

Response to referee #2:

We appreciate the constructive and valuable comments by referee #2 and are very grateful for suggestions regarding the setup and assumptions. We fully agree that longer integration periods at different climate zones of the Earth and an evaluation with real observations are finally needed to assess the applicability of this type of data assimilation for global land surface data assimilation. Certainly, this is a valuable long-term goal, but both from a technical and scientific point of view it reaches far beyond the scope of this paper.

From a technical point of view, the data assimilation experiments demand very high computational resources. The most expensive component is the atmospheric component of the TerrSysMP system in combination with the need to integrate 40 ensemble members. The suite of experiments for one seven-day period at one location, as it is presented within the manuscript, requires one month of simulation time at our high-performance computing center. Obviously, experiments on seasonal or annual time-scale at various locations are not affordable.

Likewise from a scientific point of view, the use of a localized ensemble transform Kalman filter (LETKF) for fully-coupled data assimilation at the land-atmosphere interface is at a very early stage. To the best of our knowledge, we are the first to explore the potential of the LETKF to improve the soil moisture analysis by assimilating the atmospheric boundary temperature at screen-level. At least in the numerical weather prediction community this is a very timely question, as even recent publications (Carrera et al., 2019; Muñoz-Sabater et al., 2019) still question, whether atmospheric boundary layer observations can be used to improve the analysis and forecast of the soil moisture.

Bearing in mind the idealized setup and the limited integration period, this study contains relevant contributions to the scientific community. As a proof-of-concept, the study reveals the potential of the LETKF to advance soil moisture analyses with atmospheric boundary layer observations. In particular, it highlights the superiority of the LETKF compared to commonly used simplified extended Kalman filter (SEKF) methods for this type of data assimilation. As a consequence, we have chosen to analyze these results more in-depth to showcase why and what we could expect for future work regarding the assimilation of atmospheric boundary layer observations into the land surface with advanced data assimilation techniques.

Following the raised major concerns, we will clearly indicate this idealized proof-of-concept scope of the study in the motivation and will state explicitly that further research steps are needed – as outlined by the concerns – to prove the applicability of the LETKF in real global land data assimilation systems. To additionally clarify that this study is a proof-of-concept, we will change the title to “Ensemble-based data assimilation of atmospheric boundary layer observations improves the soil moisture analysis in idealized limited-area experiments”. We hope that this adds clarity to the scope of this study.

Answers to the major comments:

- We use a heterogeneous setup where each grid point has its own soil conditions, based on a single simulation with a spin-up time of 6 years and a similar model configuration as our simulations. Our setup is representative for mid-latitudes and spans a variety of soil conditions, ranging from quite dry conditions to quite wet conditions. To analyze the results with regard to different soil conditions, we have splitted up the potential assimilation impact into different regimes in Figure 9 in the manuscript. In all of these regimes, we see a positive assimilation impact during daytime, though the highest impact can be found in the

mixed regime. In the end, our setup is surely beneficial for this type of data assimilation but includes a heterogeneous mixture of soil conditions

- As indicated above in the general statement, our study is a proof-of-concept study, where we showcase of what might be possible in the future. In addition, our simulations have a high computational cost. We thus restricted the simulation timeframe to these seven days.
- Since the data assimilation system is at a very early stage, it would be quite difficult to apply it directly to realistic scenarios in hindcast experiments. These experiments are likely to need other extensions to the data assimilation like other ensemble inflation methods or an adaptive localization. They are not implemented yet within the data assimilation system as it is in a non-operational stage. In addition, the study is a proof-of-concept and we think that such hindcast experiments are out-of-scope for this study.
- To improve the clarity of the results, we will streamline the language.

Specific comments within the manuscript:

