The authors thank all three anonymous reviewers for their useful comments, which will help improve the manuscript. Each comment is repeated in black text here; our responses are given in blue text and changes to the manuscript are given in green. A marked-up version of the new manuscript showing all changes is also provided. Line numbers in our responses refer to this marked-up document.

Reviewer 1:

The author demonstrates the need to use PTFs for LSMs and propose to use DA to calibrate PTF parameters with COSMOS-UK soil moisture measurements. The calibrated PTF parameters for Cosby PTFs were used to run JULES, and a better match with in-situ SM measurements was found. Although the structure of the manuscript is clear, there are some unclear points needed clarification.

1. In the conclusion, the author claimed that "Calibrating PTFs for the soils on which they are to be used and at the scales at which they are applied, rather than on small-scale field or lab soil samples, will ultimately improve the performance of land surface models." First of all, I agreed with the author that the LaVEnDAR DA framework was used to calibrate the Cosby PTF parameters (k1-k12). On the other hand, there is a very strong assumption the author is making here, which is that they deemed the soil texture information as from HWSD is the one very close to the in-situ conditions. This is not always true as demonstrated by the work below: Zhao, H., Zeng, Y., Lv, S. & Su, Z. 2018, Analysis of soil hydraulic and thermal properties for land surface modeling over the Tibetan Plateau, Earth system science data. 10, 2, p. 1031 This actually means that the better match between predicted SM and the COSMOSUK SM measurement, as demonstrated in this study, can be achieved with any other soil texture information input (e.g., SoilGrids, or FAO-UNESCO). But then, this is very dangerous then, as it will lead to a speculation that the in-situ measured soil information is not important . . . . . .

This work is based on the assumption that the soil texture data is correct, and we have made this clearer in the manuscript by adding the following text at line 181.

We assume that the soil texture values from the HWSD are correct; they are not changed during the data assimilation process. We used a global soil dataset rather than any locally available soil texture observations to ensure that our method has the potential for extension to areas without local measurements. Other open source global soil texture products are also available (e.g. SoilGrids Hengl et al (2017)). We acknowledge that there may be discrepancies between the HWSD and local measurements (e.g. Zhao at al (2018)), but our choice to use the HWSD here follows recent successful integration of soil texture data from the HWSD with JULES in studies such as Martinez de la Torre (2019), Ritchie et al (2019) and Ehsan Bhuiyan et al (2019)

2. For the subsections 3.2 & 3.3, they are not independent. Furthermore, the subsection titles seem need further critical thinking (see specific comments). 'Effect of Data Assimilation on . . . . . .' does not reflect the contents and seems not justified, especially when the k1-k12 were used as the state vector, which is supposed to be updated with DA and therefore the soil physics properties via Eq. 2-11.

We have added text to the start of sections 3.2 and 3.3 to make clearer the distinction between direct updating of the state vector (k1-k12) and subsequent adjustments to the JULES soil physics parameters:

Line 261: The data assimilation algorithm in this study acts directly on the PTF constants k1- k12 which make up the state vector. The resulting changes to the JULES soil physics parameters through equations (2) - (11) are presented here in section 3.2. Figures 8 and 9 show changes to the eight JULES soil physics parameters used for the topsoil and subsoil layers respectively. (Section 3.3 shows how the underlying PTF constants are updated).

Line 277: In this section we present the changes to the 12 PTF constants k1 - k12. These updates are the direct result of applying the data assimilation algorithm.

3. How were the COSMOS-UK SM measurements calibrated is not clear. It is understood that there were previous publications. However, some specific descriptions on how the CRNP measurements were calibrated in the table3 will help readers to understand why this or that station works. The relevant part of discussion on this is too thin.

We have added more detail about the calibration process in section 2.2, line 117.

The CRNS at each site counts fast neutrons within the sensor's footprint. These counts are corrected for local meteorological conditions using in situ measurements and also background neutron intensity using data from a neutron monitoring station (Evans et al., 2016). The corrected counts are then calibrated for site-specific soil properties determined from destructive soil sampling conducted after site installation. Soil samples were collected from each site following Köhli et al. (2015) and were returned to UKCEH for laboratory analysis. The results were used to determine reference soil moisture, lattice and bound water, bulk density and organic matter for the day of sampling, and are subsequently used to derive soil water content from the corrected CRNS counts.

The following comments from reviewer 1 were provided as annotations to a pdf.

Line 30: Please be consistent with the unit used.

We have changed 12 ha to 120,000m^2 throughout the manuscript.

Line 28. Make here a paragraph.

We have made a new paragraph here.

Line 38. well, one set of pedotransfer functions? What about spatial heterogeneity.

The pedotransfer functions should be applicable to any area over which soil texture information is available.

There is recently a paper on assimilating CRNS signal into a LSM utilizing Particle Filter:
Mwangi, S., Zeng, Y., Montzka, C., Yu, L., & Su, Z. (2020). Assimilation of cosmic-ray neutron counts for the estimation of soil ice content on the eastern Tibetan Plateau. Journal of geophysical research : Atmospheres, 125(3), 1-23. [e2019JD031529]. https://doi.org/10.1029/2019JD031529.
This citation has been added at line 49.

Line 48: assimilate

This has been changed

Line 55: deployed to

This has been changed to '..introduce the metric we deployed to measure how well....'

Line 57: in

We have replaced 'to' with 'in'

Line 77:

We have changed Jules to JULES

Line 116: 'unit' to be consistent.

We have changed 12 ha to 120,000m^2

Line 155: ??

We have add text to clarify the meaning of the 75m D86 value at line 155:
The observed depth changes with soil moisture and with distance from the CRNS instrument; here we have used the reported observation depth at 75m from the CRNS. For each day, we calculate a depth-adjusted JULES soil moisture estimate, SM_{depth}, depending on the 75m observation depth value, D86, provided for that day, such that..

Line 170: how to select? Randomly?

Yes, these are randomly selected.

Line 172: Are there soil texture information from COSMOS-UK sites? During the whole process, the soil texture information does not change, right? Please clarify.

Limited soil texture information is available at COSMOS-UK sites. We chose to use a globally available soil texture product in order to test the ability of the model to work in areas where local soil information is not available.

The soil texture information is assumed to be correct and we do not update it during the data assimilation process. We have added text to clarify this at line 179; see also our response to Reviewer 1's major comment no. 1.

Line 200: why? In step4, you mentioned you run for a 2 year time window. Any specific reason for this? Please clarify.

We use only observations from 2017 in the data assimilation algorithm and show that the resulting changes to the PTFs allow the JULES soil moisture to better match observations from both 2017 and 2018. The better match to observed data from 2018, which has not been included in the algorithm, strengthens our conclusions that the updated PTFs represent the physical processes better than the original.

Figure 2: what period of data you are using for data assimilation should be specified in this schematic.

We have added this information to the caption of figure 2.

In this study only observations from 2017 (at each site) were used in the assimilation algorithm.

Line 239: At least 10 out of 16 sites (the last one is not visible or they are the same?), the posterior 'r' is smaller than the priori 'r', which seems a systematical slight deterioration of correlation coefficients. This reviewer suggested the authors to dig deeper on this and clarify.

The reviewer is correct - there is a slight deterioration of the correlation coefficient at most sites. We will clarify this by replacing text at line 239 with:

..although there is a slight deterioration of the correlation coefficient at the majority of the sites. Despite this, the reduction in r is very small compared to the overall improvement in the KGE metric at all sites, and the prior and posterior r values are all greater than 0.8 at sites with a typical mineral soil

Line 244: This is not very clear. This reviewer is wondering if the COSMOS-UK CRNP were all calibrated? as such, the water held on the canopy of trees should be removed from the CRNP measurement. Otherwise, the COSMOS-UK CRNP measurement, at least at this site, should not be used.

The soil moisture measurements are calibrated at each site; we will add text to clarify this in section 2.2 (see response to your major comment no. 3). The presence of a large number of coniferous trees at Gisburn Forest potentially makes the calibration less reliable and we suggest that this, along with high organic content of the soil, contributes to the difficulty of fitting JULES to the observations. We will clarify this from line 244 by amending the text to read as follows:

.. which is likely due to the fact that there are a large number of trees at this site. The presence of aboveground biomass may make the site-specific calibration less reliable than at other sites (Baatz et al. (2014)). The high organic carbon content of the soil at Gisburn Forest likely also contributes to this as our chosen PTF is designed to work best with mineral soils. Interception is another processes which potentially complicates the calibration at sites with vegetation, although the authors of Bogena et al (2013) report that water intercepted by the canopy constitutes a negligible amount of the water detected in the CRNS footprint, even in coniferous forests.

Line 260: What the author compared in Figure 8 is actually not the effect of data assimilation on soil physics parameters, but part of the data assimilation itself. The 50 perturbed soil physics parameters, k1-k12 (strictly speaking, this should be PTF parameters), deemed as the state vector in this study, will be definitely updated after data assimilation. The perturbation or update of these k1-k12 values will definitely lead to changes of soil physics properties, via Equation 2-11. As such, it seems this section title is saying "effect of data assimilation on 'state vectors' ". Such saying will mislead readers. Since by its nature and definition, data assimilation already includes 'the update of state vectors'.

We have added text at the start of sections 3.2 and 3.3 to make clearer the distinction between direct updating of the PTF constants in the state vector (K1-K12) and the resulting changes to the JULES soil physics parameters. See also response to your major comment no. 2.

Line 273: This reviewer would suggest to show the results as well.

Unfortunately the soil temperature data we have is not measured at depths which correspond exactly with the JULES layers. For this reason, though we have compared the two datasets informally for consistency, we do not feel they are suitable for publication.

Line 276: See my comments on the subtitle '3.2'. These two are really not independent.

We have added text to the start of sections 3.2 and 3.3 to make this clearer; see our response to major comment no. 2.

Figure 8: the figure title is not mentioned in the main text.

We refer to figures 8 and 9 throughout section 3.2. We have also added the following text to the start of section 3.2 to make clear the difference between the two:

Figures 8 and 9 show changes in the eight JULES soil physics parameters used for the topsoil and subsoil layers respectively.

Line 292: Remove

The word ‘values’ has been removed.

Figure 9: The symbol in the main text is different from the figure title. Please make it consistent.

We have provided parameter names and corresponding symbols in table 1. We have now also added the parameter names to text in the section 3.2 to make the analysis easier to follow.

