Manuscript Number: gmd-2019-301

Title: A multirate mass transfer model to represent the interaction of multicomponent biogeochemical processes between surface water and hyporheic zones (SWAT-MRMT-R 1.0)

Authors: Yilin Fang, Xingyuan Chen, Jesus Gomez velez, Xuesong Zhang, Zhuoran Duan, Glenn E. Hammond, Amy E. Goldman, Vanessa A. Garayburu-Caruso, and Emily B. Graham

Type: Second Submission (First review by this referee)

Recommendation: Publish

Overview:

The manuscript describes the synthesis of three previously described models (NEXSS, SWAT and PFLOTRAN) into a coherent framework (SWAT-MRMT-R) that tracks hydrologic and biogeochemical processes at the watershed scale (and possibly larger) with reach scale resolution. Hyporheic processes, both transport and reactive, are explicitly included. The capabilities of the SWAT-MRMT-R model are demonstrated by its application, in a numerical study, to the Hanford watershed of the Columbia River. The fate of nitrogen solute is evaluated under several different scenarios.

General comments:

The study of solute fate at watershed and basin scale or even global scales has been an area of increasing interest of late and the Fang et. al. manuscript is a significant contribution to that effort. Overall, the manuscript is will written and well organized. Objectives are clearly stated, and the research has met the stated goals. Conclusions are well constrained by the observations and data. In fact, I would like to congratulate the authors for resisting the temptation (if such temptation was ever present) to describe this work as a predictive model. I see a bit of an alarming trend within our community to do a purely numerical study and call it a predictive model. This is, in my view, a significant overreach. Your work is a significant contribution as it stands. And with some development and field validation could evolve to a predictive model that has real-world impact.

My recommendation is to publish. I feel that the manuscript could be published as it stands, but I do have some suggestions and comments that are worth considering.

NEXSS is not explicitly integrated into your modeling framework. However, NEXSS or something quite similar is essential to the successful implementation of the model. NEXSS does not seem to be readily accessible (maybe I am looking in the wrong place). If your goal if to deploy this framework to other researchers, then it would be quite useful to either make NEXSS more readily available or to provide a bit of guidance as to how the necessary information could be synthesized for large scale studies.

Overall you do a good job of describing the limitations of your modeling framework. There is one other factor that I think deserves some mention, even though it may seem completely obvious. The way that this model is parameterized with multiple reaches each possibly with multiple storage zones, transfer rates and reaction rates, means that, at the outlet, there are possibly a multitude of parameterizations that can yield the “right” answer – most of them for objectively the wrong reason. As such, if this model is to be used in real-world, large-scale studies then validation at multiple points within the study area should be strongly considered and recommended.

I have some minor suggestions which are listed below.

Specific comments (need to be addressed in the narrative or explain why there is no need to revise):

1. Author listing – I believe that Velez should be capitalized.
2. Line 15: "A two-step reactions for denitrification and an aerobic respiration reaction are assumed to represent…" There is a mismatch in tense. Could be modified as: "A two-step reaction *sequence* for denitrification and an aerobic respiration reaction *is* assumed to represent…" or something similar.
3. Lines 92 – 95: the wording is a bit ambiguous. I believe that you are saying:
   - solute reaction equations are solved by the Newton-Raphson method
   - hydrologic transport is solved by operator splitting
   Please clarify for readability.
4. Section 2.4: These are questions/suggestions about future efforts that likely arise from choices that were necessarily made to facilitate the present study.

   Does SWAT surface water module include denitrification include denitrification? Recent studies have shown this to be significant in high-order, turbid streams.

   For future iterations of the model, it would be interesting to include NO_3^- -→ N_2O↑ as this is a significant reaction in large rivers, mostly n the water column but also in the HZ.
5. Line 160 – 169: The transition from the discussion of SWAT to PFLOTRAN is a bit abrupt. Suggest the following revision:

   In SWAT, dissolved nutrients are transported with the water and those sorbed to sediments are allowed to be deposited with the sediments on the bed of the channel (Neitsch et al., 2011). PFLOTRAN is an open source, massively-parallel reactive multiphase flow and multicomponent transport code. It has well-established documentation (https://www.pflotran.org/documentation/). Nutrient transport and reactions in SWAT are solved sequentially. We modified the explicit time-stepping algorithm in the original code for in-stream chemistry so the resulting nonlinear system of equations from the transformations taking place within the stream water and storage zones are simulated simultaneously with the implicit time stepping through the Newton Raphson method in batch mode (i.e., no transport) of the PFLOTRAN (Lichtner et al., 2017) model.
6. Line 223: Replace "[L] is the elevation of the free surface elevation at" with "[L] is the free surface elevation at"
7. Line 277- 279: For the seasonal flow scenario, the application of NEXSS is clearly defined. For the BASE and MRMT is seems a bit ambiguous. Is it annually averaged over the same period? Maybe I missed the it earlier in the paper, but it would be useful to make a clear distinction at the same point in the manuscript.
8. For Figure 4 which compares the BASE scenario to the MRMT scenario, it would be useful to add markers to one of the traces so that it would be visually obvious that the two traces follow essentially the same path.