



1     **Assimilating Shallow Soil Moisture Observations into Land Models**  
2                                   **with a Water Budget Constraint**

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13 **Abstract**

14       Incorporating observations of shallow soil moisture content into land models is an  
15 important step in assimilating satellite observations of soil moisture content. In this  
16 study, several modifications of an ensemble Kalman filter (EnKF) are proposed for  
17 improving this assimilation. It was found that a forecast error inflation-based  
18 approach improves the soil moisture content in shallow layers, but it can increase the  
19 analysis error in deep layers. To mitigate the problem in deep layers while maintaining  
20 the improvement in shallow layers, a vertical localization-based approach was  
21 introduced in this study. During the data assimilation process, although updating the  
22 forecast state using observations can reduce the analysis error, the water balance  
23 based on the physics in the model could be destroyed. To alleviate the imbalance in  
24 the water budget, a weak water balance constrain filter is adopted.

25       The proposed weakly constrained EnKF that includes forecast error inflation and  
26 vertical localization was applied to a synthetic experiment and two real data  
27 experiments. The results of the assimilation process suggest that the inflation  
28 approach effectively reduce both the short-lived analysis error and the analysis bias in  
29 shallow layers, while the vertical localization approach avoids increase in analysis  
30 error in deep layers. The weak constraint on the water balance reduces the degree of  
31 the water budget imbalance at the price of a small increase in the analysis error.

32  
33 **Keywords**

34 soil moisture, water balance, data assimilation, forecast error inflation, vertical  
35 localization

36



37 **1. Introduction**

38 Soil moisture content is one of the most important variables that affect the water  
39 cycle and energy balance through land-atmosphere interactions, especially  
40 evaporation and precipitation (Han et al. 2014; Kumar et al. 2014; McColl et al. 2019;  
41 Pinnington et al. 2018). Adequate knowledge of the horizontal and vertical  
42 distributions of soil moisture could improve weather and climate predictions  
43 (Delworth and Manabe 1988; Pielke 2001). Alongside snow cover, soil moisture  
44 content is an important component of the meteorological memory of the climate  
45 system over land (McColl et al. 2019; Robock et al. 2000; Zhao and Yang 2018). It is  
46 also a primary water resource for the terrestrial ecosystem and affects runoff (GUSEV  
47 and Novak 2007).

48 There are several ways to estimate the soil moisture content. Land surface  
49 models can provide temporally and spatially continuous estimates of the soil moisture  
50 content, but these estimates are limited by the uncertainty in the models' parameters,  
51 errors in the forcing data and imperfect physical parameterizations (Bonan 1996; Dai  
52 et al. 2003; Dickinson et al. 1993; Oleson et al. 2010; Yang et al. 2009). Compared  
53 with the results of models, in-situ observations of the soil moisture content provide  
54 more accurate profiles (Bosilovich and Lawford 2002; Dorigo et al. 2011; Robock et  
55 al. 2000); however, networks of in-situ observations are usually too sparse to estimate  
56 the soil moisture content on a regional scale (Gruber et al. 2018; Loizu et al. 2018).  
57 Satellite remote sensing retrievals could provide soil moisture content data on regional  
58 scales (Bartalis et al. 2007; Crow et al. 2017; Entekhabi et al. 2010; Kerr et al. 2010;  
59 Lu et al. 2015; Njoku et al. 2003), but they are only available for the shallow layer of  
60 the soil and the quality is poor in vegetated area (Pinnington et al. 2018; Yang et al.  
61 2009).



62 A much better approach to improving estimates of soil moisture contents on  
63 regional scales is to constrain land model prediction by assimilating data from  
64 large-scale remote sensing observations of the soil moisture content (Crow and Loon  
65 2006; Crow and Wood 2003; Reichle and Koster 2005). The assimilation of passive  
66 microwave measurements (brightness temperatures) into land surface models can  
67 successfully increase the spatial and temporal coverage by interpolation and  
68 extrapolation to unobserved times and locations, and also provide various land surface  
69 state and flux estimates with reduced uncertainty (De Lannoy and Reichle 2016;  
70 Reichle et al. 2017). Therefore, land surface data assimilation has significantly  
71 improved the utility of surface soil moisture data sets (Crow et al. 2017; Lu et al. 2012;  
72 Lu et al. 2015), and can further improve land surface model initial conditions for  
73 coupled short-term weather prediction (Chen et al. 2014; Santanello et al. 2016; Yang  
74 et al. 2016).

75 A good estimate of the forecast error covariance matrix is crucial for the  
76 compromise between uncertain observations and imperfect model predictions in data  
77 assimilation (Anderson and Anderson 1999; Miyoshi 2011; Miyoshi et al. 2012; Wang  
78 and Bishop 2003). For the Ensemble Kalman Filter (EnKF) assimilation method, the  
79 forecast error covariance matrix is estimated using the sample covariance matrix of  
80 the ensemble forecasts (Dumedah and Walker 2014; Evensen 1994; Han et al. 2014).  
81 However, it is usually underestimated due to sampling and model errors, which can  
82 eventually result in filter divergence (Anderson and Anderson 1999; Constantinescu  
83 et al. 2007; Yang et al. 2015). To address this problem, it suggests that the forecast  
84 covariance matrix be multiplied by an inflation factor (Dee and Da Silva 1999; Dee et  
85 al. 1999; Li et al. 2012; Zheng 2009). This approach is referred to as inflation, and it  
86 becomes particularly important when the error in the model is large (Bauser et al.