Reviewer 2

This paper clearly and neatly shows a study on optimizing constants in the underlying Cosby pedotransfer functions used by JULES model via assimilating daily-averaged COSMOS-UK soil moisture data through LaVEnDAR data assimilation approach. With calibrated values for PTFs constants, the paper shows updated soil hydraulic parameters representing on field scale and comparison results to those on small (~cm) scale. With 'vsat' updated being large and 'satcon' and 'sathh' being small, underestimations of soil moisture shown as prior are corrected and simulated soil moisture as posterior shows consistency to in situ measurements. The proposed method in this paper is an alternative attractive way to contribute to improving soil water flow and heat transport simulations by land surface models. I have four major comments and few mirror comments on the manuscript. I would suggest the consideration of accepting this paper after the author addresses major comments.

The authors thank the reviewer for their useful comments

Major comments

1. At line 188, "The daily soil moisture measurements we use are averaged from 30 minute soil moisture measurements. . .. . .uncertainty in the daily values is approximately 20%. We have inflated this here to 50% observation error. . .. . .in fact there will likely be intra-site correlations between observation errors due to site-specific instrument calibration." Here "uncertainty in the daily values is approximately 20%", what does uncertainty mean? Is it the standard deviation of soil moisture at a daily scale or 20% is an estimate accounting for the conversion from neutron counts to soil moisture? Is inflated 50% observation error as a result of an optimized one, how? How can it be proved that inflated error accounts for intra-site correlations between observation errors due to site-specific instrument calibration?

We will make this clearer. The quoted 20% error refers just to observed variance in the half hourly soil moisture values used to calculate the daily mean. The subsequent inflation of observation error was motivated by the fact that not doing so lead to a degradation of the results at all sites. We only speculate that observation error inflation is necessary due to intra-site correlations between observation errors due to site-specific instrument calibration, but as the reviewer notes, errors in the conversion to neutron counts to soil moisture will also be important here. We will change the text from line 188 to clarify:

The daily soil moisture measurements we use are averaged from hourly soil moisture measurements; analysis of the data shows that the standard deviation of the hourly data around the daily mean is approximately 20%. We have inflated this here to 50% observation error; we note that similar observation error covariance inflation techniques have been used in e.g. assimilation of satellite observations in numerical weather prediction (Fowler (2018), Hilton(2009)). The reason for inflating the observation error is essentially because we found that smaller observation error values impacted negatively on the posterior soil moisture results. We suggest that inflation of the observation error is necessary here to compensate for otherwise neglected sources of error (e.g. the error in converting neutron counts to soil moisture) and for the assumption of uncorrelated observation error; in fact there will likely be intra-site correlations between observation errors due to site-specific instrument calibration.

2. In Fig. 3, posterior shows matching to in situ measurements except for the underestimation of soil moisture during the soil wetting period (around 2018-04 and 2018-11), why? Is it related to PTFs structure itself? Compared to Fig. 3, please in Fig. 4, it is better to give numbers such as the correlation coefficient and RMSE.

Across the 16 sites there are variations in how well the posterior JULES estimates match the data; we see a 'global' improvement (i.e. across all 16 sites) across the two years but there are some parts of the data which fit better than others. We have not examined possible physical causes for each case. We will provide prior and posterior RMSE values and correlation coefficients in the captions of figures 4 and 6. Correlation coefficients are also given for each site in figure 7.

3. At line 181, it is mentioned that soil texture information for each site was taken from the Harmonised World Soil Database (HWSD) (Fischer et al., 2008). As soil texture information is a base for obtaining optimized constants for pedotransfer functions, how about the quality of HWSD compared to in situ measurements? Fig. 8 and Fig. 9 show almost the same values for topsoil and subsoil, soil profile in the site is homogenous or because of used HWSD product? How do the optimized constants for pedotransfer functions and associated soil moisture change with different soil texture inputs? Additionally, please if available, add (measured) soil constituents for each site in Table 3.

Other reviewers also questioned our use of the HWSD. Unfortunately, we do not have access to local sand, silt, clay fractions so we can't add those to table 3. Additionally, we wanted to make sure our method would work when only global dataset information such as from the HWSD was available. The similarity of the results in figs 8 and 9 is indeed due to the fact that the HWSD textures were very similar but we cannot comment on how well this matches the real situation. We plan to add text from line 181 to clarify our choice to use the HWSD:

We assume that the soil texture values from the HWSD are correct; they are not changed during the data assimilation process. We used a global soil dataset rather than locally available soil texture observations to ensure that our method has the potential for extension to areas without local measurements. Other open source global soil texture products are also available (e.g. SoilGrids Hengl et al (2017)). We acknowledge that there may be discrepancies between the HWSD and local measurements (e.g. Zhao at al (2018)), but our choice to use the HWSD here follows recent successful integration of soil texture data from the HWSD with JULES in studies such as Martinez de la Torre (2019), Ritchie et al (2019) and Ehsan Bhuiyan et al (2019)

4. At line 294, "The new distributions allow the model to access higher soil moisture values, potentially correcting for a deficiency in supporting datasets, parameter values or process representation in JULES", please clarify supporting datasets, do you mean the deficiency of soil properties dataset?

We will clarify this statement from line 294 to read:

The new distributions allow the model to access higher soil moisture values, potentially correcting for a deficiency in parameter values, process representation in JULES, or in supporting datasets (such as soil texture information or driving meteorological data).

Minor comments

1. In Table 1, the unit of satcon, Ks shall be kg m-2 s-1. Please check.

This has been corrected.

2. In Table 3, for the last cell, please complete the phrase “mineral (soil) with very high organic content”. Please explain the difference between Grassland/heath and Grassland.
   Where we have indicated grassland/heath there are a few shrubs present at the site. We have clarified this in the table caption.
3. In Fig. 10, what does the blue line mean?
   The blue line shows the original value of the constant as in table 2, we have added this to the caption of fig 10.
4. Please keep the citation consistent, for example, (Best et al. (2011),Brooks and Corey (1964)), (Cosby et al., 1984; Marthews et al., 2014). At line 168, Gupta et al. (2009); Knoben et al. (2019)
   Thanks for flagging this - we have made this consistent.
5. Please replace "in-situ" by "in situ", which follows the convention that Latin phrases should not be hyphenated (e.g. "in situ", not "in-situ").
   We have corrected this throughout the manuscript.

Reviewer 3

General Comments:

Authors present an approach which combines soil moisture predictions from the JULES land surface model with in-situ field scale observational data measured by cosmic ray neutron sensors of 16 sites. Cosby et al. (1984) pedotransfer functions were used to compute soil hydraulic parameters for the JULES model. The manuscript shows that JULES model performs better in the prediction of soil moisture if the constants of the pedotransfer functions are calibrated based on field-scale soil moisture observations. This way soil physics parameters of the JULES are not directly optimized. The manuscript presents a new approach to improve performance of JULES model in soil moisture prediction. It is a high quality research, has interesting results and is well structured. Only one aspect could be explicitly clarified, if soil textural information was derived from a course resolution raster dataset in the presented analysis. If that is the case, it would be important to discuss how uncertainty of soil textural data influences the performance of the prior JULES run.

The authors thank the reviewer for their comments.

Specific Comments

1. Title, L126, L252 and L262: In most of the text COSMOS-UK observations was mentioned as field-scale observations, except in the title, L126, L252 and L262, where large-scale is written. It might be better to call it field-scale. Please revise entire text to be consistent in using filed-scale and large-scale. L126: In the above text COSMOS-UK observations was mentioned as field-scale observations, here “large-scale” is written. It might be better to call it field-scale. Please revise it.

We have revised the use of ‘large scale’ to ‘field scale’ throughout the paper.

2. L84-90: Reference of equations 8-11 is not clear, could you please clarify it or add the reference?

We have clarified the sources of these equations with extra text after equation 11 (line 96):

Equations (8) and (9) are rearrangements of equation (2) at fixed values of matric suction corresponding to the wilting and critical points. Equation (10) is a linear combination of the assumed heat capacities of sand, silt and clay, weighted by their relative fractions, and equation (11) is as given in Dharssi et al (2009).

3. L80: In the original Cosby et al. (1984) paper (Table 4 on page 686), the multiple linear regression of the "Absolute value of the soil matric suction at saturation" uses silt% and sand%, but the equation 6 of the manuscript includes clay% and sand%. Please recheck the equation or add further reference if a modified version of Cosby et al. (1984) pedotransfer functions are used.

   Table 2: The constants needs a further check, compared to Table 4 of Cosby et al. (1984), because of the following. It is not clear: - why k2 and k3 are multiplied by 100; - why k4 is divided by 100 and in the same time the original values of k5 and k6 are kept; for predicting volumetric water content in m3/m3: also k5 and k6 has to be divided by 100 or do you consider sand and clay content as g/g (not weight %); - why k7, k8, k9 constants differ from the original constants, please note that in the original PTF silt% and sand% are the predictors as mentioned above, please clarify in the text why the constants differ from that of Cosby et al. (1984); - why k11 and k12 are multiplied by 100, do you consider sand and clay content as g/g (not weight %)? If you find after the check that constants of Cosby PTF is are those are built in the JULES model it might be helpful to check those also in the model code. Please add the units and fraction limits of clay, silt and sand content in line 91.

The differences in the values of constants between Cosby et al (1984) and here are in part due to conversions of units (from e.g. inches per hour to kg m^{-2} s^{-1} for Ksat). As the reviewer notes, we have used clay and sand as predictors in all equations, using the fact that $f_{sand} + f_{silt} + f_{clay} = 1$; this also changes the value of some of the constants. The PTF constant values we have given here match those in table 1 of Marthews et al (2014) with a small exception. While Marthews et al (2014a) express clay, sand and silt fractions as percentages, we use fractions (i.e. in Marthews et al, $f_{sand} + f_{silt} + f_{clay} = 100$). This means that the multipliers given for f_{sand} and f_{clay} are 100 times larger in our version. We have added a reference to Marthews et al (2014) at line 102:

The values of the constants given here match those in Marthews et al (2014a) (with soil fraction multipliers adjusted for fraction, rather than percentage, of soil by weight).

To clarify, the PTF is not built into the JULES code; users are required to provide values for the soil physics parameters, but can calculate these via any choice of PTF (or other method).