- Page 1:
 - As indicated within the final answer, the whole introduction will be changed in the revised version of the manuscript. This will then include a more gentle entry into the manuscript.
- Page 2:
 - In the new introduction, we will clarify that land surface models are often viewed as providing lower boundary fluxes for the atmospheric model component in numerical weather prediction. We instead promote with our modelling setup that a fully-coupled land-atmosphere system can be also advantageous for numerical weather prediction.
- Page 3:
 - In our revised introduction, we will clarify the step going from the SEKF to the LETKF and its consequences.
 - Our study is more focused on the aspect of SEKF compared to the LETKF than on weakly-coupled vs strongly-coupled data assimilation. The additional aspect of improving the soil moisture analysis with strongly-coupled assimilation is only a small additional result. Thus, we will remove the paragraph explaining the advantages of strongly-coupled data assimilation, instead we will elaborate more about the differences between SEKF and LETKF in our new introduction.
 - Our data assimilation system does not preserve the mass and energy balance within the soil or atmosphere. COSMO for the atmospheric component of the modelling system is a limited-area model that is driven by lateral boundary conditions given by another model (in our case COSMO-DE from the German meteorological service). As a consequence, there is always an income and outcome of mass and energy at the lateral boundaries within the atmosphere. In addition, we aim at time-scales of numerical weather prediction where other effects than preserving mass and energy come into play, e.g. correctly representing the incoming solar radiation. We have thus decided to neglect the conservation of mass and energy in our data assimilation system for simplicity. Nevertheless, on a global and much longer time-scale it might be necessary to take the conservation of mass and energy into account.
 - Our setup is a synthetic and idealized setup, representing typical conditions in the midlatitudes. In the midlatitudes, we have only small areas with water surfaces (only 10 % of our surfaces in CLM are bare soil that also includes urban areas). These areas thus have only a small effect on the results.
 - Will be corrected into stem area index, this was our mistake.
- Page 5:
 - We will clarify that the used setup for the SEKF is similar to a typical numerical weather prediction (NWP) setup. As our results clearly shows, the 2-metre-temperature is at most affected by the soil moisture during daytime and noon. We thus expect here the largest

assimilation impact. In a correlation analysis, we have seen the highest correlation of the temperature at noon with the soil moisture at 00:00 UTC the night before. Because the soil moisture influences the sensible heat flux, the soil moisture has an impact on the diurnal cycle of the 2-metre-temperature. As a consequence, perturbations from the soil moisture are propagated to the atmosphere throughout the day. This asynchronous impact is mirrored with our SEKF setup.

- As our SEKF setup is similar to NWP setups, we use here the static diagonal background covariances as it is used at the ECMWF for operational soil moisture data assimilation (“IFS Documentation CY47R1 - Part II: Data Assimilation”, 2020). It is true that a dynamic background covariance that also depends on the soil moisture itself might be beneficial for data assimilation, as our results with the LETKF indicate. Since we mirror with the SEKF a common approach in NWP, we have kept the covariance static.
- Page 6:
 - As only perturbations of our ensemble, we use initial soil moisture and soil temperature perturbations. These perturbations lead to differences in a order of magnitude of 0.3 K within the temperature at 10 meters height, as can be seen in Fig. 1 in this answer below. The observational error of the 2-metre-temperature is often in an order of magnitude of 1 K or even more for operational data assimilation. Using such large errors within our synthetic 2-metre-temperature would lead to a small signal-to-noise ratio; the signal would be then overshadowed by the noise. We reflect this by using smaller observational errors with a magnitude of 0.1 K. This guarantees that our 2-metre-temperature observations have a meaningful information content about the soil conditions.
- Page 7:
 - We explain the coupling between COSMO and CLM in section 2.1, where we also explain how the data is upscaled by averaging from the finer CLM grid to the coarser COSMO grid. For more information, we have referred to Shrestha et al. (2014). The COSMO fields are bilinearly interpolated to the CLM grid. In our revised manuscript, we will introduce a new second section, where explain our idealized twin experiments. This new second section will also include an overhauled description of the COSMO-CLM coupling.
 - Our assumption of spatial correlations within perturbations of the soil moisture reflect the dependence of the soil moisture on precipitation. Since errors and uncertainties within the precipitation can have similar correlation lengths, we use implicitly the assumption of larger precipitation events before the start of our simulation. Because we have perturbed the soil moisture saturation instead of the volumetric soil moisture directly, our setup catches local circumstances that also influence the porosity. The soil moisture perturbations itself have a much finer structure as can be seen in Fig. 6 (a) in the manuscript.
 - The Kalman filters would have problems if the ensemble mean is far away from the nature run and if this is not represented within the B-matrix. This case would be then similar to having biases within the soil moisture.
 - We will answer the question about the perturbations and the spin-up time within the new second section with the overhauled idealized experiment description. To showcase that the soil perturbations are already propagated into the atmosphere after the first day, we will there introduce a novel figure that would look similar to the Fig. 1 in this answer below.
- Page 8:
 - We will clarify our experiments and what is updated in these experiments in a revised experimental description.
- Page 10:

- We understand that the soil moisture saturation within Figure 3 of the manuscript is somewhat misleading. Here, the spatially-averaged soil moisture saturation is shown. Since we use heterogeneous soil conditions, there is a mixture of various soil moisture saturations across our area. To reflect this, we will revise Figure 3 of the manuscript and will replace the averaged soil moisture saturation with new subfigure where we show the percentage of binarized soil conditions in our area.