87 2018; El Gharamti et al. 2019; Liang et al. 2012; Raanes et al. 2019; Wu et al. 2013).  
88 Therefore, it could work well in this situation because of the enormous errors in the  
89 land model.

90 In this study, a scheme for assimilating synthetic and in-situ shallow observations  
91 of the soil moisture content into land models was developed based on EnKF method,  
92 which can provide a foundation for further satellite data assimilation. For the synthetic  
93 experiment, the CLM 4.0 (Version 4.0 of the Community Land Model, (Lawrence et  
94 al. 2011; Oleson et al. 2010)) was used to generate the “true values” and the CoLM  
95 (Common Land Model, (Dai et al, 2003)) was selected as the forecast operator. The  
96 differences in these two models are referred to the model error in an imperfect land  
97 surface model. The inflation factors are estimated at every observation time step  
98 during the assimilation process by minimizing the  $-2\log$ -likelihood of the difference  
99 between the forecast and the observation (Liang et al. 2012; Zheng 2009). For  
100 assimilating observations near the surface only, such inflation approach can improve  
101 the estimates of the forecast error statistics in shallow soil layers but may artificially  
102 enlarge the forecast error statistics in deep soil layers. To avoid the possibility of  
103 decreasing the quality of the estimates in deep soil layers, a vertical localization with  
104 weighting of observations is adopted (Janjić et al. 2011). In this approach, a  
105 localization function multiplies the weights on the components of the state vector  
106 according to the distance from state layer to the observation. Moreover, the method  
107 based on the maximum likelihood estimation was proposed to estimate the optimal  
108 localization scale factor. These steps can result in a better prediction of the soil  
109 moisture content in the deep layers.

110 A major objective of soil moisture data assimilation is to address biases in  
111 models and observations (Koster et al. 2009; Reichle and Koster 2004). In this study,



112 we only assume that models could be biased, while the soil moisture observations are  
113 assumed to be unbiased. Moreover, the soil moisture observations are restricted in  
114 shallow layer, so there is no observation available to correct the modeled soil moisture  
115 biases in deep layers. If one only removes the bias in shallow layer, it would introduce  
116 error in model dynamics. Therefore in this study, we still use traditional bias-blind  
117 data assimilation framework. Nevertheless, the analysis error is further decomposed to  
118 a short-lived error (random error) and a bias (system error). It demonstrates that the  
119 proposed scheme can reduce the both for soil moisture in shallow layer.

120 In addition to improve assimilation accuracy, this study also focuses on the  
121 imbalance in the water budget that occurs during the process of assimilating the soil  
122 moisture data. The terrestrial water budget is a key part of the global hydrologic cycle.  
123 A better understanding of the budget can help us to improve our knowledge of  
124 land-atmosphere water exchange and related physical mechanisms and therefore, can  
125 improve our ability to develop models (Pan and Wood 2006). Generally speaking,  
126 analyses do not conserve the water budget due to inconsistencies between predictions  
127 made by models and observations (Li et al. 2012; Pan and Wood 2006; Wei et al. 2010;  
128 Yilmaz et al. 2011; Yilmaz et al. 2012). It is really a problem if the water balance is  
129 violated in a systematic manner (for example, model is biased), which suggests a  
130 trouble in data assimilation. Pan and Wood (2006) proposed a method based on a  
131 strong constraint to reincorporate the water balance. However, this method  
132 redistributes the error among the different terms in the water budget, which could  
133 result in unrealistic estimates (Pan and Wood 2006; Yilmaz et al. 2011).

134 To overcome this shortcoming, Yilmaz et al. (2011) proposed using a weakly  
135 constrained ensemble Kalman filter (WCEnKF) to reduce the imbalance in the water  
136 budget. In a synthetic study, they concluded that the accuracy of a WCEnKF-based



137 analysis is close to that of an EnKF-based analysis but the water budget balance  
138 residuals are much smaller than that of an unconstrained filter. Nevertheless, the  
139 observations of the soil moisture content cover the entire column, and a perfect model  
140 was used in their studies. This is not generally true, especially when only satellite  
141 observations are assimilated. In this study, the experiments were further designed to  
142 assimilate surface observations into an imperfect land model.

143 The structure of this paper is arranged as follows: The data and models used in  
144 this study are described in section 2. The details of the WCEnKF-based method that  
145 incorporates inflation and vertical localization (WCEnKF-Inf-Loc) are provided in  
146 section 3. The experimental designs and evaluations of synthetic and real data  
147 experiments are set in sections 4 and 5. The primary results of the synthetic and real  
148 experiments are given in section 6. The discussion and conclusion comprise sections 7  
149 and 8.