The units for f_{sand} etc are fraction by weight, i.e. dimensionless, and we have added this to the text at line 96.

4. L104: Please list meteorological data required by JULES to derive soil moisture prediction.

We have added this information (line 104).

The required input variables are: air pressure, air temperature, humidity, downward fluxes of shortwave and longwave radiation, precipitation and wind speed.

5. L110-112: Please consider that CHIMN, PORTN, HARTW, LULLN are mineral soils too based on Table 3, therefore the sentence starting with "The Cosby pedotransfer function . . ." needs to be revised.

We have revised sentence from line 129 to read:

The Cosby pedotransfer function was designed to work for mineral soils, and the CRNS calibration is most reliable at sites with minimal vegetation. We therefore consider that the first seven sites listed in table 3 are those at which the JULES model can be expected to provide a good match to observations via our chosen PTF; soil types and land cover at the remaining sites mean that JULES may not be able to represent the observed soil moisture time series as accurately.

6. Table 3: Instead of the basic soil description it would be more informative to provide soil taxonomical information, i.e. name of soil suborders (USDA, Soil taxonomy) or reference soil groups with principal qualifiers (WRB, 2014). If soil taxonomical information cannot be added, soil texture, organic carbon content and bulk density of topsoil and subsoil could be shown, if that is available for the COSMOS-UK sites.

   L120: Are measured soil chemical and physical properties available for the COSMOSUK sites.

Unfortunately we do not have access to any further soil texture, chemical and physical properties, or taxonomical information for the soils at COSMOS-UK sites.

7. L119-120: sentence starting with "We have used . . ." is repetition of the first part of the sentence starting with "In this paper . . ." in line 95-96.

We feel that it is useful to remind the reader of this at this point in the paper.

8. L147: The reference for LaVEnDAR is given, but it might be helpful for the readers if a very short description of the data assimilation technique would be given in the text.

We have added the following short description of the algorithm at line 147:

LaVEnDAR optimises k1 to k12 here by minimising a cost function with two terms. The first term is a measure of the difference between the observed and modelled soil moisture, and the second term is a measure of the difference between prior and posterior values of k1 to k12.

9. L155: Please add the meaning of "75m" or delete it if it is not important.

We will clarify this by adding the following text at line 155:

The observed depth changes with soil moisture and with distance from the CRNS instrument; here we have used the reported observation depth at 75m from the CRNS. For each day, we calculate a depth-adjusted JULES soil moisture estimate, SM_{depth}, depending on the 75m observation depth value, D86, provided for that day, such that..

10. L148: Is not measured soil texture available at the COSMOS sites? Uncertainty of texture taken from the Harmonised World Soil Database (HWSD) can be high, because its resolution is 30 arc-second. If texture is derived from a course resolution dataset the lower performance of prior JULES run can come from the uncertainty of clay, silt and sand content. It would be interesting to analyse the performance of prior JULES run at a site where measured soil texture can be used in the Cosby pedotransfer functions. If there is no measured soil texture data, better resolution national soil texture maps or 250 m resolution SoilGrids could provide more accurate soil textural information than HWSD does. Please consider to rerun analysis based on a more accurate soil texture dataset or explain why HWSD was used. It would be good to highlight importance of using measured soil texture if that is available.

Reviewers 1 and 2 made similar comments. We used a global soil texture dataset here because we wanted to make sure our method would work when local measurements are not available, and in fact we do not have soil texture data for the COSMOS sites, only the broad descriptions given in the COSMOS-UK user guide (v2). We feel that rerunning the experiments using an alternative soil texture database would lead to an interesting comparison with the work here, but is out of the scope of this paper, which aims to demonstrate a new method for calibrating PTF constants. We have added text from line 181 to explain our choice to use the HWSD:

We assume that the soil texture values from the HWSD are correct; they are not changed during the data assimilation process. We used a global soil dataset rather than any locally available soil texture observations to ensure that our method has the potential for extension to areas without local measurements. Other open source global soil texture products are also available (e.g. SoilGrids Hengl et al (2017)). We acknowledge that there may be discrepancies between the HWSD and local measurements (e.g. Zhao at al (2018)), but our choice to use the HWSD here follows recent successful integration of soil texture data from the HWSD with JULES in studies such as Martinez de la Torre (2019), Ritchie et al (2019) and Ehsan Bhuiyan et al (2019)

11. L188: Does it mean that higher observation error was used when results of soil moisture predictions was assessed than the error computed based in the measured data? The reasoning of it is not clear, could you please describe it? Sorry if I miss something.

The inflation of observation error is for use in the LaVEnDAR algorithm and is a reasonably common technique in data assimilation. We will clarify this with the following text from line 188:

The daily soil moisture measurements we use are averaged from hourly soil moisture measurements; analysis of the data shows that the standard deviation of the hourly data around the daily mean is approximately 20%. We have inflated this here to 50% observation error; we note that similar observation error covariance inflation techniques have been used in e.g. assimilation of satellite observations in numerical weather prediction (Fowler (2018), Hilton(2009)). The reason for inflating the observation error is essentially because we found that smaller observation error values impacted negatively on the posterior soil moisture results. We suggest that inflation of the observation error is necessary here to compensate for otherwise neglected sources of error (e.g. the error in converting neutron counts to soil moisture) and for the assumption of uncorrelated observation error; in fact there will likely be intra-site correlations between observation errors due to site-specific instrument calibration.

12. Figure 2. Maybe the following could be added: - Data assimilation (LaVenDAR), - 16 sets of field-scale obs,

We have updated the schematic in figure 2 to include these suggestions

13. L185: Please add which software was used to compute the metrics and prepare plots.

We will add this information at line 221.

We used python 3.7.1 to calculate metrics and prepare plots.

14. L233: Please add under Materials and methods section which method was used to analyse if difference was significant.

We used 'significant' in a non-mathematical sense here. We will replace 'significant' with 'marked' in line 233.

15. L205-206: It would be informative to roughly add the soil organic content of MOORH site, if measured value is available that would be the best. Could you please add reference to the CRNS regarding soil organic carbon content and texture that can be reliably measured?

Unfortunately we do not have any further reliable information about the soil organic content at MOORH.

16. L244: It could be mentioned that it is a disadvantage that CRNS measurement considers water held on the canopy to be soil moisture. Is there any solution for correcting the COSMOS soil moisture values if that happens?

Soil moisture measurements are calibrated at each COSMOS-UK site, and this aims to correct for water stored on vegetation. However, vegetation makes the calibration less reliable for a number of reasons. We will add text from line 244 to make this clearer

.. which is likely due to the fact that there are a large number of trees at this site. This means that the presence of aboveground biomass may make the site-specific calibration less reliable than at other sites (Baatz et al. (2014)). The high organic carbon content of the soil at Gisburn Forest likely also contributes to this as our chosen PTF is designed to work best with mineral soils. Interception is another processes which potentially complicates the calibration at sites with vegetation, although the authors of Bogena et al (2013) report that water intercepted by the canopy constitutes a negligible amount of the water detected in the CRNS footprint, even in coniferous forests.

17. Figure 8. Please add soil depth that you consider topsoil.

The depths are 0 - 35cm and 35cm – 300cm for topsoil and subsoil layers respectively. We have added assumed depth information to the captions of figures 8 and 9.

18. L240: Do you think the profile-scale measurements could be successfully used in the presented data assimilation method?

An alternative approach would have been to use point scale measurements in our experiments. However, point sensors only measure the soil moisture in a very small area and are therefore not representative of the soil moisture on the scales that JULES is typically used. We see from point sensors at COSMOS-UK sites that sensors quite close to each other can measure quite different soil moisture values due to their different very localised conditions. We chose to use field-scale measurements here in order to average out the local variations in observed soil moisture and to better match the scales over which JULES is typically used.

19. L274: The code is available only for those who are registered for a Met Office account, it might be mentioned.

We have added text to clarify this.

Technical Corrections:

L91: . . . where fclay, fsilt and fsand are fractions of clay, silt and sand in the soil . . .

L143: Do you mean: “the value given in table 2”? Please revise it.

L193: . . . high soil organic carbon content . . .

L229: . . . 12 PTF . . .

Thank you for spotting these errors, which we have corrected.

New References:

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Using data assimilation to optimize pedotransfer functions using ~~large-scale in-situ~~ field scale in situ soil moisture observations.

Elizabeth Cooper[1], Eleanor Blyth[1], Hollie Cooper[1], Rich Ellis[1], Ewan Pinnington[3], and Simon J. Dadson[1,2]

[1]UK Centre for Ecology and Hydrology, Wallingford, UK.
[2]School of Geography and the Environment, South Parks Road, Oxford OX1 3QY
[3]National Center for Earth Observation, Department of Meteorology, University of Reading, Reading, UK

Correspondence: Elizabeth Cooper (elicoo@ceh.ac.uk)

Abstract. Soil moisture predictions from land surface models are important in hydrological, ecological and meteorological applications. In recent years the availability of wide-area soil-moisture measurements has increased, but few studies have combined model-based soil moisture predictions with ~~in-situ~~ in situ observations beyond the point scale. Here we show that we can markedly improve soil moisture estimates from the JULES land surface model using field scale observations and data assimilation techniques. Rather than directly updating soil moisture estimates towards observed values, we optimise constants in the underlying pedotransfer functions, which relate soil texture to JULES soil physics parameters. In this way we generate a single set of newly calibrated pedotransfer functions based on observations from a number of UK sites with different soil textures. We demonstrate that calibrating a pedotransfer function in this way can improve the performance of land surface models, leading to the potential for better flood, drought and climate projections.

