Geosci. Model Dev. Discuss., 8, C3947–C3950, 2016
www.geosci-model-dev-discuss.net/8/C3947/2016/

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.

G. Tang et al.

tangg@ornl.gov

Received and published: 3 February 2016

We appreciate the referee's review comments.

Comment: This is a technical paper that deals with numerical issues arising upon coupling of reactive transport models to global land surface models. Upon accepting this review, I assumed that the paper would focus on biogeochemical mechanisms, but this is not at all the case. The title is quite misleading, as this manuscript is not about codes that represent biogeochemistry in global land surface models in more mechanistic ways, but rather about possible numerical issues that arise during this coupling and how to solve them. Therefore, the intended audience is unclear. Yet, the

manuscript will not be of general use for researchers that are interested in the types of biogeochemical mechanisms to be represented in LSMs. Because of that, I am not sure whether this paper fits the scope of the journal.

Response: We agree that the title is a bit misleading. It is revised to (highlighted in page 1 in the marked version, supplement to response to referee 1):

"Using reactive transport codes to provide biogeochemistry representations in land surface models: A proof of concept with CLM-PFLOTRAN 1.0"

We also agree that this manuscript focuses on numerical issues. However, the numerical issues rise because we switch from explicit to implicit methods to better represent nonlinearity, and mechanistic representation requires explicit representation of nitrogen limitation on immobilization and uptake. Both are small but critical steps toward increasingly mechanistic representation of soil biogeochemistry. The manuscript exemplifies the need to 1) represent every rate limiting processes explicitly for flexibility and robustness; and 2) avoid discontinuities in rate formulae with respect to concentrations. In addition, it shows that complex rate formula, such as the empirical N2O production rate that was assumed to be proportional to labile carbon, and was formulated as a function of decomposition rate of Lit1C, Lit2C, Lit3C, Lit1N, lit2N, Lit3N, SOM1, SOM2, SOM3, SOM4, and ammonium concentration, brings in complex nonlinear relationship that may require small time step size to step through. It is desirable to simplify these rate formulae unless the sophistication is dictated by real physical or chemical requirements. We think this information, and the proof of concept of using RTM in CLM are useful and interesting for researchers who are interested in improving the representation of soil biogeochemistry. As our models become more mechanistic, which generally means more nonlinear, implicit methods will become more common, and these results will help guide that development.

GMD description for development and technical papers includes:

"These papers describe technical developments relating to model improvements such

as the speed or accuracy of numerical integration schemes as well as new parameterisations for processes represented in modules."

We are directly addressing speed and accuracy of a numerical integration schemes. In addition, it also includes:

"Development and technical papers usually include a significant amount of evaluation against standard benchmarks, observations, and/or other model output as appropriate."

for which we compare our predictions with CLM.

For these reasons, we think this manuscript fits in the scope of this journal, and has a potential to be very useful in the future for the land surface model community.

Comment: My main concern is that, based on the current manuscript it is not possible to recreate the analyses, as I do not fully understand how this coupling has really been implemented, nor the specifics of the CLM-PFLOTRAN simulation.

Response: We understand the challenge in reproducing the analyses as compiling and running CLM is nontrivial, and adding PFLOTRAN does not make it easier. We agree that the description about the coupling is concise. However, we do provide the source code, the scripts and directions to reproduce the results, which is available at

`http://web.ornl.gov/filedownload?ftp=e;dir=uP12a3zaPC7j`

We are happy to assist the reviewers and interested users to reproduce the results.

Comment: Also, it is not clear how the results have to be used – should one implement all these procedures (clipping, scaling, log) and select one of them based on the parameter settings?

Response: We fully agree that this was not clear in the original submission. We make significant changes to the manuscript to clarify it. In the abstract, we add

"Overall, log transformation can be used for accuracy while loosening STOL, using clipping or scaling can increase efficiency"

In the summary and conclusion section, we add

"To cover a wide range of many orders of magnitude concentrations in soil biogeochemistry and for accuracy and robustness, the modelers can start with the log transformation method. If it is desirable to reduce the computational time, STOL can be loosened, and clipping can be used without log transformation. The scaling method is another option but with strict STOL requirement. As the accuracy is checked and logged in CLM for carbon and nitrogen mass balance, the modelers can assess the tradeoff between efficiency and accuracy in CLM-PFLOTRAN and select their optimum."

Comment: Finally, have the authors thought about higher order backward schemes – do they have the same defects as the backward euler method?

Response: Yes, we do believe the same issues would come into play. PFLOTRAN currently uses the backward Euler method and does not have an option for higher order methods.

Please also note the supplement to this comment:
http://www.geosci-model-dev-discuss.net/8/C3947/2016/gmdd-8-C3947-2016-supplement.pdf

---

Interactive comment on Geosci. Model Dev. Discuss., 8, 10627, 2015.