150

## 151 **2. Models and data**

### 152 2.1 Study area and in-situ stations

153 The study area is located in the Mongolian Plateau and comprises approximately  
154 9352 square kilometers between 46° and 46.5° N and between 106.125° and 107° E.  
155 The dominant biome is grassland, and no river flows through the area (see Figure 1).

156 The soil moisture content and related meteorological and hydrological parameters  
157 are monitored by automatic stations maintained by the Coordinated Enhanced  
158 Observing Period Asian Monsoon Project (CEOP AP) (Bosilovich and Lawford 2002;  
159 Lawford et al. 2004). The CEOP AP was launched by the World Climate Research  
160 Programme (WCRP) to develop an integrated global dataset that can be used to  
161 address issues relating to water and energy budget simulations and predictions,



162 monsoon processes and the prediction of river flows. More details can be found at  
163 <http://www.ceop.net>. In this study, observations of the soil moisture content from two  
164 stations, the Bayantsagaan Station (BTS 46.7765 N, 107.14228 E) and the  
165 Delgertsgot Station (DGS 46.12731 N, 106.36856 E), were used to validate the  
166 assimilation method. At the BTS, the soil moisture content is measured every half  
167 hour at 3, 10, 20 and 40 cm below the surface. At the DGS, measurements are made at  
168 depths of 3, 10, 40 and 100 cm with the same frequency. Only the observations made  
169 at 6:00 am (same with the overpass time of SMOS satellite) are assimilated, while the  
170 others are used for validation.

171

## 172 2.2 Forcing data

173 In this study, both synthetic and realistic experiments were conducted to explore  
174 the accuracy of the assimilation schemes. In the synthetic experiments, the  
175 simulations were driven by forcing data (including radiation, wind, pressure, humidity,  
176 precipitation and temperature) from the 0.125x0.125 ERA-Interim dataset (Dee et al.  
177 2011) that had been scaled down to provide a temporal resolution of one hour.

178 In the realistic experiments, the forcing data comprised hourly measurements of  
179 the wind speed, near-surface air temperature, relative humidity precipitation and  
180 surface pressure at local stations (the BTS and DGS). The downward shortwave and  
181 longwave radiation data used were from model output time series data for the study  
182 area provided by the Japanese Meteorological Agency (Huang et al. 2008).

183

## 184 2.3 Models

185 The Common Land Model (CoLM) developed by Dai et al. (2003) is a  
186 third-generation land surface model. It combines the best features of three successful



187 models: the Land Surface Model (LSM, (Bonan 1996)), the Biosphere-Atmosphere  
188 Transfer Scheme (BATS, (Dickinson et al. 1993)) and the 1994 version of the Chinese  
189 Academy of Sciences/Institute of Atmospheric Physics model (IAP94, (Dai et al.  
190 2003)), and is being further developed. The primary characteristics of the model  
191 include 10 unevenly spaced soil layers (see Table 1), one vegetation layer, 5 snow  
192 layers (depending on the snow depth), explicit treatment of the mass of liquid water,  
193 ice and phase changes within the system of the snow and soil, runoff parameterization  
194 following the TOPMODEL concept, a tiled treatment of the sub-grid fraction of the  
195 energy and water budget balance (Dai et al. 2003) and a canopy  
196 photosynthesis-conductance mode that describes the simultaneous transfer of CO<sub>2</sub> and  
197 water vapor into and out of the vegetation. The model parameters include data on the  
198 global terrain, elevation, land use, vegetation, land-water mask and hybrid  
199 FAO/STATSGO soil types from the USGS, which are available at a resolution of 30  
200 arc seconds.

201 Version 4.0 of the Community Land Model (CLM 4.0) (Lawrence et al. 2011;  
202 Oleson et al. 2010) is the land surface parameterization used with the Community  
203 Atmosphere Model (CAM 4.0) and the Community Climate System Model (CCSM  
204 4.0). The CLM 4.0 includes bio-geophysics, the hydrologic cycle, biogeochemistry  
205 and the dynamic vegetation. CLM 4.0 simulates the bio-geophysical processes in each  
206 sub-grid unit independently and maintains its own prognostic variables. The  
207 parameters used in the CLM4.0 differ from those used in the CoLM. For example, the  
208 soil texture data are derived from the IGBP soil data, and the land use data are derived  
209 from the UNH Transient Land Use and Land Cover Change Dataset  
210 (<http://luh.umd.edu/>).

211 In addition to using different parameters, the two models have different structures.



212 For example, a model of groundwater-soil water interactions (Niu et al. 2007; Niu et  
213 al. 2005) has been incorporated into the CLM 4.0, while zero water flux at the bottom  
214 of a soil column is assumed in the CoLM. In addition, the CLM 4.0 has the same  
215 vertical discretization scheme as the CoLM (see Table 1), which makes comparing the  
216 results of the two models convenient.

