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The impact of land model structural, parameter, and forcing errors on the characterization of soil moisture uncertainty

V. Maggioni¹, E. N. Anagnostou¹, and R. H. Reichle²

¹Department of Civil and Environmental Engineering, University of Connecticut, Storrs, CT, USA ²Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, MD, USA

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Correspondence to: V. Maggioni (viviana@engr.uconn.edu)

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Abstract

A sensitivity analysis is conducted to investigate the contribution of rainfall forcing relative to the model uncertainty in the prediction of soil moisture by integrating the NASA Catchment Land Surface Model (CLSM), forced with hydro-meteorological data, in the

- ⁵ Oklahoma region. This study depicts different sources of uncertainty, namely, errors in the model input (i.e., rainfall estimates from satellite remote sensing observations) and errors in the land surface model itself. Specifically, rainfall-forcing uncertainty is introduced using a stochastic error model that generates reference-like ensemble rainfall fields from satellite rainfall products. The ensemble satellite rain fields are propagated
- through CLSM to produce soil moisture ensembles. Errors in CLSM are modeled with two different approaches: either by perturbing model parameters using the generalized likelihood uncertainty estimation (GLUE) technique or by adding randomly generated noise to the model prognostic variables. While the first method only addresses parametric uncertainty, the second one addresses both structural and parametric uncer-
- tainty. Despite this, a reasonable spread in soil moisture is achieved with relatively few parameter perturbations through GLUE, whereas the same ensemble width requires stronger prognostic perturbations with the standard random perturbation method. The probability of encapsulating the reference soil moisture simulation increases when the rainfall forcing uncertainty and the model uncertainty approaches are combined (com-
- ²⁰ pared with using only rainfall uncertainty). This improvement is more significant when using the GLUE technique to perturb CLSM parameters as opposed to perturbing the CLSM prognostic variables.

1 Introduction

Soil moisture is a key variable of the land surface water budget. It has an impact on water, energy and biogeochemical cycles; thus, it plays a major role in many research fields, such as hydrology, agriculture and ecology. As the availability of in-situ





measurements is scarce, global soil moisture data rely on satellite retrievals (e.g., Njoku et al., 2003; Kerr et al., 2010; Entekhabi et al., 2010) and land surface model (LSM) simulations (e.g., Wood et al., 1992; Koster et al., 2000). LSM soil moisture predictions can be enhanced by assimilating near-surface satellite soil moisture obser-

- vations through a land data assimilation system (LDAS). Often, such systems utilize ensemble-based techniques to update LSM soil moisture predictions in response to satellite observations of near-surface soil moisture (e.g., Reichle and Koster, 2005). Proper characterization of the uncertainty in the LSM soil moisture predictions is crucial for the optimal assimilation of the observed near-surface soil moisture data (Reichle
- et al., 2008). Advancing hydrologic prediction uncertainty goes beyond soil moisture data assimilation. As discussed in Vrugt et al. (2008), to improve hydrologic modeling, it is necessary to quantify the individual error sources in order to identify which parts of the model can potentially be improved. Moreover, uncertainty characterization can provide the decision makers with a better measure of accuracy and precision of model
 predictions (Benke et al., 2008).

A common approach for model uncertainty estimation is the Generalized Likelihood Uncertainty Estimation (GLUE) method, introduced by Beven and Binley (1992). GLUE does not consider an optimum model parameter set, but assumes that several parameter sets can have equal likelihood to be accepted ("equifinality" assumption). GLUE is implemented by performing a large number of model runs with different combinations

- Implemented by performing a large number of model runs with different combinations of parameter values. By comparing model outputs to a reference (e.g., observations), each combination of parameters is assigned a likelihood value. Then, the total sample of simulations is split into behavioral and non-behavioral parameter sets, based on a cutoff threshold. GLUE has found application in several fields; including conceptual
- rainfall-runoff modeling (Lamb et al., 1998; Hossain et al., 2004), distributed hydrologic modeling (McMichael et al., 2006), land surface modeling (Hossain and Anagnostou, 2005), and radar-rainfall estimation (Tadesse and Anagnostou, 2005).

On the other hand, a common technique to introduce modeling uncertainty in land assimilation systems is by directly adding randomly generated noise to the model





prognostic variables, representing errors in model structure and parameters (in addition to perturbations in model forcings; Reichle et al., 2007). The present study applies both approaches for a complete analysis of the contribution of model uncertainty to the prediction of soil moisture fields.

