Author's response to gmd–2013–170: A variational data–assimilation system for soil–atmosphere flux estimates for the Community Land Model (CLM3.5)

We thank Adrian Sandu for being the editor for this paper. In the revised version, we changed the article according to the suggestions of the referees. The following text contains our answers to the referees:

We are very grateful to both referees for their valuable suggestions and questions, which substantially helped to improve our manuscript. Please find below our responses to Referee 1:

1. Page 6611, equation (1): I suggest to insert a subscript i to both the observation operator H and the observation error covariance R and modify subsequent references to H and R accordingly. In the paragraph following eq. (1), explain that B is a representation in the data assimilation system of the (unknown) background error covariance matrix. Insert also a brief justification of why in the present study B has been specified as diagonal. It is well-recognized that proper specification of the background error statistics is a major issue in 4D-Var. See also recent efforts on hybrid ensemble/4D-Var data assimilation at NWP centers.

Answer: The subscript i will be added to the observation operator H and the observation error covariance R. We thank the reviewer for pointing this out, particularly since we noticed that our description of **B** was not accurate. In fact, the description of the covariance formulation is written for an older version and the set-up of this study includes off-diagonal non-zero elements of the background (forecast) error covariance matrix **B** . Details are revealed below in the paragraph included. We deleted the sentence with the diagonal B and replaced it by the following section:

"In this study, **B** includes the vertical correlation, while cross-covariances between temperature and humidity are not taken into account. With these two parameters and 10 soil layers, **B** is a symmetric 20×20 two-block diagonal matrix, which can be factorised in a Σ diagonal matrix of standard deviations and a correlation matrix **C** to read $\mathbf{B} = \Sigma\,\mathbf{C}\,\Sigma$. We assume that the vertical correlation increases with depth, following the same reasoning which designs the vertical grid spacing to increase with depths. Therefore, we argue that the variable layer thickness can be taken as units. Adopting a Gaussian covariance model for the correlation, dependent on distance in terms of model layer units, elements of **C** then read

$$C_{ij} = \exp\left(-\frac{1}{2}\frac{(i-j)^2}{l^2}\right). \tag{1}$$

Here i and j are the soil layer indices, and l is the correlation lengths in terms of layers. In our case we found best results with $l = 2$.

2. Equation (2): there should be no summation on the first term (Jb x0-gradient)

Answer: This will be corrected. The summation on the first term will be deleted.

3. Page 6612:20 I dont get what this means $M_i* := H^T$. It should be $M_i* := M_i T$. Also, boldface fonts should be used for M_i and its adjoint.

Answer: This will be corrected as suggested by the reviewer.

4. Section 3.2.1 on validation of the adjoint code should be substantiated by incorporating the numerical outcomes from the validation tests. Otherwise, this section has no significance, as all the material presented here is standard.

Answer: We agree with the reviewer. We missed to include the practical outcome of the tests. We included in the text the following paragraph, which concludes the subsection: The advantage of the tangent linear method is that the equivalence of the adjoint and tangent linear can be validated exactly. On the other hand, there is still the problem that the automatic differentiation tool may engender the same error for both calculations. In our case, we used TAPENADE as adjoint and tangent linear compiler. We also applied the finite difference method for validation. Applying both the finite difference method and the tangent-linear method, it could be verified that our adjoint code development of the core of CLM is correct. In more detail, it came out that there is less difference than 1 per mill between the exact tangent linear and the difference method if the choice of δx is appropriate. In case of the CLM plant respiration, it was found by this double checking procedure, that the highest TAPENADE optimisation level gave erroneous results. In reducing the optimisation, the correctness of the code could be directly proven.

Please find below our responses to Referee 2:

1. On line 26, page 6606, the authors mention that the fluxes of interest cannot be obtained by either model or measurements, could the authors expand on why is this the case? one or two sentences, or an appropriate citation, will sufice.

Answer: We see that the presentation is confusing. Originally, the sentences following the location mentioned above were thought as explanation. However, we were not clear here. For a domain, which is covered by a numerical grid, our statement holds simply because all models have errors, only some of which are known in statistical terms, as is the case for measurements, which are typically sparse in case of in situ type instrumentation, or coarse in case of space borne sensors.

We included the following split text:

"All models are imperfect, and in prognostic mode errors at grid points are known in statistical terms at best, rather than exactly."

...