We believe that these answers and the proposed changes reflects the review of referee #2. Together with the proposed changes based on the review of referee #1, we think that this will increase the comprehensibility of our manuscript.

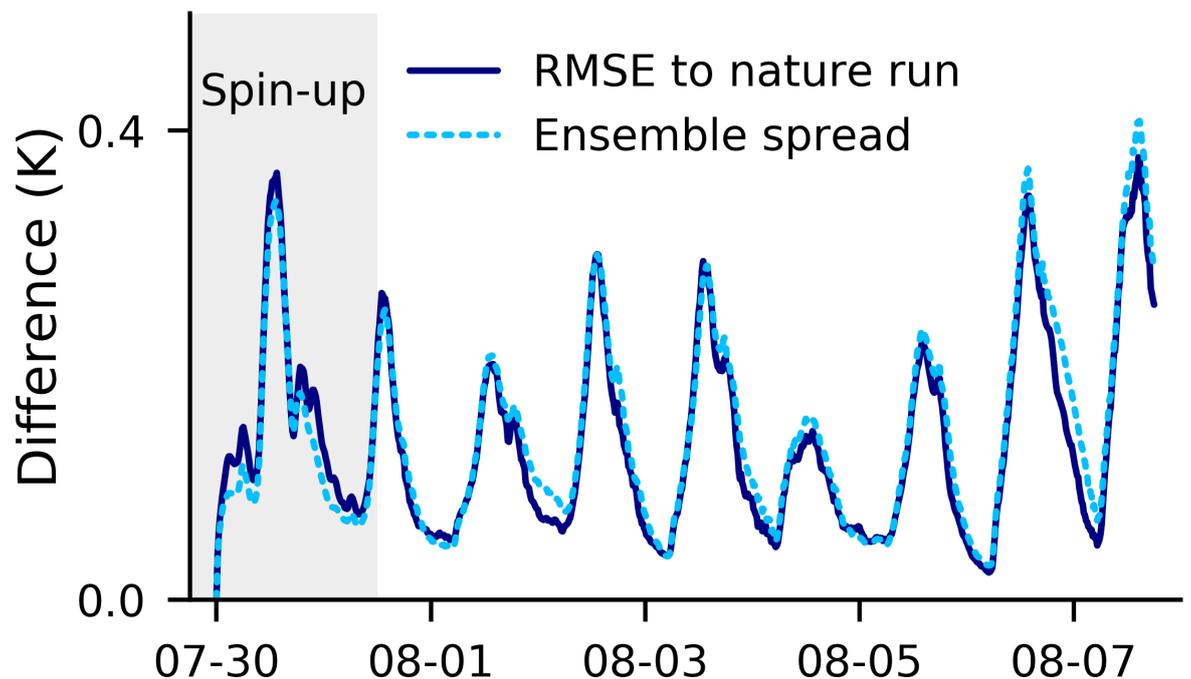


Figure 1: The spatially-averaged RMSE of the ensemble mean to the nature run and spatially-averaged standard deviation within the open-loop ensemble for the temperature in COSMO at 10 meters height.

Carrera, M. L., Bilodeau, B., Bélair, S., Abrahamowicz, M., Russell, A., & Wang, X. (2019). Assimilation of Passive L-band Microwave Brightness Temperatures in the Canadian Land Data Assimilation System: Impacts on Short-Range Warm Season Numerical Weather Prediction. *Journal of Hydrometeorology*, 20(6), 1053–1079. <https://doi.org/10.1175/JHM-D-18-0133.1>

IFS documentation CY47R1—Part II: Data assimilation. (2020). In *IFS Documentation CY47R1*. ECMWF. <https://doi.org/10.21957/0gtybbwp9>

Muñoz-Sabater, J., Lawrence, H., Albergel, C., Rosnay, P., Isaksen, L., Mecklenburg, S., Kerr, Y., & Drusch, M. (2019). Assimilation of SMOS brightness temperatures in the ECMWF Integrated Forecasting System. *Quarterly Journal of the Royal Meteorological Society*, 145(723), 2524–2548. <https://doi.org/10.1002/qj.3577>