REPLY TO THE REFEREE #1 (RC1) -- gmd-2023-135

We would like to firstly thank the anonymous referee #1 for the careful reading of the paper and the comments/suggestions. Please find hereafter our point by point reply to the referee's comments which enhance certainly the quality of our paper.

The paper titled "The community-centred aquatic biogeochemistry model unified RIVE v1.0: a unified version for water column" presents a unified version of the RIVE model for the water column, which includes formalisms for various ecological and biochemical components such as bacterial communities, primary producers, zooplankton, nutrients, inorganic carbon, and dissolved oxygen cycles. The unified RIVE model is open-source and has been implemented in Python 3 to create pyRIVE 1.0, and in ANSI C to create C-RIVE 0.32. The paper also discusses the validation of the organic matter degradation module through the simulation of batch experiments and compares the comparability of pyRIVE 1.0 and C-RIVE 0.32 by modelling a river stretch case study. The RIVE model described in this paper is state-of-the-art, the model description is generally very detailed, and the open-source implementation of the model in different programming languages is very meaningful and useful for geoscience modellers. As the importance of process-based models is increasingly recognized to uncover the underlying mechanisms behind water quality metrics, this study and its described model are very timely and valuable. While the model code and its metadata are well organized (which is the most important for a model development paper), the model descriptions and some details (text, equations, figures, and language) in the manuscript need to be improved (see my comments below). I therefore suggest minor revisions before acceptance for publication.

Major comments and questions:

1. RIVE is one of the most state-of-the-art water quality models in the world, with its particularly strong functions in simulating biogeochemical processes, multiple variables together, spatio-temporal changes, and changes with different factors. Some recent studies propose the idea that some conventional water quality models may be too complex, e.g. Jackson-Blake et al. (Water Resource Research). Although I myself fully believe the complexity and strengths of the RIVE model go hand in hand, I was just wondering: do you have some existing test or experimental examples, to roughly show that the processes/kinetics/environmental factors/or variables built in RIVE are necessary or important or advantageous for a better performance? Or show the contrary, that omitting some of them will cause poorer simulations/performance/understanding? If this is possible, can you add a paragraph for this in the discussion?

   Complexity can be understood in terms of the large number of variables represented and interacting with each other. The RIVE model is a multi-element, multi-form model and the kinetics it represents inevitably incorporate a large number of parameters. This is especially true as the RIVE model has opted for an explicit representation of the living communities (bacteria, phytoplankton, zooplankton, etc.) involved in the carbon and nutrient cycles. The model has thus become more complex over time and the addition of new processes (and therefore new parameters) has, as far as possible, been systematically based on experimental work in the laboratory or in the field to reduce the ranges of uncertainty around the kinetic parameters.

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

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

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

The above information has been added in the discussion (Section 4.2).

2. Given the complexity of the model, user-friendly documentation and tutorials would be helpful for users who are new to this field or the model. Can you possibly include the documentation in the archive of the model? For example, are you going to add the publication of this paper to the archive of the model?

   The publication of this paper will be added to the Gitlab depositories (https://gitlab.in2p3.fr/rive, https://gitlab.com/gtransp/c-rive). In addition, we are currently developing some user-friendly and interactive notebooks (jupyterlab) dedicated to the use of the RIVE code. These will be freely available. Because they are likely to change over time (and the training we provide on the RIVE model), we prefer to store them in the Gitlab repositories. For more documentation and tutorials, one can consult the website (https://www.federation-fire.cnrs.fr/rive/) and the Gitlab depositories.

3. Is phytoplankton dynamics in the RIVE also dependent on temperature? If so, please mention it in a suitable place, e.g. Line 40 and section 2.3.1. Similar questions for other processes: do you also consider temperature? This should be mentioned earlier in the text to better inform readers.

   Yes. The phytoplankton dynamics dependent on temperature and other activities of living species also. The parameter values at water temperature T°C are weighted by a temperature function using the parameter values determined at 20 °C in laboratory. We revised the equations by integrating the water temperature function and clarified water temperature effect in the text.

4. I guess “state variable” means evaluating output variables from elemental and process balances. Or maybe I misunderstand this? This needs to be explained at the beginning of the text.

   To make things clearer, when introducing the first diagram of RIVE (HSB, Fig. 1) we explain that the state variables are represented by **circles** and represent either concentrations or stocks entering and leaving the (biogeochemical) processes. The biogeochemical processes are represented by **squares**.

5. Section 2 Line 92-101: Can you clarify whether the community-centred RIVE simulated different dynamics across different locations and times/periods? This information is not mentioned, so not clear to readers.

   The applications of the RIVE model are presented in introduction (Line 62-77 in revised version). The RIVE model has simulated successfully a large variety of freshwater systems across the world. These applications were carried out for different networks and scales as well as various degrees of anthropogenic impacts in a wide climatic gradient.

6. Some terms used in equations are not explained in terms of their meaning and unit. Please thoroughly check and add explanations incl. units for all terms used in all equations.