"Observations are also error affected, with only statistical information available. In situ measurements are typically sparse for soil, especially for deeper soil layers, while space borne sensor footprints are coarse, valid for skin layers only, and with long revisit times."

2. On line 20, page 6607, the authors make the following claim: "More precisely, initial values have a high impact on the forecast skill, while, at the same time, are insufficiently well known." Im somewhat troubled by this sentence since it is known that the dependence of the forecast to the initial condition is severly degraded over the simulation time for a number of weather models. More precisely, the concept of chaos is brought to mind, which suggests that a meteorological model has a forecast limit of about two weeks. Afterwards, as chaos theory indicates, any miniscule perturbation in the initial condition provides a forecast that is almost completely dissasociated from the initial condition. I would recommend rephrasing this sentence to include the idea of a time-window for which the forecast is still highly dependent on the initial condition.

Answer: The time window is decisive on which parameter is controlling the model evolution, e.g. meteorological seasonal forecasts influenced by sea surface temperature, air quality forecasts by emissions, dependent on reactivity of constituent, and so on. Here, for our soil simulation and for initial values to be important, we stay in the limits of minutes at the insolated skin layer, to days, at deepest model levels. This means that with increasing depth the initial values are the key parameter to be optimised by the assimilation procedure, provided, other model parameters are sufficiently well specified. In fact, the assertion of the sentence in question is not really necessary for the following. To avoid further confusion, we propose to delete the sentence.

3. On line 20, page 6610, the authors say that the 4D-Var provides a physically consistent and continuous solution, which is not the case with Kalman filter approaches. Has there been any studies that apply a Kalman filter assimilation to the CLM or similar models? If so, do any of these studies suggest that the discontinuities causes a problem in the model solution?

Answer: Most soil data assimilation studies apply Kalman filtering for practical reasons (see e.g. Hain et al. 2012 for a recent paper), accepting model discontinuities for forecasts. Our investigation has a case study analysis objective, where for flux estimates with capacities for budget integration inconsistencies (jumps of the phase space trajectories) should be limited as much as possible, and not being dependent on the observation frequency. Therefore we selected the variational approach. Batemi and Entekhabi (2012) appear to follow similar lines, when selecting a Kalman smoother for heat flux estimation, which has similar properties as the variational method in this respect. Of course, in the 4D-variational case jumps occur at the limits of the assimilation interval, but not at each observation time. We replaced the sentence by:

" In order to obtain a phase space trajectory of the model for the assimilation interval, which accounts for continuous and consistent model dynamics and related heat and soil moisture fluxes and their budgets, the adjoint model version is developed and set in a 4D-var context."

4. In section 3.2.1 the authors talk about validation of the adjoint code, presenting the various approximations that can be used for validation, but no validation results are presented. I strongly suggest including some figures or discussion on any validation experiments the authors performed. Otherwise, it is hard to judge on the accuracy of the adjoint code, even if the 4D-Var experiments seem to be working.

See our response to Reviewer 1, point 4.

5. In section 4, "Parameter Impact", the authors discuss the parameters of interest for the study, and mention the importance of sensitivity analysis to these parameters. But again, no results are shown and are only slightly discussed. I suggest including the sensitivity analysis results, since this will make this particular section more relevant for the paper.

We agree with the reviewer. Therefore, we add the following example result at the end of section 4:

To illustrate the importance of well-defined soil properties, we show results for two assimilation runs with different soil parameters. The assimilation included soil temperature and soil moisture measurements at the station Selhausen, which is located close to the station Merken and has a similar measurement setup (see Sect. 5). The simulation setup was also similar to the assimilation for the station Merken described in Sect. 5. In a first assimilation run, we used the soil type that was given in the description of the measurements, namely silt loam with 13% sand and 17% clay. The result for the soil temperature at 45 cm depth of the first run is shown in the left panel of Fig. 1. It is visible that the soil temperature is clearly overestimated in the first guess. The analysis of the soil temperature is in the same order of magnitude as the observations, but there are significant discontinuities visible at the ends of the assimilation intervals. In a second run, we changed the soil properties to 5% sand and 25% clay, which constitutes a finer soil texture but is still classified as silt loam. Using the finer soil texture, the background is closer to the observations of soil temperature at 45 cm depth, and the discontinuities in the analysis are smaller than in the first run (right panel of Fig. 1).

