Geoscientific
Model Development
Discussions

Interactive comment on "Using reactive transport codes to provide mechanistic biogeochemistry representations in global land surface models: CLM-PFLOTRAN 1.0" *by* G. Tang et al.

Anonymous Referee #1

I was expecting a very happy holiday reading of the work "Using reactive transport codes to provide mechanistic biogeochemistry representations in global land surface models: CLM-PFLOTRAN 1.0" by Tang et al. Because what the authors were trying to do is a very important step towards improved land biogeochemical modeling for earth system models. However, the deeper I dived into the paper, the more suspicious I became: have the authors really developed a tool as they promised? My suspect is based on the following major concerns I identified.

First, I was very surprised that the authors do not represent the oxygen dynamics, which is very critical for the SOM decomposition dynamics in the Artic and in the fur-

ther studies they envisioned in the paper. Likewise, this raises concern if the authors' model could actually represent denitrification in a relatively reasonable way? If CLM-PFLOTRAN can indeed represent oxygen dynamics, then how is the multiphase transport handled? In my opinion, if a RTM (reactive transport model) is to be used for reasonable soil biogeochemical modeling, the gas phase transport is a process that must be resolved, not even to say that PFLOTRAN is supposed to be a very powerful RTM. Especially, I don't see the conclusion at P10654, L10-11, "it is particularly important to have robust solution methods such as fully implicit coupling of the advection-dispersion-reaction equations" is well supported in its current form of the paper.

Second, I think there is some problem in the conceptual model that the authors use for nitrogen competition. For instance, how is it justified that nitrogen just taken up by plants will instantly be available to plant organs that needs nitrogen? Many empirical evidences seem do not support this conceptual model. I think this may be one of the reasons why CLM-CN was not successful in simulating the FACE experiments (Zaehle et al., 2014, New Phytologist). Does the authors' implementation imply such inappropriate legacy will be carried on in their future model versions? Please clarify.

Third, although the authors spent a lot of time in discussing how they could successfully avoid unphysical negative values for species like NH4 and NO3, they have to tune the residual concentrations and various error tolerances diligently even at the three sites they used to show CLM-PFLOTRAN works for their purpose. Through the lines, they indicate the log-transformation is the best among the three approaches, clipping, scaling and log-transformation, they used. However, they also reported (P10641, L25-28)that log-transformation has often needs to be teamed with clipping to avoid unphysical negative values, which then unfortunately introduces mass balance error. This makes me really worried how easily would CLM-PFLOTRAN be applied at the global scale, and not even to say that additional complexities from more sophisticated biogeochemical formulations (e.g. methane dynamics, and microbial dynamics) are to be introduced in the future. If the authors do want to convince the readers that they developed a critical

and robust tool to upgrade the biogeochemical modeling for a global model like CLM, I would highly suggest they show that their model can run at large scales or even the whole globe.

Fourth, the authors mentioned a lot about reactive transport modeling (RTM) in soil biogeochemical modeling, it is however never clear to me that whether the authors are actually using the RTM capability of PFLOTRAN. If they are only solving a batch model, then is it using PFLOTRAN a waste of effort? Or the authors did use the RTM capability of PFLOTRAN to do a 1D soil biogeochemical modeling (section 3.2 does seem to indicate so), then the authors should state this clearly and provide the 1D RTM equations they are trying to solve. Also, they should state this earlier in the paper.

Finally, I have some weird feeling for the residual concentration that the authors use to model reactant availability. According to law of mass action, and thermodynamics of chemistry kinetics (which is thoroughly discussed in Langmuir's book Aqueous Environmental Geochemistry), the residual concentration is not necessary small to stop a reaction. Therefore, the residual concentration as it is proposed here is more like a funky hack that can be avoided in other methods. They somewhere referred to the study by Grant (2013), but the authors did not explain why they used values of half saturation coefficients and residual concentrations much smaller than that in Grant (2013), which is based on Barber and Silberbush (1984), who I believe synthesized their values based on empirical observations.

Because of the above issues, I would suggest the authors do a thorough revision and resubmit their paper for further review. In my opinion, the authors are a strong team in performing such type of study, and they should be more than able to address the above concerns I identified.

Other minor comments: P10637: L7, here you mentioned number of grid cells, does it mean you are solving the biogeochemistry at least for a 1D soil column? Please clarify.

P10641, L1-6, Does the false convergence mean the implicit scheme is not problem

size scalable? For clipping, can you give some advice how one should choose a STOL to ensure correct convergence for the many grid cells in a global simulation. Or is it impossible to find such a STOL.

L10641, L15-16. This unintended consequence makes more worried how others could easily apply and extend your scaling methods for a large-scale model.

P10643, L5-8: does this mean your competition algorithm is wrong? Or is it simply a numerical artifact from implicit scheme? Will including more biogeochemical processes make this issue even more severe?

P10644, L22-25, now it does seem more processes will make the false consumption problem more severe.

P10646: L24-26, now it seems weird to me why you set o_scalar to 1. A RTM should be able to resolve gas diffusion by design, otherwise how could you claim CLM-PFLOTRAN will serve the purpose to do improved soil biogeochemical modeling, which is essentially multiphase?

L10649, L23-24: Please explain why you did not track mass balance errors, did tracking the error crash the model?

From Figures 4-6, I saw non-trivial differences when you are using the different half saturation constants, so how will you specify those parameters for a global simulation?