Biogeosciences Discuss., 9, C7172–C7181, 2013
www.biogeosciences-discuss.net/9/C7172/2013/

Biogeosciences
Discussions

Interactive comment on “Intra-aggregate CO_2 enrichment: a modelling approach for aerobic soils” *by* D. Schlotter and H. Schack-Kirchner

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Received and published: 10 January 2013

We thank referee 1 for the detailed review. The main point of criticism is the model parametrization, which indeed is kept quite simple. However, as stated by referee M. D. Novak: 'The authors objectives were focused on estimating maximum values of CO_2 concentration within aggregates. Therefore they simplified their analysis by, for example, assuming constant air-filled porosity both in both the inter- aggregate and intra-aggregate pore spaces.' Thus, the criticism concerning the parametrization of our model might have been mainly caused by some unclarity concerning the formulation of our objectives and the terminology used to describe the different CO_2 gradients (e.g. intra-aggregate CO_2 enrichment). Besides that, we agree that it would be helpful to explain the choice of our parametrization in more detail and to give a few more values on modelled increases in the CO_2 partial pressure in the air- and water-filled intra-aggregate pore space for different diffusive conductivities. In the following we address the specific comments (referee comments are printed in italics):

Abstract
- P14796/L11-12: I am thinking how it can be concluded that this level of CO_2 partial pressures is reached 'independent of water saturation' if model sensitivity to changes in soil moisture/air-filled porosities etc. were not assessed, but rather depth- and timeconstant air- and water-filled porosities were assumed?

P14796/L9-12: 'Our model predicts that for aerobic respiration (respiratory quotient=1) the intra-aggregate increase in the CO_2 partial pressure can never be higher than 0.9 kPa for siliceous, and 0.08 kPa for calcaric aggregates, independent of the level of water-saturation.' This statement is based on the very low modelled gradients in the CO_2 partial pressure inside the air-filled intra-aggregate pores. The maximum difference in the CO_2 partial pressure between the intra-aggregate pore air and the air at the aggregate surface is less than 0.003 kPa. The diffusive conductivities used for the intra-aggregate pore space in the paper are based on measured values (Sexstone et al. 1985, Sierra et al. 1995). If these values were reduced by 90 % (divided by 10), the maximum difference in the CO_2 partial pressure between the intra-aggregate pore air and the air at the aggregate surface would increase to 0.02 kPa. This is still very low, but should be considered in the conclusions. The difference between the CO_2 partial pressure in the air-filled intra-aggregate pores and the maximum value in the water-filled intra-aggregate pores is limited to approximately 0.9 kPa in siliceous soil and 0.08 kPa in calcaric soil, because it is limited by the maximum decrease in the in the O_2 partial pressure. Changing the percentage of air-filled intra-aggregate pores just leads to changes in the size of the intra-aggregate space with low CO_2 gradients, but it can not lead to higher maximum intra-aggregate CO_2 partial pressures. Thus, in the statement cited in the beginning, only the maximum value for the intra-aggregate increase in the CO_2 partial pressure in calcaric soils should be changed from 0.08 kPa to 0.1 kPa (=0.02 kPa in the air-filled intra-aggregate pores + 0.08 kPa in the water-filled intra-aggregate pores).

- P14796/L16-17: Please test this statement by conducting further model simulations as advised in the general comments.

The statement concerning the CO_2 storage is discussed in the comments to P14805/L22-27 and P14807/L16-24.

- P14797/L9-11: I find this concept of 'water-filled intra-aggregate pores' somewhat too simplified. While, in general, this is the tendency water- and air-contents inside aggregates change considerably with drainage conditions (Carminati et al., 2008). Please adapt this statement to make it less general.

The consideration of air-filled parts inside aggregates is one of the main issues of our model. To include parts with air-filled pore space and parts with water-filled pore space we assigned air and water to the different slices. However, as discussed above, the CO_2 gradients inside the air-filled intra-aggregate pores are very low. Thus, the main CO_2 gradients are between the air-filled inter- or intra- aggregate pores and the water-filled pores inside the aggregates. In sentence P14797/L9-11 we only mentioned the gradient between the air-filled inter- aggregate pores and the water-filled intra-aggregate pores. To avoid confusions regarding the setup of our model we could also mention the gradients between the air-filled intra-aggregate pores and the water-filled intra-aggregate pores. However, the difference between air-filled pores in intra-aggregate and inter-aggregate space is marginal.

