~

2.1.1 OM ~~repartition or share~~ partitioning parameters~~The OM repartition~~ : from total organic carbon to six OM fractions

The OM partitioning parameters are a novelty added in C-RIVE. Indeed, former version of C-RIVE did not include any parameter to define the ~~repartition~~ partitioning of OM into DOM and POM and then further into their corresponding fractions $DOM_{1,2,3}$ and $POM_{1,2,3}$ ~~. The following five parameters are introduced to represent the repartition of OM:~~

$$t = \frac{DOM}{TOC}$$

215

$$b_1 = \frac{BDOM}{DOM}$$

$$s_1 = \frac{DOM_1}{BDOM}$$

220 $$b_2 = \frac{BPOM}{POM}$$

$$s_2 = \frac{POM_1}{BPOM}$$

where, ~~TOC: total organic matter or carbon (=~~ (see Fig. 1 for the definitions). In the recent development of C-RIVE, the total organic carbon (TOC) is initially divided into dissolved (DOM ~~+~~) and particulate (POM) ~~$mgCL^{-1}BDOM$: biodegradable~~
225 ~~DOM (= $DOM_1 + DOM_2$)$mgCL^{-1}BPOM$: biodegradable POM (= $POM_1 + POM_2$) $mgCL^{-1}$~~forms by t ~~: ratio between dissolved and total organic matter~~ parameter (Fig. 1). Then, DOM is divided into biodegradable (BDOM) and refractory (DOM_3) fractions by b_1 ~~: ratio between biodegradable DOM and DOM~~ parameter. Then, thanks to s_1 ~~: ratio between~~ parameter, BDOM is further divided into (i) DOM_1 as the limiting substrate (rapidly biodegradable DOM ~~and biodegradable DOM~~ in 5 days) and (ii) DOM_2 (slowly biodegradable DOM in 45 days). POM is similarly divided into its constituent
230 fractions using b_2 ~~: ratio between biodegradable POM and POM~~ and s_2 ~~: ratio between rapidly biodegradable POM and biodegradable POM~~

parameters. The equations concerning these five parameters and that of OM degradation are accessible in supplementary material section A3. To further clarify, ~~$DOM_{1,2,3}$ and $POM_{1,2,3}$ were state variables in the former version of C-RIVE. They used to be forced information provided by user. They are now defined by the proposed repartition model which has~~
235 ~~the above-mentioned five parameters. The~~ the only required forced information is TOC that comes from experimental data. Therefore, the five OM ~~repartition parameters~~ partitioning parameters (t, b_1, b_2, s_1, s_2) give us the possibility to conduct a

sensitivity analysis to quantify their influence on ~~the output of C-RIVE namely~~ DO concentration. ~~Thanks to~~ Given this model, we can ~~have~~ take into account for boundary conditions, per say river inflows, varying $DOM_{1,2,3}$ and $POM_{1,2,3}$ ~~depending~~ fractions that depend on the values of the five parameters ~~in a specific river~~ t, b_1, s_1, b_2 and s_2.

240   ~~figurehOM repartition into the six fractions of dissolved and particulate matter in terms of the five repartition parameters, namely, t, b_1, s_1, b_2, s_2 figure~~

2.1.2   Parameters for SA and ~~bibliographical review of~~ their variation ranges

~~Following the parameterization, the~~ The influence of 17 parameters ~~as listed in~~ on oxygen concentrations are evaluated in ~~the SA. This includes~~ this study (Tab. 1). Various types of parameters are identified: two physical parameters that account for

245   O_2 re-aeration; seven bacterial parameters that account for bacteria growth, mortality, and respiration; three OM degradation parameters ~~that demonstrate OM kinetics~~; and five OM ~~share parameters that represent the repartition of TOC into smaller dissolved and particulate fractions~~ partitioning parameters (Fig. 1).

Before proceeding to a SA, it is necessary to specify the range of variation of ~~these parameters according to the existing literature. As indicated in , the~~ each parameter according to ~~a~~ a prior distribution based on former knowledge. Those distributions

250   are assumed to be uniform within a range, whose definition relies on a literature review. The range of variation of the ~~repartition~~ partitioning and degradation parameters (Tab. 1) is selected based on a detailed bibliographical review ~~, which is discussed and tabulated thoroughly in Hasanyar et al. (2020, 2021) , while the variation of physical and bacterial parameters is retrieved from Wang et al. (2018)~~ (Hasanyar et al., 2020, 2021; Wang et al., 2018). Table 1 also includes the range of variation of TOC, which represents the total organic matter input in the model due to the boundary conditions and varies from 1 to 10 ~~mgCL~~ mgC

255   L^{-1} under low flow ~~(also retrieved from Hasanyar et al. (2020)). However, phytoplanktonic parameters are not included in this study because they exert an influence only during algal bloom periods (Wang et al., 2018), whereas this study is conducted under non-bloom situations where heterotrophic activity is dominant~~ (Hasanyar et al., 2020).

Table 1. List of the parameters accounted for in the sensitivity analyses and their corresponding ranges of variation

Parameter	Description	Min. Val.	Max. Val.	Unit	References
TOC	Total organic carbon	1	10	[mgC L^{-1}]	
OM partitioning parameters					
t	ratio between dissolved and total organic matter (DOM/TOC)	0.4	0.9	[-]	
b_1	ratio between biodegradable DOM and DOM (BDOM/DOM)	0.1	0.5	[-]	
b_2	ratio between biodegradable POM and POM (BPOM/POM)	0.1	0.5	[-]	
s_1	ratio between rapidly biodegradable DOM and BDOM (DOM_1/BDOM)	0.4	0.95	[-]	Hasanyar et al. (2020, 2021)
s_2	ratio between high biodegradable POM and BPOM (POM_1/BPOM)	0.4	0.95	[-]	
OM degradation parameters					
K_s	constant of semi saturation for bacterial substrate uptake	0.02	0.15	[mgC L^{-1}]	
K_{DOM2}	constant of semi saturation for the hydrolysis of DOM_2	0.2	1.5	[mgC L^{-1}]	
$k_{hyd,max}$	coefficient of the hydrolysis of DOM_2 to DOM_1	0.25	0.75	[h^{-1}]	
Bacterial parameters					
$T_{opt,hb}$	optimum temperature for bacterial growth	15	30	[°C]	
σ_{hb}	standard deviation of temperature function for bacterial growth	12.75	21.25	[°C]	
$V_{sed,hb}$	settling velocity of bacteria	0	0.1	[m h^{-1}]	
$K_{O_2,hb}$	Half-saturation constant for dissolved oxygen	0.375	0.625	[mgO$_2$ L^{-1}]	Wang et al. (2018)
$\mu_{max,hb}$	maximum growth rate of bacteria	0.01	0.07 [*]	[h^{-1}]	
Y_{hb}	bacterial growth yield	0.03	0.5	[-]	
$mort_{hb}$	bacterial mortality rate	0.01	0.08	[h^{-1}]	
Physical parameters					
K_{navig}	re-aeration coefficient due to navigation	0	0.05	[m h^{-1}]	
K_{wind}	re-aeration coefficient due to wind	0.885	1.475	[m h^{-1}]	

[*] The upper limit identified by Wang et al. (2018) is decreased from 0.13/h to 0.07/h in order to avoid complete DO depletion in simulations longer than 5 days

2.2 Case study

The synthetic case developed by ~~Wang et al. (2018)~~ Wang et al. (2018) is adapted for the application of ~~SA methods~~ SAs on C-RIVE parameters during a low-flow period (Fig. 2). It is a river stretch with a width of 100 m and a length of 1000 m representing the Seine river. The low-flow period is ~~identified~~ characterized with a discharge of 80 ~~m^3/s based on the data at Bougival station during the summer season~~ m^3 s^{-1}. The simulation period is ~~set at~~ 45 ~~days~~ day-long in order to be coherent with the experimental protocol of the BDOM measurement (Servais et al., 1995)~~where it is considered as the threshold between the biodegradable and refractory fractions of TOC in a batch experiment. On the other hand~~, that considers 45 days as a limit between refractory and slowly biodegradable organic matter. Moreover, a 45-day simulation period is also necessary for studying the long-term effect of TOC degradation ~~.~~ on river metabolism.
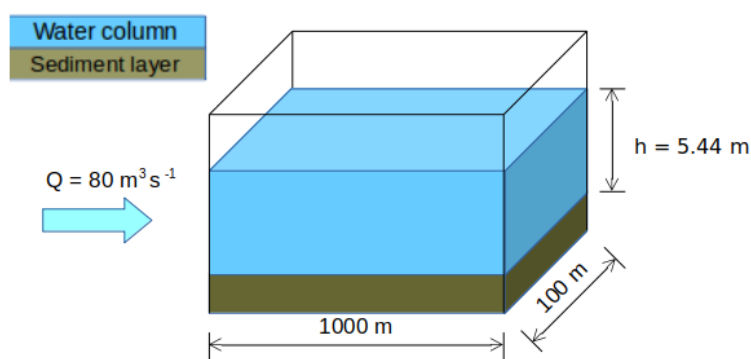
Figure 2. Synthetic scheme representing a reach of the Seine river. (modified from Wang et al. (2018)).

Considering the discharge and the wet section, the numerical experiment can be viewed as a lagrangian one, where we follow a river body along a river network of the above mentioned dimension with a speed of 0.14 m s^{-1}.