217

### 218 3. Methods

#### 219 3.1 Forecast and observation systems

220 Using notation similar to that used by Yilmaz et al. (2011), the forecast system  
221 can be written as

$$222 \quad \mathbf{y}_{n,t}^f = \mathbf{M}_{n,t-1}(\mathbf{y}_{n,t-1}^a), \quad (1)$$

223 where  $t=1, \dots, T$  is the time index,  $n=1, \dots, N$  represents an ensemble member (in this  
224 study, the ensemble size is set to 100),  $\mathbf{M}_{n,t-1}$  is a CoLM forced by the  $n$ -th perturbed  
225 atmospheric forcing, and  $\mathbf{y}$  is a state vector containing 126 variables. The superscript  
226 “ $f$ ” and “ $a$ ” specify the forecast and analysis, respectively.

227 Let  $\mathbf{x}$  be the state variables related to the water budget, that comprises of **SM** and  
228 **SIC** (the soil moisture content and the soil ice content in % at the 10 vertical levels  
229 listed in Table 1), CWC and SWE (the canopy’s water content and the snow water  
230 equivalent in  $\text{kg/m}^2$ ). In this study, only  $\mathbf{x}$  is updated by data assimilation, while the  
231 model propagates changes to the other variables over time.

232 For the traditional EnKF, the forecast error covariance matrix  $\mathbf{P}_t$  is  
233 obtained from the ensemble of their anomalies,

$$234 \quad \mathbf{P}_t = \frac{1}{N-1} \sum_{n=1}^N \left( \mathbf{x}_{n,t}^f - \frac{1}{N} \sum_{j=1}^N \mathbf{x}_{j,t}^f \right) \left( \mathbf{x}_{n,t}^f - \frac{1}{N} \sum_{j=1}^N \mathbf{x}_{j,t}^f \right)^T. \quad (2)$$

235 To avoid overestimation of the co-variability between shallow observations and soil



236 moistures deeper than a threshold layer  $s$ , the following vertical localization function  
237 with weighting of observations  $\rho_s$  (Janjić et al. 2011) will be applied on  $\mathbf{P}_t$ , i.e.,

$$238 \quad \rho_s(l) = \exp(-\mu_s |d_l - d_o|) \quad (3)$$

239 where  $l$  represents for the  $l$ -level soil layer,  $d_l$  and  $d_o$  represent the depths of  
240  $l$ -level soil layer and observation, respectively.  $|d_l - d_o|$  is the Euclidian distance  
241 between the two layers.  $\mu_s$  is estimated by minimizing the following mean square  
242 error between vertical localization function Eq (3) and a step function with threshold  
243 layer  $s$ ,

$$244 \quad M(\mu) = \sum_{l \leq s} [\exp(-\mu |d_l - d_o|) - 1]^2 + \sum_{l > s} [\exp(-\mu |d_l - d_o|)]^2 \quad (4)$$

245 The estimated  $\mu_s$  is listed in Table 2.

246 The observations of the soil moisture content are collected at a depth of 3 cm at  
247 6:00 am every day (denoted by  $o_t$ ). The observation system is defined as

$$248 \quad o_t = \mathbf{h}\mathbf{x}_t + \varepsilon_t, \quad (5)$$

249 where observational operator  $\mathbf{h}$  is a 22-dimensional vector which linearly interpolated  
250 the soil moisture at depths of 2.8 cm and 6.2 cm to depth of 3 cm,  $\mathbf{x}_t$  represents the  
251 true values of the state variables related to the water budget at the time step  $t$  and  $\varepsilon_t$   
252 is the observational error with mean zero and variance  $R_t$ . Since, the main objective  
253 of this study is for methodology related to linear observational operators. Choosing  
254 the linear interpolation as observational operator is only for convenience.

255

### 256 3.2 Assimilation with water budget constraint

257 Assimilating data on the soil moisture content usually results in an imbalance in



258 the water budget. To reduce this imbalance, a weak constraint on the water budget  
 259 (Yilmaz et al. 2011) is adopted in this study. The ensemble water budget residual at  
 260 time step  $t$  can be expressed as

$$261 \quad r_{n,t} \equiv \beta_{n,t} - \mathbf{c}^T \mathbf{x}_{n,t}^a, \quad (6)$$

262 where

$$263 \quad \beta_{n,t} = \mathbf{c}^T \mathbf{x}_{n,t-1}^a + Pr_t - Ev_{n,t}^f - Rn_{n,t}^f, \quad (7)$$

264 where  $\mathbf{c}$  is a 22-dimensional vector that converts the units to millimeters ( $mm$ ) and  
 265 adds up the states in  $\mathbf{x}$ , the diagnostic variables  $Pr_t$ ,  $Ev_{n,t}^f$  and  $Rn_{n,t}^f$  ( $mm$ ) are  
 266 scalars specifying the states of the precipitation, evapotranspiration and runoff,  
 267 respectively, in each pixel.