Materials and methods
- P14799/L5-6 and L11/12: Please include references for these statements.

These statements are based on Schack-Kirchner (2012) (cited in line 5). Indeed, this citation is not clearly assigned to the mentioned statements and should thus be added to the statements.

- P14802/L4: Was this 'cylinder diffusion model' newly developed by the authors, or is there a reference?

We developed the cylinder diffusion model ourselves. Maybe we should express this more clearly, e.g. in P14804/L11-13.

- P14802/L5-7: While this is shown in Fig. 3, please be explicit here about which proportion of air and water you assumed for the intra-aggregate pores.

The pores in the middle slice of the cylinder were defined as air-filled, the pores in the other slices of the cylinder were defined as water-filled (Fig. 3). As the cylinder consists of 23 slices and the porosity (30 %) is uniformly distributed, this means that 1/23 of the intra-aggregate pores are air-filled and 22/23 are water-filled. Indeed it might be a good idea to mention these values in the text.

- P14804/eq.8: Is there a reference to include for this equation?

The diffusion equation for cylinder geometry can e.g. be taken from: Marsal (1976): Die numerische Lösung partieller Differentialgleichungen in Wissenschaft und Technik. Bibliographisches Institut AG, Mannheim, Wien, Zürich.

Results
- P14805/L8-10: I suppose that this statement depends strongly on the assumed depth distribution of mainly total porosity, inter-aggregate porosity and diffusion coefficients, which were assumed to be depth constant in this study. Please test this statement and expand on this by adding further model scenarios as advised in the general comments. Currently, assuming depth-constant soil porosities and diffusion coefficients and exponentially decreasing soil respiration rates, this result given here seems to be quite obvious to me.

P14805/L8-10: 'The difference between the maximum pCO_2 values inside the aggre-

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gates and the pCO_2 values in the inter-aggregate air, i.e. the intra-aggregate pCO_2 increase, decreases with decreasing respiration and thus with increasing depth (Fig. 8).' This statement might be obvious, but it is most likely realistic.

For aerobic respiration, the maximum possible increase in the CO_2 partial pressure in the intra-aggregate pore space is limited by the maximum possible drop in the O_2 partial pressure inside the aggregates. This drop can never be higher than from atmospheric values at the surface of the aggregate to (almost) zero inside the aggregate. In the model scenario presented in our paper (Fig. 8) this case occurs in the topsoil. With increasing depth, the CO_2 partial pressure in the inter-aggregate pores increases and the O_2 partial pressure decreases. The strength of the decrease in pO2 depends on the depth profile of the diffusion coefficient for the bulk soil and the respiration rate. As expressed by the reviewer, the diffusion coefficients for the bulk soil usually decrease with increasing depth because of decreasing inter-aggregate porosity and increasing fractions of water-filled pores.

Thus, instead of assuming a constant diffusion coefficient we could have also chosen a depth profile with decreasing diffusion coefficients for the bulk soil. However, as long as the O_2 partial pressure inside the aggregates does not drop to values close to zero, the intra-aggregate increase in CO_2 is not influenced by the O_2 partial pressure at the aggregate surface. In the model scenario presented in our paper, the decrease in the O_2 partial pressure in the inter-aggregate pores is fairly slow. Thus, in connection with the typical decrease in respiration with depth, the O_2 partial pressures inside the aggregates below the soil surface are relatively high, which means that the modelled intra-aggregate O_2 and CO_2 gradients do not depend on the partial pressure in the inter-aggregate pores, but only on the respiration rate and the diffusive conductivity of the aggregates.

When assuming a strong decrease in the diffusion coefficient for the bulk soil with increasing depth, the stronger decrease in the O_2 partial pressure in the inter-aggregate pores could lead to a scenario where the O_2 partial pressure at the aggregate surface is too low to allow for aerobic respiration with the given respiration rate. To avoid anaerobic conditions, the respiration rate would need to be reduced, leading to a lower CO_2 enrichment inside the aggregates.