2.2.1 Initial conditions

~~A non-bloom low-flow situation (large heterotrophic bacteria biomass presence in the river) is considered to represent the low-flow period. Table 2 lists the~~ The initial concentrations for both water and sediment compartments ~~that~~ (Tab. 2) are set based on the mean concentrations of the simulations at Bougival station during the 2007-2012 period (Vilmin et al., 2016) except for water temperature (depending on summer season), DO (depending on oxygen solubility), POM and DOM fractions (depending on the TOC concentration and ~~share~~ partitioning parameters), and phytoplankton and bacterial biomass (depending on a post-bloom condition). ~~Indeed, the sum of $DOM_{1,2,3}$~~ As far as organic matter is concerned, TOC is first defined and then distributed into its DOM and ~~$POM_{1,2,3}$ is equal to the desired TOC, but they are distributed among the six fractions based~~

on the five ~~OM share~~ POM fractions depending on the values of the five OM partitioning parameters (t, b_1, s_1, b_2, s_2). The hyporheic exchanges (between groundwater and river) are ignored in this work because the contribution of groundwater to ~~downstream rivers is well known to be~~ a downstream river (Strahler order > 6), such as the Seine river at the crossing of the Paris urban area, is negligible with respect to the discharge of ~~large rivers (Strahler order > 6)~~ the river itself. For the Seine river the groundwater contribution along a 100 km is around 1 m^3 s^{-1} with respect to the Seine discharge amounting for 80 m^3 s^{-1} during severe low flow conditions (Pryet et al., 2015).

2.3 Sensitivity analysis strategy

~~The objective is to identify different scenarios under which the SA has to be conducted in order to detect the influential parameters under a summer low-flow condition. Therefore~~Before defining in detail the SA, a coarse pre-analysis consisting in forward simulations of the C-RIVE model is ~~first conduced with extreme values of a small number of representative parameters~~conducted with extreme parameter values. Then, ~~the necessary scenarios~~ various SA are developed to assess the assumptions and conclusions put in place in the pre-analysis.

2.3.1 Pre-analysis of the model ~~under parameter~~ with extreme ~~limits~~parameter values

First, we need to select certain parameters for the pre-analysis. We consider $\mu_{max,hb}$, $mort_{hb}$ and Y_{hb} as they were found to be influential in the study of Wang et al. (2018) under non-bloom situations. However, to decrease the number of parameters, $mort_{hb}$ and $\mu_{max,hb}$ are represented together as a single parameter called "net growth (NG)."

$$Net\ Growth\ (NG) = \mu_{max,hb} - mort_{hb}$$

Fixing $mort_{hb}$ = 0.02 ~~/h~~h^{-1} at its reference value and $\mu_{max,hb}$ ranging between 0.022 h^{-1} and 0.07 ~~/h, net growth was found to range~~ h^{-1}, the net growth ranges from 0.002 h^{-1} to 0.05 ~~/h~~h^{-1} while the range for Y_{hb} is taken from Table 1. ~~On the other hand, as the OM share~~As the OM partitioning parameters are not C-RIVE inputs, we consider BDOM to represent them in the model. Its range is ~~calculated in~~given by Eq. (1)-(2) ~~in order to be statistically independent based on the TOC repartition diagram (Fig. ??)~~ as follows:

$$BDOM_{min} = TOC_{ref} * t_{ref} * b_{1,min} \tag{1}$$

$$BDOM_{max} = TOC_{ref} * t_{ref} * b_{1,max} \tag{2}$$

Here, TOC_{ref} is a reference TOC value and fixed at 5 ~~mgCL~~mgC L^{-1} (considered as the baseline concentration of TOC in the Seine river (Vilmin et al., 2016)), the reference t (t_{ref}) = 0.7 is the average value of t variation range and b_1 is taken from Table 1. This way BDOM varies following b_1 only and therefore remains statistically independent from the other parameters.

Table 2. Initial concentrations of the simulations

No	Species	$C_{ini,water}$	$C_{ini,sediment}$	Unit
1	NH_4	0.12	0.33	[mgN L^{-1}]
2	NO_2	0.04	0.04	[mgN L^{-1}]
3	NO_3	7	4.54	[mgN L^{-1}]
4	TSS	16.82	95010	[mg L^{-1}]
5	PO_4	0.1	0.27	[mgP L^{-1}]
6	O_2	8.62	6.65	[mgO$_2$ L^{-1}]
7	HB	0.023	0.016	[mgC L^{-1}]
8	PP	0.010	0.003	[mgC L^{-1}]
9	DOM_1	f(TOC, partitioning parameters)	0.12	[mgC L^{-1}]
10	DOM_2	f(TOC, partitioning parameters)	1.28	[mgC L^{-1}]
11	DOM_3	f(TOC, partitioning parameters)	1.94	[mgC L^{-1}]
12	POM_1	f(TOC, partitioning parameters)	44	[mgC L^{-1}]
13	POM_2	f(TOC, partitioning parameters)	696	[mgC L^{-1}]
14	POM_3	f(TOC, partitioning parameters)	2555	[mgC L^{-1}]
15	T_{mean}	22.4 ± 3.0		°C

Eight simulations pertaining to eight different combinations of the minimum and maximum values of the net growth, its associated yield and BDOM are launched (Table 3) and accordingly for each combination, the evolution of DO, DOM_1, DOM_2, and BDOM is plotted (Fig. 3).

Therefore, eight simulations pertaining to eight different combinations of the minimum and maximum values of these three parameters are conducted () and accordingly for each combination, the evolution of DO , DOM_1, DOM_2, and BDOM is

Table 3. ~~Combinations~~ Definition of the ~~three parameter values for~~ eight single simulations achieved with extreme values of biodegradable dissolved organic matter, net growth of bacteria community and its associated yield

Sim. No.	BDOM	Net growth	Y_{hb}
1	0.35	0.05	0.03
2	0.35	0.002	0.03
3	1.75	0.05	0.03
4	1.75	0.002	0.03
5	1.75	0.05	0.5
6	1.75	0.002	0.5
7	0.35	0.05	0.5
8	0.35	0.002	0.5

310 ~~plotted (Fig. 3). In order to discriminate easily among the eight plots of single simulations using their titles, any parameter name written in capital or small letters means that its maximum or minimum value is used, respectively in that particular simulation. For example, plot 3 (BDOM NG y), that corresponds to simulation 3 in , is a simulation where the maximum values of BDOM and net growth and the minimum value of Y_{hb} are used.~~

~~As can be observed in Fig. 3,~~ From the pre-analysis, we hypothesize that:

315   1. The net growth is one of the most influential parameters on DO because all simulations on the left side with a high net growth demonstrate significant depletion of DO than those on the right side having low net growth rates.

   2. DO is sensitive to BDOM under high net growth conditions. This could be observed by comparing simulations 3 ~~(BDOM NG y), and~~ 4 ~~(BDOM ng y), 5 (BDOM NG Y)~~ under high net growth condition) with simulations 4 and 6 ~~(BDOM ng~~ 320 ~~Y) have high BDOM where all except simulation 6 demonstrate considerable DO depletion. This shows the importance of BDOM in the depletion of DO. The reason for lack of depletion in 6 could be attributed to the combination of~~ under low net growth condition) (Fig. 3).