268 The cost function used to estimate the state variables with the weak water budget  
 269 constraint (Eq. (6)) is

$$270 \quad J_{n,t}(\mathbf{x}) = (o_t - \mathbf{h}\mathbf{x})^T R_t^{-1} (o_t - \mathbf{h}\mathbf{x}) + (\mathbf{x} - \mathbf{x}_{n,t}^f)^T \mathbf{P}_{s,t}^{-1} (\mathbf{x} - \mathbf{x}_{n,t}^f) \\ + (\beta_{n,t} - \mathbf{c}^T \mathbf{x})^T \varphi_t^{-1} (\beta_{n,t} - \mathbf{c}^T \mathbf{x}), \quad (8)$$

271 where

$$272 \quad \varphi_t = \frac{1}{N-1} \sum_{n=1}^N \left( \beta_{n,t} - \frac{1}{N} \sum_{j=1}^N \beta_{j,t} \right) \times \left( \beta_{n,t} - \frac{1}{N} \sum_{j=1}^N \beta_{j,t} \right)^T \quad (9)$$

273 is an estimate of the variance of  $\beta_{n,t}$  and  $\mathbf{P}_{s,t}$  represents a forecast error  
 274 covariance matrix defined by

$$275 \quad \mathbf{P}_{s,t} = \left[ \sqrt{\lambda_t} \right] [\boldsymbol{\rho}_s] \mathbf{P}_t [\boldsymbol{\rho}_s] \left[ \sqrt{\lambda_t} \right]. \quad (10)$$

276 where  $\mathbf{P}_t$  is defined as Eq. (2);  $[\boldsymbol{\rho}_s]$  is a diagonal matrix which localizes the soil  
 277 moisture error (i.e. it is  $\boldsymbol{\rho}_s$  defined by Eq. (3) for the soil moisture contents and 1 for  
 278 other variables).  $[\sqrt{\lambda_t}]$  is also a diagonal matrix which inflates the forecast soil



279 moisture error (i.e. it is a scalar  $\lambda_t$  for the soil moisture contents and 1 for other  
 280 variable).  $\lambda_t$  is estimated by minimizing the  $-2\log$ -likelihood of the difference  
 281 between the forecast and the observation (Dee and Da Silva 1999; Liang et al. 2012;  
 282 Zheng 2009),

$$283 \quad -2L_{s,t}(\lambda_t) = \ln(\mathbf{h}\mathbf{P}_{s,t}\mathbf{h}^T + R_t) + (o_t - \mathbf{h}\mathbf{x}_t^f)^T (\mathbf{h}\mathbf{P}_{s,t}\mathbf{h}^T + R_t)^{-1} (o_t - \mathbf{h}\mathbf{x}_t^f). \quad (11)$$

284 The estimated forecast error inflation factor is denoted as  $\hat{\lambda}_t$ . The perturbed analysis  
 285 states of the variables related to water budget can be derived by minimizing Eq. (8),  
 286 which has the analytic form

$$287 \quad \mathbf{x}_{n,t}^a = \mathbf{x}_{n,t}^f + \mathbf{P}_t^a \mathbf{h}^T R_t^{-1} (o_t + \varepsilon_{n,t} - \mathbf{h}\mathbf{x}_{n,t}^f) + \mathbf{P}_t^a \mathbf{c} \varphi_t^{-1} (\beta_{n,t} - \mathbf{c}^T \mathbf{x}_{n,t}^f), \quad (12)$$

288 where  $\varepsilon_{n,t}$  is generated from a normal distribution with mean zero and variance  $R_t$ ,  
 289 and its error covariance matrix is

$$290 \quad \mathbf{P}_t^a = (\mathbf{h}^T R_t^{-1} \mathbf{h} + \mathbf{P}_t^{-1} + \mathbf{c} \varphi_t^{-1} \mathbf{c}^T)^{-1}, \quad (13)$$

291 For estimating the optimal threshold layer, define the  $-2\log$ -likelihood of the total  
 292 difference between the forecasts and the observations,

$$293 \quad L_s \equiv \sum_{t=1}^T (-2L_{s,t}(\hat{\lambda}_t)). \quad (14)$$

294 The optimal threshold layer  $\hat{s}$  is selected as the smallest number  $s$  such that  $L_s$  is  
 295 the minimum of  $\{L_2, L_3, \dots, L_{s+1}\}$ . The final analysis state is the selected corresponding  
 296 to the optimal threshold layer  $\hat{s}$ . The complete assimilation procedure is shown in  
 297 Figure 2.

298

## 299 4. Synthetic experiments

### 300 4.1 Experimental design



301 To investigate the performance of the WCEnKF-based method that incorporates  
302 inflation and vertical local decomposition, synthetic experiments were performed  
303 using the CoLM. Unlike the “perfect model” assumption used in Yilmaz et al. (2011),  
304 the assumptions of this study are accounted for the error in the model, especially the  
305 structural error. Because there were structural differences in the models of the water  
306 cycle (see section 2.3) used in the two models, CLM 4.0 was used to generate the  
307 “true values” (i.e., to perform a reference run) for the synthetic experiments and  
308 CoLM was selected as the forecast operator (i.e., to perform an open-loop run).  
309 Therefore, the CLM 4.0 and the CoLM were both integrated on a  $0.125^\circ$  grid (see  
310 Figure 1 for the locations) with a time step of one hour. The assimilation time was set  
311 to 6:00 am every day. The assimilation experiments were conducted with 4 scenarios:  
312 a weakly constrained ensemble Kalman filter (WCEnKF), a weakly constrained  
313 ensemble Kalman filter with inflation (WCEnKF-Inf), a weakly constrained ensemble  
314 Kalman filter with inflation and localization (WCEnKF-Inf-Loc) and an ensemble  
315 Kalman filter with inflation and localization (EnKF-Inf-Loc).

