Comment on "BioRT-Flux-PIHM v1.0: a watershed biogeochemical reactive transport model" by Wei Zhi et al.

Topical Editor decision

Received: 21 Sep 2021

Dear Editor Min-Hui Lo:

Thank you for your speedy handling of our manuscript. We have done another round of editing, including:

1) Removed some outdated references and updated with some new references.
2) Removed some redundancy in the text.
3) Added some explanations (e.g., Nash Sutcliffe efficiency, what kind of spatial data) for clarity.
4) Added a Table S7 and a brief summary for model validation performance as suggested.
5) Added a Zenodo DOI in the section of Code availability.

1. Although the authors have mentioned the verification of the BioRT model in the revised manuscript (The BioRT module had been verified against CrunchTope under different transport and reaction conditions (Figures S1 – S7 in SI), the performance and verification of the model can be further improved. Especially, this is a Model description paper, so it will be helpful for the readers and users if the authors can provide some statistics in the main text (maybe at the discussion section?) for the performance of BioRT compared to CrunchTope (maybe a summary table from those materials in SI?)

Response: Thank you for the comments. We have added model performance statistics in the section of 4. Numerical scheme and model verification (Line 394 – 397) and a summary Table S7 in the section of S3.4 Validation performance summary.

Line 394 – 397: "Table S7 shows an average percent bias and Nash Sutcliffe efficiency (NSE) of 1.1% and 0.98, indicating a robust performance for a variety of solutes under different transport and reaction conditions."

S3.4. Validation performance summary

Model validation performance for above-mentioned cases using percent bias (PBIAS) and Nash Sutcliffe efficiency (NSE) is summarized in Table S7. The optimal

value of PBIAS is 0, with low-magnitude values indicating accurate model simulation (Moriasi et al., 2007). Positive values indicate model underestimation bias, and negative values indicate model overestimation bias. NSE ranges between $-\infty$ and 1, with NSE = 1 being the perfect fit (Moriasi et al., 2007).

Table S7. Model validation performance

Process	Transport	Species	PBIAS (%)	NSE
Phosphorus (Fig S2, S3)	Advection-only	H^+	3.1	0.96
		Cl^-	1.0	0.99
		TP	1.0	0.99
		HPO_4^{2-}	-2.3	0.99
		$H_2PO_4^-$	1.7	0.99
		H_3PO_4	4.6	0.95
	Advection + diffusion + dispersion	H+	2.7	0.97
		Cl^-	-0.27	1.0
		TP	-0.20	1.0
		HPO_4^{2-}	-3.2	0.98
		$H_2PO_4^-$	1.4	0.99
		H_3PO_4	4.5	0.96
Carbon (Fig S5)	Advection + diffusion + dispersion	O_2(aq)	2.2	0.98
		NO_3^-	-1.4	0.99
		SO_4^{2-}	-0.2	0.99
		HCO_3^-	1.1	0.99
		N_2(aq)	2.0	0.98
		H_2S(aq)	2.5	0.98
Nitrogen (Fig S7)	Advection + diffusion + dispersion	O_2(aq)	2.2	0.99
		NH4+	1.5	1.0
		NO3-	-1.3	0.98
		N2(aq)	1.8	0.99

2. Please remove the reference from the abstract (GMD - Submission (geoscientific-model-development.net)).

Response: Removed as suggested. Thanks.

3. Please provide the doi from zenodo for the data and code section. (https://www.geoscientific-model-development.net/policies/code_and_data_policy.html)

Response: The DOI from Zenodo has been added to the code section (Line 739 – 742).

Line 739 – 742: “Code availability. The current model release (BioRT-Flux-PIHM v1.0) is archived at: https://doi.org/10.5281/zenodo.3936073. Documentation, source code, and examples are available at GitHub repository: https://github.com/Li-Reactive-Water-Group/BioRT-Flux-PIHM.

4. The authors have responded to original reviewer #2 that the Nash Sutcliffe efficiency has been removed. However, the revised manuscript L660-661 (The model outputs followed the general trend of stream DOC measurements (NSE = 0.55 for monthly DOC) still has NSE with only the abbreviation. Would you please address this carefully?
Response: Thanks for the catch. We have defined NSE on the first appearance (Line 395) and added an explanation in the text on Line 618 – 622.

Line 618 – 622: “The model outputs followed the general trend of stream DOC measurements with the model evaluation index NSE of 0.55 for monthly DOC concentration (Figure 10a). NSE ranges from $-\infty$ to 1.0 (i.e., perfect fit) with values greater than 0.5 considered good performance for monthly water quality model (Moriasi et al., 2015) “

5. L487: “It requires much more data and can be computationally expensive but can be used to identify “hot spots” of biogeochemical reactions within a watershed”. What kind of data? Please be more specific.
Response: Thanks for the comment. We have revised the paragraph and added some explanations for spatial data on Line 443 – 446.

Line 443 – 446: “Alternatively, a complex domain can be set up to track “hot spots” of biogeochemical reactions using many grids with explicit representation of spatial details (e.g., topographic map, river network, land use map, soil and geology map, mineral distribution).”

Reference:

Moriasi, D. N., Arnold, J. G., Van Liew, M. W., Bingner, R. L., Harmel, R. D., and Veith, T. L.: Model evaluation guidelines for systematic quantification of accuracy in watershed simulations, T Asabe, 50, 885-900, 2007.
Moriasi, D. N., Gitau, M. W., Pai, N., and Daggupati, P.: Hydrologic and water quality models: Performance measures and evaluation criteria, T Asabe, 58, 1763-1785, 2015.