   3. DO is not sensitive to BDOM under low net growth ~~and a high yield due to which BDOM is not consumed. However, comparing~~ rates. Comparison of simulations 6 ~~(BDOM ng Y)~~ and 7 ~~(bdom NG Y), we observe~~ demonstrate that even a 325 ~~lower~~ high BDOM coupled with ~~high~~ low net growth (simulation ~~7) has more~~ 6) has less effect on DO than a ~~high BDOM coupled with low net growth (simulation 6). This shows the interaction effect of BDOM with net growth parameters and the fact that despite BDOM being the primary requirement for depletion of DO, the net growth needs to be high in order to demonstrate the influence of BDOM and provide the means for its consumption which would result in DO depletion. Moreover, the difference between two horizontally adjacent simulations is in the net growth, which is maximum for the left-hand simulations and minimum for those on the right and as a result, all simulations on the left side with a~~ low
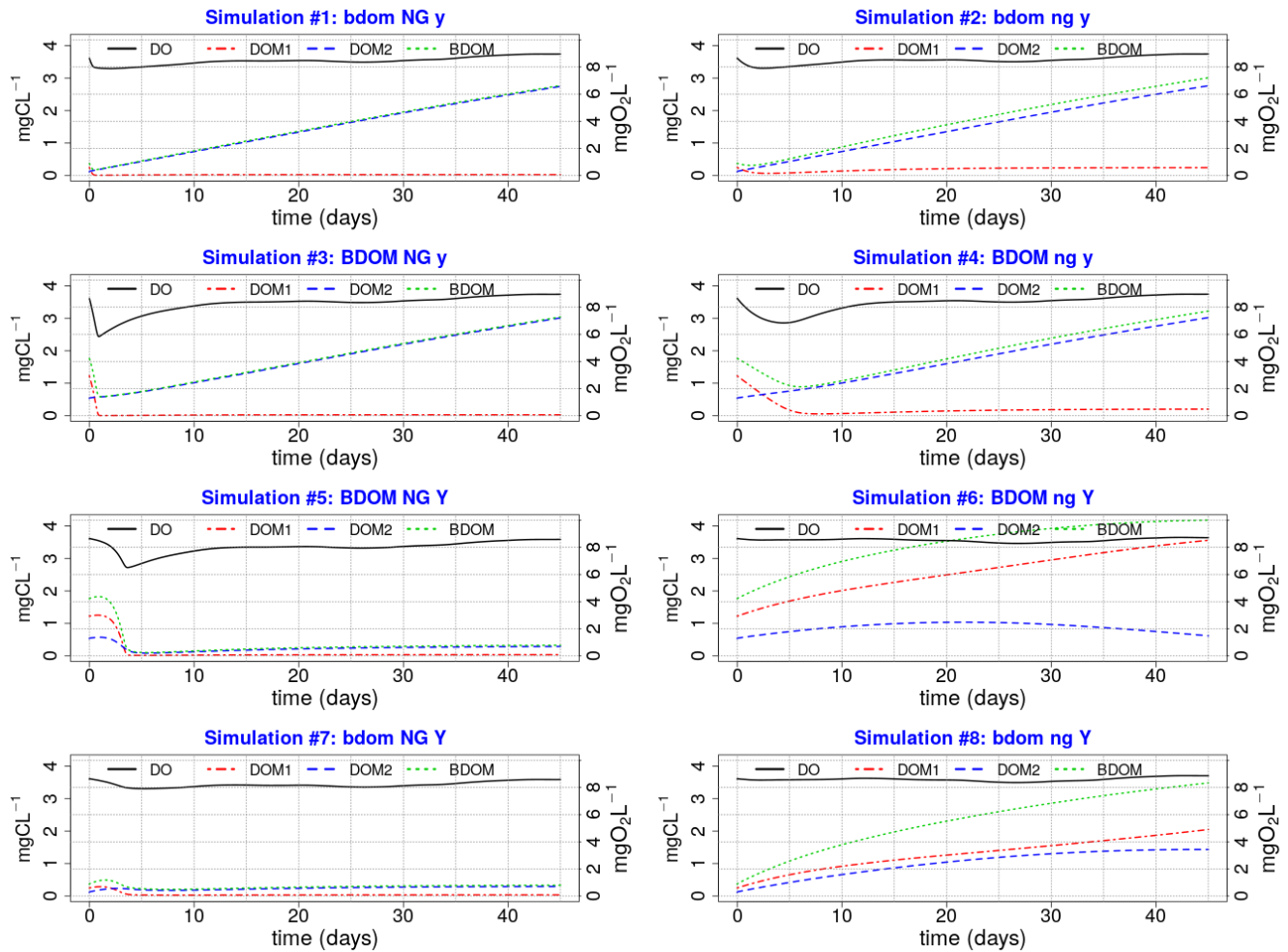
Figure 3. Eight plots of single simulations; (XX yy ZZ) Any parameter name written in capital or small letters means that its maximum or minimum value is used, respectively, in that specific single simulation. For example, plot #3 (BDOM NG y) that corresponds to simulation #3 in Table 3 is a simulation where the maximum values of BDOM and net growth and the minimum value of Y_{hb} are used

330   BDOM coupled with high net growth demonstrate more depletion or consumption of DO than those on the right side. This shows the influence of net growth parameters ($\mu_{max,hb}$, $mort_{hb}$) on the model at low flow. (simulation 7) .

2.3.2 Sensitivity analysis scenario development Understanding river metabolism controls with multiple sensitivity analyses

Having performed the pre-analysis, we understood the importance of BDOM and that of the net growth parameters such
335   that BDOM is needed primarily in order to be consumed so that DO could be depleted. And then we discern that BDOM consumption is high when net growth is at its highest value. Therefore, the following three different sensitivity analysis

~~scenarios whose parameters are detailed~~ Three sensitivity analyses (SAs) are derived to test the former three hypotheses. The detail of each SA parameterization is available in Table 4 ~~need to be conducted~~.

The first SA is conducted by assuming the general influence of net growth parameters in the pre-analysis, and in order to have a broader view of the model sensitivity with respect to all the model parameters. Based on the pre-analysis, we observed that the main effect due to BDOM is linked to high net growth rates, therefore, we can assume that the effect of parameters other than net growth parameters is demonstrated when they are coupled with a high net growth condition. In addition, since a significant interaction (the difference between the first and total sensitivity indices) is observed between net growth parameters in Wang et al. (2018), they are assumed to be hiding the influence of other parameters. ~~Therefore, in order to confirm these two assumptions and to observe the influence of other parameters, we~~ We therefore implement a second SA where net growth parameters are fixed at its highest value. This SA removes the possibility of ~~interaction~~ interactions among net growth and other model parameters. It results in a better evaluation of the model sensitivity with respect to the parameters whose influences might be hidden by the dominant and interacting parameters.

The third SA is performed to verify the second SA assumption that parameters other than net growth exert their influence only under a high net growth condition, and thus the same parameters could be deemed non-influential under a low net growth situation. ~~therefore the~~ The net growth parameter is fixed at its lowest value. ~~The~~

To summarize, the settings for the three SAs are as follows:

1. **First SA (All parameters included)**: There are 17 defined parameters (Table 1 & Table 4) in the model, the simulation period is **45 days**. It is repeated for each TOC concentration from 1 to 10 ~~times for every TOC concentration of 1-10 mgCL^{-1}~~ mgC L^{-1}, with a 1 mgC L^{-1} increase step.

2. **Second SA (Fixed high net growth)**: The ~~net growth parameters are fixed as follows:~~

$$\textit{Fixed high net growth} = \textit{High bact. growth rate } (\mu_{max,hb} = 0.07/h) - \textit{Bact. mortality rate } (mort_{hb} = 0.02/h)$$

influence of twelve parameters is evaluated (Table 4). The bacteria net growth rate is fixed to its maximum value using the highest value of the bacteria growth rate ($\mu_{max,hb}$= 0.07 h^{-1}) and a mortality rate of 0.02 h^{-1}. Furthermore, to decrease the computational cost of the model, the three OM ~~share~~ partitioning parameters (t, b_1 and b_2) from the first SA are narrowed to BDOM and BPOM whose variation ranges are calculated based on the following Eq. (3)-(6) ~~as follows~~:

$$BDOM_{min} = TOC * t_{ref} * b_{1,min} \qquad (3)$$

$$BDOM_{max} = TOC * t_{ref} * b_{1,max} \qquad (4)$$

$$BPOM_{min} = TOC * (1 - t_{ref}) * b_{2,min} \qquad (5)$$

$$BPOM_{max} = TOC * (1 - t_{ref}) * b_{2,max} \tag{6}$$

~~Here TOC varies between 1-10, therefore, similar to the first SA, this SA is repeated~~

370   Where, t_{ref} is set to 0.7. TOC varies between 1 and 10 ~~times corresponding to each TOC case. The~~ mgC L^{-1}, with a 1 mgC L^{-1} increase step. The time length is set to 5 days accordingly to the pre-analysis~~also~~, which demonstrated that BDOM or precisely the substrate (DOM_1) ~~is~~ was consumed in less than 5 days under the high net growth condition (simulations 1, 3, 5 & 7)~~, therefore imposing a **5 days** simulation period. Twelve parameters are evaluated under this scenario ()~~.

375   3. **Third SA (Fixed low net growth)**: The influence of twelve parameters is evaluated (Table 4). This SA is conducted in a similar way ~~to~~ than the second SA except that this time $\mu_{max,hb}$ is fixed at a lower value of 0.022 ~~/h~~ h^{-1} in order to simulate a very low net growth rate condition ~~as follows:~~

$$Fixed\ low\ net\ growth = Low\ bact.\ growth\ rate\ (\mu_{max,hb} = 0.022/h) - Bact.\ mortality\ rate\ (mort_{hb} = 0.02/h)$$

~~Similar to the second SA, this~~ of approximately 0.002 h^{-1}. This SA is also ~~repeated 10 times and implemented under~~
380   implemented for a **5-day** ~~simulation period . Twelve parameters are also evaluated under this scenario ()~~period of time and repeated 10 times to simulate TOC ranging from 1 to 10 mgC L^{-1}.

2.4   ~~Sensitivity analysis methodology~~

Each of the three aforementioned SAs is implemented based on an innovative SA methodology initially proposed in Wang et al. (2018) and adopted in this study, where the influence of input parameters (X) is evaluated on the C-RIVE model according to
385   the variations of a large set of DO simulations (model output, Y). The ~~followings steps are pursued in this approach:~~

~~**Input parameter identification**: Initially, a set of D input parameters () are identified with their corresponding ranges of variation (). **Parameter sampling and model input creation**: Saltelli's extension of the Sobol sequence (Saltelli, 2002) implemented in PYTHON SALIB package (Herman and Usher, 2017) is employed to create different combinations of the input parameters, which are designed to produce optimized simulations and efficient analysis results. Considering a sample~~
390   ~~size of 10,000 (N) (needed for stable results based on Nossent et al. (2011)), a matrix with a size of N(2D+2) × D is created for each SA scenario where every row represents one set of input parameters for the model.~~

~~**Model simulation**: In this step, the model inputs are launched into C-RIVE for the simulation period considered with a 1-min time step. As an output, a DO time series matrix with a size of $N(2D + 2) \times M$, where M is the number of output time steps based on a 15 min output time step^1, is created corresponding to each input matrix created in the previous step.~~

~~[1]M = 45- or 5-day simulation period × 24 hrs × 3600 min / (1-min simulation time step × 15-min output time step) = 4230 or 480 depending on the simulation period, respectively~~