316 Synthetic observations were obtained by interpolating  $\mathbf{SM}_t$  to a depth of 3 cm  
317 and adding noise with a normal distribution ( $N(\mu=0, \sigma=0.5\%)$ ). The initial state  
318  $\mathbf{x}_0$ , was generated by running the CoLM from October 1, 2002 to June 1, 2003. Each  
319 component of the initial state was perturbed using an independent standard Gaussian  
320 random variable times 5% of magnitude of the component. The forcing data were  
321 perturbed in the manner described in Yilmaz et al. (2011). The synthetic experiments  
322 were conducted from June 1, 2003 to October 1, 2003. The state variables for each  
323 pixel were updated independently.

324



325 4.2 Validation statistics

326 4.2.1 Model error and bias

327 The model errors are defined as the difference between the actual values and the  
328 model's predictions based on true initial values, and the bias is the average of the error  
329 in the model during the relevant period. Let  $x_t$  denote the true values of the soil  
330 moisture content at time  $t$  for a location and vertical soil layer.  $x_t^M$  denotes the model  
331 predicted soil moisture from the true state at the previous time step  $t-1$ . The model's  
332 bias and error variance for one step can be written as

333 
$$b_M = \frac{1}{a_{ts}} \sum_{t=1}^{a_{ts}} (x_t^M - x_t), \quad (15)$$

334 
$$v_M = \frac{1}{a_{ts}} \sum_{t=1}^{a_{ts}} (x_t^M - x_t)^2, \quad (16)$$

335 where  $a_{ts}$  is the number of time steps over which the observations made at 6:00 am  
336 each day are assimilated.

337 4.2.2 Validation of analysis soil moisture

338 The true soil moisture content values from 7:00 am to 5:00 am next day are used  
339 to validate analysis states. For a location and vertical soil layer, let  $x_{t,h}$  be the true  
340 soil moisture content at hour  $h$  on day  $t$ , and  $x_{t,h}^f$  represent the forecasted soil  
341 moisture content at hour  $h$  from analysis state  $x_t^a$  at 6:00 am on day  $t$ . The analysis  
342 bias is defined as

343 
$$b_a = \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h}). \quad (17)$$

344 The analysis error variance is defined as



$$\begin{aligned} v_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h})^2 \\ &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h} - b_a)^2 + b_a^2 \end{aligned} \quad (18)$$

(See Appendix A for the proof)

#### 4.2.3 Water balance

Following Yilmaz (2011), the water budget imbalance at location is evaluated using the water balance residual,

$$R = \frac{1}{Na_{ts}} \sum_{t=1}^{a_{ts}} \sum_{n=1}^N r_{n,t} \quad (19)$$

351

### 5. Real data experiments

In addition to the synthetic experiments, experiments in which the soil moisture content observed at the DGS and BTS were assimilated into the CoLM were conducted. In these experiments, the value of soil moisture was extracted from the output of the Global Land Data Assimilation (GLDAS)/CLM 2.0 model, which has been integrated continuously since 1979 (Rodell et al. 2004), and used to initialize the CoLM. Then, the model was run from October 1, 2002 to June 1, 2003. The states obtained at the end of the period were used as the initial states. In these experiments, the initial perturbation scheme, observation error variance, assimilation frequency and assimilation time were adopted from the synthetic experiments. The forcing data sets were in-situ observed; they were much more accurate than the ERA-Interim reanalysis data and were not perturbed.

In the realistic assimilation experiments, the truth is not known. Observations of the soil moisture content at hours not assimilated (7:00 am to 5:00 am next day) were used for validation. The analysis bias is estimated as



$$\begin{aligned}
 B_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - o_{t,h}) \\
 &\approx \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h}))
 \end{aligned} \tag{20}$$

and the analysis error variance is estimated as

$$\begin{aligned}
 V_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - o_{t,h})^2 \\
 &\approx \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h}) - B_a)^2 + B_a^2 + C
 \end{aligned} \tag{21}$$

where C is a constant which is independent of prediction schemes (See Appendix B for the proof)

Finally, the water balance residual is defined similar to Eq. (19).

