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Interactive comment on "An inversion approach for determining production depth and temperature sensitivity of soil respiration" *by* R. N. C. Latimer and D. A. Risk

Anonymous Referee #1

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The manuscript presents a synthetic data study on how model inversion could help determine soil CO_2 production parameters (in particular, temperature sensitivity and production depth) from field measurements avoiding error sources of existing approaches, and how field measurement configurations could be optimized to serve best such an inversion effort.

The follwing general comments are numbered according to the BGD review criteria list, their explanations are given in the detailed comments below.

This is (1) a highly relevant question within the scope of BG, and (2) fairly original (meaning not completely novel but an important step towards a model that is sim-

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ple enough to be used operationally across groups). The conclusions are (3) worth publishing, but with respect to the simplicity of the model at least one of them (the comparatively low usefulnes the authors found for surface flux measurements) might be somewhat premature (5). The scientific methods are (4) sound, but not everywhere outlined clearly enough, which should be changed to ensure reproducibility (6), this applies especially to three subsections of section 2 (13). The authors make clear their own contribution (7) but related previous work could in places (e.g. inversion, temperature sensitivity determination problem) be referenced more comprehensively (14). The title very well reflects the contents (8), although the authors might want to add some scope towards what appears to be theri future study plans (validation/sensitivity study with synthetic data vs. appliocation to field data). The abstract is complete and correct (9), except for a clarity issue with respect to the possible combination of surface flux and in-soil concentration measurements. The language is very fluent (11) and most of the presentation is clear (10), except for a part of the model set-up description (13). There is one missing symbol explanation in an Equation (12) and no supplementary material (15).

Detailed comments:

P10138L06: maybe insert something like "and/or *in-soil* concentrations" (to keep readers from mistaking the "surface" for relating to both the fluxes and the concentrations). Concerning the "and/or", see also comment on P10146 / Table 2.

P10139L05: maybe insert 'mainly' (think of macrobiota) ?

P10139LL27: maybe replace "normally" by "frequently" or "often"

P10140L12: 'Though not done to date...': This has been done at least once (Bauer et al. 2012, Biogeochemistry 108:119–134).

P10140L24: "Working exclusively with synthetic...": While this is a strength (in giving the MS a very clear scope) it is also a weakness - so much can go wrong when

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applying an approach only tested on synthetic data to the real word. While the first approach has the advantage that we know the truth, the second (in which this is often not the case) can add important information on the robustness of the approach that even adding noise to the synthetic data often cannot mimic. Think e.g. of the pressure pumping discussion (Takle et al. 2004, Agric. Forest Meteorol. 124:193-206), which might underlie also the fact that to my knowledge no group succeeded so far in deriving efflux from soil concentration profiles only without using surface flux (chamber) measurements for calibration. Is there any chance to add a brief case study with field data?

P10141L06: Are there any plans to make any of these versions available to the public?

P10141L11: 1 m and 100 layers: The way it is written now, it sounds as if those settings were hard-coded very deep inside the model. Is this true? If not, I would recommend a rephrasing that indicates: Here we have the way the model describes physical processes, and there we have the settings used for this particular study.

P10141L19: Same as above: The formulation leaves unclear whether the model a) is constrained to parameterizing the temperature time series as a few sine waves, b) similar but could be run on real-world temperature time series after Fourier transformation (i.e. can use a very large number of sine waves efficiently), or c) is prepared to "eat" real-world temperature time series already (as would be desirable for an inversion model) and transform (if necessary) them itself, but this feature wasn't used for the current study.

Near Eq. 2, though it is trivial, for completeness the symbol t should be described (must be time, and if important for the model implementation, also an added phase lag for the respective sinewave).

Eq. 2-3: Do I get it right that this is meant for soil thermal properties that do not change with depth?

Eq. 4: Again, this is a reasonable choice for a single synthetic study but for future applications of the model (think e.g. of agricultural sites which are more likely to have a depth-indepenendet source accross the tillage horizon) it would be good to learn that the model is modular, and that this profile shape is the particular choice done for this study.