Table 4. The parameters considered in each of the four sensitivity analyses

	1st SA	2nd SA	3rd SA
OM partitioning parameters	t	BDOM	BDOM
	b_1	BPOM	BPOM
	s_1		
	b_2		
	s_2		
OM degradation parameters	K_s	K_s	K_s
	K_{DOM2}	K_{DOM2}	K_{DOM2}
	$k_{hyd,max}$	$k_{hyd,max}$	$k_{hyd,max}$
Bacterial parameters	$T_{opt,hb}$	$T_{opt,hb}$	$T_{opt,hb}$
	σ_{hb}	σ_{hb}	σ_{hb}
	$V_{sed,hb}$	$V_{sed,hb}$	$V_{sed,hb}$
	$K_{O_2,hb}$	$K_{O_2,hb}$	$K_{O_2,hb}$
	Y_{hb}	Y_{hb}	Y_{hb}
	$\mu_{max,hb}$		
	$mort_{hb}$		
Physical parameters	K_{navig}	K_{navig}	K_{navig}
	K_{wind}	K_{wind}	K_{wind}
total number of parameters	17	12	12

395 ~~demonstrates the ensemble of 260,000 =N(2D+2)DO simulations of TOC = 5 mgCL^{-1} in the second SA scenario (TOC = 5 mgCL^{-1} is used in this study to represent the TOC range of 1-10 mgCL^{-1} and to show the results in case they are similar across all TOC concentrations).~~

~~figurehEnsemble of the 260,000 DO simulations for TOC = 5 mgCL^{-1} in the second SA scenario figure~~

~~**Dimensionality reduction**: The empirical orthogonal function (EOF) method is an adaptation of principal component~~
400 ~~analysis (PCA) to study a phenomenon that changes with a continuous variable, such as time, and is applied to transform the output data from one coordinate system into another by introducing new uncorrelated (orthogonal) variables (principal components) (Jolliffe and Cadima, 2016). EOF is adopted to transform the model output, which is a DO times series matrix composed of M columns into a smaller matrix where each simulation can be represented by a linear combination of EOFs. The coefficients of this linear combination are indeed orthogonal projections that maximize the variance while transforming the data~~
405 ~~from a higher-dimensional space into a lower one. The way EOF decreases dimensionality is such that it ranks the components based on the maximized variance. In other words, most of the information is kept in the first few components, thereby making it possible to reduce the number of dimensions without losing a considerable amount of information (Wold et al., 1987). In~~

this study, the first k EOF elements that constitute at least 99% of the total model variance are considered to represent each single simulation of the DO time series as shown for TOC = 5 mgCL^{-1} in the second SA (Fig. **??**a), where four (k) significant EOFs are found such that the first EOF (EOF_1) represents almost 55% of the total variance. b illustrates the evolution of the eigenvalues of the four (k) EOFs with time, which are consequently used to represent each simulation in terms of the k new coordinates . Thereby, an $N(2D+2) \times M$ matrix is converted into a new matrix of $N(2D+2) \times k$, which will be subjected to the Sobol SA method. The R $prcomp$ function is used to conduct the EOF analysis. figureha) Cumulative sum of EOF variances and b) time evolution of four (k) significant EOFs for TOC = 5 mgCL^{-1} in second SA figure

Sobol sensitivity analysis: The Sobol SA method (Sobol, 1993; Saltelli et al., 2010) is applied in this study to evaluate the sensitivity of the model output against the input parameters. It is a variance-based method that classifies the parameters based on their contribution to and/or influence on the total variance of the model output (Brookes et al., 2015). It is a convenient method to be used for SA of complex models that involve interactions between parameters. In this method, the model output (Y) is expressed as a function of D parameters:

$$Y = f(X) = f(X_1, ..., X_D),$$

such that the model output could be decomposed by elementary functions:

$$f(X) = f_0 + \sum_{i=1}^{D} f_i(X_i) + \sum_{i=1}^{D-1} \sum_{j=i+1}^{D} f_{ij}(X_i, X_j) + ... + f_{1,...,D}(X_1, ..., X_D)$$

Here f_0 is the expectation of the model output and each one of the elementary functions have a zero mean and can be computed by integration:

$$f_0 = \int_{[0,1]^D} f(X) d_X$$

$$f_i(X_i) = -f_0 + \int_{[0,1]^{D-1}} f(X) d_{X \sim i}$$

$$f_{ij}(X_i, X_j) = -f_0 - f_i(X_i) - f_j(X_j) + \int_{[0,1]^{D-2}} f(X) d_{X \sim (ij)}$$

On the other hand, the total unconditional model variance could be defined as:

$$V(Y) = \int_{[0,1]^D} f^2(X) d_X - f_0^2$$

Thereby, the total unconditional variance of the model can be expressed as:

$$V(Y) = \sum_{i=1}^{D} V_i(X_i) + \sum_{i=1}^{D-1} \sum_{j=i+1}^{D} V_{ij}(X_i, X_j) + ... + V_{1,...,D}(X_1, ..., X_D)$$

where, V_i is the partial variance of the i_{th} parameter and V_{ij} is the interaction effect of the i_{th} and j_{th} parameters. The partial variance is calculated as:

$$V_{i_1,...,i_s} = \int_0^1 ... \int_0^1 f_{i_1,...,i_s}^2(X_{i_1},...,X_{i_s})dX_{i_1},....dX_{i_s}$$

where $s = 1,...,D$ and f_i is an elementary function. Therefore, the first-order Sobol SA indices can be computed as follows:

$$S_i = \frac{V_i}{V}$$

S_i is also called as the "main effect" because it represents the contribution of a single input parameter i on the total variance. The total sensitivity index (S_{Ti}), also called "global effect," is another index that represents the sum of the first-order index (S_i) and the effect of the interaction between the parameters and is calculated as follows:

$$S_{Ti} = S_i + \sum_{j \neq i} S_{ij} + ...$$

here, $S_{ij} = \frac{V_{ij}}{V}$ is called the "second-order index" and measures the interaction between a pair of parameters X_i and X_j. Therefore, the sum of second-order interactions of any parameter X_A with other parameters (X_B, ..., X_D) is considered to represent the second-order index of each parameter (S_2) as follows:

$$S_{2,A} = \sum_j S_{Aj}$$

Since the output of previous step is a matrix of k vectors corresponding to the k EOFs, the Sobol indices of parameters are initially calculated k times for each EOF and then added while being weighted by the variance of the corresponding EOF. necessary steps pursued for SA are summarized in supplementary material section B.

The total computation time from step 1 to 5 Each SA is 12 h for each TOC case of the first SA, after using a parallel code in PYTHON and dividing the simulations in several groups to decrease the computational cost using 20 processors (performed with a Python script that computes on an Intel(R) Xeon(R) E5-2640 and frequency of 2.40 (20 cores @ 2.4 GHz). The computation time is 3 h for each TOC case of computational time is 12h per TOC value for the first SA, while it is reduced to only 3h per TOC value for the second and third SA, which clearly demonstrates the gain in time compared with the first SA. ones.

3   Results

This section presents the results of the three Sobol SAs during a summer low-flow period. The influential parameters of each analysis are discussed in the following paragraphs.

3.1 First SA: All parameters
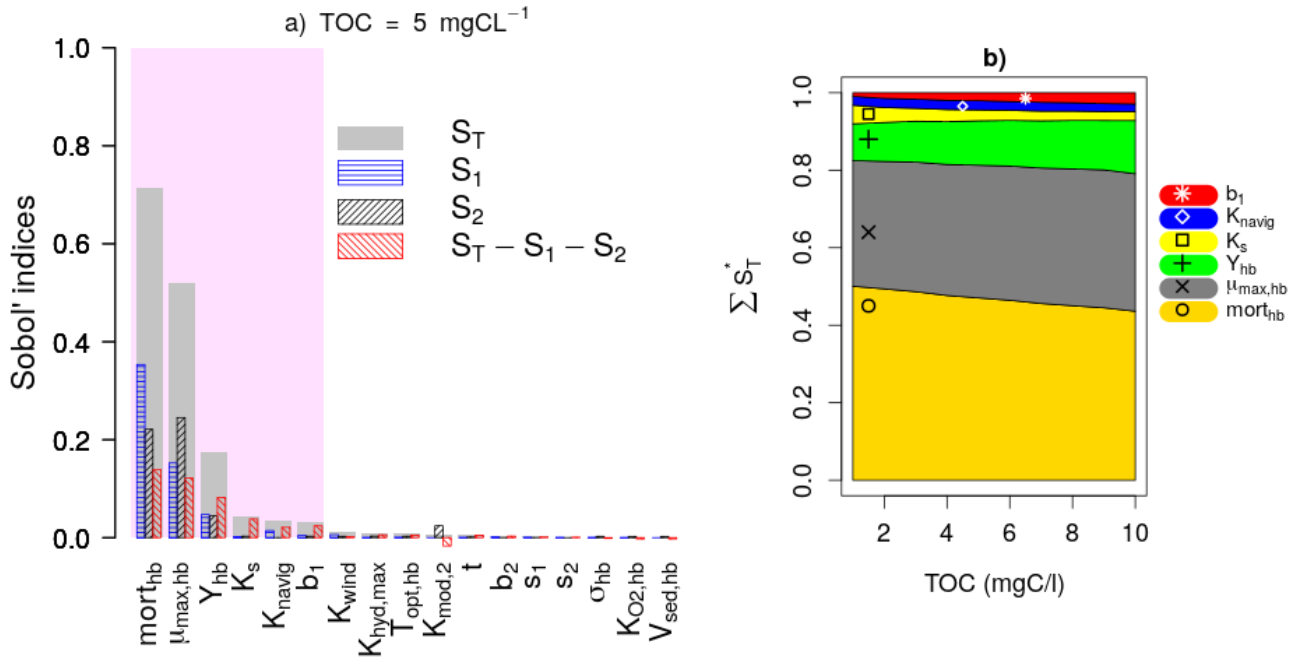
Figure 4. Sobol SA results of **first SA: All parameters** (a) Sobol SA results for TOC = 5 mgCL^{-1}; (b) Evolution of the normalized total sensitivity indices of the influential parameters with TOC

460 Figure 4a presents the results of the Sobol SA method ~~on~~ for TOC = 5 mgCL^{-1}. It is expressed by a bar plot of the total sensitivity (S_T), first-order sensitivity (S_1), and second-order sensitivity (S_2) indices of the parameters. The higher-order sensitivity indices are also calculated in terms of the difference between the total and the first- and second-order indices (S_T-S_1-S_2). The parameters are ranked based on their S_T and the most influential parameters are shown by the shaded area, which includes parameters constituting 95% of the total variance of the model output. ~~However, this~~ As the first SA is conducted ~~on~~

465 ~~different TOC values of 1-10~~ for TOC values ranging from 1 to 10 mgCL^{-1}, ~~and therefore in order to summarize all of the results together~~ which corresponds to ten runs. For each run, the evolution of the normalized total sensitivity indices (S_T^*) of the six most influential parameters ~~with TOC is presented in~~ is plotted (Fig. 4b).