   Done. We added explanations for all terms.

7. Please consider revising the expression of ions in all flowcharts. In these flow charts, gas forms (e.g., “O2” and “CO2”) and ions (e.g. “NO2” and “NO3”) are used together, but in fact “NO2” can mean a gas form, but obviously here “NO2” is only used to mean “NO2-” in this paper.

   Done. The ions (PO_4^{3-}, NH_4^+, NO_2^-, NO_3^-) have been revised in the figures 2, 3, 5, and 6. We keep O2, CO2, N2, N2O for gas forms.

8. The sentences of this manuscript are generally too long and a bit hard to read, particularly for those who may not be so familiar with this model. Some examples: The 1st sentence of the abstract is as long as three lines: “*Research on mechanisms of organic matter degradation, bacterial activities, phytoplankton dynamics, and other processes has led to the development of numerous sophisticated water quality models since one of the first in 1925, based on first order kinetics for organic matter degradation*”. The 2nd and the 3rd Another typical example is a 4-line sentence spanning Line 25-28: “*While the role of microorganisms in the degradation of organic matter has been acknowledged since the end of the 19th century, an important limitation of this type of representation is that the microbiological nature of the organic matter degradation process and the bacterial population dynamics intrinsically involved are completely obscured, being implicitly taken into account only through a biodegradability constant of OM and its dependence on temperature.*”. I suggest revising each of such long sentences into 2-3 short ones throughout the entire manuscript, to make the text more readable.

Thank you for your kindly remark. The long sentences have been shortened throughout the entire manuscript.

Minor comments:

1. Title and Line 19: The tile mentions “aquatic biogeochemistry model”. “Aquatic” can be broad and include freshwater, coastal and marine water. Does this model version simulate both freshwater and marine biogeochemistry? If only for freshwater, I suggest changing this term in the entire paper.

   Thank you for your remark. “Aquatic” is replaced by “freshwater”.

2. Line 4: This sentence is a little confusing: RIVE is certainly community-centred now, especially via this paper. However, this sentence reads like RIVE has been community-centred since its development in 1994...

   The RIVE model has been community-centered since its development in 1994 (Billen et al., 1994). The microorganism’s activities (phytoplankton, bacteria, and zooplankton) were implemented subsequently.

3. Line 5: "has since been integrated ..." should be changed to either "has since then been integrated ..." or "has subsequently been integrated ..."

   Done. The sentence is changed to “has subsequently been integrated…”

4. Line 8 (and elsewhere in the manuscript): Do you mean merely “comparability”, or “comparability and compatibility”?

   We compared the results (river stretch simulation, Section 3.3) produced by two implementations of unified RIVE v1.0 (pyRIVE 1.0 and C-RIVE 0.32). In this case, the results demonstrated their comparability. The question of the compatibility of unified RIVE v1.0 with other software should be examined case by case.

5. Line 19: add “and” or “or” between “lake” and “reservoir”; same for Line 62.

   Done. “or” is added.

6. Line 40-41: please add “of phytoplankton” before “growth” to make it more clear.

   Done.

7. Line 46-60: Since there is a Table A1 that summarizes RIVE applications, please cite the table in this paragraph.

   Done.

8. Line 53: Please add ”simulating” before “hydro-biodynamic functioning”

   Done.

9. Line 75: please add the reservoir/river basin name or location for the stagnant systems here,

   Done. Reservoir/lake name and location have been added.

10. Line 80: “Python 3” is mentioned here. Or does it work for all Python 3 versions? If not, could you please add more information here? like “Python 3 (py3.x-py3.y)”, Because Python 3.9 has been quite different from previous versions in many aspects.

    pyRIVE 1.0 has been successfully tested with python 3 versions up to 3.10 release. The information has been added when introducing pyRIVE 1.0 (Line 87 – 88 in revised version).

11. Line 89: Can you clarify here which aspects are evaluated among different implementations? e.g. performance? Running speed?

    Done. We clarify it by adding “programming languages, performance - comparability”.

12. Line 100-101: RIVE does seem to have applied development for sediment dynamics. Perhaps better to clarify this sentence to “While RIVE model does have applications for sediment dynamics and its interaction with the water column (refs xx and xx), relevant community-centred efforts need to be made in future work, which is not the focus of this study.”

    Done. Some references have been added.

13. Line 104: plural: polymers

    Done.

14. Line 105: remove “which” here. Using both “but” and “which” is not correct here.

    Done.

15. Line 107: “uptake” is generally not used as a verb. “takes up” or “utilizes” may be not suitable.

    Yes, the word “absorbs” is used.

16. Line 157: Please add the full name for “NH4+” at its 1st appearance in the text.

    Done.

17. Line 173: Please note that “AUQAPHY” is used here; but in Line 39, “*Aquaphy*” is used; in Figure 3 caption, “Aquaphy” is used.

    Done. We use now “AQUAPHY” in upper case everywhere in the paper.