1 Introduction

Soil moisture is an important physical variable, significant in agriculture (Pinnington et al., 2018), flood events (Koster et al., 2010; Berghuijs et al., 2019), and processes related to weather and climate (Seneviratne et al., 2010). Land surface models such as the Joint UK Land Environment Simulator (JULES) can be used to make predictions of soil moisture, and generally rely on empirical pedotransfer functions (PTFs) to relate readily available or easy-to-measure soil characteristics such as soil texture to the soil hydraulics parameters required by the model ~~(see e.g.Van Looy et al. (2017)).~~ (e.g., Van Looy et al., 2017)

There are a number of different types of pedotransfer function, as noted in Van Looy et al. (2017) and Hodnett and Tomasella (2002), with different inputs and outputs depending partly on the requirements of the chosen land surface model. In 'class' approaches, soil types are clustered into groups, and hydraulic model parameters are then obtained from a look-up table (Wösten et al., 1999); this results in discrete soil hydraulics parameter sets. Alternatively, continuous pedotransfer functions take soil characteristic information from each sample of interest and apply the function to produce continuous soil hydraulics parameter sets ~~(e.g.Cosby et al. (1984) , Hodnett and Tomasella (2002) , Schaap et al. (2001)).~~ (e.g., Cosby et al., 1984; Hodnett and Tomasella, 2002; Schaap et al., 2001) .To date, pedotransfer functions have been derived by fitting to results from field or laboratory experiments on point or small-scale soil samples (cm to m), despite the fact that land surface models are generally applied at larger (field to km) scales. The recent development of novel ~~in-situ~~ in situ techniques for measuring soil moisture over field, rather than point scale presents an opportunity to test whether land surface models, in conjunction with commonly used pedotransfer functions, are able to reproduce field-scale soil moisture observations.

In this paper, we have compared JULES soil moisture predictions with soil moisture observations from the COSMOS-UK dataset (Stanley et al., 2019); these observations are measured by cosmic ray neutron sensors (CRNS) over a footprint of up to ~~12 ha~~120,000m^2. We have then used the LaVEnDAR four dimensional ensemble variational data assimilation framework (Pinnington et al., 2020) to combine COSMOS-UK soil moisture observations at 16 sites with equivalent JULES soil moisture estimates. We have thereby optimized constants in the Cosby pedotransfer function (Cosby et al., 1984). This results in a newly calibrated set of pedotransfer functions based on field-scale soil moisture observations across 16 sites with a range of soil types. This approach allows us to test whether we can improve the performance of the model by optimising the pedotransfer functions for larger scales using field-scale soil moisture observations. Our approach also allows comparison of the soil hydraulics parameters generated using ~~large-scale~~ field scale ($\sim$ hundred metre) soil moisture measurements with those generated by the original pedotransfer functions, which are based on small-scale ($\sim$ cm) measurements. We chose to optimize the pedotransfer functions rather than directly optimizing soil physics parameters to better ensure physically consistent parameter sets; this approach also has the advantage that we can assimilate observations from all sites simultaneously to produce one set of pedotransfer functions applicable at all sites and beyond.

Larger scale soil moisture measurements are also increasingly available from satellite products and these have been used to good effect in data assimilation frameworks with land surface models ~~in e. g. Pinnington et al. (2018) , Liu et al. (2011) , De Lannoy and Reichle (2016) and Yang et al. (2016) .~~ (e.g., Pinnington et al., 2018; Liu et al., 2011; De Lannoy and Reichle, 2016; Yang et al., 2016) . The advantage of the CRNS measurements used here is that they provide a more direct soil moisture measurement than those from satellites. CRNS soil measurements are also representative of depths of approximately 10 to 30cm, compared to the top 5 to 10 cm for satellite retrievals.

An alternative approach to ~~assimilation of~~ assimilate CRNS soil moisture measurements into land surface models is taken in Brunetti et al. (2019)~~and Han et al. (2015) ~~, Han et al. (2015) and Mwangi et al. (2020) . These studies ~~both~~ use neutron counts from CRNS instruments as observations, combined with the method presented in Shuttleworth et al. (2013) to map modelled soil moisture estimates into equivalent neutron counts. In this study we instead directly compare modelled and CRNS derived soil moisture.

The rest of the paper is organised as follows: in section 2 we outline the JULES land surface model and the COSMOS-UK data used in this study; we also describe the data assimilation experiment we have performed and introduce the metric ~~by which we have measured~~ we deployed to measure how well the model fits the observations. In section 3 we present results, showing that we can use COSMOS-UK observations from 2017 to improve the fit between the JULES model output and observations over two years at all the sites we included. We discuss our results in the context of changes ~~to~~ in the JULES soil physics parameters in section 4. In section 5 we conclude that it is possible to optimise pedotransfer functions for field scale soil moisture measurements, and that this markedly improves the fit of JULES soil moisture estimates to COSMOS-UK observations.

2 Methods

2.1 JULES land surface model

JULES uses the Darcy-Richards equation to model soil hydraulic processes (Best et al., 2011), so that the downward water flux, W, between adjacent soil layers is given by

$$W = K\left(\frac{\partial \Psi}{\partial z} + 1\right) \tag{1}$$

where Ψ is the soil matric suction, K is the soil hydraulic conductivity and z is distance from the soil surface in the vertical direction.

JULES provides two options for representing the relation between soil water content, θ, matric suction, and hydraulic conductivity; in this paper we use the Brooks and Corey soil physics option ~~(Best et al. (2011) , Brooks and Corey (1964)),~~ (Best et al., 2011; Brooks and Corey, 1964) , where we assume

$$\frac{\theta}{\theta_s} = \left(\frac{\Psi}{\Psi_s}\right)^{-\frac{1}{b}} \tag{2}$$

and

$$\frac{K}{K_s} = \left(\frac{\theta}{\theta_s}\right)^{2b+3}. \tag{3}$$

In equations (2) and (3), θ_s, K_s and Ψ_s are values of soil moisture, hydraulic conductivity and soil matric suction at saturation; b is a soil-dependent constant with a value usually determined through a pedotransfer function. The soil physics parameters used in the implementation of Brooks and Corey soil physics in JULES are briefly described in table 1; more details are available in Best et al. (2011) or JULES user guide. (2020).

The values of the eight soil physics parameters outlined in table 1 are generally calculated via a set of pedotransfer functions. Here we use the Cosby pedotransfer functions, which have the following mathematical formulation, (Cosby et al., 1984; Marthews et al., 2014b)

$$b = \kappa_1 + \kappa_2 f_{clay} - \kappa_3 f_{sand} \tag{4}$$

$$\theta_s = \kappa_4 - \kappa_5 f_{clay} - \kappa_6 f_{sand} \tag{5}$$

Parameter name and symbol	Description
satcon, K_s	Hydraulic conductivity at saturation (~~kgm^{-2}~~kgm^{-2}s^{-1})
sathh, Ψ_s	Absolute value of the soil matric suction at saturation (m)
vsat, θ_s	Volumetric water content at saturation (m^{3}m^{-3})
vcrit, θ_{crit}	Volumetric soil moisture content at -33kPa (critical point) m^{3}m^{-3}
vwilt, θ_{wilt}	Volumetric soil moisture content at -1500kPa (wilting point) m^{3}m^{-3}
b	Exponent in soil hydraulic characteristic
$hcap$	Dry soil heat capacity (J m^{-3}K^{-1}).
$hcon$	Dry soil thermal conductivity (W m^{-1}K^{-1}).

Table 1. Soil physics parameters

$$\Psi_s = 0.01 \times 10^{\kappa_7 - \kappa_8 f_{clay} - \kappa_9 f_{sand}} \tag{6}$$

$$K_s = 10^{-\kappa_{10} - \kappa_{11} f_{clay} + \kappa_{12} f_{sand}} \times \frac{25.4}{3600} \tag{7}$$

$$\theta_{crit} = \theta_s \left(\frac{\Psi_s}{3.364} \right)^{1/b}, \tag{8}$$

$$\theta_{wilt} = \theta_s \left(\frac{\Psi_s}{152.9} \right)^{1/b} \tag{9}$$

$$h_{cap} = (1 - \theta_s)(\cancel{2.376}2.373 \times 10^6 f_{clay} + 2.133 \times 10^6 f_{silt} + 2.133 \times 10^6 f_{sand}) \tag{10}$$

$$h_{con} = 0.025^{\theta_s} \times 1.16^{f_{clay}(1-\theta_s)} \times 1.57^{f_{sand}(1-\theta_s)} \times 1.57^{f_{silt}(1-\theta_s)} \tag{11}$$

where f_{clay}, f_{sand} and f_{silt} are fractions of clay, sand and silt in the soil~~.~~, by weight. Equations (8) and (9) are rearrangements of equation (2) at fixed values of matric suction corresponding to the wilting and critical points. Equation (10) is a linear combination of the assumed heat capacities of sand, silt and clay, weighted by their relative fractions, and (11) is as given in Dharssi et al. (2009) . The values of the constants κ_1 to κ_{12} usually used in equations (4) to (11) are those given in Cosby et al. (1984); we present them in table 2. These values are empirically determined from 1448 small soil samples (cm dimensions) taken from 23 states in the United States (for further details of the soil samples and sampling methods see Rawls (1976) and Holtan (1968)). The values of the constants given here match those in Marthews et al. (2014a) (with soil fraction multipliers adjusted for fraction, rather than percentage, of soil by weight).

Constant	**Value from Cosby et al. (1984)**
κ_1	3.10
κ_2	15.70
κ_3	0.3
κ_4	0.505
κ_5	0.037
κ_6	0.142
κ_7	2.17
κ_8	0.63
κ_9	1.58
κ_{10}	0.6
κ_{11}	0.64
κ_{12}	1.26

Table 2. Values of the constants commonly used in the Cosby pedotransfer functions

JULES requires meteorological driving data to produce soil moisture estimates. The required input variables are: air pressure, air temperature, humidity, downward fluxes of shortwave and longwave radiation, precipitation and wind speed. In this paper we have used half-hourly meteorological observations measured at COSMOS-UK sites as driving data; in this way we can use JULES to give soil moisture predictions at any COSMOS-UK sites with sufficiently complete meteorological data.

JULES provides estimates of soil moisture at various depths; in the standard configuration used here these correspond to four layers, with depths [0,10cm], [10cm to 35cm], [35cm to 100cm] and [100cm to 300cm]. The JULES layers are often referred to by their thicknesses, which are 10cm, 25cm, 65cm and 200cm respectively. Here, we refer to the soil moisture estimates for the four layers as SM_{10},SM_{25},SM_{65} and SM_{200}.