~~figurehSobol SA results of~~ **~~first SA: All parameters~~** ~~(a) Sobol SA results for TOC = 5 mgCL^{-1}; (b) Evolution of the normalized total sensitivity indices of the influential parameters with TOC figure~~

470 ~~figurehResults of (a) Second SA: Fixed high net growth; (b) Third SA: Fixed low net growth figure~~

~~According to Fig. 4b, the three bacterial parameters of~~ DO is controlled by the bacterial mortality rate ($mort_{hb}$), maximum bacterial growth rate ($\mu_{max,hb}$), and bacterial yield (Y_{hb})~~exert the most influence on DO evolution, and~~, whatever the TOC concentration ~~, they represent the majority of the model sensitivity~~ (Fig. 4b). By increasing TOC, we observe a gradual decrease

in the influence of $mort_{hb}$, but an increase in the influence of Y_{hb}. This result obtained over the 45-day simulation period (Fig.
475 4) confirms the assumption made in the pre-analysis step (sec 2.3.1) regarding the overall dominance of bacterial parameters in long-term low-flow periods.

Apart from the constant of navigation (K_{navig}), which is a physical parameter, the other two influential parameters (K_s, b_1) are OM-related parameters that were introduced in this study. K_s seems to be more important in lower TOC concentrations compared to b_1 whose influence increases in higher TOC concentrations.

480 ~~On the other hand, these results~~ These results also confirm the assumptions made in the pre-analysis step that the dominant parameters tend to hide the influence of other parameters. Observing the second-order (S_2) and higher-order sensitivity (S_T-S_1-S_2) indices of $mort_{hb}$, $\mu_{max,hb}$ and Y_{hb} in Fig. 4a, very strong interactions can be highlighted between these parameters, i.e., a significant portion of their total sensitivity indices is due to their internal interactions. ~~On the other hand,~~ b_1 and K_s ~~also exert an influence due to their~~ exert their influence only through higher-order ~~interaction~~ interactions with these three
485 parameters. ~~Thus, in order to see what happens behind net growth parameters, and in order to observe the dominant parameters under two extreme conditions of high and low net growth rates, the second and third SAs are conducted by fixing the $mort_{hb}$, $\mu_{max,hb}$ parameters under the notion of net growth rate.~~

~~Moreover~~In the first SA, the three OM parameters (t, s_1 and s_2) are found to be non-influential, which means they can be excluded from SA by fixation in the second and third SA while calculating the variation ranges of BDOM and BPOM (Eq.
490 (1)-(4)). Finally, the inclusion of b_1 among influential parameters out of the five OM parameters ~~confirms~~ validates the selection of the BDOM concentration instead of other OM components in the pre-analysis step.

3.2   Second SA ~~: Fixed~~ under high bacteria net growth rate

~~Based on Fig. 5a which depicts the results of the second SA, it is shown that~~ The bacteria yield, Y_{hb}, and BDOM are the most influential parameters under high net growth rate conditions (Fig. 5a). This is due to the fact that the bacterial community
495 manages to consume most of BDOM under a high net growth condition and then at some point, BDOM becomes a limiting factor for their growth. This result confirms the assumption made in the pre-analysis that the influence of parameters other than net growth parameters will be displayed if they are studied under a high net growth condition. The other important parameters are K_{navig} and K_s whose influence is reduced by ~~increased~~ increase in TOC. Moreover, very small interactions are observed between the parameters because almost all of their global influence stem from their main effects ($S_T \approx S_1$ for each parameter),
500 which once again confirms the previous consideration that interactions are related to the effect of a varying net growth rate.

3.3   Third SA ~~: Fixed~~ under low bacteria net growth rate

The results of the third SA (Fig. 5b) reveal that Y_{hb} ~~is a predominantly~~ only is the influential parameter under a low net growth rate condition across ~~all~~ whatever the TOC concentrations. This is due to the fact that, with such a low net growth rate, the bacterial community hardly grows at all and ~~therefore BDOM is~~ BDOM is subsequently not a limiting factor for
505 ~~bacterial growth as there is not enough bacterial activity under a low net growthrate condition~~such a small bacterial growth.
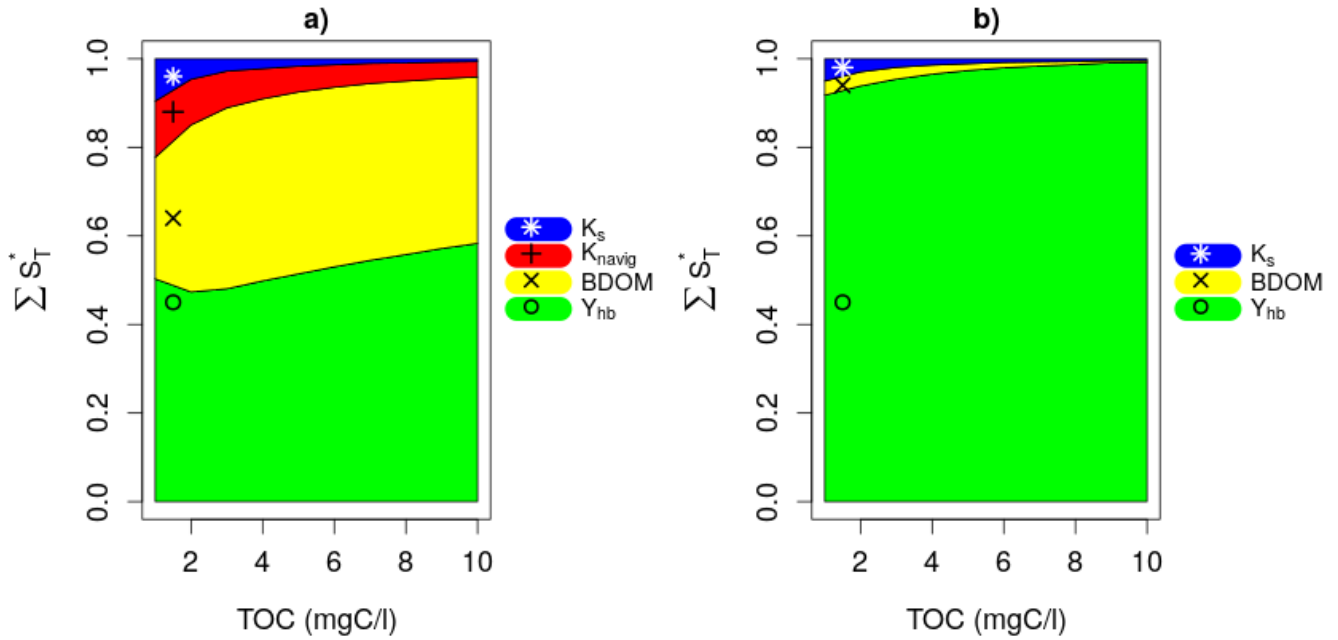
Figure 5. Results of (a) Second SA: Fixed high net growth; (b) Third SA: Fixed low net growth

This result ~~verifies~~ confirms the assumption made in the second SA by displaying all previous influential parameters except Y_{hb} as non-influential.

~~In observing the role of BDOM, we conclude that by increasing the net growth rate,~~ Finally, the second and third SA show that the influence of BDOM ~~increases. Here, we need to highlight that the actual upper limit of net growth is 0.11/h (Wang et al., 2018) compared to the current value of 0.05/h because the upper limit of $\mu_{max,hb}$ is reduced in in order to prevent complete DO depletion of simulations that occur due to the combination of extreme values in Sobol sampling. Therefore, it can be envisaged that BDOM may have a greater influence under the actual range of~~ on DO increases with an increasing bacteria net growth rate.

510

4 Discussion

515 In this section, we ~~highlight answers to the proposed research questions and~~ propose first synthesize of our results, before analyzing the limitations in terms of physical processes accounted for. We then discuss what consequences do our results have on water quality monitoring in urban areas and on data assimilation.

4.1 Hierarchy of the most influential parameters on DO during low flow period

This study confirms that over a 45-day post-bloom summer low-flow period and whatever the TOC concentration, the bacterial
520 net growth rate ~~represented by $mort_{hb}$, $\mu_{max,hb}$~~ and Y_{hb} control the DO evolution. This is in ~~accordance~~ agreement with the findings of the study by Wang et al. (2018), which was conducted over a 4-day simulation period. However, the mentioned bacteria physiological parameters are not sufficient to describe DO variation because the OM ~~repartition~~ partitioning parameter, b_1, and the OM degradation parameter, K_s, are also influential at low flow under a high bacteria net growth rate.

