Anonymous Referee #1

- We appreciate the referee's comments on our manuscript, which have helped us to clarify several key points. These comments are reproduced below, with our response to each provided as a bullet point.

The paper investigates the benefits of data assimilation of remotely sensed soil moisture in the Catchment land model on three different time scales and therefore fits within the scope of the journal. The authors find that assimilation significantly reduces errors at every study site for all time scales, in particular also for long-term events. Further analysis on observation-bias correction parameters shows, that the estimation of rescaling parameters from only one year of data record will not considerably reduce the average benefit, but can increase local errors. The paper is well-written and in general well organized, but a more detailed description of the study approach would make the paper easier comprehensible:
1) It does not get clear in the Introduction and in the Methods if the decomposed soil moisture was assimilated into the model separately, or if the soil moisture time series were assimilated and the results decomposed afterwards for analysis.

- In response to Referee #1 & #2, Section 2.2, which introduces the data assimilation experiments has been expanded to more fully describe the assimilation experiments. This includes explicitly stating that the assimilation experiments use 'only the original AMSR-E time series data, and not the decomposed time series'.

2) It would greatly improve clarity to describe the two methods of rescaling (CDF and Interactive linear) in the Methods section as in the current draft the linear rescaling is first mentioned in section 3.4. Furthermore, a short explanation on the rescaling experiment with short data records in the Methods section would be useful.

- The details of the two rescaling methods, and the rescaling experiment with short data records, has been expanded and moved into the expanded Section 2.2.

3) It would be good to give the definition (for example the one of page 7985, lines 26-28) and an equation for the ubMSE in the methods section.

- An equation for the ubMSE has been added to Section 3.5, together with a sentence pointing out that the ubMSE is also known as the variance of the error.

More information about the dealing with scaling differences between the soil moisture datasets would be interesting, as differences in the results might be influenced by differences in spatial scaling.
1) ARS sensors: Which and how many sensors were used for each study site? What is the size of the respective areas covered by the sensors?

- Section 2.1 has been expanded to provide more details of the in situ data used. This includes stating that there were between 8 and 15 sensors averaged at each site, covering an area roughly equivalent to the AMSR-E observations. The specific numbers of sensors and approximate area for each watershed have also been added to Table 1.

2) How many grid cells of AMSR-E and the Catchment model did you use /are surrounding each site? How did you deal with differences in the number of grid cells and their resolution (0.25° vs. 9km)?

- A single grid cell was used for each site. This has been made clearer in Section 2, by changing 'the grid cells surrounding each site' to the 'grid cells encompassing each site'. We do not explicitly deal with the difference between the 9 km model grid and the 25 km AMSR-E grid, beyond rescaling the observation time series prior to assimilation. While the difference in spatial support between the model and the AMSR-E observations could be better accounted for by averaging multiple model grid cells, in this example the resulting model time series would be very similar to the present time series for a single grid cell. This is because the model physics do not explicitly account for soil processes at multiple spatial scales, and likely do not represent the specified spatial support of the grid cells very well. Spatial variation present in the model soil moisture is derived from the atmospheric forcing or surface parameters (topography, vegetation, soil parameters). In these experiments, the forcing (from MERRA, at 0.5 degrees) is at much coarser resolution, and any sub-25 km variability will be contributed by the surface parameters, which do not have sharp gradients within the ARS Watershed sites.

3) If more than one grid cell was used for each site, how were the single time series for each site created?

- A single grid cell was used.

Specific and technical comments
Eq. 1: ak and bk are not defined

- ak and bk are the coefficients that will be selected to fit the function to the data. This has been clarified at the introduction of equation 1:
  'Formally, for some observed time series, y, the a_k and b_k coefficients in the decomposed form function, $\hat{y}$, are fit for some selection of integers k_i:'

P. 7987-7988, lines 28/1-2: '. . .differences that are addressed by the CDF-matching. . .' You used linear rescaling for the Ayy results, is that right? Then this formulation might be confusing. The same applies for p. 7992, line 8

- CDF-matching was used for Ayy. This was not at all clear in the first submission, and has been made much clearer in the expanded Section 2.2.

Page 7989, line 25: Delete one ‘significantly’

- Done.

References: Most references give the numbers of the pages on which they appear in the text after the year. However, this has not been done consistently.

- These numbers seem to have been added by the copy editors. We will coordinate with them to ensure a consistent approach.

Fig. 6: Which method of decomposition was used for these time series? Would there be a difference to the other decomposition method (even though Fig.2 did not show significant differences)?

- Harmonic decomposition was used. This is now specified in the caption.

Anonymous Referee #2

- We appreciate the referee's comments on our manuscript, which have helped us to clarify several key points. These comments are reproduced below, with our response to each provided as a bullet point.

The authors analyze biases between AMSR-E, Catchment model, and in-situ SMs at three different time scales ' subseasonal (short), seasonal, and long term – and investigates the impacts of assimilating rescaled AMSR-E SM into the Catchment model. SM-DA showed consistent improvement of SM at all time scales at four ARS sites. It is also shown that rescaling for one-year model-observation can result in updated SM worse than open loop SM.
This paper deals with an important emerging question in land data assimilation (multi-scale biases between different 'measurements') and how SM-DA affects individual time components when SM is scaled at a lumped time scale. The manuscript is well writ- ten and tables/figures concisely summarize results. I recommend that this manuscript should be accepted for publication after addressing comments listed below.
1. In the Introduction, the authors mention a possibility of model-observation biases varying at different time scales citing Su and Ryu (2015). It naturally leads to an expectation that the authors rescale sub-seasonal – long-term time components separately, but AMSR-E SM is rescaled for the lumped time scale in both control and treatment cases. It needs to be clarified in Introduction that the main focus this work is analyzing the effects of SM-DA with a lumped rescaling on updated SM at multiple time scales. It would also be good to add discussions about rescaling individual time components separately.

- The focus on rescaling with bulk statistics is now specified in the introduction:
  'We have then used this decomposition to examine the differences between remotely sensed and modeled soil moisture at each time scale, and how assimilating bulk-rescaled soil moisture observations impacts the model soil moisture at each time scale.'

- As noted below, Section 2.2 of the methods has been expanded to better introduce the assimilation experiments, and so this is specified here again.

- The possibility of rescaling at separate time scales is left for later work, however this possibility is now pointed out in the conclusions:
  'This could perhaps be avoided by rescaling the observations separately at each time scale using the decomposed time series produced in this study, or using other methods that distinguish scaling characteristics at different time scales (e.g., Su and Ryu, 2015).'

2. It is written in Section 2.2 that a CDF-matching is used to rescale the observations, but it was later in the Result, Section 3.4, that I found that actually a linear model using mean and variance was used. The authors need to move this specific description to the Methods section because the use of mean-variance-based linear rescaling can influence the rescaling results discussed in the earlier sections.

- In response to Referee #1 & #2, Section 2.2, which introduces the data assimilation experiments has been expanded to more fully describe the assimilation experiments. This includes introducing the rescaling methods, and clarifying that all presented experiments used CDF-matching.
- It is later noted as a point of curiosity that the experiments were repeated with mean/variance rescaling, and very similar results were obtained:
  'This suggests that for the particular examples in this study, the CDF-matching operator could be approximated by a linear rescaling, in which only the mean and variance of the model are matched, as in Scipal et al, 2008. To confirm this, the assimilation experiments were repeated using linear rescaling of the AMSR-E observations in place of CDF-matching. The results (not shown) were indeed very similar to the CDF-matching experiments, in terms of the rescaled observations and the assimilation output.'

3. The basis for using linear rescaling in place of CDF-matching is that variance distribution across time scales did not vary after CDF-matching. This argument should be strengthened with more specific supports. For example, CDF-matching can be a more robust choice for non-stationary time series or when model and observation pdfs feature very different symmetry.

- All presented experiments used CDF-matching. See bullet above.

4. Was the mean perturbed ensemble (open loop) compared with the unperturbed single run? Please make sure the perturbation of soil moisture was done without unfairly penalizing the perturbed background predictions.

- This was done early in the experiments. The greatest deviation between a single unperturbed run and the mean of the model ensemble was at Walnut Gulch, during periods when the soil moisture nears the lower boundary (since the boundary limits the -ve ensemble deviation, the ensembles becomes biased). However, these deviations had a near-negligible effect on the evaluation statistics, and were deemed acceptable.

5. In Figure 6c, changes between M and Ac in SM_seas looks unrealistically substantial. With given AMSR-E SM pattern at LR shown in Figure 2, neither rescaling nor Kalman

update would likely to make that large difference. Please double check the data to ensure the correctness.

- The plotted time series are correct. The evidence for them can be seen in Figure 1c. The AMSR-E observations have a consistent and sharp single peak in the seasonal cycle, while the Catchment model has annual maxima that occur at different times of year that are often maintained for longer. Hence, the assimilation reduced the maxima to one per year (while over-exaggerating its magnitude). The real issue here is likely that the notion of a mean seasonal cycle does not describe the model behavior very well.

More specific comments - Page 7977, 'due to very low observation counts over the study period at the other sites': Please provide more information about the data scarcity in these sites (e.g., % of period the root-zone SM is available).

- There are no observations below the surface layer at Walnut Gulch and Reynolds Creek. At Little Washita, the 5-60 cm observations are available from 2007 onwards (giving too short a period to adequately sample inter-annual variations in this study). This information has been added into Section 2.1.

