Improving JULES Soil Moisture Estimates through 4D-En-Var Hybrid Assimilation of COSMOS-UK Soil Moisture Observations

Response to Anonymous Referee #1 – Visweshwaran et. al (2025) doi:10.5194/egusphere-2024-3980

The authors thank the reviewer for their insightful comments. Below we list each comment and have numbered them for ease of reference. Our responses are provided below in purple. References are as cited in the manuscript or provided in each response.

1) A big part of the methodology and the monitoring data set have been presented already in Cooper et al., 2021a (https://doi.org/10.5194/hess-25-2445-2021). The second scenario of the manuscript seems to be very similar to this work published by the manuscript's second author as main author. It is using the same land surface model JULES, the same pedotransfer functions including the same starting parameter values, the same 16 cosmic-ray neutron locations out of the about 50 sites of the COSMOS-UK network, the same year for the data assimilation and the same following year for the forecast, and the same ensemble size. The 4D-En-Var assimilation method outlined in the manuscript is depicted already in Pinnington et al. (2020), also including a combination of parameter vector and state vector, and seems to be part of LAVENDAR already together with JULES.

Thank you for this comment. Pinnington et al. (2020) developed the LAVENDAR framework and later applied for **parameter estimation** in JULES for Toth PTF constants (Pinnington et al., 2021). Cooper et al. (2021a) applied this framework for **parameter estimation** to optimize Cosby pedotransfer function (PTF) constants. However, their implementation focused solely on parameter estimation and **did not include any state estimation**. Here we introduce a novel extension by incorporating **joint state-parameter estimation** by modifying the algorithm to incorporate the state vector alongside the parameter vector in an augmented approach, enabling a more comprehensive data assimilation scheme. This dynamically adjusts both soil moisture initial conditions and soil hydraulic parameters (through PTF constants) within the 4D-En-Var assimilation framework.

To assess the impact of simultaneously updating both states and parameters (Scenario 3 in our results) and to understand how the model responds to this approach, it is necessary to compare it against state-only (Scenario 1) and parameter-only (Scenario 2) estimation. We acknowledge that this distinction was not clearly articulated in the introduction and conclusion sections and we will revise these.

2) While the study presented in the manuscript does go somewhat further by now also applying the data assimilation method to include the initial soil moisture state, it does not describe the methods and results of the manuscript on basis of the existing work but as an unclear mix with vague formulations of origin. These publications are cited but often rather as context. A clear distinction between existing work and own work is necessary. Maybe there are reasons to use exactly the same setting as before, though using another data set and approach could contribute more novelty, but this needs to be discussed and rectified. Also results should be discussed on basis of existing work, not in a diffuse way. To give one simple example, in the conclusions, second paragraph, the manuscript presents that KGE has improved from 0.33 to 0.66 for the parameter-only assimilation, which is identical to the statement in the conclusion of Cooper et al. (2021a) that 'we see an

improvement in the average KGE metric from 0.33 (range 0.10 to 0.69) before data assimilation to an average of 0.66 after data assimilation'. It should be referred to the previous result and made clear that this finding is identical to this previous result and why or to be discussed how it nevertheless may be different and why.

As noted in our response to Comment 1, we will revise the introduction and conclusion sections to clarify the distinction between this study and previous work such as Cooper et al. (2021a). To assess the impact of simultaneously updating both state and parameter estimates (Scenario 3) and to enable a direct comparison with state-only (Scenario 1) and parameter-only (Scenario 2) assimilation, we deliberately use the same observation data (COSMOS-UK in-situ observations), assimilation period (2017), forecast period (2018), land surface model (JULES), PTF selection (Cosby). The prior values of the PTF constants follow Cosby et al. (1984) and Marthews et al. (2014), consistent with previous applications in JULES and other land surface models. To ensure that all three scenarios in this study are run using exactly the same model configuration and processing, we repeat the parameter-only assimilation experiment rather than relying on results from Cooper et al. (2021a). Re-running the experiment avoids the risk of introducing uncertainty due to possible differences in implementation or processing steps.

In addition, for the benefit of readers, we include Scenario 2 in this work so that the comparison across all three scenarios can be followed within a single study, without requiring reference to previous work. After performing the experiment, we observe that the results for Scenario 2, including KGE and RMSE, are identical to those reported in Cooper et al. (2021a), and this will be clearly stated and referenced in the revised manuscript.