2.2 COSMOS-UK soil moisture data

The COSMOS-UK project comprises a network of soil moisture monitoring stations across the United Kingdom, providing long-term soil moisture measurements at around 50 sites. Data for 2013 to 2017 are available in the EIDC archive ~~(Stanley et al. (2019))~~(Stanley et al., 2019) . Soil moisture observations are made using an innovative Cosmic Ray Neutron

Sensor (CRNS) instrument at each site; these provide a measurement of soil moisture over an area of up to ~~12 ha~~ 120,000m^2 (30 acres) (Antoniou et al., 2019; Evans et al., 2016). The CRNS at each site counts fast neutrons within the sensor's footprint. These counts are corrected for local meteorological conditions using in situ measurements and also background neutron intensity using data from a neutron monitoring station (Evans et al., 2016) . The corrected counts are then calibrated for site-specific soil properties determined from destructive soil sampling conducted after site installation. Soil samples were collected from each site following Köhli et al. (2015) and were returned to UKCEH for laboratory analysis. The results were used to determine reference soil moisture, lattice and bound water, bulk density and organic matter for the day of sampling, and are subsequently used to derive soil water content from the corrected CRNS counts. The majority of sites explored in this study are grasslands and it is therefore expected that CRNS soil moisture results are not significantly affected by seasonal changes in biomass (Baatz et al., 2014) .

We have used daily-averaged soil moisture data from 16 COSMOS-UK sites as observations in this paper. The sites were selected based on completeness of soil moisture and meteorological data over a three year period from 2016-2018 and are listed in Table 3, with details of land cover and broad soil descriptions taken from Antoniou et al. (2019). Locations of the sites are shown in figure 1. For more details of each of the sites, see Antoniou et al. (2019). The Cosby pedotransfer function was designed to work for mineral soils~~and we~~ , and the CRNS calibration is most reliable at sites with minimal vegetation. We therefore consider that the first seven sites listed in table 3 are those at which the JULES model can be expected to provide a good match to observations via our chosen PTF; soil types and land cover at the remaining sites mean that JULES may not be able to represent the observed soil moisture time series as accurately.

Both the depth and the footprint over which the CRNS measure soil moisture change with soil moisture ~~(Evans et al. (2016) ; Köhli et al. (2015) Antoniou et al. (2019))~~(Evans et al., 2016; Köhli et al., 2015; Antoniou et al., 2019) , with the footprint and depth of the measurement both becoming smaller as soil moisture increases. The COSMOS-UK dataset includes estimates of the depth over which each daily soil moisture value is valid, known as a $D86$ value. Measurements of several other environmental variables are made at COSMOS-UK sites, using a suite of instrumentation. These include point soil moisture and temperature measurements at various depths in the soil, and meteorological variables. We have used half-hourly ~~in-situ~~ in situ meteorological data from the COSMOS-UK dataset as driving data for the JULES model.

2.3 Data assimilation

Data assimilation is a group of methods in which information from models and observations is combined in order to give the best estimate of the state of a physical system and/or model parameter values. In this paper we have used the four-dimensional ensemble variational data assimilation technique, LaVEnDAR, which is introduced in Pinnington et al. (2020) and is based on Liu et al. (2008). We use LaVEnDAR ~~here~~ to optimise 12 constants, κ_1 to κ_{12}, in the Cosby pedotransfer functions (eqns (4) to (11)) based on estimates of soil moisture from JULES and corresponding ~~large-scale~~ field scale observations of soil moisture from COSMOS-UK. ~~The~~ LaVEnDAR optimises κ_1 to κ_{12} here by minimising a cost function with two terms. The first term is a measure of the difference between the observed and modelled soil moisture, and the second term is a measure of the difference between prior and posterior values of κ_1 to κ_{12}.

Sitename and abbreviation	Land cover	Soil description
Cardington (CARDT)	Grassland	Typical mineral soil
Bickley Hall (BICKL)	Grassland	Typical mineral soil
Crichton (CRICH)	Grassland	Typical mineral soil
Waddesdon (WADDN)	Grassland	Typical mineral soil
Hollin Hill (HOLLN)	Grassland	Typical mineral soil
Easter Bush (EASTB)	Grassland	Typical mineral soil
Rothamstead (ROTHD)	Grassland	Typical mineral soil
Chimney Meadows (CHIMN)	Grassland	Calcereous mineral soil
Sheepdrove (SHEEP)	Grassland	Mineral soil; fairly high organic carbon content
Porton Down (PORTN)	Grassland	Highly calcereous mineral soil
Hartwood Home (HARTW)	Grassland/woodland	Typical mineral soil
Gisburn Forest (GISBN)	Coniferous forest	Mineral soil; high organic carbon content
Chobham Common (CHOBH)	Heath	Highly variable soil
Lullington Heath (LULLN)	Grassland/heath	Highly calcareous mineral soil
Moorhouse (MOORH)	Grassland/heath	Mineral soil with very high organic content
Sourhope (SOURH)	Grassland	Mineral soil with very high organic content

Table 3. COSMOS-UK sites selected for this study. 'Heath' indicates some shrubs are present at the site.

The values of κ_1 to κ_{12} are assumed to be constant in time and space; the same values are used across all sites to generate soil JULES moisture estimates via the pedotransfer functions.

2.4 Experimental details

In order to use COSMOS-UK data with JULES outputs in the LaVEnDAR scheme, we require both sets of soil moisture values to correspond to the same soil depth. We have therefore devised a weighted depth approach, in which we extract from each JULES prediction an average soil moisture corresponding to the UK-COSMOS ~~$D86$~~ observed depth. The observed depth changes with soil moisture and with distance from the CRNS instrument; here we have used the reported observation depth at 75m from the CRNS. For each day, we calculate a depth-adjusted JULES soil moisture estimate, SM_{depth}, depending on the 75m ~~$D86$ value~~observation depth value, $D86$, provided for that day, such that

$$SM_{depth} = \begin{cases} SM_{10}, & \text{if } D86 \leq 10\text{cm}, \\ \frac{10}{D86}SM_{10} + \frac{(D86-10)}{D86}SM_{25} & \text{if } 10\text{cm} < D86 \leq 35\text{cm}, \\ \frac{10}{D86}SM_{10} + \frac{25}{D86}SM_{25} + \frac{(D86-35)}{D86}SM_{65}, & \text{if } 35\text{cm} < D86 \leq 65\text{cm}, \end{cases} \tag{12}$$

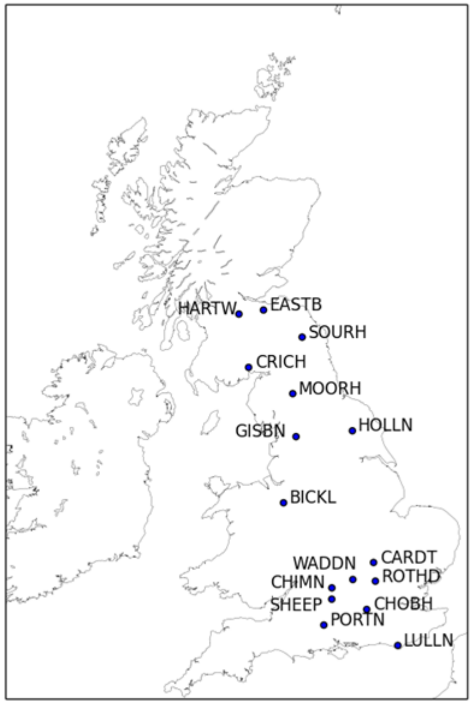

Figure 1. Locations of COSMOS-UK sites used in this study

where SM_{10}, SM_{25} and SM_{65} are the JULES predicted soil moisture values from the [0,10cm], [10cm to 35cm] and [35cm to 100cm] layers respectively, and the D86 value is given in cm. In this way, thickness-weighted contributions to the soil moisture are taken from every JULES layer which would be wholly or partly contained within the D86 depth. We have not taken the COSMOS-UK variable footprint into account in this study.

In this paper we have used an ensemble size of 50, as in related experiments in Pinnington et al. (2020) and Liu et al. (2008). In order to implement the LaVEnDAR scheme we

1. Generated a 50-member ensemble of each of the 12 PTF constants κ_1 to κ_{12}. These were obtained by sampling from a Gaussian distribution centred on the value given in table ~~3~~2, with standard deviation equal to 10% of the mean. This standard deviation value was chosen fairly arbitrarily; future work could assess the sensitivity of the results to the values chosen for each PTF constant.

2. Assembled 50 unique sets of 12 constants κ_1 to κ_{12}.

3. Used each unique set of constants in equations (4) to (11) to generate 50 sets of soil physics parameters for each site. Soil texture information for each site was taken from the Harmonised World Soil Database (HWSD) (Fischer et al., 2008)

4. Used the soil parameter sets to run 50 realisations of JULES at each of our selected sites over a 2 year time window to create a prior ensemble of 50 soil moisture time series per site.

5. Used the LaVEnDAR scheme to generate a new, posterior ensemble of values for each of the 12 PTF constants, taking into account COSMOS-UK soil moisture observations from 2017. Here, we assumed uncorrelated observation errors of 50 % of the mean soil moisture value at each site.

6. Used the new posterior ensemble of PTF constants to generate 50 posterior sets of soil physics variables at each site.

7. Ran 50 posterior realisations of JULES at each site to create posterior soil moisture time series.

These steps are also shown in schematic form in figure 2.

We assume that the soil texture values from the HWSD are correct; they are not changed during the data assimilation process. We used a global soil dataset rather than any locally available soil texture observations to ensure that our method has the potential for extension to areas without local measurements. Other open source global soil texture products are also available, e.g., SoilGrids (Hengl et al., 2017) . We acknowledge that there can be discrepancies between the HWSD and local measurements (e.g., Zhao et al., 2018) but our decision to use the HWSD here follows recent successful integration of soil texture data from the HWSD with JULES in studies such as Martínez-de la Torre et al. (2019) , Ritchie et al. (2019) and Ehsan Bhuiyan et al. (2019) .

We have assumed a high observation error value in this experiment. The daily soil moisture measurements we use are averaged from ~~30 minute~~ hourly soil moisture measurements; analysis of these data shows that ~~uncertainty in the daily values~~ the standard deviation of the hourly data around the daily mean is approximately 20%. We have inflated this here to 50% observation error~~as we~~ ; we note that similar observation error covariance inflation techniques have been used in e.g. assimilation of satellite observations in numerical weather prediction (Fowler et al., 2018; Hilton et al., 2009) . The reason for inflating the observation error is essentially because we found that smaller observation error values impacted negatively on the posterior soil moisture results. ~~Inflation~~ We suggest that inflation of the observation error ~~here compensates for the~~ is necessary here to compensate for otherwise neglected sources of error (e.g. the error in converting neutron counts to soil moisture) and for the assumption of uncorrelated observation error; in fact there will likely be intra-site correlations between observation errors due to site-specific instrument calibration. ~~We note that similar observation error covariance inflation techniques have been used in e.g. assimilation of satellite observations in numerical weather prediction (Fowler et al. (2018) , Hilton et al. (2009)). We have used~~

We have used COSMOS-UK measurements from 2017 only in our data assimilation experiments, but compared the prior and posterior JULES runs from 2017 and 2018 with observations.