## 6. Results

In the synthetic experiments, the magnitudes of the model's bias and error were calculated using Eqs (15) and (16), respectively, and are shown in Figure 3. It shows that the model's bias was almost negative from Figure 3a. The negative bias in the surface layer was the result of a combination of a lower surface roughness and a larger leaf area index in the CoLM; these values led to more soil evaporation and more canopy interception and could result in a smaller amount of water infiltrating the soil than the amount modeled using the CLM 4.0. In the CoLM, the porosity of each layer was less than it was in the CLM 4.0, which retained less water and contributed to the negative bias of the upper 9 layers. However, the magnitude of the bias increased to 2% in the bottom layer. The significant difference between the two models at the bottom layer could be ascribed to their different boundary conditions. Interactions between the soil moisture content and the ground water at the bottom of the soil column were modeled in the CLM 4.0 (Oleson et al. 2010) but not in the CoLM. The error in each



388 model (Figure 3b) fluctuated in a manner similar to that of the model's bias. Unbiased  
389 observations are necessary for correcting bias in a model, which is not possible in  
390 many realistic applications, especially in assimilating remote sensing retrievals. Since  
391 satellite observations of the soil moisture content of deep layers are unavailable, only  
392 removing the bias in shallow layers would introduce error in model dynamics.

393

#### 394 6.1 Forecast error inflation and vertical localization

395 In the synthetic experiments, the study domain comprised 40 pixels. Each point in  
396 the grid-scale threshold layer, the localization scale factor  $\mu_s$ , was determined  
397 independently. Therefore, totally 9 sets of experiments with different localization  
398 scale factor (see Table 2) were conducted separately. Among these experiments, the  
399 "optimal" case for each pixel was defined as the case in which the column averaged  
400 analysis error (Eq. (18)) was minimized (shown in Figure 4). According to Figure 4a,  
401 the corresponding threshold layer  $s$  of  $\mu_s$  was generally between 5 and 6 in both  
402 cases, which could be ascribed to the homogeneous soil texture and land cover. In the  
403 WCEnKF-Inf-Loc, there were 19 pixels in which the threshold layers were "optimal,"  
404 and the layers selected in the other pixels were suboptimal (most were roughly one  
405 layer away from the "optimal" case). As shown in Figure 4b, the spatial average of the  
406 root analysis error variance (Eq. (18)) of the WCEnKF-Inf-Loc (4.09%) was  
407 comparable with the optimal value (3.84%) even though  $s$  was not selected on the  
408 basis of minimizing the analysis error.

409 The spatial average of the root analysis error variance in each layer in the  
410 schemes with (WCEnKF-Inf-Loc and WCEnKF-Inf) and without (WCEnKF)  
411 inflation are displayed in Figure 5a. Above 62.0 cm, the analysis errors of the schemes  
412 without inflation were substantially larger than those of the schemes with inflation for



413 the synthetic experiments. This suggested that inflation provided a better estimate in  
414 the layers close to observation. When no inflation was performed, the accuracy of the  
415 soil moisture content was barely improved over that of the simulation case (shown in  
416 Figure 5a).

417 By comparing the schemes with (WCEnKF-Inf-Loc) and without (WCEnKF-Inf)  
418 vertical localization, the impact of this approach on the assimilation accuracy in each  
419 layer is shown in Figure 5a. Because the threshold layer of the localization function  
420  $\rho_s$  was layer 6 (36.6 cm) for 28 of the pixels (see Figure 4a), the spatial average of  
421 root analysis error variance of the results of the WCEnKF-Inf-Loc is almost identical  
422 to that of the results of the WCEnKF-Inf for depths above 36.6 cm. In contrast,  
423 inflation increased the analysis error in the soil moisture content of the deep layers in  
424 the WCEnKF-Inf. In this model, the sample error covariances of the moisture contents  
425 of shallow and deep soil were inflated by a factor greater than 6 (the average inflation  
426 factor was 6.25). This could lead to larger assimilation errors for deep soil moisture  
427 profiles in the WCEnKF-Inf. Therefore, inflation should be used with vertical  
428 localization to reduce the spurious covariance resulting from the covariance  
429 inflation-based approach.

430 As it was in the synthetic experiments, vertical localization (WCEnKF-Inf-Loc)  
431 was helpful in avoiding erroneous estimates of the soil moisture contents at lower  
432 levels (in the WCEnKF-Inf). A comparison of the analysis error at a depth of 3 cm  
433 (i.e., the depth of the assimilated observations was 3 cm) in the models with  
434 (WCEnKF-Inf and WCEnKF-Inf-Loc) and without (WCEnKF) inflation showed that  
435 the inflation technique significantly reduces the analysis error at the depth at which  
436 observations are made.

437 In the real data experiments, the spatial averages of root analysis error variance



438 in each layer (Eq. (21)) are shown in Figures 6a and 7a. To validate the effect of the  
439 vertical localization, the results of the “optimal” (based on the minimum analysis error  
440 at the four observation sites) and WCEnKF-Inf-Loc were compared. In the  
441 experiments using the data from the DGS, the threshold,  $s$ , was set to layer 2 (2.8 cm)  
442 for the “optimal” case and layer 5 (21.2 cm) for the WCEnKF-Inf-Loc. However, the  
443 analysis error in the two models at each layer in which observations were made  
444 remained comparable. In the experiments using the data from the BTS, the value of  $s$   
445 was set to 3 (6.2 cm) in both models, which resulted in equivalent analysis errors.

