**Geoscientific
Model Development
Discussions**

## *Interactive comment on* "CLM4-BeTR, a generic biogeochemical transport and reaction module for CLM4: model development, evaluation, and application" *by* J. Tang et al.

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We thank the positive and comprehensive comments from the reviewer. We address the comments carefully below.

*I am aware that different (sub-)disciplines might have different terminologies, but I object using throughout the manuscript the term 'tracer' as synonym for any (reactive) chemical species.*

Reply: One of our motivations for the presented development is to design a model to couple the belowground biogeochemistry with the atmospheric biogeochemistry and transport processes. Therefore, in order to be consistent with the terminology used by

the atmospheric tracer transport modeling community, we believe 'tracer' is a proper terminology that could avoid some ambiguities in our future development and application of the model, while balancing the terminology used by the belowground biogeochemistry community who are working at various spatial and temporal scales.

*The coupling between the different model parts needs to be introduced in a better way. Which part is simulating which processes, and which information is exchanged between the different parts? Here a schematic or flow chart type figure might be helpful – Figure 1 is not suitable for this. The entire concept should also be comprehensible for readers not familiar with CLM4. It is also not clear what the mentioned 'hierarchy of subsurface biogeochemical models' is supposed to be.*

Reply: We recognized that the major development of CLM4 has been documented by many publications spread in the literature (for a list of relevant publication, see http://www.cesm.ucar.edu/publications/bibliography.html). Thus we consider Figure 1 as sufficient to present a complementally description to those existing developments. We agree that we should describe in a more straightforward way how the different components of CLM4 are tied to our new development presented in this study. So we added a few sentences to cover this description. We also clarified what the phrase 'hierarchy of subsurface biogeochemical models' means in the revision. Briefly, we designed our new module with the flexibility to use subsurface chemistry models with different complexities, spanning those that use explicit representation of microbial community population dynamics (e.g., trait-based microbial decomposition model) to those that uses simple first order parameterizations (e.g., CENTURY model).

*There is a certain inconsistency in introducing the new module. It is supposed to be a generic biogeochemical module but its description is limited/focussing to/on a certain set of processes. Some clarification would be needed here: which processes are/can be considered (e.g.,. which are the 'physical, biophysical, chemical, biochemical, and biological dynamics' mentioned on P 2710, L 19), which are the limits of flexibility etc.? It would be helpful to have such general issues described first before going into details.*

Reply: We revised our introduction to more clearly indicate the range of processes that can be integrated in the model. Broadly, because CLM4-BeTR was designed to be as general as possible, biogeochemical process that can be represented as a function of soil moisture, soil temperature, soil aqueous or gaseous advection, or soil structure can be included, as well as interactions with microbes.

*The model considers (1D) vertical transport, only. Some words on how this can be implemented in the simulation of large scale systems with horizontal resolution would be helpful.*

Reply: CLM4 currently has no capability to move tracers horizontally in surface water or groundwater. However, the model does calculate these water fluxes, so we have integrated the capability to simulate horizontal tracer transport once the proper horizontal flux treatments are integrated in CLM. We also added some guidelines on how to implement our new development in models that have horizontal resolutions.

*There is a large number of biogeochemical models for subsurface systems available in the literature. Some discussion to which extent the presented module and its underlying concept are similar or different to these models would be useful.*

Reply: We added some discussion on the difference between our developments and other existing developments in the revision.

*The shown analytical solutions provide a good reference for the conservative transport of species, but the accuracy of the model for reactive transport is not shown. One could use numerical results from an existing biogeochemical model to generate some references to test the presented module.*

Reply: We agree with the reviewer that a more rigorous evaluation for the accuracy of our development should compare its results with that from an existing reactive biogeochemical model, which has already been well evaluated. However, for a couple of reasons, we recognize that such a comparison is currently not feasible for the CLM4 model

we are trying to improve. For instance, we do not have access to a high-resolution reactive biogeochemistry model that has similar components being represented in CLM, e.g. vegetation dynamics, boundary layer parameterization, permafrost dynamic and many others. As a matter of fact, our development is in parallel with the development of a few high-resolution reactive biogeochemistry models for the NGEE-Arctic experiment. In the future we plan a comprehensive evaluation of CLM components, including soil physics (mass and energy flow), snow dynamics, and belowground biogeochemistry, under different setups with these high resolution models and new datasets from the NGEE and other relevant projects.