2.5 Metrics

In order to assess how well our prior and posterior JULES runs match COSMOS-UK observations we require a metric. Here we have used the Kling-Gupta efficiency metric, as described in Gupta et al. (2009) ~~; Knoben et al. (2019)~~ and Knoben et al. (2019) ,

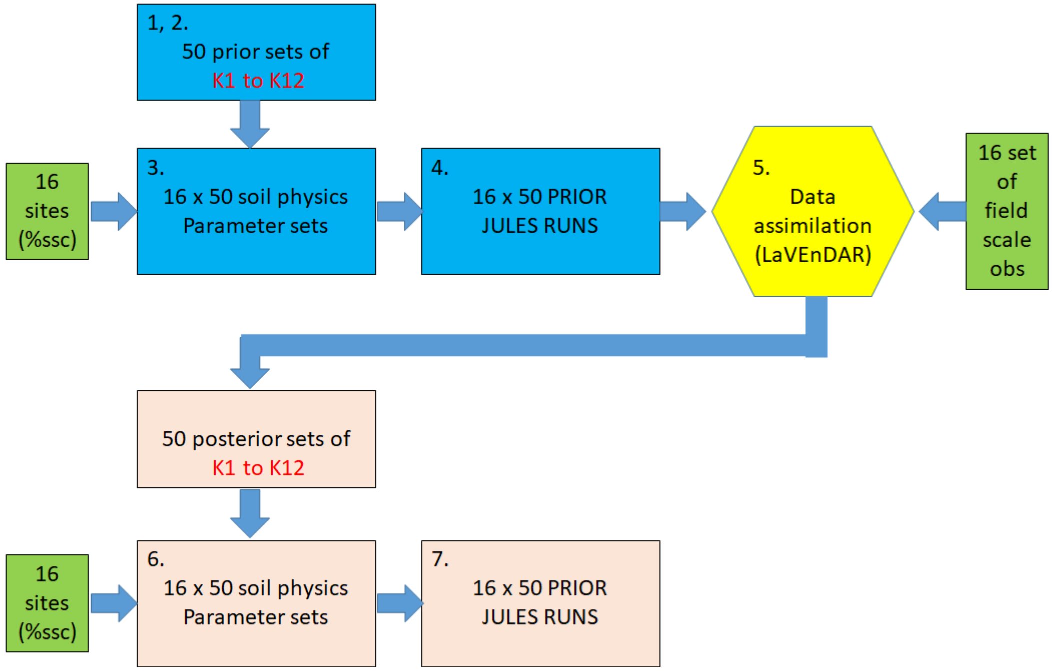

Figure 2. Schematic showing data assimilation experimental design; %ssc refers to site specific fractions of sand, silt and clay in the soil. In this study only observations from 2017 (at each site) were used in the assimilation algorithm.

to compare the goodness of fit between observed and modelled (ensemble mean) soil moisture times series. The Kling Gupta efficiency (KGE) is given by

$$KGE = 1 - \sqrt{(1-r)^2 + (1-\alpha)^2 + (1-\beta)^2}, \tag{13}$$

where

$$\alpha = \frac{\sigma_{model}}{\sigma_{obs}} \tag{14}$$

and

$$\beta = \frac{\mu_{model}}{\mu_{obs}}. \tag{15}$$

In equations (14) and (15), μ_{model} and μ_{obs} are mean values of the modelled and measured soil moisture time series respectively; σ_{model} and σ_{obs} are the standard deviations in the modelled and observed soil moisture time series. The value of r is the Pearson correlation coefficient between the model and the observation time series data, and can vary between -1 (anti-correlation) and 1 (perfect correlation), with score of 0 indicating no correlation. The value of α reflects how well the spread in the modelled soil moisture values matches that of the observations, with a value of 1 corresponding to perfect matching. Equation (15) shows that the value of β represents bias between the model and observations, with a value of 1 indicating zero bias. Since α and β can be larger or smaller than 1, the value of the KGE can range between 1 (perfect model fit to data) to very large negative values. In Knoben et al. (2019) the authors argue that while in some studies a threshold of KGE $\geq$0 has been used to denote 'good' model performance, a lower threshold of KGE $\geq$-0.41 is required for the model to perform better than a mean persistence forecast. We used python 3.7.1 to calculate metrics and prepare plots.

3 Results

3.1 Effect of data assimilation on JULES soil moisture predictions

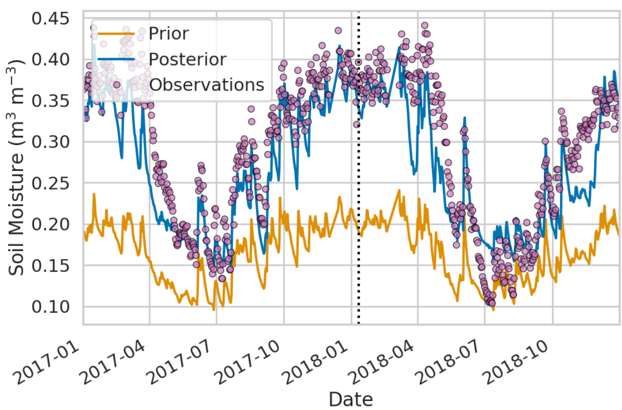

Figure 3. Observed and modelled (ensemble mean) soil moisture time series at Bickley Hall (BICKL). The dotted line separates the period over which observations used for assimilation (2017) from the period in which no observations have been assimilated (2018).

Figures 3 to 6 show measured and modelled soil moisture time series for 2017 and 2018 at two representative COSMOS-UK sites. In all cases the modelled soil moisture series is the ensemble mean. These figures show that the JULES runs using posterior PTF constants produce soil moisture estimates which are a better match to the observations than the JULES runs using the prior PTF constants. Figures 3 and 4 show results from Bickley Hall (BICKL), which is a site at which we expect soil moisture to be well represented by JULES via the Cosby PTF (this site has a typical mineral soil). Figures 5 and 6 represent results from a site at which the high organic content of the soil and the presence of trees means that we do not expect our JULES setup to match the observations so successfully.

Figure 7a shows the KGE values for prior and posterior JULES runs at all 16 sites included in our study. These metrics show how closely the prior and posterior JULES runs match the observations over the period of 2017 and 2018 before and after assimilation of observations from 2017. Figure 7a shows that data assimilation ~~makes fits to observations significantly better~~ markedly improves the fit to observations at all sites according to the Kling Gupta metric; all the analysis Kling-Gupta efficiency scores are closer to the ideal value of 1 than the prior values. We note that for all sites, the match between model and measurements is better in 2017 and 2018 even though only observations from 2017 were used in the optimization process.

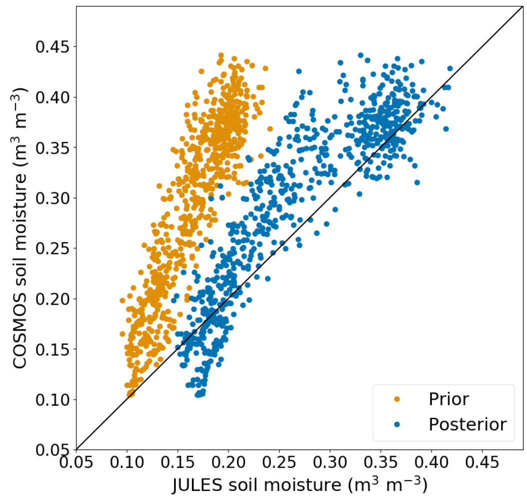

Figure 4. Observed vs modelled (ensemble mean) soil moisture at Bickley Hall (BICKL) for prior and posterior JULES runs. Diagonal line shows 1:1 perfect correspondence line. The correlation coefficient at this site changed from 0.93 (prior) to 0.94 (posterior) and the rmse reduced from 0.13 (prior) to 0.03 (posterior).

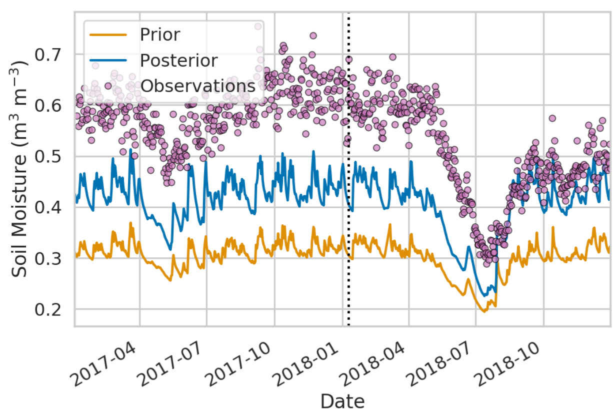

Figure 5. Observed and modelled (ensemble mean) soil moisture time series at Gisburn Forest (GISBN). The dotted line separates the period over which observations used for assimilation (2017) from the period in which no observations have been assimilated (2018).