Conducting the Sobol' SA for 5-days under a high bacterial net growth rate condition demonstrated the significant influence
525 of BDOM and Y_{hb} at low flow. This is in connection with the findings of Hullar et al. (2006); Crump et al. (2003) that emphasized the importance of BDOM on bacteria population. This result is also in accordance with Bailey and Ahmadi (2014) who consider the model boundary condition as influential on DO but they do not specify which portion of the OM neither do they conduct their study at low flow. Nevertheless, this work is the first quantitative recognition of the role of BDOM on DO evolution that illustrates BDOM as the most influential fraction of the total organic matter entering a river system from its
530 boundary conditions.

4.2 Limitations of the sensitivity analysis

This study is conducted under carbon source conditions where TOC ~~is varied between 1-10 mgC /L~~ varies between 1 and 10 mgC L^{-1}. It is also assumed that a carbon sink condition never happens. Indeed, carbon depletion would preclude the possibility to quantify the influence of the carbon on the DO concentration. Therefore the upper limit of $\mu_{max,hb}$ is reduced from 0.13
535 ~~/h~~h^{-1} to 0.07 ~~/h~~h^{-1} so as to avoid depletion of both carbon and oxygen during the simulation period.

~~On the other hand~~Moreover, since C-RIVE currently lacks the radiation effects of bacteria population, this process is not considered in this work. Nevertheless, it is recommended to be considered in future researches as radiation is found to damage the bacteria DNA impacting their growth and oxygen intake rates (Matallana-Surget and Wattiez, 2013). This phenomenon could be included in the model in a simplistic approach either by increasing bacterial mortality or decreasing its growth rate
540 by a given factor. However, it is necessary to find experimental data in order to ~~find this factor because~~ quantify the effects of radiation that also depend on the type of bacterial community (Fernandes et al., 2021).

4.3 Consequences of the results on water quality monitoring in urban areas

Rivers are highly sensitive to urban outflows at low flow (Seidl et al., 1998a; Huang et al., 2017) due to their low diluation capacity at this period of the year. Moreover, the construction or renewal of sanitary facilities, such as WWTP and CSO during

545 transient events, induce changes in water quality due to changes in DOM, and BDOM concentrations (Servais and Garnier, 1993; Seidl et al., 1998b). As a result, this induces potential shifts in bacterial communities, which have been found to be related to ~~DOC~~ DOM source and its biodegradability (Hullar et al., 2006; Crump et al., 2003) such that an increase in BDOM is considered to increase the diversity of bacterial populations (Landa et al., 2013). Even et al. (2004) therefore ~~recommend~~ recommended a regular reassessment of the influential bacterial parameters. The sampling frequency in the monitoring sta-

550 tions should be set-up not only considering the temporal variability of the variable of interest, but also integrating possible successions of species.

~~On the one hand, our~~ Our study provides the list of important parameters for water quality modeling at low flow. ~~On the other hand, these parameters are dynamic (varying with time). Thus in urban areas submitted to large WWTP outflows, continuous monitoring networks would be able to provide up-to-date values of parameters that influence the water quality.~~

555 ~~Considering the results of this study which introduce initially several~~ For the bacterial parameters (mortality rate, maximum growth rate and growth yield)~~as having the most influence on DO evolution~~, we propose the implementation of regular bacterial community sampling campaigns in the framework of the water quality monitoring program. Samples should thus be taken in river waters upstream from the major urban areas, and in the effluents of major WWTPs and CSOs.

~~Then~~Finally, considering the importance of BDOM at low flow periods, we propose the addition of BDOM measure-

560 ment in the existing and new monitoring stations. ~~These~~ Innovative methods such as specific ultraviolet absorbance at 254 nm ($SUVA_{254}$) and fluorescence spectroscopy (Parlanti et al., 2000, 2002; Goffin et al., 2017) could be proposed for high frequency measurement of OM and BDOM specifically. The monitoring stations shall be dense ~~and capable of characterizing~~ enough in space so that they could characterize the upstream tributary rivers and the outflow of anthropogenic sources such as WWTP and CSO~~because an appropriate spatial resolution (Polus et al., 2010)~~. Such a spatial density and consideration

565 of point and non-point pollution sources ~~(Dixon et al., 1999; Do et al., 2012)~~ are necessary to cover all BDOM sources ~~. On the other hand, innovative methods such as specific ultraviolet absorbance at 254 nm ($SUVA_{254}$) and fluorescence spectroscopy (Parlanti et al., 2000, 2002; Goffin et al., 2017) could be proposed for high frequency measurement of OM and BDOM specifically~~(Dixon et al., 1999; Polus et al., 2010; Do et al., 2012).

4.4 Consequences of the results on data assimilation (DA) in water quality modeling

570 ~~Coupling water quality models with data assimilation techniques allows to avoid relying on a continuous water quality monitoring.~~

Data assimilation is a method that combines observation data and physically based modeling in a statistical framework. It consists in sequentially updating the model parameters so that the output of the model will match the observation at each time step (Carrassi et al., 2018). These techniques not only estimate the evolution of influential parameters thanks to observation

575 data such as that of DO, but also provide enhanced simulation results of state variables.

The first assimilation tool that uses the particle filter technique (a statistical technique where numerous simulations are launched instead of one single simulation and are weighted based ~~on~~ upon how well they reproduce the observed data) to couple with a water quality model is the ProSe-PA software (Wang et al., 2019b; Wang, 2019a; Wang et al., 2022). While

studying a dry year using this software, mismatches were found between simulated and observed DO ~~in~~ during low-flow periods (Wang et al., 2022). These mismatches were assumed to be due to insufficient biodegradable organic matter loading in the model caused by underestimated BDOM inputs to the Seine river. Therefore, based on our SA results, we can confirm that hypothesis and propose the incorporation of BDOM (the most influential OM-related parameter through the b_1 parameter) as a new component of ProSe-PA. It will facilitate not only the estimation of BDOM, but also ~~consequently~~ improves the simulation results subsequently.

Another consequence of our results is that ~~in accordance with the results of the second and third SA,~~ it would be appropriate to fix one or both of the $mort_{hb}$ and $\mu_{max,hb}$ parameters during data assimilation in order to facilitate parameter identification. In addition, the model of OM ~~repartition~~ partitioning (Fig. ~~??~~1) shall be explicitly included in the data assimilation software~~and BDOM from each~~. The description of BDOM in each major organic matter source (tributary river, WWTP, and CSO) should also be independently represented in the DA scheme ~~due to their distinct~~ because each source brings its own specific contribution of organic matter and heterotrophic bacteria in urban rivers (Garnier et al., 1992; Servais and Garnier, 1993; Seidl et al., 1998b).

~~Finally, we can conclude that once a water quality model capable of data assimilation is validated and its uncertainties are suitably reduced, it can provide acceptable estimates of water quality variables in periods when monitoring is not possible or at locations where accessibility is an issue (Reis et al., 2015; Jiang et al., 2020). In other words, while the approach of PIREN-Seine (https://www.piren-seine.fr/en) research program followed laboratory incubation experiments (Servais et al., 1995), it appears today that the coupling between measurement networks and modeling makes it possible to approach the functioning of the systems in a more dynamic way (Wang et al., 2022).~~

5 Conclusions

The objective of this work was to investigate the role of organic matter loadings to river systems and the physiology of bacteria in river metabolism during a summer non-bloom low-flow period. New parameters were introduced to account for ~~repartition~~ partitioning and degradation of OM. Then, the sensitivity of the C-RIVE model was analyzed against the newly introduced and the already existing model parameters. The following conclusions can be drawn from this study:

– The Sobol sensitivity analysis method proved very efficient in the identification of influential parameters on DO evolution in the C-RIVE model. Then, by fixing the interaction-inducing parameters, the influence of other parameters was assessed. This methodology may also be of interest for future sensitivity analysis where parameter interactions may hide the effect of other parameters;

– The river metabolism is dominated by bacterial activity at low flow during summer non-bloom periods. As a consequence, the net growth rate of bacteria~~composed of~~, that combines their maximum growth rate ($\mu_{max,hb}$) and mortality rate ($mort_{hb}$), is the most important parameter under different TOC concentrations; therefore, it is essential to have a better estimation of the variation ranges of the growth and mortality rates of bacterial communities;

- Model response is very sensitive to the biodegradable share of DOM (BDOM) contributed by the boundary conditions. The effect of this parameter prevails at higher bacteria net growth rates occurring during summer low-flow periods when the organic matter ~~attributable to human pressure~~ brought by urban outflows is abundant in the river;

- ~~The river metabolism is dominated by bacterial activity at low flow during summer non-bloom periods;~~

615
- Water quality monitoring networks shall continuously measure the influential parameters of this study in order to provide the water quality models with update values;

- More frequent sampling of autochtonous bacteria communities upstream and downstream of major urban areas and in majors WWTP and CSO effluents will be of considerable interest to validate time varying parameter values estimated by data assimilation frameworks;

620
- The results of this study provide a list of influential and non-influential parameters. The latter can be fixed at their average or preferred value as per the literature, and the former can be introduced to the data assimilation tools in order to estimate their temporal evolution ~~thanks to the~~ with assimilation of high-frequency ~~observed DO data;~~ DO data.

