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Comment

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.

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We thank the referee for spending valuable time in reviewing our manuscript and providing detailed comments. We are gratified that the referee recognized that what we were trying to do is “a very important step towards improved land biogeochemical modeling for earth system models”. We share the referee’s intermediate-term vision of land-surface models that take full advantage of PFLOTRAN’s reactive transport capability, including oxygen dynamics and gas and liquid phase transport running at the global scale.

However, it is important to recognize that CLM and PFLOTRAN are both complex

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codes based on incompatible numerical formulations, and that merging these two codes in a robust and reliable way requires several implementation hurdles be overcome. This manuscript focuses on reconciling the numerical schemes (explicit for CLM and implicit for PFLOTRAN and other major RTMs). In addition, we demonstrate that the coupled CLM-PFLOTRAN produces predictions that are consistent with the widely used CLM carbon-nitrogen model (proof of concept). This is an important first step toward that longer term vision.

Now that the numerical issues are resolved and the implementation is in good shape, we are in the position to activate the full range of capability in PFLOTRAN. Research using this new capability is ongoing and will be reported in future publications that focus on science results instead of numerical implementation issues. This manuscript is the first of several that demonstrate the use of reactive transport models (RTM) in land surface models.

We revise the manuscript to further clarify the scope at first to address the main comments 1, 2, and 4. For main comments 3 and 5, we add a paragraph in the summary and conclusion section to address concerns about numerical issues. Finally, we provide detailed responses to each of the comments. The revisions are highlighted in the marked version (supplement to this comment) and a clean final version (supplement to comments by referee 2) is also uploaded. These revisions improve the manuscript and we value the referee's help.

Response to comments 1, 2, and 4: clarify the scope (R1)

We recognize that the original title, and to a lesser extent the abstract, did not properly convey the scope of the work. We revise the title to

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

(page 1 in the marked version).

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We also revise the abstract to

“We explore coupling to a configurable subsurface reactive transport code as a flexible and extensible approach to biogeochemistry in land surface models. A reaction network with the CLM-CN decomposition, nitrification, denitrification, and plant uptake is used as an example. We implement the reactions in the open-source PFLOTRAN code and couple it with the Community Land Model (CLM). To make the rate formulae designed for use in explicit time stepping in CLM compatible with the implicit time stepping used in PFLOTRAN, the Monod substrate rate-limiting function with a residual concentration is used to represent the limitation of nitrogen availability on plant uptake and immobilization. We demonstrate that CLM-PFLOTRAN predictions are consistent with CLM4.5 for Arctic, temperate, and tropical sites.

Switching from explicit to implicit method increases rigor but introduces numerical challenges. Care needs to be taken to use scaling, clipping, or log transformation to avoid negative concentrations during the Newton iterations. With a tight relative update tolerance (STOL) to avoid false convergence, an accurate solution can be achieved with about 50% more computing time than CLM in point mode site simulations using either the scaling or clipping methods. The log transformation method takes 60–100% more computing time than CLM. The computing time increases slightly for clipping and scaling; it increases substantially for log transformation for half saturation decrease from 10^{-3} to 10^{-9} mol m⁻³, which normally results in decreasing nitrogen concentrations. The frequent occurrence of very low concentrations (e.g. below nanomolar) can increase the computing time for clipping or scaling by about 20 %, double for log transformation. Overall, log transformation can be used for accuracy while relaxing STOL, using clipping or scaling can increase efficiency.

As some biogeochemical processes (e.g., methane and nitrous oxide reactions) involve very low half saturation and thresholds, this work provides insights for addressing non-physical negativity issues and facilitates the representation of a mechanistic biogeochemical description in earth system models to reduce climate prediction uncertainty.”

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as highlighted in page 2-3 in the marked version. These revisions further clarify the scope of this work. Following-up research on oxygen dynamics and gas phase transport (comment 1), plant nitrogen allocation (comment 2), and using full capability of PFLOTRAN (comment 5) is under way, but is beyond the scope of this manuscript.

Response to comments 3 and 5: clarify the numerical issues (R2)

We add in the abstract (highlighted in page 2 of the marked version):

“Overall, log transformation can be used for accuracy while relaxing STOL, using clipping or scaling can increase efficiency”

In the conclusion and summary section (page 10653 between the first and second paragraphs), we add the follow paragraph (highlighted in page 26 in the marked version) to address the referee’s concerns.