3) Features of cosmic-ray neutron sensing are partly wrong and even contradictory within the manuscript. For example, in line 30 the horizontal footprint size is specified as 'approximately 25 to 30 hectares', in line 112 then 'an area up to 120,000 m^2', which is only half of the former.

Thank you for pointing out this inconsistency. The horizontal footprint size of the cosmic-ray neutron sensing (CRNS) instrument spans approximately 12 hectares (i.e., 120,000 m^2). We will revise line 30 accordingly.

4) Also, the depth specifics are not explained adequately and the fourth, deepest layer of the JULES model actually is not linked to the soil moisture observation by cosmic-ray neutron sensing at all, and the third layer likely only sometimes. And, the equations used for a weighted average of model layer soil moisture values to compare to the observed soil moisture (Cooper et al., 2021a, Pinnington et al., 2021) is a mere average accounting for the different layer thicknesses but not accounting for the strongly decaying weight with depth of cosmic-ray neutron sensing.

We will clarify the depth ranges of the JULES soil layers in the revised manuscript. While we acknowledge that the weighted averaging operator used does not explicitly account for the depth-dependent sensitivity of cosmic-ray neutron sensing, previous studies (Cooper et al., 2021a; Pinnington et al., 2021) have shown this operator to be effective in practice.

We have also tested more complex operators and found that the data assimilation results were not particularly sensitive to the choice of operator. The weighted averaging approach is also computationally cheaper and thus more suitable for future application of the data assimilation system to larger problems. The sensing depth of the COSMOS instrument varies with soil moisture but does not extend to the deepest JULES layer (Evans et al., 2016; Antoniou et al., 2019), which is why this layer is excluded from the weighted averaging. However, assimilation updates still reach deeper layers through strong vertical correlations in the background error covariance.

Reference:

Evans, J. G., Ward, H. C., Blake, J. R., Hewitt, E. J., Morrison, R., Fry, M., Ball, L. A., Doughty, L. C., Libre, J. W., Hitt, O. E., Rylett, D., Ellis, R. J., Warwick, A. C., Brooks, M., Parkes, M. A., Wright, G. M. H., Singer, A. C., Boorman, D. B., and Jenkins, A.: Soil water content in southern England derived from a cosmic-ray soil moisture observing system – COSMOS-UK, Hydrol. Proc., 30, 4987–4999, https://doi.org/10.1002/hyp.10929, 2016.

Antoniou, V., Askquith-Ellis, A., Bagnoli, S., Ball, L., Bennett, E., Blake, J., Boorman, D., Brooks, M., Clarke, M., Cooper, H., Cowan, N., Cumming, A., Doughty, L., Evans, J., Farrand, P., Fry, M., Hewitt, N., Hitt, O., Jenkins, A., Kral, F., Libre, J., Lord, W., Roberts, C., Morrison, R., Parkes, M., Nash, G., Newcomb, J., Rylett, D., Scarlett, P., Singer, A., Stanley, S., Swain, O., Thornton, J., Trill, E., Vincent, H., Ward, H., Warwick, A., Winterbourn, B., and Wright, G.: COSMOS-UK user guide: users' guide to sites, instruments and available data (version 2.10), Tech. Rep.,Wallingford, http://nora.nerc.ac.uk/id/eprint/524801/, 2019.

5) Furthermore, the error estimate for the observations does not account for the relation between hourly values and a daily value for this cumulative measurement nor the Poisson distribution of its uncertainty instead of a Gaussian.

The analysis of the data showed that the standard deviation of the hourly values around the daily mean is approximately 20% (as mentioned in lines 258–262). However, we have inflated the observation error to 50% of the daily mean observation to account for multiple sources of uncertainty, including the conversion of neutron counts to soil moisture, the averaging of hourly measurements to a daily scale, and temporal (intra-site) observation error correlations arising from persistent calibration or environmental effects at a given site. We also recognize the presence of representation errors (Janjić et al., 2018), which may result from differences in scale between the model and the observations, or simplifications in the observation operator.