*The forest soil example demonstrates the potential of the model, but to my opinion the discussion of the differences between the production and effluent fluxes is a bit too extensive (and/or might be directed in a slightly different direction): most differences are actually quite small and it is not very surprising that $CO_2$ released at a given depth needs some time to reach the atmosphere. In turn the time lag between peaks of production and of effluent fluxes could serve as consistency check of the results using the considered length scales and transport dynamics. When using different $CO_2$ species according to their origin, how was it ensured that reactive processes depending on the (total) $CO_2$ concentration are expressed properly?*

Reply: We agree with the reviewer that more detail is needed to highlight our point that production does not in general equal surface efflux. In the revision, we stressed that this discrepancy was mostly manifested at sub-daily time scale for the Harvard forest site we applied the model to. When using different $CO_2$ species according to their origin, we assumed there were no interactions between these different $CO_2$ species, an assumption that is widely used to model isotopic trace gas transport. This last point is also supported by the fact that there is no chemical interaction between these different $CO_2$ species.

*P 2706, L 15: Point (1) is actually not shown. The results appear reasonable but their accuracy is not demonstrated.*

Reply: See our previous description on the parallel model development for the NGEE project.

*P 2708, L 25f: This statement is not true in general. There are plenty of biogeochemical models able to simulate specially resolved and simultaneously various complex reactive transport processes in the subsurface.*

Reply: We agree, but there are few that are integrated with a global climate model. We have corrected the statement to reflect this caveat.

*P 2713, Equation 8: Is it correct to integrate the reaction part only once for a $\Delta t/2$ time step?*

Reply: We corrected this typo in the revision.

*P 2714, L 1-14: As species are only coupled via the reactions they are involved in but their transport is not depending on other species, it should not matter anyway in which order the transport of different species is simulated within a time step.*

Reply: In theory, the order should not matter. However, when the problem is treated numerically, particularly with large time steps, the operator splitting error will arise, which says the order does matter. We implemented the Strang split approach in a way that tries to minimize the numerical error from operator splitting.

*P 2714, L 17ff: How is the water distribution determined? Further up (L 3) it is stated that Richards' equation is used for the flow simulation. This implies that the water saturation is dynamically determined and that there cannot be explicit wetting fronts somewhere inside a grid layer but gradual variations in water saturations following the numerical discretization scheme. In any case, Figure 2 is not very comprehensive.*

Reply: CLM4 determines water distribution through multiple steps. First, the vertical distribution of soil moisture is updated with infiltration, evaportranspiration, and drainage. Then lateral drainage and interaction with the aquifer is carried out to update the water table. Occasionally, the diagnosed water can be within a grid cell rather

than at the interface of two consecutive numerical grids. We designed our approach to account for this situation. We also hope our approach will be useful for models that can accurately resolve the wetting front.

*P 2715, Equation 11: Explain A, B, and $\Delta z_a$, j, b. Also, when considering different diffusion coefficients for each species, diffusion would have a chromatographic effect. This is ok for the aqueous phase and for low concentration species in the gas phase but for major gas phase species (e.g., $O_2$ and $N_2$) this would lead to a variation of the soil air composition and the partial pressure of the gas phase would vary in space (also in the absence of any other processes). Does the advective gas phase transport account for that or is such variation of soil air composition avoided otherwise?*

Reply: For well-aerated condition we adjusted the overall soil gas pressure to atmospheric pressure. When the surface soil surface is ice-frozen, the gas pressure is allowed to build up and all gases are mixed vertically (such that the detailed transport mechanism is not important).

*P 2717/2718: Not being familiar with CLM4 this passage and Figure 3 are not understandable. Provide a more comprehensible description of the used assumptions.*

Reply: We put a more straightforward description in the revision.

*P 2720, L 15: What is a 'tracer tracking capability'? The ability to compute the spatio-temporal distribution of species and their fluxes is an inherent feature of every reactive transport model.*

Reply: We agree that the ability to compute the spatio-temporal distribution of species and their fluxes is an inherent feature of every reactive transport model. However, it is a new feature for large-scale land models, such as CLM4. We stress this capability and hope this will stimulate more similar developments to improve climate models.

*P 2721, L 4: Are these velocities correct? If yes, the transport would be diffusion dominated, which is not the common case in soil systems. With such water flow veloc-*

*ities ($10^{-7}$ m/s is less than 1 cm per year) there would hardly any drainage of rainfall precipitation and no groundwater recharge.*

Reply: the velocities are correct. $10^{-7}$ m/s equals about 3.7 m/year, so there is sufficient drainage and groundwater recharge happening for tracer loss through those pathways.

*P 2722, L 7ff: Provide more details: reactions, processes etc. Are there any sinks for $CO_2$ considered, is the interaction of $CO_2$ with water chemistry considered?*

Reply: In the soil, there is no biological sink of $CO_2$. We considered the dissolution of $CO_2$ into water. However, the dynamic evolution of pH and the interaction of $CO_2$ with different cations are not currently accounted for.