- Page 7984, 'AMSR-E could be expected a prior to have a larger fraction of . . . in the remotely selected observations': This a prior expectation (relatively large SMshort Var over SMseas Var) contradicts somehow 'exaggerated seasonal cycle' of AMSR-E at Little Washita and Little River. Need discussion on this contradiction.

- The point that we were attempting to make was that before looking at the data, we could expect AMSR-E to have large SMshort variance fraction, due to measurement noise but that this turns out not to be the case because of its very large seasonal cycle. Unfortunately, our use of ' a priori' in the sentence was confusing, given it's use in assimilation terminology. The relevant sentence has been edited to make this clearer: 'One might expect AMSR-E to have a larger fraction of variance at SMshort, due to measurement noise from the remote sensor. However, ...'

- Page 7988, line 1: 'forecast' to 'predicted'

- Left as is. We prefer 'forecast' in this setting, since this is consistent with the use of observation minus forecast (O-F) terminology in data assimilation. However, we do acknowledge that the 'forecast' referred to here is not a free forecast such as might be used in an operational setting, and is instead a rather tightly constrained one day prediction intended to be used as the background in the data assimilation.

Interactive comment from Imtiaz Dharssi

- We appreciate Dr Dharssi taking the time to comment on our manuscript. His comments are reproduced below, with our response to each provided as a bullet point.

This is an interesting paper which demonstrates that assimilation of satellite derived surface soil moisture (SSM) measurements improves the soil moisture analysis compared to an open-loop control that has no data assimilation. I humbly ask the following questions:
1) A discussion of the practical applications of the research described by the manuscript would be very useful. Do meteorological reanalysis systems such as the Modern Era Retrospective-analysis for Research and Applications (MERRA) assimilate satellite derived surface SSM measurements? If not, what is the reason? Similarly, do Numerical Weather Prediction (NWP) centres operationally assimilate satellite derived soil moisture?

- The opening sentences of the introduction have been rephrased to insert citations of the soil moisture assimilation literature, to provide the reader with any necessary background on soil moisture assimilation. Additionally, in the conclusions it has been noted that the outcome of these experiments suggests that the representation of the surface climate in reanalyses could benefit from the assimilation of long soil moisture data records.

2) How does the skill of the open-loop simulation in this research compare to soil moisture analyses from the ECMWF ERA Interim? Would it be possible to provide values of temporal and anomaly correlation between model open-loop and ARS in-situ soil moisture? From figure 6, it appears that the model open-loop poorly captures the seasonal and inter-annual variations in soil moisture at the Little River site and I wonder if this is a common problem.

- The Catchment model used here is an established model that has been presented and evaluated on many occasions (Reichle et al, 2007; Liu et al, 2011; Draper et al, 2012; De Lannoy et al 2014), most often using the correlation / anomaly correlation. The evaluation metric used in this manuscript is the unbiased Mean Square Error with respect to the ARS in situ soil moisture. This is provided for the model open loop, and discussed at length in the manuscript. The use of an alternative approach to evaluation (partitioning into time scales) has indeed highlighted that the open loop does struggle to capture some of the seasonal and inter-annual variations (as does the AMSR-E data), and while it would be very interesting to check whether this is a common problem in other models, this is beyond the scope of the current study.

L24P7986 says the site is Little Washita which I presume is a typo.

- Yes, this has been fixed.

My comments should not be interpreted, in any way, as a criticism of the manuscript.

Manuscript, with changes tracked.

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\begin{document}\hack{\sloppy}

\title{The impact of near-surface soil moisture assimilation at subseasonal, seasonal, and inter-annual time scales}

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\runningtitle{Soil moisture assimilation time scales}

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\begin{abstract}
Nine years of Advanced Microwave Scanning Radiometer -- Earth Observing System (AMSR-E) soil moisture retrievals are assimilated into the Catchment land surface model at four locations in the US. The assimilation is evaluated using the unbiased Mean Square Error (ubMSE) relative to watershed-scale in situ observations, with the ubMSE separated into contributions from the subseasonal (SM$_{\mathrm{short}}$), mean seasonal (SM$_{\mathrm{seas}}$) and inter-annual (SM$_{\mathrm{long}}$) soil moisture dynamics. For near-surface soil moisture, the average ubMSE for Catchment without assimilation was (1.8\,$\times$\,10^{-3}\,m^{3}\,m^{-3})^2, of which 19\,{\%} was in $\mathrm{SM}_{\mathrm{long}}$, 26\,\% in SM$_{\mathrm{seas}}$, and 55\,\% in SM$_{\mathrm{short}}$. The AMSR-E assimilation significantly reduced the total ubMSE at every site, with an average reduction of 33\,\%. Of this ubMSE reduction, 37\,\% occurred in SM$_{\mathrm{long}}$, 24\,\% in SM$_{\mathrm{seas}}$, and 38\,\% in SM$_{\mathrm{short}}$. For root-zone soil moisture, in situ observations were available at one site only, and the near-surface and

root-zone results were very similar at this site. These results suggest that, in addition to the well-reported improvements in SM$_{\mathrm{short}}$, assimilating a sufficiently long soil moisture data record can also improve the model representation of important long term events, such as droughts. The improved agreement between the modeled and in situ SM$_{\mathrm{seas}}$ is harder to interpret, given that mean seasonal cycle errors are systematic, and systematic errors are not typically targeted by (bias-blind) data assimilation.

Finally, the use of one year subsets of the AMSR-E and Catchment soil moisture for estimating the observation-bias correction (rescaling) parameters is investigated. It is concluded that when only one year of data is available, the associated uncertainty in the rescaling parameters should not greatly reduce the average benefit gained from data assimilation, although locally and in extreme years there is a risk of increased errors.

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\introduction

Many studies have demonstrated that assimilation of remotely sensed near-surface soil moisture observations can improve modeled soil moisture, with improvement typically measured by temporal agreement with in situ observations \citep{ReichleD09108, Scipal1101, Bolten57,DraperL04401}. Typically, the remotely sensed soil moisture observations are assimilated using a~bias-blind assimilation of observations that have been rescaled to have the same mean and variance as the model forecast soil moisture \citep{ReichleL19501,Scipal1101}. This approach is designed to avoid forcing the model into a~regime that is incompatible with its assumed (likely erroneous) structure and parameters, while also avoiding the inadvertent introduction of any observation biases into the model \citep{ReichleL19501}. The assimilation can then correct for random errors in the model forecasts \citep{ReichleL19501}. Here ``random'' errors are defined as errors that persist for less than the time scale used to -- subjectively -- define the

bias in the mean.

Traditionally, observation rescaling is based on the maximum available

coincident observed and forecast data record

\citep{ReichleD09108,Scipal1101,DraperL04401}, effectively defining the bias over the same period. The rescaled

observations will then retain the signal of all observation-forecast

differences occurring at time scales shorter than the data record, which for a multi-year data record would include differences spanning the subseasonal, seasonal and inter-annual time scales. Assimilating these rescaled observations then has the potential to improve the model soil moisture at each of the aforementioned time scales, and yet bias-blind soil moisture assimilation is often implicitly assumed to target only the random errors occurring at the relatively short subseasonal time scales.

At subseasonal, seasonal, and inter-annual time scales, different physical processes control the true soil moisture and errors in soil moisture estimates.

Most notably, in many locations seasonal scale variability is dominated by the mean seasonal cycle (the annually repeating variability), and any errors in the mean seasonal cycle will be systematic, with causes such as incorrect separation of the soil and vegetation moisture signals from remotely sensed brightness temperatures, or errors in the land surface model vegetation

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dynamics. In contrast, variability at subseasonal and inter-annual time scales is rarely dominated by repeating cycles, and is more typically associated with transient atmospheric forcing events. Specifically, rapid time scale (daily) soil moisture dynamics are driven by factors such as individual precipitation events and changes in cloud cover, while longer time scale (seasonal-plus) dynamics are driven by changes in the atmospheric supply and demand for moisture \citep{Entin11865}. Soil moisture errors at subseasonal scales could then be caused by factors such as atmospheric noise in remotely sensed data, or errors in the daily meteorology of the model atmospheric forcing, while inter-annual scale errors could be caused by factors such as drift in the remote sensor calibration, or incorrect representation of atmospheric drought conditions in the atmospheric forcing.

The differing nature of soil moisture errors across time scales has unexplored consequences for data assimilation. Most notably, the systematic nature of errors in the mean seasonal cycle is problematic. Theoretically, (bias-blind) data assimilation is not designed, nor optimized, to correct for systematic errors. More practically, if the systematic differences are not due to model errors (i.e., are caused by observation errors, including representativity errors), then assimilating such information can seriously degrade model performance.

Additionally, the time scale dependence of soil moisture errors may also be

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problematic for the use of bulk parameters, intended to correct systematic differences across all time scales, for observation rescaling. Even within relatively short time scales (up to about one month), \cite{Su17} showed that the multiplicative

((differences in standard deviation) and additive (differences in mean) components of the systematic differences between modeled and remotely sensed soil moisture differ across time scales. They highlight that this lack of stationarity cannot be adequately addressed by using bulk statistics to estimate observation rescaling parameters.

Consequently, in this study we have decomposed modeled, remotely sensed, and in situ soil moisture into separate time series representing soil moisture dynamics at subseasonal, mean seasonal, and inter-annual time scales.