Code availability. Name of software : C-RIVE

Contact address: nicolas.flipo@minesparis.psl.eu

625
Year first available: 2019

Program language: ANSI C

Operating system: Linux

Software access: Deposit in progress

Availability and cost: Open source

630
Licence: Eclipse Public Licence v2.0

Author contributions. The author contributions are as follows:

The calculations were designed by all authors;

The calculations were executed by Masihullah Hasanyar;

The results were analyzed by all authors;

635
The first draft of the article was drafted by Masihullah Hasanyar, and then it was revised and corrected by all authors;

And finally Nicolas Flipo did the search for funding;

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References

Bailey, R. T. and Ahmadi, M.: Spatial and Temporal Variability of In-Stream Water Quality Parameter Influence on Dissolved Oxygen and Nitrate within a Regional Stream Network, Ecological Modelling, 277, 87–96, https://doi.org/10.1016/j.ecolmodel.2014.01.015, 2014.

645 Billen, G.: Protein Degradation in Aquatic Environments, in: Microbial Enzymes in Aquatic Environments, edited by Brock, T. D. and Chróst, R. J., pp. 123–143, Springer New York, New York, NY, https://doi.org/10.1007/978-1-4612-3090-8_7, 1991.

Billen, G., Lancelot, C., Becker, E., and Servais, P.: Modelling Microbial Processes (Phyto- and Bacterioplankton) in the Schelde Estuary, Hydrobiological Bulletin, 22, 43–55, https://doi.org/10.1007/BF02256781, 1988.

Billen, G., Garnier, J., and Hanset', P.: Modelling Phytoplankton Development in Whole Drainage Networks: The RIVERSTRAHLER Model

650 Applied to the Seine River System, Hydrobiologia, 289, 119–137, https://doi.org/10.1007/BF00007414, 1994.

Billen, G., Garnier, J., Ficht, A., and Cun, C.: Modeling the Response of Water Quality in the Seine River Estuary to Human Activity in Its Watershed over the Last 50 Years, Estuaries, 24, 977, https://doi.org/10.2307/1353011, 2001.

Billen, G., Garnier, J., and Rousseau, V.: Nutrient Fluxes and Water Quality in the Drainage Network of the Scheldt Basin over the Last 50 Years, Hydrobiologia, 540, 47–67, https://doi.org/10.1007/s10750-004-7103-1, 2005.

655 Boudreau, B. P.: Diagenetic Models and Their Implementation, vol. 134, Springer, 1997.

Brookes, V. J., Jordan, D., Davis, S., Ward, M. P., and Heller, J.: Saltelli Global Sensitivity Analysis and Simulation Modelling to Identify Intervention Strategies to Reduce the Prevalence of Escherichia Coli O157 Contaminated Beef Carcasses, PLoS One, 10, 1–22, https://doi.org/10.1371/journal.pone.0146016, 2015.

Carrassi, A., Bocquet, M., Bertino, L., and Evensen, G.: Data assimilation in the geosciences: An overview of methods, issues, and perspec-

660 tives, Wiley Interdisciplinary Reviews: Climate Change, 9, e535, https://doi.org/10.1002/wcc.535, 2018.

Cho, J., Her, Y., and Bosch, D.: Sensitivity of Simulated Conservation Practice Effectiveness to Representation of Field and In-Stream Processes in the Little River Watershed, Environmental Modeling & Assessment, 22, 159–173, https://doi.org/10.1007/s10666-016-9530-6, 2017.

Cho, K. H., Pachepsky, Y., Ligaray, M., Kwon, Y., and Kim, K. H.: Data Assimilation in Surface Water Quality Modeling: A Review, Water

665 Research, 186, 116 307, https://doi.org/10.1016/j.watres.2020.116307, 2020.

Cox, B.: A Review of Currently Available In-Stream Water-Quality Models and Their Applicability for Simulating Dissolved Oxygen in Lowland Rivers, The Science of The Total Environment, 314-316, 335–377, https://doi.org/10.1016/S0048-9697(03)00063-9, 2003.

Crump, B. C., Kling, G. W., Bahr, M., and Hobbie, J. E.: Bacterioplankton Community Shifts in an Arctic Lake Correlate with Seasonal Changes in Organic Matter Source, Applied and Environmental Microbiology, 69, 2253–2268, https://doi.org/10.1128/AEM.69.4.2253-

670 2268.2003, 2003.

Demars, B., Thompson, J., and Manson, J.: Stream Metabolism and the Open Diel Oxygen Method: Principles, Practice, and Perspectives, Limnology and Oceanography: Methods, 13, 356–374, https://doi.org/10.1002/lom3.10030, 2015.

Dixon, W., Smyth, G. K., and Chiswell, B.: Optimized Selection of River Sampling Sites, Water Research, 33, 971–978, https://doi.org/10.1016/S0043-1354(98)00289-9, 1999.

675 Do, H. T., Lo, S.-L., Chiueh, P.-T., and Phan Thi, L. A.: Design of Sampling Locations for Mountainous River Monitoring, Environmental Modelling & Software, 27-28, 62–70, https://doi.org/10.1016/j.envsoft.2011.09.007, 2012.

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, Environ Sci Pollut Res, 25, 23 451–23 467, https://doi.org/10.1007/s11356-016-7096-0, 2018.

680   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, Ecological Modelling, 173, 177–196, https://doi.org/10.1016/j.ecolmodel.2003.08.019, 2004.

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

Fernandes, A., Oliveira, A., Soares, R., and Barata, P.: The Effects of Ionizing Radiation on Gut Microbiota, a Systematic Review, Nutrients, 13, 3025, https://doi.org/10.3390/nu13093025, 2021.

Flipo, N.: Modélisation intégrée des transferts d'azote dans les aquifères et les rivières : Application au bassin du Grand Morin, Ph.D. thesis,
690   CIG, 2005.

Flipo, N., Even, S., Poulin, M., Tusseau-Vuillemin, M.-H., Ameziane, T., and Dauta, A.: Biogeochemical Modelling at the River Scale: Plankton and Periphyton Dynamics: Grand Morin Case Study, France, Ecological Modelling, 176, 333–347, https://doi.org/10.1016/j.ecolmodel.2004.01.012, 2004.

Flipo, N., Rabouille, C., Poulin, M., Even, S., Tusseau-Vuillemin, M.-H., and Lalande, M.: Primary Production in Headwa-
695   ter Streams of the Seine Basin: The Grand Morin River Case Study, Science of The Total Environment, 375, 98–109, https://doi.org/10.1016/j.scitotenv.2006.12.015, 2007.

Garnier, J. and Benest, D.: Seasonal Coupling between Phyto- and Bacterioplankton in a Sand Pit Lake (Creteil Lake, France), Hydrobiologia, 207, 71–77, 1990.

Garnier, J., Billen, G., Servais, P., and Servais, P.: Physiological Characteristics and Ecological Role of Small and Large Sized Bacteria in a
700   Polluted River (Seine River, France), Arch. Hydrobiol. Beih., 37, 83–94, 1992.

Garnier, J., Billen, G., and Coste, M.: Seasonal Succession of Diatoms and Chlorophyceae in the Drainage Network of the Seine River: Observation and Modeling, Limnology and Oceanography, 40, 750–765, https://doi.org/10.4319/lo.1995.40.4.0750, 1995.

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

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., Némery, J., Billen, G., and Théry, S.: Nutrient Dynamics and Control of Eutrophication in the Marne River System: Modelling the Role of Exchangeable Phosphorus, Journal of Hydrology, 304, 397–412, https://doi.org/10.1016/j.jhydrol.2004.07.040, 2005.

710   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 of Marine Systems, 128, 62–76, https://doi.org/10.1016/j.jmarsys.2012.04.001, 2013.

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.: Ecological Functioning of the Seine River: From Long-Term Modelling Approaches to High-Frequency Data Analysis, in: The Handbook of Environmental Chemistry, pp. 1–28, Springer Berlin Heidelberg, 2020.

Garvey, J. E., Whiles, M. R., and Streicher, D.: A Hierarchical Model for Oxygen Dynamics in Streams, Can. J. Fish. Aquat. Sci., 64, 1816–1827, https://doi.org/10.1139/f07-144, 2007.

Goffin, A., Guérin, S., Rocher, V., and Varrault, G.: Caractérisation de l'évolution de la matière organique dissoute de l'amont à l'aval de l'agglomération parisienne pendant une année hydrologique par spectrométrie de fluorescence 3D, Tech. rep., PIREN-Seine phase VII, 2017.

Hasanyar, M., Flipo, N., Romary, T., Wang, S., and Yari, A.: Rôle de la matière organique dans le métabolisme des rivières à bas débit, PIREN-Seine phase 8 - Technical report, PIREN-Seine, 2020.

Hasanyar, M., Flipo, N., Romary, T., and Wang, S.: A review of water quality variables and parameters characterizing organic matter in world rivers., manuscript in preparation, available upon request from masihullah.hasanyar@mines-paristech.fr, 2021.

Herman, J. and Usher, W.: SALib: An Open-Source Python Library for Sensitivity Analysis, Journal of Open Source Software, 2, 97, https://doi.org/10.21105/joss.00097, 2017.

Huang, J., Yin, H., Chapra, S., and Zhou, Q.: Modelling Dissolved Oxygen Depression in an Urban River in China, Water, 9, 520, https://doi.org/10.3390/w9070520, 2017.

Hullar, M. A. J., Kaplan, L. A., and Stahl, D. A.: Recurring Seasonal Dynamics of Microbial Communities in Stream Habitats, Applied and Environmental Microbiology, 72, 713–722, https://doi.org/10.1128/AEM.72.1.713-722.2006, 2006.