*P 2723, Section 4.1: If the purpose is to demonstrate the accuracy of the numerical scheme one should show first results with a sufficiently high spatial resolution. If a specific coarse distribution is still acceptable would also depend highly on the dynamics of the considered processes and the resulting spatial gradients. From the examples shown here one should not make any general conclusions concerning the spatial and temporal resolution needed for other potential applications.*

Reply: We revised the tone of our conclusion to be consistent with this reasonable assertion.

*P 2725, Section 4.3: Why is $CO_2$ form the atmosphere considered as a potential source for an efflux of $CO_2$ into the atmosphere?*

Reply: $CO_2$ can intrude into the soil from the atmosphere. This mechanism is important in explaining, for example, the 18O isotopic content of atmospheric $CO_2$ (Tans, 1998; Riley et al. 2002). Our tagged $CO_2$ simulation could potentially provide a way to check how useful the isotopic measurements are for understanding belowground biogeochemistry.

*P 2725, L 16 – P 2726 L 11: As mentioned above, this passage can be shortened.*

*In turn some words on the $CO_2$ mass balance saying if all of the produced $CO_2$ is leaving the system towards the atmosphere would be helpful. I am also wondering if the mentioned discrepancies depend on the used discretization scheme.*

Reply: we agree that the mentioned discrepancies depend on the applied discretization scheme. However the discrepancy should be robust, as some other studies also identified similar discrepancies (Moncrieff and Fang, 1999). The significance of such a discrepancy depends on how one interprets empirical studies, which are used to parameterize the soil $CO_2$ production. As a result, the impact of the discretization scheme is less important than the uncertainty from the parameterized soil biogeochemistry.

Other minor comments, which we carefully addressed in the revised manuscript: *P 2706, L 8ff: Sentence unclear. Or does it mean that the model considers water based advective transport of dissolved species : : : ?*

*P 2706, L 18: What are 'seasonal cycles of soil physics and biogeochemistry'?*

*P 2707, L18ff: This passage is correct but should be shortened.*

*P 2708, L 5: Clarify: 20 cm depth?*

*P 2708, L 5ff: The 'characteristic time' eventually depends on the process not on the model.*

*P 2708, L 9: Do not start sentences with 'And'.*

*P 2708, L 22: No new paragraph here*

*P 2709, L 1: Reword or clarify: a system with four species is not really complex. P 2709, L 5: 'sportive species'?*

*P 2709, L 11f: Again, in general there are models considering fast and slow processes. They might not have been used in the given context.*

*P 2709, L 23f: Clarify: the consideration of 'ocean, atmosphere : : :' is a feature of the*

*CESM1.0 model not of the module presented here.*

*P 2711, L 4ff/Equation 1: This equation is known in the literature as advection-diffusion-reaction equation.*

*P 2711, L 11: Introducing diffusivies for solid species is rather odd. Some explanation is give later on in the manuscript, but this explanation (or some reference to it) should be given already here.*

*P 2711, L 15: It sounds not very handy if the positive z direction is upward. Also, further down in the manuscript (P 2721, L 2) the positive velocity direction is downward.*

*P 2711, L 16ff: This statement is not clear.*

*P 2712, L 3ff: The purpose of this passage is not clear.*

*P 2714, L 16: Change to ': : : Crank-Nicolson approach (e.g., Pruess et al., 1986) : : :'.*

*P 2716, L 20f: Not clear.*

*P 2719, L 1f: To me the term 'diagnostics' does not make sense here.*

*P 2719, L 2: Change to ': : : fluxes along different : : :'.*

*P 2719, L 9: If the presented concept is supposed to be generic, why considering a fixed number of soil layers with a given thickness here?*

*P 2719, L 26: 'considered prognostically'?*

Reply: we carefully integrated those comments in our revised paper.

References

Moncrieff J.B.; Fang C, A model for soil $CO_2$ production and transport 2: Application to a florida Pinus elliotte plantation, Agricultural and Forest Meteorology, 1999

Riley, W. J., C. J. Still, M. S. Torn, and J. A. Berry, A mechanistic model of $H_2^{18}O$ and

$C^{18}OO$ fluxes between ecosystems and the atmosphere: Model description and sensitivity analyses, Global Biogeochem. Cycles, 16(4), 1095, doi:10.1029/2002GB001878, 2002.

Tans, P. P. (1998), Oxygen isotopic equilibrium between carbon dioxide and water in soils. Tellus B, 50: 163–178. doi: 10.1034/j.1600-0889.1998.t01-1-00004.x