We have then used this decomposition to examine the differences between remotely sensed and modeled soil moisture at each time scale, and how assimilating bulk-rescaled soil moisture observations impacts the model soil moisture at each time scale.

The decomposition is achieved by fitting each soil moisture time series with harmonic functions specified to target the mean seasonal cycle (SM_{seas}), and the subseasonal (SM_{short}) and inter-annual (SM_{long}) dynamics. By fitting the appropriate harmonic functions to each time series, we can separate the total mean square error of each soil moisture time series into contributions from each time scale. This is a~much more targeted evaluation of soil moisture dynamics at the physically relevant time

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scales than is usually undertaken. Standard evaluation methods focus on bias-blind metrics, such as the correlation or unbiased Root Mean Square Error (ubRMSE, which is calculated after removing the long term mean difference \citep{Entekhabi832}). Both of these are sensitive to soil moisture time series variability at all time scales. While anomaly correlations (R_{anom}), are also used to exclude the seasonal cycle, this is not done consistently, and does not allow the total error to be broken into contributing time scales. Depending on how the anomalies are calculated, R_{anom} measures subseasonal scale errors (anomalies defined relative to a~simple moving average, as in Dorigo et~al., 2015), or a~combination of inter-annual and subseasonal scale errors (anomalies defined relative to the mean seasonal cycle over multiple years, as in Draper et~al., 2012).

In the second part of this study, we also explore the impact on the assimilation of using short time periods for observation bias correction. When first introducing Cumulative Distribution Functions (CDF)-matching to rescale remotely sensed soil moisture prior to assimilation, \citet{ReichleL19501} showed that for Scanning Multi-channel Microwave Radiometer (SMMR) soil moisture observations (1979--1987), reasonable rescaling parameters could be estimated using a~single year of data. We repeat

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their investigation using the more modern Advanced Microwave Scanning Radiometer-Earth Observing System (AMSR-E) data set, and also extend their investigation by providing a~more statistically robust analysis of the impact of using single-year scaling parameters in the assimilation. This part of the study is motivated by the recent launch of the NASA's Soil Moisture Active Passive (SMAP) mission \citep{Entekhabi704}, as it will address the consequences of using short records to rescaling the observations during the early phases of the SMAP mission.

\section{Data and methods}%s2

Nine years of surface soil moisture retrievals from AMSR-E X-band data (Owe et~al., 2008) have been assimilated into the Catchment land surface model \citep{Koster24809}, at four locations in the US. The impact of the assimilation on the model skill is measured by comparison to watershed-scale in situ soil moisture observations collected by the Agricultural Research Service (ARS) of the United States Department of Agriculture (Jackson et~al., 2010). Each of these data sets is first described below (Sect.~\ref{sec:tseries}), followed by a~discussion of the assimilation approach (Sect.~\ref{sec:assim}) and the method used to decompose soil moisture time series into subseasonal, seasonal, and inter-annual time scales (Sect.~\ref{sec:fit_meth}).

\subsection{The soil moisture data sets\label{sec:tseries}}%s2.1

For over a~decade the ARS has been collecting near-surface (5cm) soil moisture observations, at least hourly, using dense networks of in situ sensors at four watershed scale sites in the US: Reynolds Creek (RC), Walnut Gulch (WG), Little Washita (LW), and Little River (LR). near-surface (5cm)

Given that we will focus on evaluating variance, we have not supplemented the ARS observations with observations from single sensor networks, such as SCAN \citep{Schaefer2073}. Unlike the locally dense in situ measurements from the ARS networks, the variance (and mean) of observations from single sensors cannot be assumed representative of the coarse scale soil moisture from Catchment and AMSR-E.

Level 3 Land Parameter Retrieval Model (LPRM) X-band AMSR-E near-surface soil moisture retrievals at 0.25{\degree} resolution were obtained for the grid cells encompassing the center of each watershed site in Table~\ref{tab:sites_locn}. At X-band the observations relate to a~surface layer depth slightly less than 1\,\unit{cm}. Only the descending (1:30\,a.m.\,LT) overpass has been used to avoid possible differences in the climatological statistics of day- and night-time observations. The sites were explicitly selected by ARS to avoid possible radio frequency interference and proximity to permanent open water, and the AMSR-E

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soil moisture retrievals were screened to remove observations with X-band vegetation optical depth above 0.8.

NASA's Catchment land surface model was run over the 9\,\unit{km} EASE grid cells encompassing the center of each watershed site, using atmospheric forcing fields from Modern Era Retrospective-Analysis for Research (MERRA; Rienecker et~al., 2011) and recently improved soil parameters \citep{Lannoy957}. The model initial conditions were first spun-up from January~1993 to January~2002 using a~single member without perturbations. The ensemble (including perturbations) was then spun-up from January to October~2002 (see Sect.~\ref{sec:assim} for details of the ensemble). For both the model open loop and data assimilation model output, the ensemble average near-surface (0--5\,\unit{cm}) and root zone (0--100\,\unit{cm}) soil moisture is then reported.

Daily ARS and Catchment time series were generated by sampling each at the approximate time of the descending AMSR-E overpass (1:30\,a.m.\,LT). Initially each time series spanned the AMSR-E data record, rounded down to nine full years from October~2002 to September~2011, however the Little River root-zone soil moisture observations are not available before January~2004, and were truncated to the seven years from October~2004 to September~2011. Also, there were just 21 ARS observations at Reynolds Creek in the last year of this period, and so the Reynolds Creek time series were truncated to the eight years from October~2002 to September~2010. The ARS and

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AMSR-E sensors can only measure liquid soil moisture, and all data have been screened out when the Catchment model indicates frozen near-surface conditions. Since the Reynolds Creek site is frozen for an extended period each winter, liquid soil moisture is not well defined there during winter, and the Reynolds Creek time series have then been truncated to remove winter, defined from 1 December to 10 March (the period during which the Catchment surface is continuously frozen for at least three of the eight years of the Reynolds Creek record).

\subsection{The assimilation experiments}\label{sec:assim}%s2.2

The assimilation experiments were performed using a~one-dimensional bias-blind Ensemble Kalman Filter, with the same set-up and ensemble generation as in \cite{Liu750

Prior to assimilation, the AMSR-E observations were rescaled using CDF-matching \citep{ReichleL19501}. For each experiment a single set of bulk CDF-matching parameters were used (i.e., the rescaling is applied only to original AMSR-E time series, and not to the decomposed time series). In the baseline assimilation experiments, the CDF-matching parameters were calculated using the maximum available nine year AMSR-E data record, following standard practice.

This nine year AMSR-E record is the longest remotely sensed soil moisture record available from a~single satellite sensor, and soil moisture assimilation experiments using newer satellites, or a modeling system with limited archives, are limited to shorter time periods for observation rescaling. To establish the potential consequences of using a shorter data record, a second set of experiments was conducted, in which the rescaling parameters were estimated using the 12 month periods starting in consecutive Octobers (but assimilating the full eight or nine year near-surface soil moisture data record listed in Table~\ref{tab:sites_locn}). \citet{ReichleL19501} also tested the use of one year periods for rescaling soil moisture from SMMR. In contrast to their approach, we do not use ergodic substitution (of spatial sampling for temporal sampling) when estimating the rescaling parameters with a~single year of observations, since with more modern remote sensors, this is no longer necessary to obtain a~sufficient sample size. Additionally, for the assimilation of Soil Moisture Ocean Salinity retrievals, \citet{LannoySUB} found ergodic substitution degraded the estimated CDFs, by introducing conflicting information from neighboring grid cells, possibly due to the higher spatial resolution, compared to SMMR.

The benefits of each assimilation experiment have then been compared to that of the Catchment model open loop ensemble mean, in which the same ensemble generation parameters were used, and no observations were assimilated. The improvement from the open loop is measured using the unbiased Mean Square Error (ubMSE) of the resulting model soil moisture, with respect to the ARS in situ observations. For data set X compared to in situ data I, both of length n, the ubMSE is calculated as:

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\text{ ubMSE}=\frac{1}{n}\Sigma_{i=1,n}(X_i-I_i-\langle X-I\rangle)^2

\end{align}%enew

where $\langle . \rangle$ indicates the temporal mean. The ubMSE is also referred to as the variance of the errors in X, however we use the ubMSE terminology for consistency with commonly used unbiased \textit{root} mean square error (ubRMSE) in the soil moisture literature

\citep{Entekhabi832}. We do not apply the square root here to take advantage

of the additive property of the variance of independent time series. However to aid interpretation the ubMSE equivalent to the common

ubRMSE target accuracy of 0.04\,\unit{m^{3}\,m^{-3}} is indicated in

the relevant plots.

\subsection{Decomposition of soil moisture time series} \label{sec:fit_meth}%s2.3

We wish to decompose each soil moisture (SM) time series into separate

components representing soil moisture dynamics at the subseasonal

(SM_{short}), seasonal (SM_{seas}),

and inter-annual (SM_{long}) time scales. Variability

in a~time series at specific time scales can be isolated by fitting

a~function made up of the sum of sinusoidal functions. Formally, for

some observed time series, y, the a_k and b_k coefficients in the decomposed form $\hat{y}$ are fit for

some selection of integers k_i:

\begin{align}

&\hat{y}(t)=a_0 + \Sigma_{k=k_1,k_2,{\ldots}}a_k \sin \left(\frac{2\pi

kt}{n}\right) + b_k \cos \left(\frac{2\pi kt}{n}\right)\label{eq:cos_sin},

\end{align}%e1

where t is the time step and n is the length of the time series.