18. Line 182: Please revise: “The most common way of measuring phytoplankton biomass is using the chlorophyll a concentration”.

Done.

19. Line 183-189: This part may be misleading. Please consider moving the last sentence that mentions "the initial proportions of different constituents are fixed and used to determined …." to be before the sentences describing the detailed proportion numbers.

    Done. We move the sentence "The initial proportions of different constituents (F, R, S) are fixed (Lancelot et al., 1991). They are only used to determine the initial concentrations of the three cellular constituents and the concentrations of the three cellular constituents in incoming water fluxes for each phytoplankton species." before the sentences describing the detailed proportion numbers (Line 206 – 208 in revised version).

20. Line 188: "external inflows" is very confusing. Can you revise it to make the meaning clearer?

    Done. "external inflows" is replace by "incoming water fluxes".

21. Line 216: Please add the full term for "N", "P" and "Si" at the first-time use of the abbreviation.

    Done.

22. Line 216-217: This sentence is unnecessarily wordy: "The nutrients can potentially limit phytoplankton growth if their quantities are insufficient".

    Done. Thanks for your proposition.

23. Line 216 and 223: I understand the authors want to mean "DIN", "DIP", and "DSi", but the use of [N], [P] and [Si] may mean "TN", "TP" and "TSi", respectively. Need to clarify these uses to change to the correct terms.

    Done. The "DIN", "DIP", and "DSi" are used in the equation (17).

24. Line 258: "Disappearance" seems not the most suitable expression here. Please consider "consumption" or another word.

    "Disapperance" has been replaced by "Extinction".

25. Line 311, 581: Nutrient cycling

    Done.

26. Line 315-316: Maybe need to specify whether C, N, P, and Si are dissolved inorganic forms. Or are they not?

    No, they are not. In fact, we use the Redfield-Conley ratio C:N:P:Si = 106:16:1:42 (Redfield et al., 1963; Conley et al., 1989) to determine the composition of living species and organic carbon in terms of carbon (C), nitrogen (N), phosphorus (P) and

silicon (Si). They are used to transform organic carbon (e.g. mgC L-1) to nitrogen (mgN L-1), phosphorus (mgP L-1) or silicon (mgSi L-1).

27. Line 387: Here water temperature appears for the first time. But I believe water temperature is (should be) used also in other processes described in other sections.

    Yes, you are right. The other processes related to microorganism's activities such as the photosynthesis of phytoplankton, growth of living species, mortality of living species depend on water temperature. The parameter values at water temperature T °C are weighted by a temperature function using the parameter values determined at 20 °C in laboratory. Water temperature effect has been clarified in the text and equations (see response to major comment 3).

28. Line 395 and Line 370-372: Sediment dynamics can be important e.g. for P dynamics and sediment oxygen demand, and RIVE has been applied for sedimentary dynamics long ago. Can you roughly mention here, e.g., through citations of RIVE with sedimentary dynamics, whether or how much the influence of excluding sediment dynamics is for this RIVE v1.0 version with a focus on the water column? For example, are P and O2 concentrations still well simulated and agree with observations?

    Citations have been added to show the influence of sediment dynamics on P/O2, and the necessary of integrating a sediment module in unified RIVE in the future.

29. Line 455: Please specify the specific item name in Appendix.

    Done. Appendix B added. Furthermore, we have segregated the parameters associated with heterotrophic and nitrifying bacteria by dividing Table B1 into two distinct tables, B1 and B2.

30. Captions of Figures 7, 8, 10: Can you add the location (or name of water system/river basin) and time (year or month or date) for the validation figures?

    Done. Added for figure 7, 8. For the figure 10, it is the output of a virtual case study to compare the performance – comparability of C-RIVE 0.32 and pyRIVE 1.0.

31. Section 3.2: Can you describe in this section a little bit the reason why DOM and SHB+LHB are selected to show validation, and validation of other state variables such as DO and nutrients are not shown?

    A sentence has been added in this section. Since only dissolved organic matter (DOM) and heterotrophic bacterial biomass are measured during the batch experiments. No DO and nutrients data are available.

32. Line 569-570: Please choose one between "such as" and "for instance"

    Done. We keep "for instance".

33. Line 568: "depend on different limitations" is confusing. Please consider the use of "limiting factors".

Done.

34. Line 673: The name of the first author is not correct for this reference.

Thank you for your remark. Author name is corrected.

References

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

Conley, D. J., Kilham, S. S., and Theriot, E.: Differences in silica content between marine and freshwater diatoms, Limnology and Oceanography, 34, 205–212, 1989.

Hasanyar, M., Romary, T., Wang, S., and Flipo, N.: How much do bacterial growth properties and biodegradable dissolved organic matter control water quality at low flow?, Biogeosciences, 20, 1621–1633, 2023.

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

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

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, 2018.

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Wang, S., Flipo, N., Romary, T., and Hasanyar, M.: Particle filter for high frequency oxygen data assimilation in river systems, Environmental Modelling & Software, p.105382, 2022.