- Rainfall is the dominant meteorological forcing input to the land surface model for soil moisture simulations. Therefore, uncertainty in the input precipitation products can have an important impact on the predicted soil moisture fields and their associated uncertainty. Hossain and Anagnostou (2006a) have proposed a stochastic error model (named SREM2D) to generate "ground truth" rainfall ensembles from satellite rainfall
 products. Hossain and Anagnostou (2006c), and recently Maggioni et al. (2011), have
- investigated the implication of using SREM2D in representing soil moisture prediction uncertainty from a land surface model forced with satellite rainfall data. They showed that soil moisture ensembles from land surface models forced with SREM2D-generated rainfall adequately capture the soil moisture error characteristics at different spatial scales.
- In addition to satellite rainfall-only uncertainty, Hossain and Anagnostou (2005) have explored the effect of the combined (model parameters and rainfall forcing) uncertainty on the simulation of soil moisture. The parametric uncertainty was represented by the GLUE technique and the rainfall forcing uncertainty was characterized by a one-²⁰ dimensional version of SREM2D. They showed that precipitation uncertainty alone can explain only part (between 20% and 60%) of the uncertainty in soil moisture prediction. This demonstrates the need for further investigation of the interaction between rainfall and model errors to optimize the use of satellite rainfall products in land data assimilation systems.
- ²⁵ This study aims at investigating the relative impact of modeling and rainfall forcing uncertainties on soil moisture fields simulated by the Catchment Land Surface Model (CLSM, Koster et al., 2000). Specifically, it builds upon the recent study by Maggioni et al. (2011) that investigated soil moisture prediction uncertainty associated with errors in rainfall forcing. The present study introduces several novelties that address





some of the limitations of the earlier work by Hossain and Anagnostou (2005). First, two different model uncertainty frameworks are compared: the GLUE technique versus the direct perturbation of model prognostic variables. Second, results are presented in terms of both surface and root zone soil moisture. Third, our study uses spatially distributed data and a spatial error model, while the study by Hossain and Anagnostou (2005) was limited to a one-dimensional simulation that used single point data, thus neglecting spatial error characteristics. Finally, we use a different land surface model (i.e., CLSM), which is part of the NASA GMAO (Global Modeling and Assimilation Office) quasi-operational Goddard Earth Observing System Model, Version 5 (GEOS-5)

¹⁰ system (Rienecker et al., 2008).

The manuscript is structured as follows. Section 2 provides a description of the area of interest and datasets. Next, Sect. 3 describes the approach followed to study how uncertainty in simulated soil moisture is affected by (a) modeling uncertainty, (b) rainfall forcing uncertainty, and (c) the combination of the two sources. Section 4 provides a discussion of results, and Sect. 5 summarizes the major findings.

2 Study area and data

The study area is the Oklahoma region in the United States. Specifically, we use a 25 km Cartesian modeling grid ranging between 100° W and 94.5° W in Longitude and 34.5° N and 37° N in Latitude (Fig. 1). The study period includes three continuous years from 1 January 2004 to 31 December 2006. The Oklahoma region offers a good coverage by the Weather Surveillance Radar 88 Doppler (WSR-88D) network (Maddox et al., 2002), multi-year satellite rainfall products and a dense network of hydro-meteorological stations from the Oklahoma Mesonet (Brock et al., 1995). The Oklahoma Mesonet provides observations with high temporal frequency from 115 automated observing stations that record several meteorological parameters (rainfall, wind, radiation, etc.) and soil moisture at depths of 5, 25, 60, and 75 cm (available ev-





quantity and quality at all four measurement depths were available only at 21 Mesonet stations as shown in Fig. 1.

Two rainfall products – the rain gauge-calibrated WSR-88D radar rainfall and the NOAA CMORPH satellite rainfall – are employed in this study and interpolated to the 25-km Cartesian grid shown in Fig. 1. Along with supplemental surface meteorological forcing data, these radar and satellite precipitation products force the land surface model at the 25-km grid resolution to generate soil moisture fields. The radar rainfall product is from the Stage IV WSR-88D precipitation estimation algorithm, which consists in a national mosaic of precipitation estimates based on observations from all WSR-88D radars across the continental US (Fulton et al., 1998). Stage IV data represent the best quality WSR-88D rainfall product available at hourly/4-km resolution and include corrections for ground clutter and anomalous propagation, vertical reflectivity profile effects and systematic variations of the reflectivity-to-rainfall relation-

- ship on the basis of bias estimates through comparisons with rain gauge observations
 (Fulton et al., 1998; Lin et al., 2005). The satellite product is the NOAA-Climate Prediction Center morphing (CMORPH) product, which is based on a unique combination of passive microwave (PMW) retrievals and Infrared (IR) data (Joyce et al., 2004). In particular, CMORPH uses motion vectors from half-hourly interval IR images to propagate the relatively high-quality precipitation estimates derived from PMW data. The
 spatio-temporal resolution of CMORPH is 8 km/half-hourly. As stated above both radar
- and satellite precipitation datasets are gridded to the 25-km grid and aggregated to a 3-hourly time step to ensure common spatial and temporal scales.