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$\frac{2\pi k}{n}$ is the (angular) frequency for a~sinusoid completing k cycles over n time steps (i.e., that has frequency k/n per time unit), and $\hat{y}$ for $k=k_\mathrm{i}$ is referred to as the $k_\mathrm{i}th$ harmonic. a_0 is the mean of y. If the time series is sampled at regular intervals and has no missing data, the sinusoids for individual harmonics are orthogonal and independent of each other. This is the basis for the discrete Fourier transform, which exactly fits Eq.~(\ref{eq:cos_sin}) to y using the first $n/2$ harmonics (i.e., $k_\mathrm{i}=1,2,3,{\ldots}n/2$). In this study, we use multiple linear least squares regression to fit Eq.~(\ref{eq:cos_sin}) to the soil moisture time series for a~sum of harmonic frequencies selected to isolate the variability at each target time scale, as described below.

We define SM_{seas} by fitting Eq.~(\ref{eq:cos_sin}) to the soil moisture time series for some combination of the annual harmonic frequencies (i.e., for k/n an integer multiple of 1\,\unit{yr^{-1}}). The frequencies higher than 1\,\unit{yr^{-1}} moderate the shape of $\hat{y}$ to account for differences in the shape of the seasonal cycle from the single sinusoid described by the first harmonic. Typically, only a~few annual harmonics are necessary to fit the seasonal cycle of geophysical variables \citep{Scharlemann1408,VinnikovL22708}. Here we define SM_{seas} to be the sum of the first two harmonics, since fitting additional harmonics did not improve the ability to predict withheld data, following the method of

\citet{Narapusetty4845}. Note that since the same annual harmonics are repeated each year, we are restricting SM_{seas} to represent only the mean seasonal cycle, and any inter-annual variability at seasonal time scales, such as anomalous vegetation growth in a~given year, will be assigned to the subseasonal or inter-annual variability, depending on its temporal characteristics.

We define SM_{long} by fitting Eq.~(\ref{eq:cos_sin}) to the soil moisture time series using the harmonic frequencies lower than 1\,\unit{yr^{-1}} that divide into the number of years in the data record (i.e., for $k/n=1/m$, $2/m$, $3/m{\ldots}(m-1)/m$, where m is the time series length in years). Finally, we define SM_{short} as the residual:

\begin{align}

&

\text{SM}_{\text{short}}=\text{SM}-\langle \text{SM} \rangle -\text{SM}_{\text{long}}-\text{SM}_{\text{seas}}\label{eq:sms}

\end{align}%e2

where $\langle \text{SM} \rangle$ is the temporal mean soil moisture. Note that, as defined here, SM_{long}, SM_{seas}, and SM_{short} are all zero-mean, since the time series mean was assigned to a_0 in Eq.~(\ref{eq:cos_sin}).

Both of the AMSR-E and ARS observed time series are incomplete (Table~\ref{tab:sites_stats}). When applied to incomplete time series,

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the sinusoids fitted by Eq.~(\ref{eq:cos_sin}) are not necessarily independent, hence the fitted SM_{seas} and SM_{long} may not be independent. We opted not to use gap-filling prior to fitting Eq.~(\ref{eq:cos_sin}), to keep the method simple, and because gap-filling would directly affect the SM_{short} dynamics. In Sect.~\ref{sec:results}, before using the decomposed time series we check for signs of strong dependence between the fitted SM_{long}, SM_{seas}, and SM_{short}, by testing whether the sum of the variances of the three time scale components differs from the variance of the original soil moisture time series. We assume that if there is little difference then any dependence between SM_{long}, SM_{seas}, and SM_{short} has only a~minimal impact on our results. Following initial investigation with this test, the number of observations used at each location is maximized by comparing only model (or assimilation) estimates to ARS in situ measurements, avoiding direct comparison of the incomplete ARS and AMSR-E time series (which would require cross-screening for the availability of both). Finally, we do not use the harmonic fit to interpolate missing data, and instead screen out the fitted SM_{long} and SM_{seas} at times when the original soil moisture was not available. Also, at Reynolds Creek, where the time series has been truncated to remove frozen winters, the length of the year used to fit the harmonics was

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similarly truncated.

For demonstration purposes, in Section \ref{sec:var_results} we decompose each soil moisture time series into similarly defined time scale components using moving averages, since moving averages are often used for calculating anomaly correlations \citep{DraperL04401,Dorigo380}. The length of the averaging windows were chosen to give close agreement with the results of the harmonic decomposition described above. For the moving average decomposition, the inter-annual soil moisture time series, $\text{SM}^{\text{MA}}_{\text{long}}$, is defined as the 181\,day moving average, and the seasonal cycle, $\text{SM}^{\text{MA}}_{\text{seas}}$, is defined for each day of the year by averaging the data from all years that fall within a~45\,day window surrounding that day-of-year. As with the harmonic approach, the subseasonal time series, $\text{SM}^{\text{MA}}_{\text{short}}$, is calculated as the residual, analogous to Eq.~(\ref{eq:sms}). The same data processing and quality control as for the harmonic decomposition is used (also without gap filling), plus the moving averages are only calculated when at least 60\,{\%} of the data within the averaging window are available.

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\section{Results}\label{sec:results}%s3

Below, the original AMSR-E, Catchment, and ARS soil moisture time series are examined (Sect.~\ref{sec:orig}), before being split into SM_{seas}, SM_{long}, and SM_{short} (Sect.~\ref{sec:decomp}). The distribution of variance across the different time scales for each soil moisture estimate is then compared (Sect.~\ref{sec:var_results}), before the observations are rescaled (Sect.~\ref{sec:cdf_results}), and the benefit of assimilating the AMSR-E data into Catchment is assessed at each time scale (Sect.~\ref{sec:assim_results}). Finally, the consequences of using a~relatively short record to rescale the AMSR-E data is examined (Sect.~\ref{sec:yearly}).

\subsection{The ARS, AMSR-E, and catchment time series}\label{sec:orig}%s3.1

Figure~\ref{fig:SM_orig} shows the original time series at each site. In general, soil moisture from in situ, modeled, and remotely sensed estimates have systematic differences in their behavior, due to representativity or structural differences between each estimate \citep{Reichle430. The most obvious difference in Fig.~\ref{fig:SM_orig} is that the mean and variance of each estimate differ (see also Table~\ref{tab:sites_stats}). Both AMSR-E and Catchment are consistently biased high compared to the ARS soil moisture. Bias values for the model range from 0.01\,\unit{m^{3}\,m^{-3}} for Little

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Washita to 0.09\,\unit{m^{3}\,m^{-3}} for Little River, and bias values for the AMSR-E retrievals range from 0.07\,\unit{m^{3}\,m^{-3}} for Reynolds Creek to 0.21\,\unit{m^{3}\,m^{-3}} for Little River. Additionally, the standard deviation of AMSR-E is two to three times larger than the other two estimates. Figure~\ref{fig:SM_orig} demonstrates that this is due to greater noise, and also a~prominent seasonal cycle at Little Washita and Little River that is not evident in the other time series.

In addition to the systematic differences in their mean and standard deviation reported above, there are more subtle differences between the soil moisture dynamics described by each estimate. For example, for both the surface and root-zone soil moisture, the ARS time series tend to show a~sharper response to individual rain events than does Catchment, with (relatively) larger peaks followed by more rapid dry down after each event. At Walnut Gulch this is particularly obvious, with ARS rapidly drying to a~well defined lower limit after each precipitation event, while Catchment has a~lesser response to individual events, and a~stronger seasonal signal.

\subsection{Soil moisture time series at each time scale}\label{sec:decomp}%s3.2

Figure~\ref{fig:decomp_LR} shows an example of the time scale decomposition, for the Catchment surface soil moisture at Little River, for both the harmonic and moving average approaches. The time series described by each method are similar in terms of the magnitude and timing of their dynamics, except that the moving average inter-annual soil moisture includes more high-frequency variability than does the harmonic version. Evaluation of soil moisture at specific time scales should ideally be based on time series separated into independent time scale components. For the harmonic method, independence between the time series at each time scale is not guaranteed since the original time series were not complete, while for the moving average method, independence is not expected.

Figure~\ref{fig:var_method} shows an example of the variance bar plots used to check for signs of dependence between the time series at each time scale, in this case for the Catchment model and the AMSR-E observations. In Fig.~\ref{fig:var_method}a, for the harmonic method, the sum of the variances at each time scale (the stacked bars) is very close (within 2\,{\%}) to the total variance of the original soil moisture time series (the white circles), falling within the 95\,{\%} confidence interval of the total variance in each case. In contrast, for the moving average method in Fig.~\ref{fig:var_method}b the sum of the variances of each time scale falls outside the 95\,{\%} confidence interval for the total time series variance at three of four sites, with a~mean difference of 8\,{\%} of the total variance (with differences ranging between 1 and 16\,{\%}), indicating strong dependence between the three components. In each case the sum of the variances of the time scale components is less than the total variance at each site, indicating positively correlated features between the moving average time scale components (since $\langle \sigma^2_{X+Y} \rangle = \langle \sigma^2_X \rangle - 2 \langle \sigma_{XY} \rangle + \langle \sigma^2_Y \rangle$). This positive correlation is intuitively expected, since an anomaly in the original soil moisture time series has the same direction of influence on both the moving averages and the residual from that moving average (e.g., in Fig.~\ref{fig:decomp_LR} note the signal of the large positive anomaly in early 2004 in both $\text{SM}^{\text{MA}}_{\text{long}}$ and $\text{SM}^{\text{MA}}_{\text{short}}$). Finally, the distribution of variance across the time scales is similar for each method, largely because the moving average window lengths for $\text{SM}^{\text{MA}}_{\text{seas}}$ and $\text{SM}^{\text{MA}}_{\text{long}}$ were selected to generate time series closely matching those from the harmonic method.