To compensate for these unaccounted error sources, we adopt an inflation approach for the observation error variance. Similar techniques have been used in other data assimilation contexts, such as in the assimilation of satellite radiances for numerical weather prediction, where inflation is applied to account for unmodelled observation error correlations (Liu et al., 2003; Stewart et al., 2008).

Regarding the use of Gaussian error probability density functions (pdfs), these are commonly used in data assimilation even though real-world pdfs may be non-Gaussian (Fowler and van Leeuwen, 2013). The Gaussian assumption leads to a quadratic loss function and a mathematically tractable minimization problem. Alternative pdfs may not preserve this property, particularly when combining different distributions with Bayes' rule. Furthermore, in our experiments, the distribution of representation errors is unknown, and the Gaussian pdf is a reasonable choice as it is the maximum entropy distribution for a given mean and covariance.

Reference:
Liu, Z. Q., & Rabier, F. (2003). The potential of high-density observations for numerical weather prediction: A study with simulated observations. *Quarterly Journal of the Royal Meteorological Society: A journal of the atmospheric sciences, applied meteorology and physical oceanography*, *129*(594), 3013-3035.

Stewart, L. M., Dance, S. L., & Nichols, N. K. (2008). Correlated observation errors in data assimilation. *International journal for numerical methods in fluids*, *56*(8), 1521-1527. https://doi.org/10.1002/fld.1636

Janjić, T., Bormann, N., Bocquet, M., Carton, J. A., Cohn, S. E., Dance, S. L., Losa, S. N., Nichols, N. K., Potthast, R., Waller, J. A., & Weston, P. (2018). On the representation error in data assimilation. *Quarterly Journal of the Royal Meteorological Society*, 144(713), 1257–1278. https://doi.org/10.1002/qj.3130

6) In respect to the definition of the Cosby's pedotransfer functions, there are also shortcomings. The manuscript refers to Cosby et al. (1984), but not everything presented is given there and seems neither

developed within the manuscript's study. Cosby et al. (1984) has reported linear relations between grain fractions and four hydraulic variables, but not the full mathematical equations as presented in 2.3. Therefore, a part of the earlier development seems to be missing. Marthews et al. (2014) could be cited *directly* in this respect, as one component. But further considerations would be helpful.

We agree with the reviewer that the full set of equations presented in Section 2.3 are not entirely as given in Cosby et al. (1984). We will revise the manuscript to directly cite Marthews et al (2014)

7) And some discussion, why this set of pedotransfer functions? Only because they have been used in the similar preceding study (Cooper et al., 2021a)? And why not start with the parameters adjusted there already? How does it compare to other pedotransfer functions as used in other studies, etc.

We chose the Cosby et al. (1984) PTFs because they are widely used, simple to apply, and commonly used with the JULES land surface model. Their formulation provides continuous functions that are well-suited for representing spatial heterogeneity in soil properties across large scale. One of the key advantages of Cosby's approach is that it relies only on soil texture information, making it a practical and efficient method, especially when direct measurements of hydraulic conductivity are unavailable. Furthermore. Lee (2005) compared different PTFs for estimating soil hydraulic conductivity and found that Cosby's PTF provided the best prediction of saturated hydraulic conductivity.

Another important reason for choosing Cosby's PTFs is their planned operational use by the UK Met Office in their land surface modelling framework. Using the same PTFs ensures our findings are aligned with practical applications and relevant for future operational use.

The reason for not choosing the parameters already estimated by Cooper et al (2021a) as a starting point is explained in our response to comment 2.

8) The title is full of abbreviations and unclear

We acknowledge the reviewer's concern about the use of abbreviations in the title. To improve clarity, we will revise the title to: *"Improving Land Surface Model Soil Moisture Estimates through Hybrid Data Assimilation of In-Situ Soil Moisture Observations."*

9) The introduction to monitoring of soil moisture starts with a general list of remote sensing sensors (and references) and rather outdated observation networks reported in 2006 and 2007. This part could be more to the point and up to date.

We will revise the introduction to make sure it is succinct and strictly relevant to this paper. We will incorporate more recent in-situ soil moisture networks alongside the existing ones to ensure the discussion remains up to date. These additions include the Murrumbidgee Soil Moisture Monitoring Network (MSMMN) (Smith et al., 2012), FR-AQUI (Aquitaine soil moisture network, France) (Jean-Pierre W, et al., 2018), the Center for Western Weather and Water Extremes (CW3E) network (Sumargo et al., 2021), and the GROW Observatory (Xaver et al., 2020).