3 Methodology

The NASA Catchment Land Surface Model (CLSM; Koster et al., 2000) constitutes the
 modeling scheme to simulate surface and root zone soil moisture in this study. The
 model uses the hydrological catchment as fundamental land surface element. Within
 each catchment, the variability of soil moisture is related to topography and to three bulk





soil moisture variables, representing equilibrium conditions associated with water table distribution, and non-equilibrium conditions near the surface. CLSM is forced by several surface meteorological variables, such as precipitation, humidity, air temperature and radiation. Precipitation data in this study are from the aforementioned WSR-88D

- Stage IV) and CMORPH products; whereas the other meteorological forcing data are extracted from the Global Land Data Assimilation Systems (GLDAS) project (Rodell et al., 2003; http://ldas.gsfc.nasa.gov), based on output from the global atmospheric data assimilation system at the NASA GMAO (Bloom et al., 2005). CLSM simulations were initialized from a spin-up integration by forcing the model with the WSR-88D (Stage IV)
 rainfall fields and by looping three times through the 3-year time series of forcing data
- (2004–2006).

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The Catchment model was demonstrated in several past studies to realistically describe soil moisture dynamics (Bowling et al., 2003; Nijssen et al., 2003; Boone et al., 2004). In a recent study, Maggioni et al. (2011) showed consistency and fairly high correlations between soil moisture anomaly time series from the OK Mesonet station observations and corresponding simulations from the Catchment model forced with WSR-88D (Stage IV) rainfall.

In this study CLSM is first forced with the WSR-88D (Stage IV) precipitation data to generate the "reference" soil moisture fields (Fig. 2). Then, CLSM simulations are performed to investigate the contributions of model and rainfall-forcing error in soil moisture

- formed to investigate the contributions of model and rainfall-forcing error in soil moisture prediction uncertainty: (i) model uncertainty alone through parameter perturbations (case M1); (ii) model uncertainty alone through prognostic perturbations (case M2); (iii) rainfall forcing uncertainty alone (case F); (iv) combination of rainfall forcing and model (through parameter perturbation) uncertainty (case M1F); and (v) combination
- of rainfall forcing and model (perturbing prognostics) uncertainty (case M2F). The uncertainty analysis is carried out in terms of both surface and root zone soil moisture values. Surface soil moisture henceforth refers to the (0–2) cm soil moisture output from CLSM and to the OK Mesonet soil moisture observations at 5 cm depth, whereas "root zone" soil moisture is defined as the (0–100) cm soil moisture CLSM output and





the corresponding depth-weighted average over the 5 cm, 25 cm, 60 cm and 75 cm OK Mesonet measurements.

Details about the different experiments are described next. Specifically, Sect. 3.1 describes the methodology used to study the model uncertainty alone (left column of

Fig. 2); Sect. 3.2 presents the setup to study rainfall forcing uncertainty alone (middle column of Fig. 2), and Sect. 3.3 illustrates the method used to analyze the combined rainfall and model uncertainty (right column of Fig. 2).

3.1 Model uncertainty

The first framework to characterize the model error (case M1 in Fig. 2) is based on GLUE. The GLUE approach finds a set of model parameters that are behavioral in the sense that they are acceptably consistent with the reference integration. It uses an informal likelihood measure to detect parts of the model parameter space that provide acceptable fits to the data. An analysis was conducted in this study to identify a small subset of parameters for which CLSM exhibits the strongest sensitivity in terms

- of simulated soil moisture effects. This was computed with respect to the "reference" soil moisture, obtained by forcing the model with radar rainfall and with the original set of parameters. Each parameter was independently scaled by multiplicative coefficients ranging from 25% to 400% of their standard values. Only one parameter at a time was perturbed with the same scaling factor for all grid cells, while keeping the
 other parameters constant; the scaled parameter was held constant for the entire 3-yr
 - integration. The ensemble members of surface and root zone soil moisture fields generated from CLSM based on each value of the parameter-scaling factor are evaluated in terms of two performance metrics: efficiency score (Eq. 1) and relative bias (Eq. 2), defined as
- 25 follows:





$$\mathsf{ES} = 1 - \frac{\frac{1}{N} \sum_{i=1}^{N} \left(\hat{\vartheta}_{i} - \vartheta_{i}\right)^{2}}{\mathsf{var}\left(\vartheta\right)}$$

Relative Bias =
$$\frac{\sum_{i=1}^{N} \left(\hat{\vartheta}_{i} - \vartheta_{i}\right)}{\sum_{i=1}^{N} \left(\vartheta_{i}\right)}$$

where $\hat{\vartheta}$ is soil moisture obtained by the perturbed simulation, ϑ is the "reference" soil moisture and *N* is the length of the time series.

