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GMDD

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Interactive Comment

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

Anonymous Referee #2

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The manuscript "CLM4-BeTR, a generic biogeochemical transport and reaction module for CLM4: model development, evaluation, and application" (gmd-2012-69) by Tang et al. presents the coupling of a land model with a new simulation module capable of modeling 1D reactive transport in soils. The manuscript introduces the new module, its underlying concepts and their numerical implementation. Model performance is tested using analytical results of two conservative transport scenarios and the model is subsequently applied for the simulation of the dynamics CO2 production and of the associated atmospheric CO2 emissions from a forest soil.

Soils represent an important compartment of terrestrial systems and the spatially resolved consideration of biogeochemical processes in this compartment is certainly needed for simulating the cycling of carbon or any element or reactive species of interest. The presented model extension is thus a significant step forward in the simulation potential of the CLM4 land model. The applied modeling concept appears technically sound and the presented simulation results support the accuracy and applicability of the model. I thus generally support publication of this study. I do however think that the presentation of the new module should be improved, that the model performance should be further verified and that some passages of the Results and discussion Section should be written more to the point.

General comments:

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.

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.

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.

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

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be helpful.

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.

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.

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 to extensive (and/or might be directed in a slightly different direction): most differences are actually quite small and it is not very surprising that CO2 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 CO2 species according to their origin, how was it ensured that reactive processes depending on the (total) CO2 concentration are expressed properly?

Specific comments:

P 2706, L 8ff: Sentence unclear. Or does it mean that the model considers water based advective transport of dissolved species . . . ?

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

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?

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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 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.

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

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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.

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

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.

P 2715, Equation 11: Explain A, B, and Δza,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?

P 2716, L 20f: Not clear.

P 2717/2718: No being familiar with CLM4 this passage and Figure 3 are not understandable. Provide a more comprehensible description of the used assumptions.

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'?

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

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

P 2722, L 7ff: Provide more details: reactions, processes etc. Are there any sinks for CO2 considered, is the interaction of CO2 with water chemistry considered?

P 2722, L 8: Not the biogeochemistry but the soil depth is discretized.

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.

P 2725, Section 4.3: Why is CO2 form the atmosphere considered as a potential source for an efflux of CO2 into the atmosphere?

P 2725, L 16 – P 2726 L 11: As mentioned above, this passage can be shortened. In turn some words on the CO2 mass balance saying if all of the produced CO2 is leaving the system towards the atmosphere would be helpful. I am also wondering if the mentioned discrepancies depend on the used discretization scheme.

Figure 4: Clarify what is shown, the x-axes have no labels.

Interactive comment on Geosci. Model Dev. Discuss., 5, 2705, 2012.