References:

Smith, Adam B., Jeffrey P. Walker, Andrew W. Western, R. I. Young, K. M. Ellett, R. C. Pipunic, R. B. Grayson, Lionel Siriwardena, Francis HS Chiew, and Harald Richter.: The Murrumbidgee soil moisture monitoring network data set, Water Resources Research, 48,7, https://doi.org/10.1029/2012WR011976, 2012.

Wigneron, Jean-Pierre, Sylvia Dayan, Alain Kruszewski, Christelle Aluome, Marie Guillot-Ehret Amen AI-Yaari, Lei Fan, Serhat Guven et al.: The aqui network: soil moisture sites in the "Les landes" forest and graves vineyards (Bordeaux aquitaine region, France), In IGARSS 2018-2018 IEEE International Geoscience and Remote Sensing Symposium, pp. 3739-3742. IEEE, https://doi.org/10.1109/IGARSS.2018.8517392, 2018.

Xaver, Angelika, Luca Zappa, Gerhard Rab, Isabella Pfeil, Mariette Vreugdenhil, Drew Hemment, and Wouter Arnoud Dorigo.: Evaluating the suitability of the consumer low-cost Parrot Flower Power soil moisture sensor for scientific environmental applications, Geoscientific Instrumentation, Methods and Data Systems, 9, 117-139, no. 1, https://doi.org/10.5194/gi-9-117-2020, 2020.

Sumargo, Edwin, Hilary McMillan, Rachel Weihs, Carolyn J. Ellis, Anna M. Wilson, and F. Martin Ralph.: A soil moisture monitoring network to assess controls on runoff generation during atmospheric river events, Hydrological Processes 35, no. 1, https://doi.org/10.1002/hyp.13998, 2021.

10) In line 56 a reference is needed, as such and also for the claim to be more accurate.

We agree that the original statement was a bit unclear and we will revise the sentence, and include references, as
"Hybrid data assimilation methods, such as Ensemble-Variational approach, combine features of both variational and ensemble techniques by using ensemble-based background error covariances within a variational framework. These methods avoid the need to explicitly compute the full model adjoint while still approximating the model trajectory over an assimilation window, offering a flexible alternative to traditional approaches (Lorenc, 2015; Poterjoy and Zhang, 2015)."

References:

Lorenc, A. C., Bowler, N. E., Clayton, A. M., Pring, S. R., & Fairbairn, D. (2015). Comparison of hybrid-4DEnVar and hybrid-4DVar data assimilation methods for global NWP. *Monthly Weather Review*, *143*(1), 212-229.

Poterjoy, J. and Zhang, F.: Systematic Comparison of Four-Dimensional Data Assimilation Methods With and Without the Tangent Linear Model Using Hybrid Background Error Covariance: E4DVar versus 4DEnVar, Monthly Weather Review, 143, 1601 – 1621, https://doi.org/10.1175/MWR-D-14-00224.1, 2015

11) Line 175: It is a bit uncalled-for to first give p a time index and then declare that it is constant in time.

We appreciate the reviewer's comment and agree that the current wording may be confusing. This will be rectified in the revised manuscript.

- In a data assimilation cycling system, where there are sequential assimilation time-windows and subsequent forecast steps, it is common to express both model states and parameters as functions of time. In a cyclic data assimilation system, parameters would be updated after each assimilation window and before the next forecast step, and in this sense they would evolve with time. Assigning a time index to the parameter vector ensures consistency with the time-dependent structure of the model state equations Thus, our notation has been designed for flexibility for future applications, with cycling in mind.
- In this study, however, we only use one assimilation window. The model parameters are assumed to be time-invariant over the data assimilation time-window, as the properties they represent (e.g., soil hydraulic parameters) are not expected to vary significantly over the one-year time-window considered.

12) Line 245 to 253 Replace N_e by the value chosen here (50), as mentioned anyway several times and as the other particular parameters are also specified as values.

We will replace N_e by 50 at the three places suggested.

13) The references contain a large number of malformed doi links.

Thank you for pointing this out. We will correct the DOI formatting.