- Figure 3 shows the above performance metrics (efficiency score and mean relative error respectively) versus the parameter value scaling factor (presented in %) for the two parameters to which CLSM showed the highest sensitivity: the Clapp-Hornberger parameter (*b*) and the soil wilting point wetness (wpwet). Metrics are computed for each grid cell and shown as boxplots, where the central mark is the median, and the
- ¹⁰ edges of the box are the 25th and 75th percentiles. Results are presented here only for the surface soil moisture, but are very similar for the root zone simulations. Efficiency score ranges between 0.88 and 1 for *b*, and it ranges from negative values to 1 for wpwet, while the relative bias varies between -0.3 and 0.1 for *b*, and between -0.3and 0.6 for wpwet.
- ¹⁵ Based on the performed sensitivity analysis, the GLUE parametric uncertainty was applied to combinations of the two most sensitive parameters: *b* and wpwet. Specifically, each set of perturbed parameter values is assigned a likelihood value; in this study it was chosen to be the efficiency score (Eq. 1), which indicates the correspondence between the model predictions and the "reference" integration. Using a cutoff
- threshold of acceptable efficiency scores, the total sample of simulations is then split into behavioral and non-behavioral parameter combinations (Fig. 4). This threshold is defined in terms of a certain allowable deviation of the highest likelihood value in the



(1)

(2)



sample, namely, only those combinations of parameters with an efficiency score higher than 80 % (70 %) for surface (root zone) soil moisture are picked to evaluate the model parameter uncertainty (case M1). This results in fourteen parameter combinations, listed in Table 1, which are used to integrate a CLSM ensemble of fourteen members.

⁵ For each ensemble member, the same parameter set is used for all grid cells in the domain and kept constant during the 3-year integration period.

Alternatively, model uncertainty can be represented by directly perturbing model prognostic variables (case M2 in Fig. 2). The three bulk soil moisture prognostic variables of CLSM are surface excess, root zone excess, and catchment deficit. How-

- ever, Reichle et al. (2007) observed that perturbations in the root zone excess might lead to biases between the ensemble mean and the unperturbed "reference" integration. Therefore, perturbations are limited to the surface excess and the catchment deficit. Each ensemble member is subject to randomly generated noise that is added to the model prognostic variables to represent errors in model structure and param-
- eters. Specifically, normally distributed additive perturbations are applied; ensemble means are constrained to zero, and time series correlations are imposed via a first-order autoregressive model. The perturbation parameter values are identical to the ones listed in Table 2 of Liu et al. (2011), and shown here in Table 2 for complete-ness. For consistency with case M1, fourteen ensemble members are produced by perturbing the two model prognostic variables.

It is worth noting that while case M1 only addresses uncertainty in the model parameters, approach M2 technically addresses both model structural and parameter uncertainty. However, the GLUE technique used in M1 provides an objective approach to characterize modeling uncertainty over data poor regions relying solely on the equifinal-

ity of model parameters determined from model sensitivity studies. M2 is a parametric approach requiring independent observations to properly characterize the parameter values of the statistical perturbation model. Moreover, the character of the ensembles generated by the M1 and M2 is very different. In the first case, each ensemble member will be biased against the reference in terms of long-term mean soil moisture at a





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variability across scales (Hossain and Anagnostou, 2006b). The input parameters for the satellite rainfall error model are shown in Table 3. In the study of Maggioni et al. (2011) it was shown that, compared to a simpler rainfall error model, SREM2D ensembles provide better encapsulation of the "reference" (WSR-88D) precipitation. In this study, CMORPH satellite rainfall is perturbed by SREM2D to produce an ensemble of twenty-four equiprobable reference-like rainfall realizations. This ensemble is used to force CLSM to obtain an ensemble of soil moisture fields that represent the rainfall forcing uncertainty (case F in Fig. 2). In the rain-forcing uncertainty alone, CLSM parameters are set to their original values.

- to determine the error propagation from rainfall forcing to the soil moisture prediction. SREM2D models the multi-dimensional error structure of satellite retrievals with spacetime stochastic formulations. The important aspect of SREM2D is its ability to model not only the spatial variability of rain rate estimation error, but also the spatial structure of the successful delineation of rainy and non-rainy areas. As real sensor data actually exhibit spatial clusters of false rain and no-rain area delineations, this characteristic makes SREM2D capable of capturing the magnitude of the satellite rainfall error and
- The SREM2D rainfall error model (Hossain and Anagnostou, 2006a) is employed here 10
- 3.2 Rainfall forcing uncertainty

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In Sect. 4 standard normal deviates of soil moisture obtained simulated by the two methods are compared to standard normal deviates of Mesonet soil moisture observations to study how the model parametric uncertainty captures the ground measure-5 ments.

given grid cell, whereas in case M2 each ensemble member is generally unbiased with

respect to the ensemble mean (or reference).