“These computational issues arise because we switch from the explicit methods to the implicit methods for soil biogeochemistry. We use small half saturation (e.g., 10^{-9}), residual concentration (e.g., 10^{-15} , slightly above machine zero), and large initial time step size (e.g., 0.5 h) to exemplify the causes of the accuracy, efficiency, and robustness issues. For the zero order rate formulae in CLM, the limitation of reactant (nitrogen in this work) availability needs to be explicitly represented for robustness and flexibility. With mechanistic representations, reaction stops or reverses when the rate limiting reactants decrease to a threshold, or when the reaction becomes thermodynamically unfavorable, nullifying the need for half saturation and residual concentration. Before our representations are sufficiently mechanistic, a small residual concentration (say 10^{-15}) serves as a safeguard to avoid failure for the log transformation method and unnecessary efficiency and accuracy loss for the clipping and scaling methods unless a smaller residual concentration is dictated by physical and chemical conditions.

For reactions with very low half saturation and residual concentrations, e.g., redox reactions involving O_2 , H_2 , and CH_4 , STOL can be set to zero to avoid false convergence,

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at the risk of potential increased computational cost. Increasing STOL (say to 10^{-12}) decreases computing time at the risk of potential accuracy loss. 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 relaxed, 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.”

These revisions clarify 1) why we examine use of small half saturation and residual concentration, 2) that we do uncover the underlying reasons for the numerical issues, and 3) that modelers can balance the accuracy and computational cost in CLM-PFLOTRAN, therefore, address comment 3 and 5.

Detailed responses:

Comment 1

Comment: 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 Arctic and in the further studies they envisioned in the paper.

Response: We agree that oxygen dynamics is critical but it is beyond the scope of this work. The work described here is a necessary first step in that direction.

Comment: Likewise, this raises concern if the authors' model could actually represent denitrification in a relatively reasonable way?

Response: Denitrification representation is detailed in Appendix A3 (p10657). We are working on more mechanistic representations.

Comment: 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.

Response: We did not explicitly represent oxygen dynamics in this work.

Comment: 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.

Response: This was not intended to be a "conclusion" of this work but rather a restatement of what we regard as a consensus in the RTM community. We add the following citations to support it (highlighted in page 27 of the marked version).

Yeh, G.T. and V.S. Tripathi, 1989, A critical evaluation of recent developments in hydrogeochemical transport models of reactive multi-chemical components. *Water Resources Research* 25, 93-108

Steeffel, C. I., et al. (2015), Reactive transport codes for subsurface environmental simulation, *Comput Geosci*, 19(3), 445-478.

Zheng, C., and G. D. Bennett (2002), *Applied Contaminant Transport Modeling*, Wiley.

Comment 2

Comment: 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.

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Response: The reviewer is correct to point out that observations of nitrogen allocation within plants between the time of uptake from the soil and incorporation into new growth are inconsistent with the notion of instantaneous allocation. Our text describing the calculation of plant N demand in CLM4 (p. 10639, lines 13-18) did not include a full description of model algorithms predicting nitrogen dynamics once plant N demand has been reconciled with plant-microbe competition and an actual uptake amount is determined. In fact, there are both carbon and nitrogen storage state variables associated with all of the plant tissue types tracked by the model (leaves, fine roots, woody tissue), as described in Oleson et al. (2013) and cited in this section of the text. We are by no means satisfied with the present level of detail in the representation of these storage and transport processes in the plant model – this is an active area of research and we have proposed some new mechanisms to augment the transport and storage representations used in CLM4, work which is currently under review at another journal. To help eliminate confusion, we modified the text to indicate the presence of the carbon and nitrogen storage pools in CLM4. Specifically, we add

“Once the plant nitrogen uptake is calculated in PFLOTRAN, it is returned to CLM, which allocates the uptake among, e.g., leaf, live stem, dead stem, etc., and associated storage pools (Oleson et al. 2013).”

as highlighted in page 12 of the marked version.

Regarding the suggestion that Zaehle et al. (2014) can be used as support for an argument against the methods used in CLM4, we agree that there are some model-data metrics explored by Zaehle et al. (2014) for which CLM4 scored poorly, but also other metrics for which CLM4 was closer to observations than most of the other models. Quoting from the abstract of that paper: “. . .none [of the 11 models] was able to simulate both the sustained 10-yr enhancement at Duke and the declining response at ORNL. . .” For example, while the response of CLM4 predicted NPP to enhanced CO₂ in the first year of the Duke and ORNL experiments was too weak at both sites, the first year response of N uptake was better than most other models. Comparing first year

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response with the final five years of the Duke and ORNL experiments, CLM4 outperformed most models on most carbon and nitrogen metrics. Our point here is that none of the models did particularly well on all metrics at both sites in all time periods, and so it seems wrong to assert that Zaehle et al. (2014) argues strongly for or against a particular treatment of the coupled carbon-nitrogen dynamics from any of the 11 models evaluated in that study.

