

Geosci. Model Dev. Discuss., author comment AC1 https://doi.org/10.5194/gmd-2021-310-AC1, 2022 © Author(s) 2022. This work is distributed under the Creative Commons Attribution 4.0 License.

Reply on RC1

Jinyun Tang et al.

Author comment on "Supporting hierarchical soil biogeochemical modeling: version 2 of the Biogeochemical Transport and Reaction model (BeTR-v2)" by Jinyun Tang et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-310-AC1, 2022

Comment: In the paper "Supporting hierarchical soil biogeochemical modeling: Version 2 of the Biogeochemical Transport and Reaction model (BeTR-v2)"", authors Tang, Riley, and Zhu develop a new version of BeTR—a model development framework enabling investigation of different levels of complexity, process representations, and numerical method implementations. The new version (BeTR-v2) implements new numerical algorithms, is said to be a more efficient software, and can be run independent from host models. To demonstrate, the soil biogeochemistry model of ELMv1-ECA was implemented in BeTR-v2. The numerical solution was compared to analytical solutions, and simulations were performed at multiple scales (single layer, 1D, and global), comparing ELM versus ELMBeTR model configurations. Global simulations were benchmarked using ILAMB. Overall, this is a nice paper presenting tools and concepts that will be of interest to the GMD readership.

Response: We appreciate the reviewer's positive assessment of our work. Based on the raised concerns, we have made changes accordingly in the submitted revision.

Comment: The most interesting result was that the different numerical implementation of ELMv1-ECA in BeTR-v2 led to substantially different predictions. Re-calibrating some of the key parameters was not sufficient to reduce these differences. I agree with the authors that this is an important source of uncertainty that is often not considered in the biogeochemical modeling community. I think this point could be better highlighted in the paper, though. For example, numerical methods as a source of uncertainty is mentioned in the middle of a list in the introduction, but not much is done to highlight or elaborate on this point (even though it becomes one of the main take-home points in the results and conclusion).

Response: Following the reviewer's suggestions, we added at the end of the abstract "We contend that earth system models should strive to minimize this uncertainty by applying better numerical solvers." In the introduction, when discussing this type of numerical uncertainty, we now write "In particular, when the differential equations of a model are approximated with inappropriate numerical solvers, the model may obtain answers that better match observations for wrong reasons because calibration may inappropriately make up for deficiencies in the model's governing equations (i.e., type-I error that gets right answers with poor model formulations). This problem can result in incorrect inference of causality and interactions between processes. For instance, Tang et al. (2015) found that the simulated evapotranspiration agreed better with observations when the

coupled equations for soil and root water exchange were purposely solved incorrectly in a sequential manner than when they were solved correctly as tightly coupled. Alternatively, if calibration cannot make up the deficiency caused by the inappropriate numerical method, one may assert that a right model formulation is wrong (i.e., type-II error that gets wrong answers with good model formulations). For example, when the 1D diffusion equation is solved with central difference in both time and space, the numerical solution actually approximates a wave equation instead, and this deficiency cannot be fixed by calibration. Both types of inference error will contribute to the uncertainty of climate-biogeochemistry feedback simulated by ESMs."

Comment: I also think several aspects of section 2 could be clarified. This is a model description paper, so developments in this new version should be at least briefly described (even if they've been detailed elsewhere). For example, how is the code "more efficient" and could more details be provided regarding the new numerical algorithms? Please briefly describe the "multiple-flux-co-limiting solver" at first mention. I also suggest to clarify Table 1. This is important for keeping model configurations straight, but was not intuitive. For example, is the best description of the BeTR configurations really "Based on src/Applications/soil-farm/v1eca". The reader is left to mine the text to understand what this means. Also, the BeTR configurations used the multiple-flux-co-limiting solver for belowground processes too, right?