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3.3 Combined uncertainty

The combined uncertainty is studied by merging the rainfall forcing uncertainty with the model uncertainty described above. Firstly, four parameter sets out of the fourteen behavioral parameter combinations were chosen to represent the model parameter uncertainty in the combined uncertainty experiment. These are: (0.50, 1.15), (0.80, (1.05), (1.25, 0.90), and (2.00, 0.80) for b and wpwet parameters, respectively, which represents the widest range of parameter values in Table 1. For each of those four sets of parameters, six ensemble members were integrated with perturbed CMORPH precipitation inputs (using the SREM2D rainfall error model), for a total of 24 soil moisture ensemble members (case M1F in Fig. 2). Secondly, another 24-member ensemble 10 of CLSM was integrated by perturbing both forcing precipitation (using SREM2D) and prognostic variables at the same time. In particular, normally distributed additive perturbations were added to the same prognostic variables as in case M2, i.e., surface excess and catchment deficit. The output from these runs is a soil moisture ensemble carrying rainfall forcing and model uncertainty (case M2F). 15

The combined uncertainty (rainfall forcing + model error) obtained with the two different methods (cases M1F and M2F) is then compared to the uncertainty introduced by only perturbing rainfall forcing (case F). To quantify the uncertainty associated with each experiment, exceedance and uncertainty ratios (defined below) are computed for both surface and root zone soil moisture. Results are described in the next section.

4 Discussion of results

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We first investigate how the modeling uncertainty determined by the two techniques encapsulates in-situ measurements from Mesonet. Next, we compare the forcing rainfall uncertainty alone to the combined modeling and rainfall forcing uncertainty through soil moisture time series plots and performance metrics.





4.1 Model uncertainty analysis

To compare the two model uncertainty approaches (M1 and M2), we focus on anomaly time series, specifically standard normal deviate time series and associated anomaly correlation coefficients, which capture the correspondence in phase between model es-

- timates and ground observations, disregarding any potential bias or differences in the variance (Entekhabi et al., 2010b). Figures 5 and 6 show standard-normal deviate daily time series of CLSM predicted surface and root zone soil moisture, and corresponding Mesonet measurements during the three years of 2004, 2005 and 2006 and for both model error approaches. Daily standard-normal deviates are computed by subtracting the 2004, 2002 means and (menthe) dimetalement of dividing by the series and dividing by the series and series and series are computed by subtracting the 2004.
- the 2004–2006 mean seasonal (monthly) climatology and dividing by the corresponding standard deviation. Specifically, Figs. 5 and 6 show standard-normal deviate time series at two representative Mesonet stations, located, respectively, in the eastern (and wetter) and western (drier) region of the study area and at the corresponding 25 km grid cell.
- Figures 5 and 6 show that variations in the model predicted soil moisture values are consistent with the Mesonet measurements as well as the associated rainfall forcing variations. Furthermore, the standard-normal deviate time series are consistent between surface and root zone soil moisture. The domain-average anomaly correlation coefficients between simulated (ensemble mean) soil moisture and the Mesonet obser-
- vations are 0.78 (0.64) for the surface soil moisture (root zone soil moisture) for both M1 and M2 modeling uncertainty approaches. At the western station (drier conditions), correlation is slightly higher than the eastern pixel case (wetter conditions). Specifically, at the eastern location the anomaly correlation coefficient is 0.53 (0.56) when modeling uncertainty is introduced by directly perturbing parameters, and 0.54 (0.56) when
- ²⁵ modeling uncertainty is assessed by perturbing model prognostic variables for surface (root zone) soil moisture. On the other hand, at the western location the anomaly correlation coefficient is 0.58 for the surface soil moisture, and it increases to 0.81 for root zone soil moisture, for both model uncertainty approaches. We can conclude





that correlation coefficients are comparable between the M1 and M2 modeling error approaches for surface and root zone soil moisture and for both rainfall climatological conditions.

Although, both model uncertainty approaches capture equally well the measurement 5 variability from Mesonet stations, when employing the GLUE technique (for both soil moisture depths) a reasonable spread in soil moisture is achieved with relatively small parameter perturbations (four perturbations). We could not obtain the same ensemble width in the model prognostic experiment using the Liu et al. (2011) parameter values for the same number of perturbations. This larger ensemble spread from GLUE approach translates into a better encapsulation of the reference (i.e., Mesonet obser-10 vations) surface and root zone soil moisture.