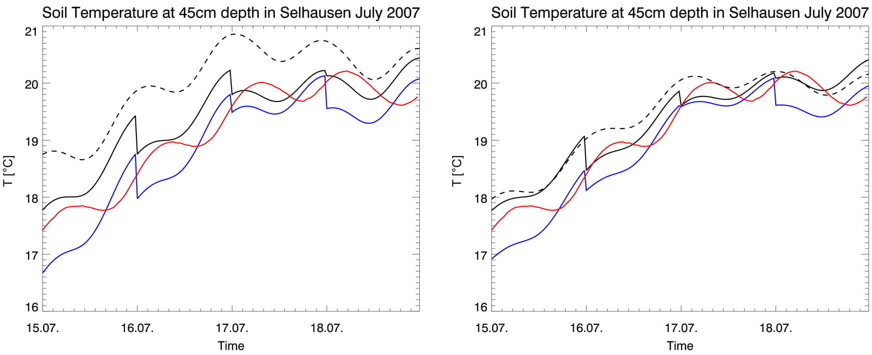

Figure 1: Soil temperature in Selhausen for 15th to 18th July 2007 at 45 cm depth. The black-dashed curve shows the control run, the black solid curve shows the CLM forecast based on the analysis of the previous day, while the blue curve depicts the analysis. Measurement values are shown as red line. The left panel shows results for the original soil composition, containing 13% sand and 17% clay. The right panel shows the respective results for a soil containing 5% sand and 25% clay.

6. On section 5.1, "Idealized Experiments" the authors choose the background and observation error covariance matrices to be similar, why were these matrices similar? What is the typical error of real observations (2-10%)? It would seem better to use an observation covariance matrix that reflex the observation error expected in real life. That way the idealized experiment would carry more credibility.

Answer: The referee is right with the remark, that the presented errors do not reflect real life conditions. Nevertheless, soil humidity measurements in the dry and saturation limits are also critical and often worse than 10%. However, for the idealized experiments the important quantity actually is the ratio between observation and background error. Since the background error is unknown here, we felt free to choose a configuration which allows for particularly easy interpretation of the results. Choosing the same errors for background and observations is however motivated by the possibility of straightforward testing of the analysis results being "half way" between the background run and the nature run ("artificial reality"), as exposed in Fig. 1 (old manuscript). We also made tests with other settings for B and R without fundamentally different results. We therefore propose to accept our test configuration, along with adding a justifying remark, included in line 16, page 6618:

".... as large as the impact of the background, which will be easily testable by an analysis right in the middle between background and virtual measurements."

Technical Corrections:

1. On line 11, page 6607, the "Nevertheless" at the beginning of the sentence seems odd. The sentence seems to follow the same idea as the previous sentence, but it begins with "nevertheless".

Answer: We will replace nevertheless with In any case.

2. On line 22, page 6610, there is a "has not discontinuities", should be "contains no discontinuities".

Answer: This will be changed as suggested.

3. In Table 1, the authors present the layer depth and thickness. Im somewhat confused since, following the table, there seems to be gaps between each layer. That is, layer 1 starts at 0.7 cm and has a thickness of 1.8 cm, which means that it goes all the way down to 2.5 cm, but layer 2 starts at 2.8 cm. There is a gap of 0.3 cm between layers 1 and 2, what is that gap? what is it filled with?

Answer: The layer depths given in Table 1 do not denote the start of the soil layer. Instead, they give the node depth that is located inside the layer. The distance of the node depths increases exponentially with soil depth. The layer interfaces lie in the middle of two node depths. The thickness is defined as the distance between two layer interfaces. The definition of the soil layers in the CLM is described by Lawrence et.al. (2008). For example, the first soil layer extends from the surface (0.0cm) down to 1.8cm depth. The node depth of this layer is 0.7 cm, and its thickness is 1.8cm. We will include the citation Lawrence et.al. (JGR, 2008) in the article to give a reference to the exact definition of the soil layers.

4. In Figure 1, what are the dotted black lines? This is not explained in the caption or main body of the manuscript. Also, due to the very slim line thickness of the plot it is hard to discern colors. Please use slightly thicker lines.

Answer: The dotted black lines indicate the assumed background error. This remark will be included in the figure caption We also will use thicker lines in this figure.

5. Figures 4-8 are also hard to read, due to their size and line thickness. I strongly suggest modifying these plots to make them clearer.

Answer: The thickness of the lines in these plots will also be increased.