Comment 3:

Comment: Third, although the authors spent a lot of time in discussing how they could successfully avoid unphysical negative values for species like NH_4 and NO_3 , 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.

Response: We think this is a misinterpretation of the results. The purpose of testing a range of half saturation, residual concentration, and tolerances is not to struggle to make it work, but to stretch the limits, and reveal why numerical issues may arise so that we can provide guidance to others in obtaining accurate, efficient, and robust solutions. Recall that our longer term goal is to include oxygen and methane dynamics, and representations of these processes have the potential to lead to very small concentrations. Thus, understanding numerical issues related to convergence and time step size with small concentrations is important for enabling more advanced applications. As stated in page 10639 line 4 in the original submission for simple tests,

“We start with $k_m = 10^{-6}$ M or mol m^{-3} , and residual concentration $=10^{-15}$ M or mol m^{-3} for plants and microbes. To further investigate the nonphysical solution negativity for the current study and for future application for other reactants (e.g., H_2 and O_2) where the concentrations can be much lower, we examine k_m from 10^{-3} to 10^{-9} in our test problems. The k_m is expected to be different for different plants, microbes, and for ammonium and nitrate. We do not differentiate them in this work as we focus on numerical issues.”

As stated in page10647 line 6 in the original submission for coupled CLM-PFLOTRAN simulations, “To assess the sensitivity of various preference levels for ammonium and nitrate uptake, and downregulation levels, we examine $k_m = 10^{-3}$ to 10^{-9} mol m⁻³.”

Namely, our goal is not to avoid negative concentration per se, but to avoid false convergence or divergence as a result of a combination of, say, close to machine zero concentrations, large initial time step size, loose STOL, etc. We identify these causes and provide solutions (R2).

Comment: 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.

Response: To clarify confusion, we add in the abstract:

“Overall, log transformation can be used for accuracy while relaxing STOL, using clipping or scaling can increase efficiency”

Clipping can introduce mass balance errors for the explicit method, as we stated in page 10640 line 16 in the original submission:

“Even though clipping avoids convergence to the negative solution, the ammonium consumption is clipped, but the PlantA (Reaction AR13) production is not clipped (spreadsheet case5), violating the reaction stoichiometry. This results in mass balance errors for explicit time stepping (Tang and Riley, 2015). For implicit time stepping, additional iterations can resolve this violation to avoid mass balance error.”

In implicit methods, this can be resolved by additional iterations. It is the false convergence, not clipping per se, that causes the mass balance error. No mass balance is introduced as long as the solution is properly converged. It can be avoided by using a small STOL, as stated in the abstract (page 10629 line 14):

“With a tight relative update tolerance to avoid false convergence, an accurate solution can be achieved with about 50% more computing time than CLM in point mode site simulations using either the scaling or clipping methods.”

and in page 10650 line 13, “Tightening STOL from 10^{-8} to 10^{-12} , the reported greater than 10^{-8} g m⁻³ mass balance errors are eliminated.”

As we mentioned in the abstract, text, and summary, the log transformation method is robust, but requires more computational cost, which increases with decreasing concentrations (R2).

Comment: 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.

Response: This is why we think this is an important issue, and go to the bottom of this issue in this manuscript. As we find the root cause, we know how to avoid the issue in more sophisticated applications. R2 discusses the tradeoff between accuracy and efficiency. We test at the Arctic, temperate and tropical sites. We are confident about the statement

“As physical half saturation ranges from 10^{-5} to 10^{-6} M for nitrogen, and the detection limits are often above 10^{-9} M, our results indicate that accurate, efficient, and robust solutions for current CLM soil biogeochemistry can be achieved using CLM- PFLO-TRAN.”

in summary and conclusion section in the original submission. We are working on methane, microbial dynamics, and global scale simulations. Again, we think they are

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beyond the scope of this work (R1). Additional response and revisions are described in earlier (R2).

Comment 4

Comment: 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.

Response: we add the following the first paragraph in page 10633 (highlighted in page 6 in the marked version):

“This work focuses on the PFLOTRAN biogeochemistry, with CLM solving the energy and water flow equations and handling the solute transport (mixing, advection, diffusion, and leaching). Here, we focus on how reactions are implemented and thus only use PFLOTRAN in batch mode (i.e. without transport). However, PFLOTRAN’s advection and diffusion capabilities are fully operational in the CLM-PFLOTRAN coupling described here.”

Comment 5

Comment: 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.