As discussed above, GLUE is a non-parametric mathematical approach founded on the concept of equifinality, namely, it identifies sets of parameters with undistinguishable model performances with respect to an optimal set of parameters. On the

other hand, the prognostic perturbation method makes assumptions on the model error 15 characteristics (i.e., standard deviation, space-time correlation, Gaussian error), which cannot be known a priori. One could argue that by increasing the variance of the error model, or by increasing the number of perturbations, we could get ensemble spreads that are similar to M1. However, determination of the M2 error model parameters would require independent observations of soil moisture that are not typically available.

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Model and rainfall forcing uncertainty analysis 4.2

In this section, the rainfall forcing uncertainty alone is compared to the combined modeling and rainfall uncertainty through time series plots and performance metrics. Figures 7 and 8 show time series of surface and root zone soil moisture ensembles during the warm season of 2005 (June to September) for the following three experiments: case F where only rainfall forcing uncertainty is introduced; case M1F which combines rainfall forcing uncertainty with model uncertainty by perturbing model parameters





(GLUE approach); and case M2F which includes rainfall forcing uncertainty and model uncertainty by perturbing prognostics. Figures 7 and 8 also include time series of reference model soil moisture, which is defined as the output from CLSM forced with unperturbed WSR-88D rainfall fields. In particular, these figures show time series for

- the same representative grid cells as in Figs. 5 and 6, one located in the wetter eastern region of the study area (Fig. 7) and one in the drier western part (Fig. 8). Figures 7 and 8 show that for both soil moisture depths, the ensemble envelope is wider when considering the combined rainfall forcing and model uncertainty through parameter perturbations (case M1F) compared to the other two cases. Moreover, soil moisture
- time series show slightly wider ensemble envelopes for the combined rainfall forcing and prognostic perturbations compared to the rainfall forcing alone uncertainty experiment. By comparing the two pixel time series, it can be inferred that more variability is observed in wetter rainfall conditions for both surface and root zone soil moisture, which is expected as soil water content variability correlates to rainfall variability and consequently exhibits stronger dependence on rainfall forcing error.

As discussed earlier, wider ensemble envelopes derived from the combined rainfall and model uncertainty will increase the probability of encapsulating the reference soil moisture simulations. Two metrics are introduced to quantify this effect. Specifically, we use the exceedance ratio (ER) metric to evaluate the ability of the ensemble integrations to encapsulate the reference predictions and the uncertainty ratio (UR) metric to evaluate the accuracy of the ensemble envelope width. These metrics are presented for the three experiments with respect to the reference modeled soil moisture. The exceedance ratio is defined as:

$$\mathsf{ER} = \frac{N_{\mathsf{exceedance}}}{N_{\mathsf{t}}}$$

where $N_{\text{exceedance}}$ is the number of times the reference soil moisture falls outside the ensemble envelope and N_{t} is the total number of times and locations. If ER is equal to 1, it means there is a 100% probability that the reference will not fall between the lower an upper bounds of the ensemble envelope, whereas if ER is close to 0, there is





(3)

a low probability that the reference exceeds those bounds, or, in other words, there is a perfect encapsulation of the reference inside the ensemble envelope.

The uncertainty ratio, on the other hand, represents the ratio of the aggregate width in the simulated uncertainty relative to the corresponding average actual uncertainty (with respect to the "reference" soil moisture):

$$UR = \frac{\sum_{1}^{N} \left(\hat{\theta}_{upper}^{i} - \hat{\theta}_{lower}^{i} \right)}{2 \times \sum_{1}^{N} \left| \hat{\theta}_{ens_mean}^{i} - \hat{\theta}_{opt}^{i} \right|}$$

5

10

where $\hat{\theta}_{upper}^{i}$ and $\hat{\theta}_{lower}^{i}$ are, respectively, the upper and lower bounds of the simulated ensemble, $\hat{\theta}_{ens_mean}^{i}$ corresponds to the ensemble mean, and $\hat{\theta}_{opt}^{i}$ represents the reference soil moisture obtained by forcing the model with unperturbed WSR-88D rainfall fields. A perfect ensemble spread has UR values equal to 1. If UR is less (greater) than 1 the ensemble is underestimating (overestimating) the model prediction error spread, which can translate in excessive (lower) weights given to observations in an ensemble-based data assimilation system.

ER and UR statistics are computed for each grid cell of the domain. Figures 9 and 10 show frequency histograms of ER and UR metrics for the surface and root zone soil moisture. The corresponding mean values of these metrics are reported in Table 4. Consistent to the time series discussed above, the lowest ER is observed for the experiment that combines rainfall forcing and model parameter uncertainties (M1F). Histograms for M1F are shifted towards significantly lower ER values where the average for surface (root zone) soil moisture is 0.39 (0.35). The complement to 1 of the exceedance ratio can also be interpreted as the ensemble ability of encapsulating the reference. Namely, the simulated ensemble has a probability of 61 % (65 %) on average of encapsulating the reference ground measurements in the case of surface (root zone) soil moisture. In comparison, the experiment that combines rainfall-forcing



(4)



uncertainties with model prognostic perturbations (M2F) exhibits only slightly reduced ER values when compared to the rainfall forcing uncertainty experiment (F). Specifically, the average exceedance ratio reduces from 0.61 (0.64) in case F to 0.54 (0.59) in case M2F for surface (root zone) soil moisture.