\subsection{Variance distribution across time scales}\label{sec:var_results}%s3.3

In Fig.~\ref{fig:var_method} the AMSR-E variance is much larger than that for Catchment (as was discussed in Sect.~\ref{sec:orig}), making it difficult to compare the relative distribution of variance across

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each time scale. Figure~\ref{fig:var_unit}a then shows the AMSR-E and Catchment variance bar plots with the total variance normalized to one, to allow direct comparison to the fraction of variance at each time scale. The same plots are also presented for the Catchment and ARS soil moisture in Fig.~\ref{fig:var_unit}b (recall we do not directly compare the ARS and AMSR-E time series, so as to avoid cross-screening their availability).

In Fig.~\ref{fig:var_unit}, the distribution of variance across time scales for each data set can be very different, and there is not a~consistent pattern across the four sites. As was previously noted from Fig.~\ref{fig:SM_orig}, AMSR-E has a~very prominent seasonal cycle at Little River and Little Washita (40--70\,{\%} of the total variance) that is not present for Catchment or ARS, for which the SM_{seas} fraction of variance is around 10--20\,{\%} in Fig.~\ref{fig:var_unit}. In contrast, at Reynolds Creek and Walnut Gulch, Catchment has a~larger fraction of its variance in the seasonal cycle (55--70\,{\%}) than does AMSR-E (20--40\,{\%}), with ARS agreeing with Catchment at Reynolds Creek only. At Walnut Gulch the greater variance-fraction in the Catchment SM_{seas} is mostly balanced by less variability in SM_{short} (30\,{\%} compared to 60\,{\%} for ARS). This is associated with the differing responses to precipitation events already noted in Fig.~\ref{fig:decomp_LR}.

One might expect AMSR-E to have a~larger fraction of

 variance at SM_{short}, due to measurement noise from the remote sensor. However, this is only the case at

Reynolds Creek, where AMSR-E has 50\,{\%} of its variance in SM_{short}, compared to 20--30\,{\%} for Catchment and ARS. At Walnut Gulch, the AMSR-E and ARS SM_{short} variance-fractions are similar (50--60\,{\%}), while the fraction for Catchment is much lower (25\,{\%}). At Little Washita and Little River the variance-fraction in the AMSR-E SM_{short} is similar to Catchment (at around 50 and 30\,{\%}, respectively) and both are much smaller than for ARS (around 70\,{\%}). At these two sites the AMSR-E SM_{short} variance-fraction may well be less than expected due to the large amount of variance in its exaggerated seasonal cycle.

For the SM_{long} variance, the patterns at Little Washita and Little River are again similar to each other. Catchment has much more variance in SM_{long} (40--50\,{\%}) than ARS (20\,{\%}) or AMSR-E (10\,{\%} or less). At the other two sites, the SM_{long} variance-fraction is similar for all data sets, except for the lower value for AMSR-E at Walnut Gulch (<10\,{\%}, compared to around 20\,{\%} for ARS and Catchment).

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\subsection{Baseline observation rescaling}\label{sec:cdf_results}%s3.4

For the baseline experiment, the AMSR-E observations were rescaled using bulk CDF-matching parameters estimated over the full data record. By design, the CDF-matched AMSR-E observations, labeled Oc, have the same mean (not shown) and variance (Fig.~\ref{fig:var_method}a) as the Catchment soil moisture. Figure~\ref{fig:var_unit} shows that the CDF-matching had little impact on the variance distributions across each time scale. This suggests that for the particular examples in this study, the CDF-matching operator could be approximated by a~linear rescaling, in which only the mean and variance of the model are matched, as in \citet{Scipal1101}.

To confirm this, the assimilation experiments were repeated using linear rescaling of the AMSR-E observations in place of CDF-matching. The results (not shown) were indeed very similar to the CDF-matching experiments, in terms of the rescaled observations and the assimilation output (for both the Oc rescaling presented in this Section, and the Oy rescaling presented in Sect.~\ref{sec:yearly}).

Recall that the distribution of the variance across each time scales was quite different for the AMSR-E and Catchment soil moisture in Fig.~\ref{fig:var_unit}. Note that large errors in the variance at one time scale (in either AMSR-E or Catchment) will affect the rescaling of the variance at other time scales. In particular, if the

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unrealistically large AMSR-E seasonal cycle at Little Washita were replaced with something more realistic, for example representing 8\,{\%} of the total variance (as in the ARS time series), then the fraction of variance in SM_{short} would increase from the current 48 to 75\,{\%}, increasing the SM_{short} variance in the CDF-matched AMSR-E from 0.0036 to 0.0054\,\unit{(m^3\,m^{-3})^2}.

\subsection{Evaluation of the baseline assimilation experiment at each time scale}\label{sec:assim_results}%3.5

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Figure~\ref{fig:mse_cat_years} shows the ubMSE for each assimilation experiment, separated into each time scale. Prior to assimilation, the average ubMSE in the near-surface soil moisture across the four sites was 1.8×10^{-3} \,\unit{(m^3\,m^{-3})^2} (giving a~ubRMSE just above the 0.04\,\unit{m^{3}\,m^{-3}} target). Close to half (55\,{\%}) of the ubMSE is in SM_{short}, with the rest split between SM_{seas} (26\,{\%}) and SM_{long} (19\,{\%}). The Ac assimilation significantly reduced the total ubMSE at each site, reducing the average near-surface ubMSE across the four sites by 33\,{\%} to 1.2×10^{-3}\,\unit{(m^3\,m^{-3})^2}, with average reductions in the near-surface layer of 52\,{\%} for

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SM_{long}, 25\,{\%} for SM_{seas}, and 22\,{\%} for SM_{short}. The baseline assimilation experiment, labeled Ac, reduced the total ubMSE at each site for all time scale components, except for SM_{seas} at Little Washita (where the model ubMSE was already relatively small).

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Root-zone soil moisture observations were available for the study period only at Little River. Both the distribution of the ubMSE across each time scale, and the relative reductions achieved from assimilation, are similar for the near-surface and root-zone layers at Little River in Fig.~\ref{fig:mse_cat_years}d~and~e, adding confidence that the model improvements reported above for the near-surface soil moisture are indicative of the performance throughout the soil profile.

To illustrate the impact of the assimilation at each time scale, Fig.~\ref{fig:assim_out_LR} compares the decomposed time series for the Catchment model and Ac assimilation experiments to that from the ARS in situ observations at Little River. The difference between the three SM_{short} time series is difficult to visually judge in Fig.~\ref{fig:assim_out_LR}d, however, the impact of the assimilation on the SM_{seas} and SM_{long} time series is clear. Figure~\ref{fig:assim_out_LR}b suggests that the large SM_{long} ubMSE reduction (by over 80\,{\%}) from the

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assimilation is due to the reduced amplitude in the

SM_{long} dynamics, although there is perhaps also an

improvement in event timing. In Fig.~\ref{fig:assim_out_LR}c, the

model seasonal cycle has an overestimated amplitude, and also includes

two maxima per year, where the ARS seasonal cycle has only one. The

assimilation exacerbates the overestimated amplitude, but also removes

the second annual maxima, resulting in an overall

SM_{seas} ubMSE reduction (by 46\,{\%}).

\subsection{Observation rescaling with a~short data record}\label{sec:yearly}%S3.6

The nine year time period used in the baseline experiment to estimate the CDF-matching parameters is longer than is often available for soil moisture assimilation experiments. Obviously, assimilating a~shorter

time period will limit the potential improvements to the model

SM_{long} (of similar magnitude to the

SM_{short} improvement in this study). The potential

benefit of an assimilation over a~shorter period may also be limited

by the increased sampling uncertainty in the estimated observation

rescaling parameters. This increased uncertainty could arise from

systematic errors due to inadequate sampling of

SM_{seas} and SM_{long}, or from

increased random errors associated with the smaller sample size.

This is tested here with nine additional experiments, labeled AyYY, in which the CDF-matching parameters are each based on a~12 month period starting on October 1. For example, experiment

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Ay03 uses CDF- matching parameters based on the 12 months of data from 1 October 2003 to 30 September 2004. Each of the nine experiments assimilates the full eight or nine year record of AMSR-E near-surface

soil moisture retrievals (including the data for the year from which the CDF-matching parameters were determined).