Eq. 5: Are the porosities assumed constant over depth and time?

To summarize most of the above comments on section 2.1, maybe it would be good to give section 2 a structure (or maybe it is already sufficient to move some information from here to the next subsection 2.2) that distinguishes more clearly between what's at the heart of the model (including any limitations on the vertical and temporal vari-ability of parameters that might result from the chosen equations) on the one hand, and parameter choices for this particular study on the other hand. For example, the time step (P10144L12) is mentioned only in 2.2 although it is probably not more or less fix than the number of layers which is already mentioned in 2.1. By the way, maybe you could comment on the interdependence between layer thickness and time step to obtain stability? Since it is mentioned later that the study used up a lot of computation time, it would be helpful to check that both values (layer thickness and time step) are not much smaller than needed for robust results.

Section 2.3: Unclear how this agrees with section 2.1. When/where/why were the sinusoidal temperature waves replaced? Capitalize "soil" at beginning of new sentence (P10145L01).

Section 2.4: Maybe one or some references on inverse modelling in soil physics and/or biogeosciences would be helpful. Have you considered the possibility to weigh obser-vations according to their reliability in the objective function (e.g. make all concentration measurements together as important as the surface flux measurements - if such com-binations were tested, see comment on Table 2. In this case it would also be important to somehow solve the arbitrarity problem arising from the different units of flux and

concentration, e.g. by normalizing differences in Eq. 9 by the magnitude or variance of the measurements). The word "pair" near the end is somewhat confusing (since you suggest in the Equation to compare more than one time series of modelled and measured values), maybe "parameter set" would be more consistent here?

Section 2.5: Again, this section, section 2.3 and section 2.1 somehow together seem to try to give a complete picture of what was actually done - but it is hard to understand, at least to me.

P10146 / Table 2: The table suggests that surface flux measurements were never tested in combination with any in-soil concentration measurements, while the wording of the abstract (especially "and/or") suggests that combinations were tested.

P10147L06: To be reproducable the noise-adding needs to be described in somewhat more detail. Did you add normally distributed random values, and were they correlated in time or not?

P10149L07: Clarify if you really want to say that deep soil or surface flux measurements worsen the results, or if they just add no or little value.

Figure 4: When using small letters in the caption, do so in the figure subpanels as well. I'm not sure, but when looking at the dependence of the Q10 estimate deviation (especially on Q10 itself), it might be more logical to look at the relative rather than the absolute error. Increases of the error with Q10 (or a part of such an increase) might otherwise be a quite trivial result of the lognormal nature of Q10 (with a lower bound at zero and theoretically infinite maximum values).

P10152L05: delete "a" from "which is a fairly high". Maybe, to avoid confusion, you should add that x μmol m-3 s-1 CO_2 production are equivalent to x μmol m-2 s-1 of efflux / column-averaged production, due to the particular choice of a 1 m deep modelling domain. I guess more readers will be more familiar with surface flux magnitudes than those of volume-related production.

Section 3.3: The title might be a bit misleading. At first I was expecting typical errorscapes from the inversion to be discussed here (i.e. how the objective function depends on the tested parameters). In fact showing those would be an interesting add-on because it would help to decide whether your inversion really needs to scan the whole parameter space, or can make use of a simple optimizer that quickly runs into the next local minimum of the objective function. What is shown instead is just a 3-D-version of what was already shown in the previous section, right? In this case maybe it should better be included into that section and shortened a bit.

P10153L08: "which soil conditions should be avoided": Better write something like "which soil conditions will be most challenging / pose the bigest problems etc.". If the ultimate motivation behind the inversion study is to characterize global variability in soil respiration parameters (see introduction), the final application cannot afford to systematically skip sites with certain properties that might make them exceptional also in terms of their respiration parameters. Rather, it should be aware that results from such sites will be associated with the largest errors.

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