- On the other hand, the UR in case M1F exhibits values that are closer to 1 compared 5 to the other experiments. In particular, the average UR is equal to 0.58 (0.45) for surface (root zone) soil moisture when perturbations are based only on the forcing rainfall, which increases to 0.65 (0.53) and 1.02 (1.08) when adding the model prognostic perturbations and model parameter perturbations, respectively. This demonstrates that in
- cases F and M2F the ensemble significantly underestimates the average actual soil moisture error, whereas in case M1F the ensemble spread is less biased and statistically closer to the average actual error. Furthermore, we note that root zone soil moisture exhibits slightly higher UR values in the case of M1F and lower UR values for cases F and M2F. This is related to the fact that variability in the forcing rainfall more directly influences the upper centimeter soil moisture, whereas variability added to the 15
- model parameters affects the prediction of both surface and root zone soil moisture variables.

In summary, the ER and UR metrics indicate that by combining model parametric uncertainty through GLUE with rainfall forcing uncertainty, variability in soil moisture prediction error can be well described. Specifically, we showed that this combination 20 increases the ability of the ensemble envelope of encapsulating the reference simulation (lower ER), without overestimating the ensemble spread (UR close to 1). On the other hand, using only rainfall perturbations, or adding prognostic perturbations to rainfall forcing perturbations, results in an underestimation of the actual soil moisture

errors (UR values significantly lower than 1) and a lower likelihood of encapsulating the 25 reference simulations (higher ER values).

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5 Conclusions

In this study we investigated the impact of rainfall forcing errors and model structural and parameter uncertainty (separately and in combination) on the prediction of soil moisture using the NASA CLSM. Firstly, we examined how ensemble prediction uncer-

- tainty encapsulates the reference ground measurements from Mesonet stations, comparing two model uncertainty approaches. The first approach, the GLUE technique, uses perturbed model parameters. The second approach adds randomly generated noise to the model prognostic variables during the land model integration. Both methods were shown to capture well the soil moisture (temporal) variations measured at
- ¹⁰ in situ Mesonet stations. However, a difference is observed in the two approaches. In fact, the GLUE technique contributed wider ensemble spread in the soil moisture time series relative to the model prognostic random perturbation method, by applying the same number of perturbations. This is compelling for different reasons. The first one is that the GLUE technique (perturbing parameters) only takes into account model
- ¹⁵ parametric error, whereas perturbing prognostics is more inclusive because it technically addresses not only parameter uncertainty, but also model structural uncertainty. The second reason is that GLUE is a well-established model uncertainty framework, based on the concept of equifinality, and independent from model calibration, while the prognostics perturbation approach is based on a priori assumptions on the model error statistics.

Next, we compared soil moisture prediction uncertainty derived from rainfall forcing uncertainty alone (case F) against uncertainty derived from combining modeling and rainfall forcing uncertainty, using both model uncertainty approaches (cases M1F and M2F). Rainfall forcing perturbations alone provided narrower ensemble envelopes of simulated surface and root zone soil moisture time series if compared to the ones

of simulated surface and root zone soil moisture time series if compared to the ones obtained by combining forcing and modeling uncertainties. For what concerns the two modeling error approaches, prognostic perturbations only added modest variability to the rainfall forcing uncertainty. On the other hand, the combined uncertainty employing





direct perturbations of model parameters (case M1F) was shown to produce the widest soil moisture ensemble envelopes relative to the other two cases, for both soil moisture depths. This is exhibited in the exceedance and uncertainty ratio metrics. The lowest exceedance ratio, metric that assesses the capability of the ensemble integrations to

- ⁵ encapsulate the reference, is observed when combining rainfall forcing and model parameter uncertainties, while the experiment that combined rainfall-forcing uncertainty with prognostic perturbations exhibited only slightly reduced ER values relative to the rainfall forcing uncertainty alone. Moreover, the uncertainty ratio, which measures the accuracy of the ensemble envelope width, is shown to be close to 1 when perturbations
- are added to the model parameters (case M1F). This demonstrates that uncertainty in soil moisture is better described by M1F, being the ensemble width closer to the model prediction uncertainty spread, defined as the difference between the ensemble mean and the reference model simulation. The accurate estimation of the soil moisture prediction uncertainty spread is encouraging towards the application of this approach in accurate estimation of this approach in accurate estimation of the soil moisture prediction uncertainty spread is encouraging towards the application of this approach in accurate estimation of this approach in accurate estimation of the soil moisture prediction uncertainty spread is encouraging towards the application of this approach in accurate estimation.
- ensemble data assimilation systems. When rainfall forcing perturbations alone (case F) or rainfall forcing and prognostics perturbations (case M2F) are considered, the uncertainty ratios are significantly lower than 1, exhibiting an underestimation of the actual errors.