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The potential uncertainty introduced by using a~single year to estimate the rescaling parameters depends on the inter-annual variability in the systematic differences between the observed and forecast soil moisture. The main systematic differences that are addressed by the CDF-matching are the differences in the observed and forecast mean and standard deviation. For demonstrative purposes, Fig.~\ref{fig:scale_params} illustrates the difference between the means, and the ratio of the standard deviations, estimated using the full data record, and using each single year. Note, however that in the presented Ay experiments the AMSR-E observations are rescaled based on the full CDF, and not just the mean and variance. In Fig.~\ref{fig:scale_params}a~there is considerable inter-annual scatter in the yearly mean differences, although by linearity the average is unbiased. The standard deviation ratio in Fig.~\ref{fig:scale_params}b also shows inter-annual variability, however the single year ratios are also biased low compared to the all-years ratio, since the single year estimates did not sample the SM_{long} variance (which was consistently a~greater fraction of the total variance for Catchment than for AMSR-E in

Fig.~\ref{fig:var_unit}a). This is particularly marked at Little River, where the average of the single year standard deviation ratios was 30\,{\%} less than when estimated using all years (since SM_{long} makes up close to 50\,{\%} of the total variance in Catchment, compared to less than 5\,{\%} for AMSR-E in Fig.~\ref{fig:var_unit}a).

Figure~\ref{fig:mse_cat_years} includes the ubMSE for the nine Ay assimilation experiments, as well as the mean ubMSE ($\langle \text{Ay} \rangle$) across all nine.

On average, assimilating the AMSR-E observations that have been rescaled using parameters estimated from a single year is beneficial. As with the Ac experiment, the $\langle \text{Ay} \rangle$ ubMSE is consistently less than that of the model at each time scale, except for SM_{seas} at Little Washita. However, for individual realizations there is an increased risk when using the single year parameters that the assimilation will not significantly improve the model, or will even significantly degrade the model. For example, at Little Washita, where the Ac experiment reduced the ubMSE by a~small but significant amount, none of the Ay experiments significantly decreased the ubMSE, and the Ay10 experiment significantly increased it.

Additionally, comparing the Ay experiments in Figure \ref{fig:mse_cat_years} to the baseline Ac experiment shows that at Reynolds Creek, Walnut Gulch, and Little Washita most of the Ay experiments resulted in larger total ubMSE than for the Ac experiment, while at Little River the opposite occurred. Overall

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there were eight Ay experiments for which the total ubMSE was significantly different (at the 5\,{\%} level) and higher than for the Ac experiment, seven for which it was significantly different and lower, and 20 where the ubMSE was not significantly changed. The differences between the Ac and Ay ubMSE are skewed, in that when the Ay ubMSE is higher, the difference tends to be greater than when it is lower. Consequently, the average reduction in the model ubMSE for the near-surface soil moisture, compared to the model with no assimilation, is slightly less for $\langle \text{Ay} \rangle$ (30\,{\%}) than for Ac (33\,{\%}).

Each instance of relatively poor ubMSE for an Ay experiment can be traced to the more extreme (i.e., unrepresentative) single year systematic differences in Fig.~\ref{fig:scale_paramsGoing through the experiments with the largest relative increase in ubMSE, experiment Ay07 at Reynolds Creek, and experiments Ay05, Ay06, and Ay07 at Walnut Gulch all have extreme standard deviation ratios, while Ay06 at Reynolds Creek and Ay10 at Little Washita have extreme mean differences. In each case, most of the increase in the ubMSE is due to increased errors in the SM_{seas} and SM_{long} components, suggesting that the SM_{short} corrections are more robust to uncertainty in the scaling parameters. Note that unrepresentative scaling parameters do not necessarily degrade the assimilation output, and in some instances are even advantageous. Most obviously, at Little River, where the single year

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standard deviation ratios were biased low (by 30\,{\%}), the Ay assimilation experiments all produced slightly lower ubMSE than the Ac experiment.

In general, the impact of errors in the rescaling of the mean value are likely under-reported here, since any introduction of biases into the model will not be directly detected by the ubMSE. Despite this, the examples cited above in which unrepresentative mean difference corrections degraded the bias-robust ubMSE highlight the potential for a~bias-free assimilation of biased observations to degrade model soil moisture dynamics.

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\conclusions

Many studies have demonstrated that near-surface soil moisture assimilation can improve modeled soil moisture, in terms of the anomaly time series used to represent ``random errors'', often implicitly assumed to represent subseasonal scale variability associated with individual precipitation events \citep{ReichleD09108, Scipal1101,DraperL04401}. Here, nine-years of LPRM AMSR-E observations were assimilated into the Catchment model, and the resulting model output evaluated separately at the subseasonal (SM_{short}), seasonal (SM_{seas}), and inter-annual (SM_{long}) time scales against watershed-scale in situ observations at four ARS sites in the US. The results show that, in addition to reducing the near-surface SM_{short} ubMSE averaged across the four sites, the assimilation also reduced the near-surface SM_{long} ubMSE. The magnitude of the reductions in SM_{short} and SM_{long} were similar (2.1×10^{-4}\,\unit{(m^3\,m^{-3})^2}, and 2.5×10^{-4}\,\unit{(m^3\,m^{-3})^2}, respectively), although this represented a~much larger relative reduction in the SM_{long} ubMSE (52\,{\%} of the model SM_{long} ubMSE, compared to 22\,{\%} for the SM_{short} ubMSE). In situ observations of the root-zone layer were available for only one site, however the similarity between the near-surface and root-zone results at this site (Fig.~\ref{fig:mse_cat_years}) is encouraging in terms our near-surface results being representative of the deeper soil moisture profile.

The reduced SM_{long} ubMSE suggests that assimilating a~sufficiently long data record of near surface soil moisture observations can improve the model soil moisture dynamics at inter-annual time scales, enhancing the model ability to simulate important events such as droughts. There is then a clear potential for reanalyses, or other long-term simulations, to benefit from the assimilation of long-term remotely sensed soil moisture records. Such long records are available from the AMSR-E satellite used here (May 2002 – Oct. 2011), and increasingly from the active microwave ASCAT series (ongoing from Oct. 2006). Carefully merged multi-satellite records, such as the 30 year record being produced by the Water Cycle Multi-mission Observation Strategy (WACMOS) project \citep{Su270, Liu280} are also now providing data records of unprecedented length. As with SM_{short}, an important caveat on this finding is it is possible that the reduced ubMSE was

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associated with reduced representativity differences compared to the in situ observations that were used to calculate the ubMSE. For example, at Little River in Fig.~\ref{fig:mse_cat_years} the substantial improvements to the SM_{long} near-surface and root-zone soil moisture gained by assimilating the AMSR-E observations were largely due to reduced SM_{long} variance. If the model's exaggerated SM_{long} was a~representativity or structural error (e.g., too strong a~signal of underlying water table), then it is not clear that the model would benefit from correcting this error, in terms of improvements to forecast skill.

Assimilating the AMSR-E observations also reduced the near-surface SM_{seas} ubMSE by 26\,{\%}, averaged across the four sites, suggesting the possibility that the assimilation was beneficial to the modeled mean seasonal cycle, despite not being designed to address systematic errors. However, even more so than for SM_{long}, the reduced SM_{seas} ubMSE could be due to reduced representativity differences, rather than a~genuine improvement to the model's ability to represent the desired physical processes. To confirm that the SM_{long} and

SM_{seas} ubMSE reductions do indicate improved model soil moisture would require evaluating the dependent moisture and energy flux forecast, and unfortunately verifying observations are not available at the study locations.

In comparing the AMSR-E and Catchment soil moisture at each time scale in this study, it became apparent that the distribution of variance across each time scale was very different between the remotely sensed and modeled soil moisture time series (Fig.~\ref{fig:var_unit}). Traditionally, observation rescaling strategies used in land data assimilation do not distinguish between variability at different time scales, and apply a~single set of bulk rescaling parameters to the full time series. Consequently, the large discrepancies in the variance at one time scale (due to errors in one of or both estimates) can have follow-on effects for the rescaling of other time scales. For example, the unrealistically large AMSR-E seasonal cycle at Little Washita caused the variability at SM_{long} and SM_{short} to be overly dampened by the bulk rescaling. This could perhaps be avoided by rescaling the observations separately at each time scale using the decomposed time series produced in this study, or using other methods that distinguish scaling characteristics at different time scales (e.g., Su and Ryu, 2015).

In addition to observation bias removal strategies that respect the time scale-dependent nature of observation -- forecast systematic differences, it may be advantageous to target only certain time scales, for example by retaining the model seasonal cycle while rescaling other time scales (e.g., \citet{DruschL15403,Bolten57}). Ultimately, whether these approaches will be beneficial will

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depend on whether the model observation differences at each time scale are caused by model or observation errors. This study is a~first effort to investigate soil moisture assimilation at specific time scales associated with different soil moisture physical processes. Looking forward, further evaluation of soil moisture at these time scales will help to identify the physical processes responsible for errors in modeled and remotely sensed soil moisture (including representativity errors in the latter), which will in turn help to refine observation bias removal strategies.

Finally, we have updated the investigation of \cite{ReichleL19501} into the use of short data records for estimating observation rescaling (CDF-matching) parameters. Nine additional assimilation experiments were performed, each with the AMSR-E observations rescaled using parameters estimated from a~single year of data. Compared to the scaling parameters estimated using the full data record, using only one year of data introduced sampling errors due to inter-annual variability in SM_{seas} and SM_{short}, and the unsampled SM_{long} variability in the parameters.