This indicates that the new values for the PTF constants allow JULES to simulate ~~large-scale~~ field scale scale soil moisture measurements better than the original (prior) PTF constants. Figure 7b shows that the prior and posterior correlation coefficients, r, are very similar at most sites, although there ~~are a number of sites at which the r value gets slightly worse following data assimilation~~is a slight deterioration of the correlation coefficient at the majority of the sites. Despite this, the reduction in r is very small compared to the overall improvement in the KGE metric at all sites, and the prior and posterior r values are all greater than 0.8 at ~~all~~ sites with a typical mineral soil. The r value stays low at Moorhouse (MOORH), perhaps because the soil

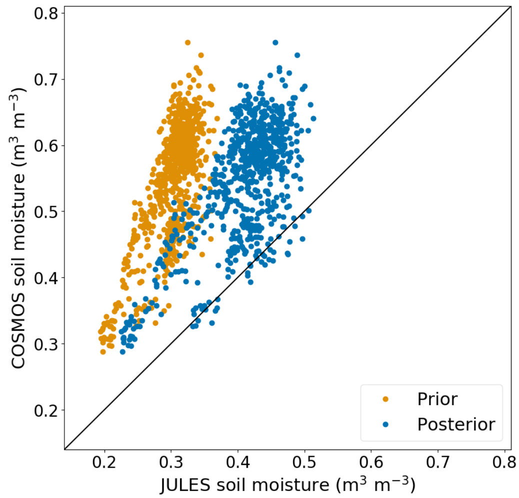

Figure 6. Observed vs modelled (ensemble mean) soil moisture at Gisburn Forest (GISBN) for prior and posterior JULES runs. Diagonal line shows 1:1 perfect correspondence line. The correlation coefficient at this site changed from 0.73 (prior) to 0.69 (posterior) and the rmse reduced from 0.25 (prior) to 0.15 (posterior).

at this site is too highly organic for the Cosby parameters to really be applicable, and for the COSMOS-UK measurements to be reliable. The r value also stays low at Gisburn Forest (GISBN), which is likely due to the fact that there are a large number of trees at this site~~and interception processes are therefore likely to be more important here~~. The presence of aboveground biomass may make the site-specific calibration less reliable than at other sites ~~; the COSMOS-UK 'soil moisture' measurement may actually include water held on the canopy of trees, which is not included in the JULES modelled soil moisture value here.~~ (Baatz et al., 2014) . The high organic carbon content of the soil at Gisburn Forest likely also contributes to this as our chosen PTF is designed to work best with mineral soils. Interception is another processes which potentially complicates the calibration at sites with vegetation, although the authors of Bogena et al. (2013) report that water intercepted by the canopy constitutes a negligible amount of the water detected in the CRNS footprint, even in coniferous forests.

Figure 7c shows that a significant contribution to improved KGE at all sites comes from improvement in the alpha component, which is much closer to the ideal value of 1 for all of the posterior JULES runs than the prior JULES runs. The alpha component represents how well the spread in the model matches the spread in the observations. We saw in time series plots such as figures 3 and 5 that the spread in JULES soil moisture was too small at all sites; our results show that the data assimilation has acted to correct this by updating the value of the PTF constants. Figure 7d shows that the beta parameter is closer to the ideal value of 1 after data assimilation than before at all sites except for Cardington, i.e. data assimilation is correcting a bias in the JULES outputs at all but one site. The prior bias at Cardington is in the opposite direction to bias at all of the other sites.

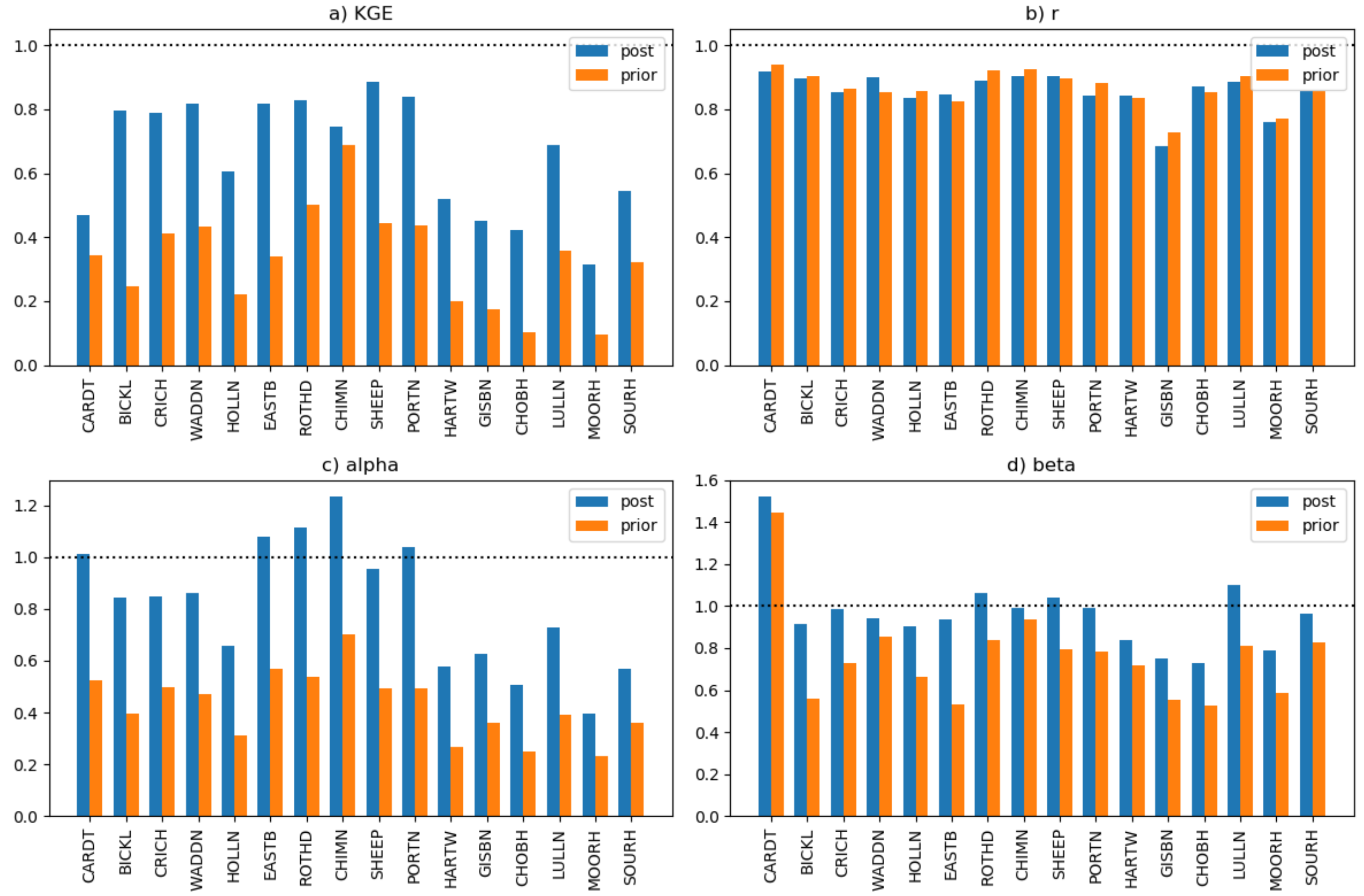

Figure 7. Kling Gupta efficiency scores for JULES runs using prior and posterior PTF variable values. Dotted horizontal lines show value of metric for perfect match between model and observation

3.2 Effect of data assimilation on JULES soil physics parameters

The data assimilation algorithm in this study acts directly on the PTF constants κ_1 - κ_{12} which make up the state vector. The resulting changes to the JULES soil physics parameters through equations (4) - (11) are presented here in section 3.2. Figures 8 and 9 show changes to the eight JULES soil physics parameters used for the topsoil and subsoil layers respectively. (Section 3.3 shows how the underlying PTF constants are updated).

Figures 8 and 9 show that the mean value of K_s (satcon) gets smaller (4 to 5 times smaller) at each site after data assimilation, and that the posterior distribution of the K_s (satcon) parameter is narrower than the prior distribution. The results in figures 8 and 9 also show that the site-to-site variability of the b parameter reduces following data assimilation; the largest mean prior values of b are reduced, and the distributions with the smallest mean values are shifted to slightly larger values. Figures 8 and 9 show that the mean value θ_s (vsat) has increased at all the sites following data assimilation, and the distribution of θ_s (vsat)

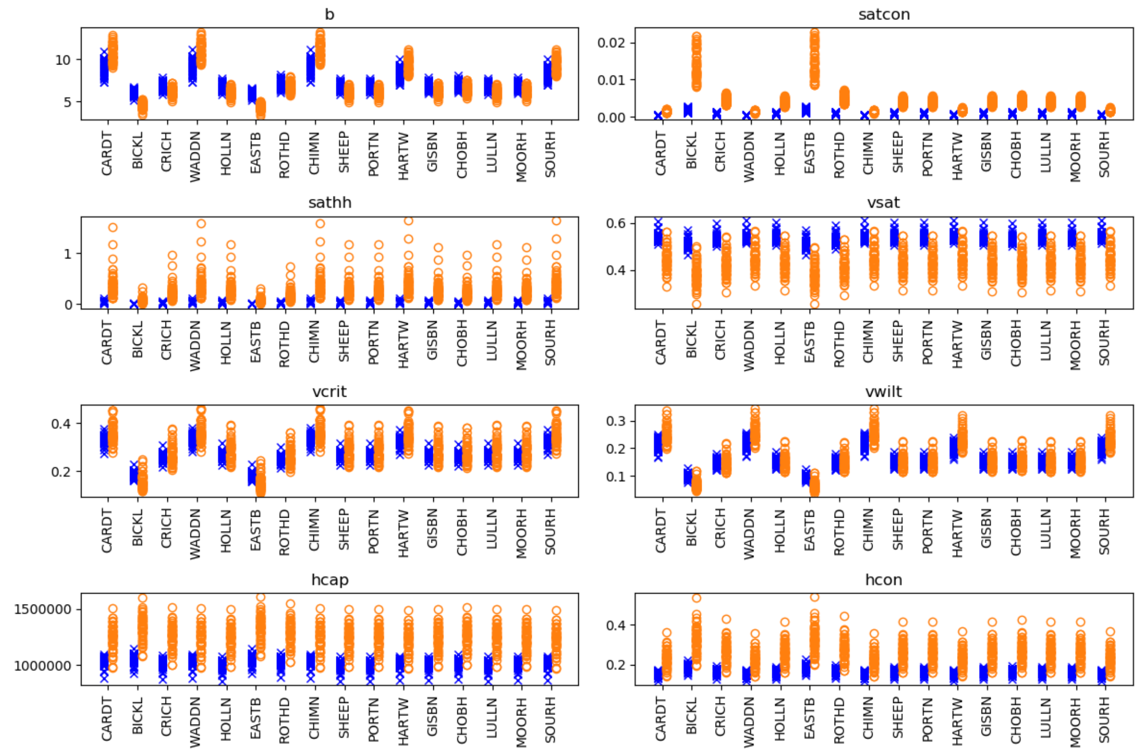

Figure 8. Ensemble prior (orange) and posterior (blue) parameter values at each site. These are 'topsoil' results, which we have assumed to correspond to the top two soil layers in JULES (0 - 35cm depth from the surface).

at each site has become much narrower. The mean values of the θ_{crit} (vcrit) and θ_{wilt} (vwilt) distributions have stayed broadly similar or increased slightly after data assimilation. We also see that at all sites Ψ_s (sathh) becomes very small ($\sim$ 30 times smaller) after data assimilation.