This study contributes to the development of the NASA Global Modeling and Assimilation Office (GMAO) land data assimilation system. In particular, it provides valuable insights about the interaction between rainfall forcing and model uncertainties in case of satellite rainfall application in land data assimilation. Along those lines, future studies should investigate the impact of rainfall and model uncertainty on the assimilation of remotely sensed soil moisture in a land data assimilation system. Moreover, other land

²⁵ surface models should be considered, as well as other regions of the world characterized by different hydroclimatic regimes need to be analyzed.





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Table 1. Combinations of parameters with efficiency score higher than 80% for surface and 70% for root zone soil moisture.

<i>b</i> /wpwet	0.80	0.90	1.05	1.15
0.50		Х	Х	Х
0.80	Х	Х	Х	Х
1.25	Х	Х	Х	Х
2.00	Х	Х	Х	



Table 2. Parameters for perturbations to the CLSM prognostic variables.

Model prognostic perturbation	Туре	Standard deviation	AR(1) time series correlation scale
Catchment deficit	additive	0.05 mm	3 h
Surface excess	additive	0.02 mm	3 h

Table 3. SREM2D input parameters.

	Units	Value
Mean of log-normal multiplicative error Standard deviation of log-normal multiplicative error	dimensionless	1.00
False alarm mean rain rate	$mm h^{-1}$	0.20
No-rain probability of detection	dimensionless	0.96
Correlation length for multiplicative error	km km	90
Correlation length for successful no-rain detection	km	70

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Table 4. Mean exceedance and uncertainty ratios for surface soil moisture (in regular font) and root zone soil moisture (in *italics*).

	Mean ER (SSM/ <i>RZSM</i>)	Mean UR (SSM/ <i>RZSM</i>)
Case F	0.61/0.64	0.58/0.45
Case M1F	0.39/0.35	1.02/ <i>1.08</i>
Case M2F	0.54/0.59	0.65/ <i>0.53</i>



Fig. 1. Map of 3-year (2004–2006) average rainfall, overlaid by a 25 km grid covering the experiment domain and locations of OK Mesonet stations (black dots). The triangular symbols represent Mesonet stations where sufficient soil moisture observations are available at four different depths during the study period Black circles highlight two locations for which soil moisture time series are shown in Sect. 4. This figure corrects for a mistake in Fig. 1b of Maggioni et al. (2011).







Fig. 2. Experimental setup showing the methodology used to investigate model uncertainty alone (left column), rainfall-forcing uncertainty alone (middle column), and rainfall-forcing uncertainty combined with model uncertainty (right column).







Fig. 3. Efficiency score – (a) and (b) – and relative bias – (c) and (d) – as a function of model parameter value deviations (presented in %). The Clapp-Hornberger parameter – (a) and (c) – and the soil wilting point wetness – (b) and (d) – parameters are shown. Scales differ for each panel.







Fig. 4. Efficiency score for different combinations of the parameter values for surface soil moisture (a) and root zone soil moisture (b). The cutoff threshold of acceptable efficiency scores is also shown.







Fig. 5. Standard-normal deviate time series for a representative Mesonet station located in the eastern region of the study area (94.845° W–36.889° N, see Fig. 1) and for the corresponding 25 km grid cell. Panels (a) and (b) illustrate model simulations in which parameters are perturbed, while panels (c) and (d) illustrate model simulations in which model prognostic variables were perturbed. Surface (a) and (c) and root zone (b) and (d) soil moisture time series are shown.















Fig. 7. Surface **(a, b, c)** and root zone soil moisture **(d, e, f)** time series during the warm season of 2005 (June to September) for the grid cell shown in Fig. 5, located in the eastern region of the study area. Panels a and d show the experiment where only rainfall forcing uncertainty is introduced; panels **(b)** and **(e)** show the experiment that combines rainfall forcing uncertainty with model uncertainty by perturbing model parameters; and panels **(c)** and **(f)** show the experiment that combines rainfall forcing by perturbing prognostics. Time series of rainfall are also shown on the second axis of each panel.







Fig. 8. Same as in Fig. 7 but for the representative 25 km grid cell shown in Fig. 6, located in the western region of the study area.















Fig. 10. Frequency histograms of Uncertainty Ratios (UR) for surface soil moisture (a) and root zone soil moisture (b).