For hindcasting/reanalysis applications, when the same short time period is used for bias parameter estimation and data assimilation, such unrepresentative parameters should not be problematic, since the rescaled observations will still be unbiased relative to the model over the length of the assimilation experiment, allowing shorter time scale errors to be corrected. However, in a~forecasting/analysis application in which the bias corrections parameters must be estimated with the available (short) data record, and then applied to future observations, unrepresentative parameters can be more problematic. Our results suggest that, when necessary, for example early in the SMAP mission, assimilating near-surface soil moisture over an extended period using single year parameters will introduce some additional uncertainty into the assimilation output, however over a~large domain the overall impact will be minor. Of the total of 35 individual assimilation realizations that we performed with single year parameters at the four locations, nine resulted in no significant change in the near-surface ubMSE compared to the open loop, and one resulted in significantly increased ubMSE (recall that the baseline assimilation significantly reduced the ubMSE at all four sites). However, averaged across all realizations, which should translate to an average across a~large spatial domain, the net impact of the single year parameters was

small, and the benefit gained from the assimilation was not practically reduced, compared to the baseline assimilation experiment.

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\begin{acknowledgements}

Thanks to Balachandrudu Narapusetty for helpful comments, USDA-ARS and Michael Cosh for providing access to the long term in situ soil moisture observations from the experimental watersheds. The

AMSR-E soil moisture retrievals were obtained from the NASA Goddard Earth Sciences Data and Information Services Center (GES DISC). This work was supported by the NASA Terrestrial Hydrology program (NNX15AB52G).

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%T1
\begin{table}[t]
\caption{Location, time period, and number of in situ network sites at each watershed.}
\label{tab:sites_locn}
\scalebox{.87}[.87]{%
\begin{tabular}{llll}
\tophline
Name (abbreviation)	& Approx. area and center location & \# sites & Time period \\
\middlehline
Reynolds Creek, surface (RC-sfc) & 150 km$^4$ (116.7{\degree}\,W, 43.2{\degree}\,N)  & 10 & Oct 2002--Sep 2010, \\
& & &excluding 1~Dec--10~Mar\\
Walnut Gulch, surface (WG-sfc) & 600 km$^4$, (110.0{\degree}\,W, 31.7{\degree}\,N) & 14& Oct 2002--Sep 2011 \\
Little Washita, surface (LW-sfc) & 350 km$^4$ (98.0{\degree}\,W, 34.8{\degree}\,N) & 15 & Oct 2002--Sep 2011 \\
Little River, surface (LR-sfc) & 250 km$^4$ (83.5{\degree}\,W, 31.5{\degree}\,N) & 8 & Oct 2002--Sep 2011 \\
Little River, root-zone (LR-rz) & as above &4 & Oct 2004--Sep 2011 \\
\bottomhline
\end{tabular}
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\begin{table}[t]

\caption{Descriptive statistics for each the data sets at each watershed.}

\label{tab:sites_stats}

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\begin{tabular}{llll}

\tophline

Data source & Number of daily data & Mean (\unit{m^3\,m^{-3}}) & Standard deviation (\unit{m^3\,m^{-3}})  \\

\middlehline

\multicolumn{4}{c}{Reynolds Creek,  surface} \\\middlehline

AMSR-E        & 1209 & 0.17 & 0.097 \\

ARS      & 1944 & 0.10 & 0.068 \\

Catchment   & 2111 & 0.16 & 0.039 \\\middlehline


\multicolumn{4}{c}{Walnut Gulch,  surface} \\\middlehline

AMSR-E        & 1960 & 0.15 & 0.067 \\

ARS      & 3282 & 0.05 & 0.023 \\

Catchment   & 3287 & 0.14 & 0.039 \\\middlehline
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\multicolumn{4}{c}{Little Washita,  surface} \\\middlehline
AMSR-E          & 1748 & 0.27 & 0.097 \\
ARS       & 2690 & 0.13 & 0.054 \\
Catchment   & 3287 & 0.14 & 0.039 \\\middlehline

\multicolumn{4}{c}{Little River,  surface} \\\middlehline
AMSR-E          & 1989 & 0.31 & 0.100 \\
ARS       & 3155 & 0.10 & 0.044 \\
Catchment   & 3287 & 0.19 & 0.049 \\\middlehline

\multicolumn{4}{c}{Little River,  root-zone} \\\middlehline
AMSR-E          & --   &  -- & -- \\
ARS       & 2808 & 0.09 & 0.036 \\
Catchment   & 2830 & 0.15 & 0.038 \\
\bottomhline
\end{tabular}
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\begin{figure}

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\caption{The ARS in situ, Catchment model, and AMSR-E remotely sensed surface soil moisture, with near-surface soil moisture at \textbf{(a)}~Reynolds Creek, \textbf{(b)}~Walnut Gulch, \textbf{(c)}~Little Washita, \textbf{(d)}~Little River, and \textbf{(e)}~root-zone soil moisture at Little River.\label{fig:SM_orig}}

\end{figure}

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\begin{figure}

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\caption{Decomposition of the Catchment near-surface soil moisture time series at Little River, using the harmonic (HA; black) and moving average (MA; cyan) methods, for \textbf{(a)}~the original time series (red dots) and the sum of $\text{SM}_{\text{long}} + \text{SM}_{\text{seas}} +$\,the long-term mean soil moisture (solid lines), and the individual components \textbf{(b)}~SM_{long}, \textbf{(c)}~SM_{seas}, and \textbf{(d)}~SM_{short}.\label{fig:decomp_LR}}

\end{figure}

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\begin{figure}

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\caption{Time series variance at each time scale, with the Catchment Model (M), original AMSR-E Observed (O), and CDF-matched AMSR-E Observed (Oc) soil moisture variances plotted for the

\textbf{(a)}~harmonic, and \textbf{(b)}~moving average decomposition methods. The circles and error bars give the variance of the original soil moisture time series, with 95\,{\%} confidence intervals (some very small confidence intervals are obscured by the plotted circles).\label{fig:var_method}}

\end{figure}

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\begin{figure}

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\caption{Fraction of variance at each time scale, obtained by normalizing the time series variance before decomposition. The Catchment Model (M), original AMSR-E Observed (O), and the CDF-matched AMSR-E Observed (Oc) soil moisture time series, cross-screened for AMSR-E availability, are plotted in~\textbf{(a)}, and the ARS In situ observations (I), Catchment model (M), and baseline assimilation (Ac) soil moisture time series, cross-screened for ARS availability, are plotted in~\textbf{(b)}. The circles give the variance of the original (normalized) soil moisture time series.\label{fig:var_unit}}

\end{figure}

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\begin{figure}

\includegraphics[width=70mm]{hess-2015-292-discussions-f05.pdf}

\caption{Error variances (ubMSE) compared to ARS in situ observations at each time scale, for the near-surface soil moisture at \textbf{(a)}~Reynolds Creek, \textbf{(b)}~Walnut Gulch, \textbf{(c)}~Little Washita, \textbf{(d)}~Little River, and \textbf{(e)}~for the root-zone soil moisture at Little River. Bars show the Catchment model open loop (M), baseline assimilation (Ac), individual Ay assimilation experiments, and the mean across the Ay experiments ($\langle \text{Ay} \rangle$). Label AyYY indicates the Ay experiment with bias correction parameters estimated from the 12\,months from 1~October of 20YY. Circles and error bars give the ubMSE and its 95\,{\%} confidence interval for the original soil moisture time series (some very small confidence intervals are obscured by the plotted circles). The dashed line at ubMSE of 1.6×10^{-3}\,\unit{(m^3\,m^{-3})^2} is equivalent to the common ubRMSE target of 0.04\,\unit{m^{3}\,m^{-3}}.\label{fig:mse_cat_years}}

\end{figure}

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\begin{figure}

\includegraphics[width=120mm]{hess-2015-292-discussions-f06.pdf}

\caption{Harmonic decomposition of the ARS In situ (I), Catchment model (M), and baseline assimilation output (Ac) near-surface soil moisture time series at Little River, showing the \textbf{(a)}~original time series, \textbf{(b)}~$\text{SM}_{\text{long}}$, \textbf{(c)}~$\text{SM}_{\text{seas}}$, and \textbf{(d)}~$\text{SM}_{\text{short}}$.\label{fig:assim_out_LR}}

\end{figure}

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\begin{figure}

\includegraphics[width=120mm]{hess-2015-292-discussions-f07.pdf}

\caption{Systematic differences between AMSR-E observations and Catchment model near-surface soil moisture, with \textbf{(a)}~the mean difference ($\langle \text{model} \rangle - \langle \text{observation} \rangle$), and \textbf{(b)}~the ratio of the standard deviations ($\sigma(\text{model})/\sigma(\text{observations})$). The parameters are estimated using all years (All), and each year separately (with label YY indicating the parameters estimated from the 12\,months from 1~October of 20YY), and the dashed lines give the mean of the YY parameters.\label{fig:scale_params}}

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Remotely sensed near-surface soil moisture observations are typically

assimilated using a~bias-blind assimilation of observations that have

been ``bias-corrected'' to have the same mean as the model forecast

soil moisture \citep{ReichleD09108,Scipal1101,Bolten57}.

Page 4: [2] Deleted	Draper	11/17/15 5:41 PM

bias. Observation-bias

correction of remotely sensed soil moisture is usually achieved by

rescaling the observations to have the same mean and variance as model

forecasts, for example by matching their Cumulative Distribution

Functions (CDFs; Reichle and Koster,

2004). Traditionally, the observation rescaling

(CDF-matching) parameters are estimated over the maximum available

coincident observed and forecast data record

\citep{ReichleD09108,Scipal1101,DraperL04401}, so that the rescaled

observations will retain a~signal of any observation-forecast

differences that occurred at time scales shorter than the data record.

For a~multi-year data record assimilating these rescaled observations

could then potentially update the model soil moisture with observed

information at subseasonal, seasonal, and inter-annual time scales.