Hutchins, M., Harding, G., Jarvie, H., Marsh, T., Bowes, M., and Loewenthal, M.: Intense Summer Floods May Induce Prolonged Increases in Benthic Respiration Rates of More than One Year Leading to Low River Dissolved Oxygen, Journal of Hydrology X, 8, 100 056, https://doi.org/10.1016/j.hydroa.2020.100056, 2020.

Jiang, J., Tang, S., Han, D., Fu, G., Solomatine, D., and Zheng, Y.: A Comprehensive Review on the Design and Optimization of Surface Water Quality Monitoring Networks, Environmental Modelling & Software, 132, 104 792, https://doi.org/10.1016/j.envsoft.2020.104792, 2020.

Jolliffe, I. T. and Cadima, J.: Principal Component Analysis: A Review and Recent Developments, Phil. Trans. R. Soc. A, 374, 20150 202, https://doi.org/10.1098/rsta.2015.0202, 2016.

Landa, M., Cottrell, M. T., Kirchman, D. L., Blain, S., and Obernosterer, I.: Changes in Bacterial Diversity in Response to Dissolved Organic Matter Supply in a Continuous Culture Experiment, Aquatic Microbial Ecology, 69, 157–168, https://doi.org/10.3354/ame01632, 2013.

Larsson, U. and Hagstrom, A.: Phytoplankton Exudate Release as an Energy Source for the Growth of Pelagic Bacteria, Marine Biology, 52, 199–206, https://doi.org/10.1007/BF00398133, 1979.

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.

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.

Martin, L.: Ecological functioning of the Seine river downstream the wastewater treatment plant "Seine Aval": experimental datas and bidimensional modeling., Ph.D. thesis, École Nationale Supérieure des Mines de Paris, Sciences of the Universe [physics], 2001.

Matallana-Surget, S. and Wattiez, R.: Impact of Solar Radiation on Gene Expression in Bacteria, Proteomes, 1, 70–86, https://doi.org/10.3390/proteomes1020070, 2013.

Nossent, J., Elsen, P., and Bauwens, W.: Sobol' Sensitivity Analysis of a Complex Environmental Model, Environmental Modelling & Software, 26, 1515–1525, https://doi.org/10.1016/j.envsoft.2011.08.010, 2011.

Odum, H. T.: Primary Production in Flowing Waters1, Limnol. Oceanogr., 1, 102–117, https://doi.org/10.4319/lo.1956.1.2.0102, 1956.

Parlanti, E., Wörz, K., Geoffroy, L., and Lamotte, M.: Dissolved Organic Matter Fluorescence Spectroscopy as a Tool to Estimate Biological

755   Activity in a Coastal Zone Submitted to Anthropogenic Inputs, Organic Geochemistry, 31, 1765–1781, https://doi.org/10.1016/S0146-6380(00)00124-8, 2000.

Parlanti, E., Morin, B., and Vacher, L.: Combined 3D-Spectrofluorometry, High Performance Liquid Chromatography and Capillary Electrophoresis for the Characterization of Dissolved Organic Matter in Natural Waters, Organic Geochemistry, 33, 221–236, https://doi.org/10.1016/S0146-6380(01)00154-1, 2002.

760   Polus, E., de Fouquet, C., Flipo, N., and Poulin, M.: Caractérisation spatiale et temporelle de la qualité des « Masses d'Eau Cours d'Eau », rseau, 23, 415–429, https://doi.org/10.7202/045101ar, 2010.

Polus, E., Flipo, N., de Fouquet, C., and Poulin, M.: Geostatistics for Assessing the Efficiency of a Distributed Physically-Based Water Quality Model: Application to Nitrate in the Seine River, Hydrol. Process., 25, 217–233, https://doi.org/10.1002/hyp.7838, 2011.

Pryet, A., Labarthe, B., Saleh, F., Akopian, M., and Flipo, N.: Reporting of stream-aquifer flow distribution at the regional scale with a

765   distributed process-based model, Water Resources Management, 29, 139–159, https://doi.org/10.1007/s11269-014-0832-7, 2015.

Quynh, L. T. P., Garnier, G., Billen, G., Thiem, L. N., and Minh, C. V.: Preminary results of riverstrahler model application to the red river system (Vietnam), Vietnam Journal of Chemistry, 47, 110, https://doi.org/10.15625/4550, 2014.

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.

770   Reis, S., Seto, E., Northcross, A., Quinn, N. W. T., Convertino, M., Jones, R. L., Maier, H. R., Schlink, U., Steinle, S., Vieno, M., and Wimberly, M. C.: Integrating Modelling and Smart Sensors for Environmental and Human Health, Environmental Modelling & Software, 74, 238–246, https://doi.org/10.1016/j.envsoft.2015.06.003, 2015.

Reusser, D. E., Buytaert, W., and Zehe, E.: Temporal dynamics of model parameter sensitivity for computationally expensive models with the Fourier amplitude sensitivity test, Water Resources Research, 47, https://doi.org/10.1029/2010WR009947, 2011.

775   Saltelli, A.: Making Best Use of Model Evaluations to Compute Sensitivity Indices, Computer Physics Communications, 145, 280–297, https://doi.org/10.1016/S0010-4655(02)00280-1, 2002.

Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M., and Tarantola, S.: Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index, Computer Physics Communications, 181, 259–270, https://doi.org/10.1016/j.cpc.2009.09.018, 2010.

780   Seidl, M., Servais, P., Martaud, M., Gandouin, C., and Mouchel, J. M.: Organic Carbon Biodegradability and Heterotrophic Bacteria along a Combined Sewer Catchment during Rain Events, Water Science and Technology, 37, 25–33, https://doi.org/10.1016/S0273-1223(97)00752-X, 1998a.

Seidl, M., Servais, P., and Mouchel, J.: Organic Matter Transport and Degradation in the River Seine (France) after a Combined Sewer Overflow, Water Research, 32, 3569–3580, https://doi.org/10.1016/S0043-1354(98)00169-9, 1998b.

785   Servais, P.: Modélisation de la biomasse et de l'activité bactérienne dans la Meuse belge, rseau, 2, 543–563, https://doi.org/10.7202/705042ar, 1989.

Servais, P. and Garnier, J.: Contribution of Heterotrophic Bacterial Production to the Carbon Budget of the River Seine (France), Microb Ecol, 25, 19–33, https://doi.org/10.1007/BF00182127, 1993.

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.

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.

Sobol, I. M.: Sensitivity Estimates for Nonlinear Mathematical Models, Mathematical modelling and computational experiments, 1, 407–414, 1993.

Staehr, P., Bade, D., van de Bogert, M., Koch, G., Williamson, C., Hanson, P., Cole, J., and Kratz, T.: Lake Metabolism and the Diel Oxygen Technique: State of the Science, Limnology and Oceanography: Methods, 8, 628–644, https://doi.org/10.4319/lom.2010.8.0628, 2010.

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.

Thibodeaux, L., Poulin, M., and Even, S.: A Model for Enhanced Aeration of Streams by Motor Vessels with Application to the Seine River, Journal of Hazardous Materials, 37, 459–473, https://doi.org/10.1016/0304-3894(93)E0101-7, 1994.

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., Garnier, J., and Billen, G.: Assessing the Effect of Nutrient Mitigation Measures in the Watersheds of the Southern Bight of the North Sea, Science of The Total Environment, 408, 1245–1255, https://doi.org/10.1016/j.scitotenv.2009.12.031, 2010.

Vanrolleghem, P., Borchardt, D., Henze, M., Rauch, W., Reichert, P., Shanahan, P., and Somlyódy, L.: River Water Quality Model no.1 (RWQM1): III Biochemical submodel selection, Water Science and Technology, 43, 31–40, 2001.

Vilmin, L.: Modélisation Du Fonctionnement Biogéochimique de La Seine de l'agglomération Parisienne à l'estuaire à Différentes Échelles Temporelles, These de doctorat, Paris, ENMP, 2014.

Vilmin, L., Flipo, N., and Poulin, M.: Le modèle de simulation biogéochimique C-RIVE, Tech. rep., PIREN-Seine, 2012.

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), Science of The 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?, ESPR, 25, 23 485–23 501, https://doi.org/10.1007/s11356-016-7109-z, 2018.

Wang, Q., Li, S., Jia, P., Qi, C., and Ding, F.: A Review of Surface Water Quality Models, The Scientific World Journal, 2013, e231 768, https://doi.org/10.1155/2013/231768, 2013.

Wang, S.: Simulation Du Métabolisme de La Seine Par Assimilation de Données En Continu, These de doctorat, Paris Sciences et Lettres, 2019a.

Wang, S., Flipo, N., and Romary, T.: Time-Dependent Global Sensitivity Analysis of the C-RIVE Biogeochemical Model in Contrasted Hydrological and Trophic Contexts, Water Research, 144, 341–355, https://doi.org/10.1016/j.watres.2018.07.033, 2018.

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, 2019b.

Wang, S., Flipo, N., Romary, T., and Hasanyar, M.: Particle Filter for High Frequency Oxygen Data Assimilation in River Systems, Environmental Modelling & Software, 151, 105 382, https://doi.org/10.1016/j.envsoft.2022.105382, 2022.

830   Wold, S., Esbensen, K., and Geladi, P.: Principal Component Analysis, Chemometrics and Intelligent Laboratory Systems, 2, 37–52, 1987.

Yang, C.-P., Lung, W.-S., Kuo, J.-T., and Liu, J.-H.: Water Quality Modeling of a Hypoxic Stream, Pract. Period. Hazard. Toxic Radioact. Waste Manage., 14, 115–123, https://doi.org/10.1061/(ASCE)HZ.1944-8376.0000021, 2010.