Respond: We revised the text by adding brief introductions of new algorithms adopted in BeTR-v2, and also clarified that the BeTR configurations used the multiple-flux-co-limiting solver for belowground processes by default. Specifically, we now write in the last paragraph of section 2.1 "Gaseous and aqueous diffusion are solved together using the dual-phase algorithm (that assumes equilibrium between gaseous and aqueous phases) with the implicit time stepping method (Tang and Riley, 2014), which is equally accurate but simpler than the treatment in BeTR-v1 that requires calculating locations of wetting fronts in the soil. Solid phase diffusion is also solved implicitly. Aqueous advection is solved using the mass-conserving semi-Lagrangian approach (Manson and Wallis, 2000), which is more accurate (by reducing numerical dispersion) than the upstream scheme used in BeTR-v1. Biogeochemical reactions are solved using the multiple-flux-co-limiting algorithm (Tang and Riley, 2016), which considers the production and consumption fluxes concurrently, so that there is no delay between nutrient mineralization and its competition by consumption fluxes within a time step, a critical feature to resolve the nutrient limitation dynamics (Tang and Riley, 2018). To ensure numerical accuracy, within each modeling time step of ELM (which is 30 minute), each solver uses the adaptive time stepping that exits when either the relative difference between solutions based on coarse time step and halved time step is less than 0.1% or when the minimum time step (30 seconds) is reached."

We also revised Table 1 based on both reviewers' suggestions:

Table 1. Summary of the configurations for the four global simulations.

Model configuration	ELMv1-ECA	ELMv1-ECA-V	ELMv1-BeTR- ECA0	ELMv1-BeTR-ECA
Code base	Default	Default		/s src/Applications/s

Soil BGC	Default	Default	Implemented ELMv1-ECA soil BGC in BeTR	Implemented ELMv1-ECA soil BGC in BeTR
Plant carbon and nutrient allocatio		Multiple-flux-co- limiting solver	Multiple-flux-co- limiting solver	Multiple-flux-co- limiting solver
Parameters	Default	Default	Default	Recalibrated

Minor comments:

Comment: P1 L14-16: This sentence is kind of vague with regard to the algorithms and structural improvements.

Respond: Now the sentence is revised as "Here, we describe the new version, BeTR-v2, which adopts more robust numerical solvers for multiphase diffusion and advection, and coupling between biogeochemical reactions, and improves code modularization over BeTR-v1".

Comment: P3 L19: change "share" to "sharing"

Response: Done.

Comment: P7 L1-3: The structure of this sentence is confusing. The analytical solutions should follow the colon, not equation 3.

Response: We revised the sentence as "As was done for BeTR-v1, two analytical solutions with different boundary conditions are employed to benchmark the numerical accuracy of the BeTR-v2 reactive transport solver that solves the following equation:".

Comment: P9 L15: Elaborate. What previous findings?

Response: We adjusted the sentence as "When using the same parameters, the reordering required by *ecacnp*caused significant differences in the simulated carbon and nutrient cycling compared to ELMv1-ECA (which confirms our previous findings in Tang and Riley (2018)), and such differences were inferred not correctable by calibration." So that it clearly says that our previous finding is "reordering causes significant differences in model simulated carbon and nutrient cycling".

Comment: P10 L18-19: "Comparing ELMv1-ECA and ELMv1-ECA"?

Response: We corrected it with "By comparing ELMv1-ECA-V and ELMv1-ECA".

Comment: Figure 1: X-axes look like the title of the panel below.

Response: We looked for other approaches, like enlarging the space among panels, or putting the labels into the panel, neither of these methods make the illustration better. Therefore, we decided to stick with the current approach.

Comment: P14: Fig 2c is not referenced in the text.

Response: Now it is properly referenced in the sentence "Accordingly, the soil CO_2 concentration builds up continuously, with a seasonal cycle that has its maximum in July and minimum in March (Figure 2c).".

Comment: Figure 3: Maybe make ELMv1-ECA a thicker line so that the reader can easily tell which model it is hidden behind.

Response: We made ELMv1-ECA a thicker line and used dash-dot line for ELMv1-ECA-V. Now the figures are more readable.

Comment: Table 2: Similar issue as above. I think one of these should be ELMv1-BeTR-ECA.

Response: Sorry for this typo, now it is corrected by identifying ELMv1-BeTR-ECA on the right side.