Short comments (SCs)

Received and published: 29 September 2020

This manuscript presented a recently developed watershed-scale biogeochemical model and its various applications for the two water-table, and DOC and nitrate at Shale Hills watershed. Currently there is an urgent need in the field for such watershed-scale reactive transport codes and the model developed in this manuscript has a wide potential to reach a broad biogeochemistry community. The manuscript is generally well organized in model materials and has done a decent job validating the model against the benchmark code CrunchTope. I enjoyed reading the most part of the manuscript yet it is lengthy and could be shortened for conciseness. I think the model presented here will be of interesting to many others who are interested in understanding the interaction of land surface, hydrological, and biogeochemical processes. Yet the manuscript also needs a major revision to reduce its length, re-organize its structure, and make some clarification. Therefore, I am supportive of its publication after the major revision.

Response: Thank you for your interests in our model. As you can see from our response to other reviewers, we have thoroughly revised the manuscript for conciseness and clarity.

Some detailed comments are listed below.

1) Figure 1 is a very nice conceptual figure. But it is not clear how the ET is calculated, i.e., what form does it has (e.g., evaporation, transpiration, or even snow sublimation). It is also not clear what does the dark green (e.g., microbe-mediated redox reactions) and shallow green (e.g., mineral dissolution and precipitation) means in the legend.

Response: The ET is the sum of evaporation, transpiration, and snow sublimation. We have added a sentence about ET method with a reference. An explanation has been added to the legend.

Line 243 – 244: "The ET is calculated by the Penman potential evaporation scheme and detailed equations can be found in Shi (2012)."

Line 170 – 171: "For BioRT, the light and dark greens refer to abiotic and biological reactions, respectively."

2) Figure 2 is a useful representation for detailed hydrological processes yet I think the author need to make it more explicitly (or highlight) in the figure about the "two water-table" concept, which is a new model development feature for this study. Does the deeper zone have ET process? How does different water flux terms relate to each other (from the water balance perspective)?

Response: Only the shallow zone has ET process. We have now revised the figure so relationships between different water fluxes are encoded in water equations (Eqn 1, 2 and Eqn S1, S2).

3) The hydrological equations are 2.5 pages long and some of them are repetitive with the same set of equation only in different layers. This section can either be shortened or moved into SI.
Response: We agree and have moved much of the content to SI.

4) Macropore and its equation are presented yet are not mentioned or discussed in the later part. Is it also a new feature for the model development, if not, consider remove it.
Response: Macropore it is part of the original Flux-PIHM so it is not new. But here we show how macropore affects the hydraulic conductivity of soil matrix. Moved to SI.

5) Equation 14, not sure how the hydrology model and bioRT coupled together, i.e., need to be more specific about which terms in this equation are from the hydrology model? Are they coupled outside the hydrology model or coupled internally?
Response: The hydrological module Flux-PIHM provides water storage $S_{w,i}$ and water fluxes q_{ij} for this equation. The solved temperature profile from Flux-PIHM is also provided to the reaction rate. They are coupled internally (see model code details at https://github.com/PSUmodeling/BioRT-Flux-PIHM).

Line 437 – 439: "BioRT reads in the model output of water and temperature from Flux-PIHM, and solves the biogeochemical reactive transport equations."

6) Consider reduce the section of 3.2
Response: Reduced substantially.

7) Line 359, not sure if this "numeric scheme" is necessary. Not very relevant to other materials.
Response: We have shortened it and added two sentences for solving the reactive transport equation, as other reviewers asked for it.

Line 413 – 417: "In BioRT, the transport step is first solved with water by the preconditioned Krylov (iterative) method and the Generalized Minimal Residual Method (Saad and Schultz, 1986). In the following reaction step, all primary species in each finite volume are assembled in a local matrix and then solved iteratively by the Crank-Nicolson and Newton-Raphson method in CVODE (Bao et al., 2017)."

8) Figure 5, what are the multiple orange ET arrows, from soil, tress, and snow?
Response: Figure 5 has been removed to condense the paper

9) Font style is not consistent in Table 1.
Response: Thanks for the catch. Changed.

10) Some references in Table 1 are missing from the reference list. For example, Leila 2020 (preprint DOI maybe?).
Response: Reference updated. Thanks.

11) Line 485, and Line 493, there seems no mentioning about how was the modeled ET calculated. Consider provide an ET equation or a reference.
Response: We have added a sentence about ET method with a reference.

Line 243 – 244: "The ET is calculated by the Penman potential evaporation scheme and detailed equations can be found in Shi (2012)."

12) I like the way Figure 6b was presented. This figure makes sense to me and the upper bound of 40% GW contribution is generally consistent with literature. One tiny thing to improve is the small font size of Figure 6a legend, especially the subscript and superscript.
Response: Slightly enlarged in font size. Thanks.

13) 5.2 Reactive Transport Example, this section already has sufficient details about N reaction. This makes me wondering whether the 3.2 section should be shortened for conciseness.
Response: The section of 3.2 has been shortened and reorganized as suggested. Much of the reaction rate related materials have been moved to sections in biogeochemical reactions and biological processes.

14) 5.3 Reactive Transport Example 2, it seems to me that the model is flexible in model domain setup. In addition to more model inputs (e.g., spatial information), what are other requirements or burdens in using a spatially explicit model.
Response: For the spatially distributed version, it takes longer time to set up the model and run the model. the computational cost can be high. In addition, the model needs more spatial data in order to represent spatial details and capture dynamics at different spatial locations.

Line 487 - 488: "It requires much more data and can be computationally expensive but can be used to identify "hot spots" of biogeochemical reactions within a watershed