Page 4: [3] Deleted	Draper	11/17/15 5:43 PM

The physical processes causing soil moisture errors at the

above-mentioned subseasonal, seasonal, and inter-annual time scales

will be quite different

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For

example

Page 5: [5] Deleted Draper 11/17/15 5:54 PM

The systematic nature of errors in the mean seasonal cycle is problematic for data assimilation.

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Consequently, due to concerns over the accuracy of the seasonal cycle in remotely sensed soil moisture, \citet{DruschL15403} suggested that soil moisture observation-bias correction for data assimilation might be better designed so that the model soil moisture seasonal cycle is retained by the assimilation, as has been done in several more recent studies \citep{Bolten57,YilmazSUB}.

In addition to the systematic nature of seasonal errors, the time scale dependence of soil moisture errors may also be more generally problematic for observation rescaling. Even within time scales less than one month, \cite{Su17} showed that the multiplicative

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To better understand the time scale dependency of near-surface soil moisture assimilation,

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. We have used this decomposition to examine the differences between remotely sensed and modeled soil moisture at each time scale, how these difference affect observation rescaling, and how assimilating the remotely sensed observations impacts the model soil moisture at each time scale

Page 6: [9] Deleted	Draper	11/17/15 5:58 PM

Page 9: [10] Deleted	Draper	11/17/15 6:02 PM

See

Table~\ref{tab:sites_locn} for the locations of each site. These observations are averaged across each network to produce a~coarse scale soil moisture observation with spatial support similar to typical remotely sensed and modeled soil moisture estimates. Observations are potentially made at every 5\,\unit{cm} from 5--60\,\unit{cm} depth, although the 5\,\unit{cm} layer typically has a~longer and more complete record than the deeper layers. In this study, the near-surface soil moisture from Catchment and AMSR-E was evaluated using the 5\,\unit{cm} ARS observations, while the root-zone soil moisture from Catchment was evaluated using the average of the 5--60\,\unit{cm} observations (including only times with data reported for all layers). The ARS root-zone soil moisture was used at Little River only, due to very low observation counts over the study period at the other sites.

Page 12: [11] Deleted	Draper	11/17/15 6:05 PM

}. We used CDF-matching

\citep{ReichleL19501} to rescale the observations prior to each assimilation experiment. The details of the time period used to estimate the observation scaling parameters are given in Sect.~\ref{sec:results}, before presenting each set of results.

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The coverage statistics for each data set in

Table~\ref{tab:sites_stats} highlight that the AMSR-E and ARS observed

time series are incomplete

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}. These systematic differences are clear in

Fig.~\ref{fig:SM_orig}

Page 23: [14] Deleted	Draper	11/17/15 6:13 PM

AMSR-E could be expected a~priori to have a~larger fraction of

variance at SM_{short}, due to measurement noise in

the remotely sensed observations.

Page 24: [15] Deleted	Draper	11/17/15 6:14 PM

The systematic differences between observed and forecast soil moisture

mean and variance (Fig.~\ref{fig:var_method}) motivate the practice of

rescaling observations to match the model forecast climatology prior

to assimilation. If this is not done, the assimilation may force the

model into a~regime that is incompatible with its assumed structure

and parameters, leading to degraded flux forecasts

\citep{LannoyW09410}.

Page 24: [16] Deleted	Draper	11/17/15 6:15 PM

Hence, the observation rescaling, and assimilation

of the resulting observations, was repeated using linear rescaling of

the AMSR-E observations in place of CDF-matching, with very similar

results in terms of the rescaled observations and the assimilation

output (for both the Oc rescaling presented here, and the Oy rescaling

in Sect.~\ref{sec:yearly}).

Page 25: [17] Deleted	Draper	11/17/15 6:17 PM

The improvement gained from assimilating the AMSR-E observations is evaluated using the unbiased Mean Square Error (ubMSE) of the resulting model soil moisture, with respect to the ARS in situ observations. We define the ubMSE as the mean square difference after removing the long-term mean bias from both data sets. This is the square of the commonly used unbiased \textit{root} mean square error \citep{Entekhabi832}. We do not use the square root to take advantage of the additive property of the variance of independent time series, however to aid interpretation the ubMSE equivalent to the common ubRMSE target accuracy of 0.04\,\unit{m^{3}\,m^{-3}} is indicated in the relevant plots.

Page 25: [18] Deleted	Draper	11/17/15 6:18 PM

In the baseline

assimilation experiment, labeled Ac, the observations CDF-matched over the full time period (Oc) were assimilated into the Catchment model.

Page 27: [19] Deleted	Draper	11/17/15 6:19 PM

The nine year AMSR-E data record used here is the longest remotely sensed soil moisture record available from a~single satellite sensor, and soil moisture assimilation experiments using newer satellites are limited to shorter time periods.

Page 28: [20] Deleted	Draper	11/17/15 6:20 PM

To

establish the potential consequences of this uncertainty, we conducted nine additional experiments, labeled Ay, with the rescaling parameters for each estimated from a~12 month period starting in consecutive

Octobers (but assimilating the full eight or nine year near-surface

soil moisture data record listed in Table~\ref{tab:sites_locn}).

Page 28: [21] Deleted	**Draper**	**11/17/15 6:20 PM**

In contrast to \citet{ReichleL19501}, we do not use ergodic

substitution (of spatial sampling for temporal sampling) when

estimating the rescaling parameters with a~single year of

observations, since with more modern remotely sensed data sets (than

the SMMR data used by Reichle and Koster, 2004) this is no longer

necessary to obtain a~sufficient sample size. Additionally, for the

assimilation of Soil Moisture Ocean Salinity retrievals,

\citet{LannoySUB} found ergodic substitution degraded the estimated

CDFs, by introducing conflicting information from neighboring grid

cells (possibly due to the higher spatial resolution, compared to

SMMR).

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Note that errors in the

rescaling of the mean value are likely under-reported here, since any

introduction of biases into the model will not be directly detected by

the ubMSE. Comparing the 35 individual Ay experiments to the baseline

Ac experiments, most of the Ay experiments resulted in larger total

ubMSE than the Ac experiment did at Reynolds Creek, Walnut Gulch, and

Little Washita, while the opposite occurred at Little River.

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}. For example,

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The result that unrepresentative mean

difference corrections can impact the ubMSE (a~bias-robust metric) is

interesting in that it demonstrates that bias-free assimilation of

biased observations can degrade model soil moisture dynamics.

Page 31: [25] Deleted **Draper** **11/17/15 6:26 PM**

Above, the assimilation of AMSR-E data that has been rescaled using

parameters estimated from a~single year, and from the full time period

were compared, showing that the average ubMSE is slightly higher when

the single year parameters were used. However, it is perhaps more

relevant to assess whether the assimilation is still beneficial when

the single year parameters are used. Figure~\ref{fig:mse_cat_years}

Page 31: [26] Deleted **Draper** **11/17/15 6:26 PM**

suggests that on average it is. As with the Ac experiment, the

$\langle \text{Ay} \rangle$ ubMSE is consistently less than that of

the model at all time scales, except for SM_{seas} at

Little Washita. However, for individual realizations there is an

increased risk when using the single year parameters that the

assimilation will not significantly improve the model, or will even

significantly degrade the model. For example, at Little Washita,

where the Ac experiment reduced the ubMSE by a~small but significant

amount, none of the Ay experiments significantly decreased the ubMSE,

and the Ay10 experiment significantly significantly increased it.

Page 33: [27] Deleted **Draper** **11/17/15 6:28 PM**

However, more so than for

SM_{short},

Page 34: [28] Deleted	Draper	11/17/15 6:30 PM

using rescaling methods that rescale each

time scale separately (e.g., Su and Ryu, 2015).

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Bolten et~al., 2010; Yilmaz et~al.,

2015

Page 36: [30] Deleted	Draper	11/17/15 6:31 PM

small, and did not practically reduce the benefit gained from the

assimilation.

Page 38: [31] Deleted	Draper	11/17/15 6:32 PM

\bibitem[{De~Lannoy et~al.(2007)De~Lannoy, Reichle, Houser, Pauwels, and Verhoest}]{LannoyW09410}

De~Lannoy,~G., Reichle,~R., Houser,~P., Pauwels,~V., and Verhoest,~N.:

{Correcting for forecast bias in soil moisture assimilation with the ensemble Kalman filter},

Water Resour. Res.,

43, W09410,

doi:\href{http://dx.doi.org/10.1029/2006WR005449}{10.1029/2006WR005449}, 2007.

Page 47: [32] Deleted	Draper	11/17/15 6:35 PM

Reynolds Creek, surface (RC-sfc) & 116.7{\degree}\,W, 43.2{\degree}\,N & Oct 2002--Sep 2010, excluding 1~Dec--10~Mar\\

Walnut Gulch, surface (WG-sfc) & 110.0{\degree}\,W, 31.7{\degree}\,N & Oct 2002--Sep 2011 \\

Little Washita, surface (LW-sfc) & 98.0{\degree}\,W, 34.8{\degree}\,N & Oct 2002--Sep 2011 \\

Little River, surface (LR-sfc) & 83.5{\degree}\,W, 31.5{\degree}\,N & Oct 2002--Sep 2011 \\

Little River, root-zone (LR-rz) & 83.5{\degree}\,W, 31.5{\degree}\,N & Oct 2004--Sep 2011
\\