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Response: we agree that it is not necessary for some methods, for example, the explicit methods as we stated in page 10631 line 7

“The limitation of nitrogen availability on plant uptake and immobilization is simulated by a demand-based competition: demands are downregulated by soil nitrogen concentration (Oleson et al., 2013; Thornton and Rosenbloom, 2005). This avoids negative concentrations and does not introduce mass balance errors (Tang and Riley, 2015) as CLM uses explicit time stepping.”

Further, in our earlier response (R2), we acknowledge that thermodynamics normally stop the reactions before a concentration goes to zero. In these cases, half saturation and residual will not be necessary. We also state that we use small values (slightly above machine precision) to test the limit of the implicit methods (R2). We add

“Before our representations are sufficiently mechanistic, a small residual concentration (say 10^{-15}) serves as a safeguard to avoid failure for the log transformation method and unnecessary efficiency and accuracy loss for the clipping and scaling methods unless a smaller residual concentration is dictated by physical and chemical conditions.”

Overall, it is not a funky hack, but a safeguard that has physical meaning: if there is no nitrogen, plants or microbes will not be able to take any.

Comment: 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.

Response: This is also addressed in response to comment 3. Again, our purpose is to resolve these numerical issues in a more general way rather than determining the values we should use in a particular application, which is why we scanned the half saturations and residual concentrations across a wide range. Recall that our long-term goal is to include oxygen and methane dynamics, which may result in very small

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concentrations, so it is important to have this basic understanding of the algorithm robustness.

Responses to the Minor Comments

Comment: 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.

Response: See response to comment 4.

Comment: 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.

Response: If STOL is zero, the false convergence discussed here can be avoided. The consequence is decreased efficiency. R2 provides discussion about the tradeoff between accuracy and efficiency.

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

Response: As described in R2, “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.”

It has been used to solve large scale models in RTM literature. Our contribution is that we find the seldom-reported implication, and ways to avoid it.

Comment: 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?

Response: We do not think that the competition algorithm is wrong. We want to have

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the freedom to try alternative algorithms. You can say it is a numerical artifact. We consider it as increasing nonlinearity, which requires small time step size to march through. Like the phase change, turbulence, combustion etc. problems, highly nonlinear problems are numerically challenging to solve.

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

Response: similar to previous response: it is because the nonlinearity in the representation becomes severe under certain conditions. The false convergence is due to a loose STOL to allow large time step size to step through a nonlinear transition.

Comment: 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?

Response: the `o_scalar` in CLM4.5 is 1 unless the methane module is turned on. As we respond to comment 1, 3, and 5 (R1), this is so.

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

Response: The sentence reads: “Numerical errors introduced due to false convergence in clipping, scaling, or log transformation are captured in CLM when it checks carbon and nitrogen mass balance for every time step for each column, and reports 10^{-8} g m⁻² errors.”

We add (highlighted in page 22 in the marked version):

“(to limit the log file size as the simulation durations are hundreds of years and the time step size is half an hour)”

The error is checked for every time step for each column in CLM, not in PFLOTRAN. If every error is logged, it will create huge log files as we ran the simulations with a

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half-hour time step for hundreds of years. Tracking the error did not crash the model unless the storage space is running out.

Comment: 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?

Response: We revise the first two sentences in the last paragraph in page 10649 from

“Except for the tropical site where the higher k_m of 10^{-3} mol m^{-3} results in lower immobilization, higher accumulation of LITN, and higher ammonium and nitrate concentrations during the spin-up (Fig. 6), the range of k_m values (10^{-6} , and 10^{-9} mol m^{-3}) generally has limited impact on the overall calculations except that the nitrogen concentrations drop lower with lower k_m values (e.g., inset in Figs. 4 e and f and 5e).”

to

“The higher k_m of 10^{-3} mol m^{-3} results in lower immobilization, higher accumulation of LITN, and higher ammonium and nitrate concentrations than k_m of 10^{-6} mol m^{-3} during the spin-up for the tropical site (Fig. 6). This is not surprising as the higher k_m of 10^{-3} mol m^{-3} poses a stricter limitation on the extent that plants and microbes can take from the soils. A range of k_m values (10^{-6} , and 10^{-9} mol m^{-3}) generally has limited impact on the overall calculations except that the nitrogen concentrations drop lower with lower k_m values (e.g., inset in Figs. 4 e and f and 5e).”

We consider that determining k_m for use in global simulations is beyond the scope of this work (R1).

Please also note the supplement to this comment:

<http://www.geosci-model-dev-discuss.net/8/C3932/2016/gmdd-8-C3932-2016-supplement.pdf>

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