Thus, by choosing a realistic depth profile for the respiration and a realistic value for the diffusion coefficient of the aggregates, we can estimate the maximum intra-aggregate CO_2 increases in a soil profile for aerobic respiration. Using diffusion coefficients for the bulk soil which decrease with depth can only lead to lower, but not to higher intra-aggregate CO_2 gradients within the soil, and therefore does not affect the conclusions of our study.

The diffusive conductivity of the intra-aggregate pore-space was also assumed to be constant over depth in our model. It is difficult to find information on depth profiles of aggregate porosity or diffusive conductivity, but assuming roughly constant values seems realistic (e.g. Sierra & Renault, 1998). Additionally, even when assuming decreasing intra-aggregate diffusive conductivities with depth, the decreasing O_2 partial pressure in the inter-aggregate pore-space would still lead to decreasing maximum intra-aggregate CO_2 gradients.

As long as there is enough oxygen available, small-scale variations in the respiration rate and / or in the diffusive conductivity of soil aggregates might lead to spot-like increasing intra-aggregate CO_2 gradients also in the deeper soil. But, as explained above, for aerobic respiration a decrease in intra-aggregate CO_2 gradients with increasing depth can be expected on the meter-scale because of decreasing maximum intra-aggregate CO_2 gradients.

- P14805/L22-27: Also this result seems to be rather obvious to me considering that the intra-aggregate pores were assumed to be nearly completely water filled. Please test and expand on this by adding further model scenarios as advised in the general comments.

The difference between the CO_2 storage calculated with the modelled intra-aggregate CO_2 partial pressures and the CO_2 storage calculated for an assumed equilibrium between the CO_2 partial pressure in the inter- and in the intra-aggregate pores only depends on the modelled intra-aggregate pCO_2 gradients. Considering that the modelled intra-aggregate CO_2 partial pressures decrease with decreasing intra-aggregate water content (because of an increased diffusive conductivity), a reduction in the percentage of water-filled intra-aggregate pores can only lead to decreasing differences between the CO_2 storages calculated with the two different procedures. Thus, the statement made in P14805/L22-27 for the presented high fraction of water-filled pores is also true for lower water-content.

- For all figures, I suggest to transfer the legends from the figures into the figures captions.

We think that the legends in the figures facilitate the understanding. However, if the editor wishes to transfer the legends from the figures into the figures captions, we will adjust the figures accordingly.

Discussion
- P14806/L25-28: In this article to which the authors of the discussion paper refer (Koehler et al., 2010), I don't find a quantitative statement in terms of 'strength' of CO_2 enrichment. The authors only make a comparative statement arguing that, at deeper depths, the inter-aggregate porosity and soil gas diffusion coefficients are smaller resulting in 'a stronger CO_2 accumulation in the intra-aggregate pores' (Koehler et al., 2010). In the current discussion paper, the authors question this suggestion by running a model with depth-constant inter-aggregate porosity and diffusion coefficients, which is in contrast to the conditions observed in the respective study (Koehler et al., 2010). The authors of the discussion paper add that 'strong CO_2 enrichment in the intra-aggregate pores at deeper depths' seems only possible if 'the respiration inside aggregates is high at these depths, or if the diffusive conductivity of the intra-aggregate pore space is extremely low'. However, again, in their model simulations they assumed that diffusion coefficients remained constant across depths. What are 'extremely low' diffusive conductivities? In the discussed study (Koehler et al., 2010), for example, soil gas diffusion coefficients at 1 m depth were around 0.5 mm2 s-1 and smaller still at 2 m depth. Is this 'extremely low'? Please revise, and test these statements with further model simulations as advised in the general comments.