Figures 8 and 9 show that h_{cap} and h_{con} change through data assimilation. However, this translates into minimal differences between the prior and post soil temperatures; both prior and post data assimilation temperature estimates are close to the ~~in-situ~~ in situ COSMOS-UK measurements (not shown).

3.3 Effect of data assimilation on pedotransfer function constants

In this section we present the changes to the 12 PTF constants κ_1 - κ_{12}. These updates are the direct result of applying the data assimilation algorithm.

Figure 10 shows prior (orange) and posterior (blue) distributions of the 12 ~~PFT~~ PTF constants, κ_1 to κ_{12}. These plots demonstrate how the dependence of the soil physics parameters on texture is changed in equations (4) to (11) via data assimilation. The values of κ_1, κ_2 and κ_3 control the magnitude of the soil physics parameter b through equation (4). The decreases of κ_2 and κ_3 after data assimilation translate to a decreased dependence of b on clay and sand fractions through equation (4). Changes

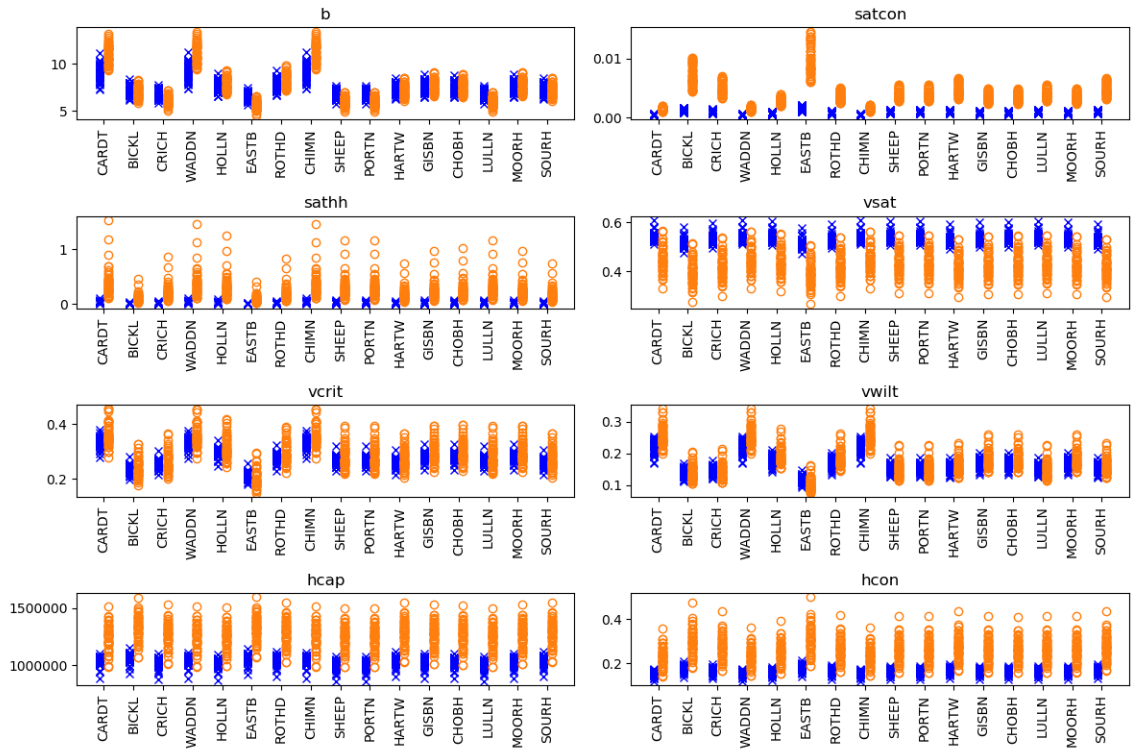

Figure 9. Ensemble prior (orange) and posterior (blue) parameter values at each site. These are 'subsoil' results, which we have assumed to correspond to the deeper two soil layers in JULES (35 - 300cm depth from the surface).

to κ_4, κ_5 and κ_6 contribute to changes to θ_s through equation (5). The large increase in κ_4 values allows larger values of θ_s to be realised after data assimilation. The parameter Ψ_s controlled by κ_7, κ_8 and κ_9. The mean value of κ_7 is greatly reduced following data assimilation, and this leads to the much smaller posterior values of Ψ_s seen in figures 8 and 9. The constants κ_{10}, κ_{11} and κ_{12} determine the values of K_s through equation (6). The shift in the κ_{10} distribution to larger values leads to the reduction in values of K_s seen in figures 8 and 9.

4 Discussion

The results in section 3.1 show that we have been able to successfully update the constants in a Cosby-like pedotransfer function based on field scale ~~in-situ~~ in situ soil moisture measurements. The new set of constants obtained in this way generate soil physics parameters at each studied COSMOS-UK site such that there is a large improvement in the match between modelled and observed field-scale soil moisture ~~values~~ at all sites.

Our results suggest that it is primarily a combination of the changes to θ_s, Ψ_s and K_s distributions which result in a better match to the observations after data assimilation. The new distributions allow the model to access higher soil moisture values,

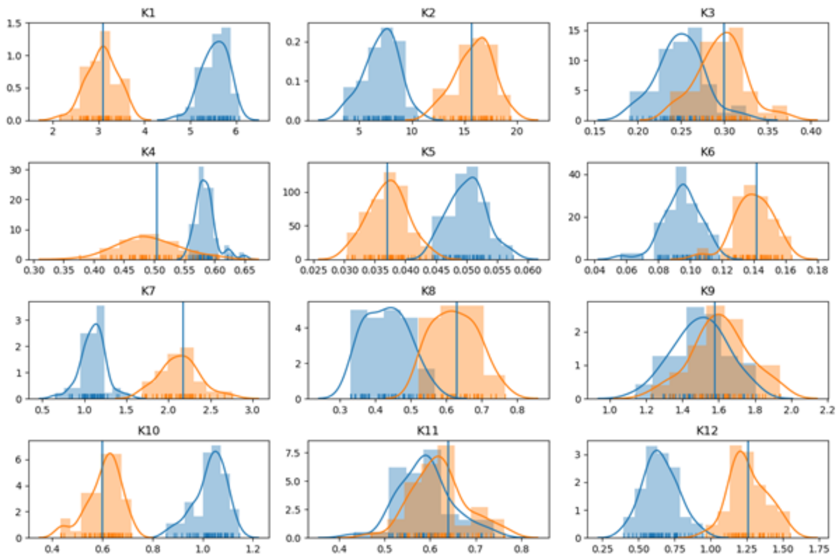

Figure 10. Prior and ~~post~~ posterior PTF ~~variable~~ constant value distributions. Orange shows prior and blue posterior. The blue line shows the original value of the constant as in table 2

potentially correcting for a deficiency in ~~supporting datasets, parameter valuesor~~ parameter values, process representation in JULES, or in supporting datasets (such as soil texture information or driving meteorological data). We suggest that the data assimilation is effectively acting to slow the drainage of water in JULES, especially close to saturation, by increasing θ_s and decreasing K_s.

The improvements seen here were obtained by assimilating all the soil moisture values across 16 sites simultaneously rather than on a per site basis. This strengthens our implicit assumption that the same physical processes can be modelled (through JULES and the Cosby pedotransfer function) for a range of different UK sites and soil types.

We note that the soil physics parameter values calculated here may not exactly match physically expected values for a number of reasons. Firstly, we have fitted to COSMOS ~~large-scale~~ field scale measurements; differences in parameter values from the prior values may therefore reflect the different scales on which they were calculated. Additionally, the COSMOS-UK soil moisture observations likely include contributions from processes which are important to soil moisture but we have not taken account of here with JULES, such as ponding of water on the soil surface, interception of water on vegetation, groundwater processes and local soil compaction. Therefore, we may be effectively parameterising for these processes (and others not included in JULES) through our new soil physics parameters. In this experiment we have mainly used grass sites, so interception is not likely to play a large role in daily averaged moisture values (JULES outputs show the amount of water intercepted to be, at most, of the order 100 times smaller than the amount of water in the top soil layer).

5 Conclusions

We have shown that it is possible to use the LaVEnDAR data assimilation framework to improve JULES estimates of soil moisture based on one year's worth of ~~large-scale~~ field scale COSMOS-UK soil moisture measurements across 16 sites. We have demonstrated improved fit to observations over a two year period at all 16 sites by adjusting the values of constants in the underlying pedotransfer function. Averaging across all the sites 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 (range 0.31 to 0.89).

The method we propose here could be used for any different choice of land surface model and/or pedotransfer function; our choice of PTF here was motivated by the fact that it is widely used and has a relatively simple mathematical formulation. Calibrating PTFs for the soils on which they are to be used and at the scales at which they are applied, rather than on small-scale field or lab soil samples, will ultimately improve the performance of land surface models. This will allow better estimates from flood forecasting models, earth system models and numerical weather prediction.

Code availability. TEXT

Data availability. TEXT

Code and data availability. The code used in these experiments is available from the MetOffice JULES repository (https://code.metoffice.gov.uk/trac/jules) under Rose suite number u-bq016. Registration required.

The LAVENDAR data assimilation first release is available here: https://github.com/pyearthsci/lavendar.

COSMOS-UK data are deposited annually in the Environmental Information Data Centre (EIDC) (eidc.ac.uk); additional data not included in the online repository are available on request (cosmos.ceh.ac.uk). https://doi.org/10.5285/a6012796-291c-4fd6-a7ef-6f6ed0a6cfa5)

Author contributions. EC, EP and RE devised the experiments, with input from EB and SD. EP created the LaVEnDAR data assimilation framework. EC and EP designed the rose-suite used here and ran the experiments. EC, RE, EP, EB and SD all contributed to analysis of results. HC provided access to COSMOS-UK data and site-specific information for model setup. EC prepared the manuscript with inputs from all co-authors.

Competing interests. The authors have no competing interests.

Disclaimer. TEXT

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