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We refer to the above cited statement, that, at deeper depths, the inter-aggregate porosity and soil gas diffusion coefficients are smaller resulting in 'a stronger CO_2 accumulation in the intra-aggregate pores' (Koehler et al., 2010). Possibly we misunderstood the term 'CO_2 accumulation in the intra-aggregate pores'. As we understood, this expresses higher CO_2 partial pressures in the intra- than in the inter-aggregate pores. If the statement in Koehler et al. (2010) only expresses that the CO_2 partial pressures in the intra-aggregate pores at deeper soil depths are higher than at lower soil depths we generally agree with this statement. As shown in figure 8, a decrease in the maximum values of the intra-aggregate CO_2 partial pressures with increasing depth can occur under certain conditions. But if e.g. the decrease in respiration with depth is slower, the maximum intra-aggregate CO_2 partial pressures would indeed increase with increasing depth (P14805/L15-18). Thus, in case we misunderstood the statement in Koehler et al. (2010), we would like to withdraw our remark.
Also, we want to stress that we can not judge the statement in Koehler et al. (2010) for the case of anaerobic respiration.
However, if the statement in Koehler et al. (2010), as we understood, expresses generally stronger increases in the CO_2 partial pressure inside soil aggregates in deeper depths compared to the topsoil, we disagree with this statement. Our model shows that, for aerobic respiration, a decrease in the intra-aggregate CO_2 gradients with increasing depth can be expected, even for decreasing diffusive conductivity of the bulk soil with depth (see comment to P14805/L8-10).
The term 'extremely low diffusive conductivities for the intra-aggregate pore space' refers to the typical values used in our model (1 % of diffusive conductivity in free air or water, P14804/L7-10). For these values and the chosen respiration profile the modelled intra-aggregate increases in pCO_2 at deeper soil depths ($<$ -0.4 m) are very low ($<$ 0.02 kPa in siliceous soil) compared to the maximum value (0.9 kPa) . If the diffusive conductivity for the intra-aggregate pore space would be reduced by 90 %, the intra-aggregate increase in pCO_2 would still be lower than 0.1 kPa. This information should possibly also be added to the results chapter.

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- P14807/L16-24: Please test this statement by further model simulations.

Indeed, the commonly observed decrease in respiration with depth is not sufficient to conclude that the difference in the total CO_2 storage calculated in the 2 different ways is negligible. To fully support our conclusion, we should also mention that the maximum possible intra-aggregate CO_2 gradients always decrease with increasing depth because of decreasing O_2 partial pressures in the inter-aggregate pores, and therefore decreasing maximum intra-aggregate pO_2 gradients (comment to P14805/L8-10).

- P14807/L29-P14808/L1: I find this statement rather speculative, please consider to revise.

P14807/L27-P14808/L1: 'But a change from aerobic to anaerobic conditions usually leads to a decrease in the microbial activity in soils (Linn and Doran, 1984; Skopp et al., 1990; Grant and Rochette, 1994), and therefore pCO_2 gradients inside anaerobic aggregates are probably not higher than in aerobic ones.'
This statement clearly is speculative. To stress this more we could e.g. change the sentence to:
'But a change from aerobic to anaerobic conditions usually leads to a decrease in the microbial activity in soils (Linn and Doran, 1984; Skopp et al., 1990; Grant and Rochette, 1994). Thus, pCO_2 gradients inside anaerobic aggregates might often be in a similar range as in aerobic ones. This assumption, however, can not be tested with our modelling approach.'

- P14808/L11-13: I think it is difficult to conclude this from the results based on the current depth-constant model parametrization for porosities and diffusion coefficients. Please test by further model simulations.

P14808/L11-13: 'Therefore, only in the highly respiring parts (topsoil) of non-calcaric soils, intra-aggregate pCO_2 gradients might cause a high variability in the soil solution chemistry on a mm-scale.' This statement indeed is not completely correct, because high intra-aggregate pCO_2 gradients could also occur in regions with low respiration

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as long as the diffusive conductivity of the intra-aggregate pore-space is low enough. However, the following statement can be concluded from our model runs, because the calculated value for the maximum intra-aggregate increase in the CO_2 partial pressure (0.9 kPa for siliceous, and 0.08 kPa for calcaric soil) is independent of the choice of the intra-aggregate diffusion coefficient: 'Therefore, only in non-calcaric soils intra-aggregate pCO_2 gradients might cause a high variability in the soil solution chemistry on a mm-scale.'

References:

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