446 Unlike the truth at all model depths are available in the synthetic experiments,  
447 the observations only available at the four depths for the two stations, which did not  
448 cover the all model layers. Therefore, the analysis error in layers deeper than the  
449 observation could not be checked.

450

## 451 6.2 The water budget constraint

452 In the synthetic experiment, the weak constraint on the water budget reduced the  
453 water balance residual significantly in each pixel and the results are shown in Figure 8.  
454 It shows that, the water balance residuals for the assimilation scheme with water  
455 budget constraint are smaller than those without water budget constraint. The forecast  
456 error covariance matrix inflation can lead to the increase of water balance residual,  
457 while the vertical localization technique (i.e. WCEnKF-Inf-Loc scheme) can restrict it  
458 in a rational range. In the WCEnKF-Inf-Loc, the spatial average of the water balance  
459 residual was 0.0742 mm, which was much less than that of the EnKF-Inf-Loc (0.2259  
460 mm). The spread of the water balance residual was also smaller in the  
461 WCEnKF-Inf-Loc, which signals a more stable water balance budget. Therefore, the  
462 weak constraint on the water budget resulted in an assimilation accuracy that was



463 comparable to that of unconstrained filters but had a much smaller water budget  
464 residual, which is consistent with the results of previous studies (Yilmaz et al. 2011;  
465 Yilmaz et al. 2012).

466 To investigate the role of the water budget constraint in the assimilation process  
467 in the synthetic experiment, the spatial averaged root analysis error variance (Eq. (18))  
468 of the schemes with (WCEnKF-Inf-Loc) and without (EnKF-Inf-Loc) the water  
469 budget constraint were compared. In the EnKF-Inf-Loc, the threshold layers were  
470 adopted from the WCEnKF-Inf-Loc. According to Figure 5a, the spatial averaged root  
471 analysis error variances of the two models were almost identical (1.83% for the  
472 WCEnKF-Inf-Loc and 2.00% for the EnKF-Inf-Loc) in the layers that were shallower  
473 than 21.2 cm. However, for the layers that were deeper than 36.6 cm, the average  
474 RSME of the EnKF-Inf-Loc (4.95%) was less than that of the WCEnKF-Inf-Loc  
475 (5.87%). This could be the compensation for the reduction in the water balance  
476 residual.

477 In the real data experiments, consistent reductions in the water budget residual  
478 were obtained from the different experiments. The water balance residuals (Eq. (19))  
479 in the EnKF-Inf-Loc at the DGS and BTS were 0.1545 mm and 0.1792 mm,  
480 respectively. In contrast, the residuals were reduced to 0.0386 mm and 0.0131 mm,  
481 respectively, at the two stations in the WCEnKF-Inf-Loc, which supports the  
482 robustness of the weak constraint on the water budget.

483

## 484 **7. Discussion**

### 485 **7.1 Covariance inflation and vertical localization**

486 In this study, the cost function used to estimate the state variables with the weak  
487 water budget constraint (Eq. (8)) consists of three parts, which are related with



488 observations, model forecasts and water residual (Yilmaz et al. 2012). It is represented  
489 as a summation of three scalars, no matter how many observations are assimilated.  
490 Therefore, inflating of one scalar (e.g., model forecasts) seems to have the similar  
491 impact as deflating another one (e.g., water residual), particularly the weights  
492 associated in this problem can be shown as function of the ratio of these three scalars.  
493 Specifically, inflation of forecast error covariance has somewhat similar impact with  
494 deflation the water balance residual covariance. Accordingly, it is plain obvious that  
495 the water balance residual of the scheme WCEnKF-Inf is larger than that of the  
496 scheme WCEnKF. According to Figures 5a-7a, the covariance inflation improved the  
497 estimates of the soil moisture content in the shallow layers independently of whether  
498 vertical localization was used. This is primarily because the observation operator,  $\mathbf{h}$ , is  
499 the linear operator that was used to interpolate the soil moisture content at depths of  
500 2.8 cm and 6.2 cm to a depth of 3 cm. Then, the likelihood function for the inflation  
501 factor (Eq. (11)) depends only on the observations and predictions of the soil moisture  
502 content in the 2<sup>nd</sup> and 3<sup>rd</sup> layers. The mean value of the inflation factor is 6.25 for  
503 WCEnKF-Inf, indicating that the initial forecast spread is not large enough. This leads  
504 to an improvement in the forecast error statistics in the shallow layers, and to further  
505 improvements in the soil moisture contents of those layers. However, the soil moisture  
506 contents of the deep layers are not directly related to the inflation factor. Inflating the  
507 forecast errors in the deep layers leads to an overestimation of the corresponding  
508 forecast error covariance, and could lead to larger analysis errors in the deep layers  
509 (see WCEnKF-Inf in Figure 5a). Therefore in this study, the vertical localization  
510 approach was developed to prevent soil moisture over fitting for deep layers. Using all  
511 observations for shreshold  $s$  is only for model selection (from the 10 layers), not for  
512 fitting parameter. When vertical localization is used, the soil moisture contents of the



513 deep layers are not significantly updated. Consequently, larger errors are avoided in  
514 the deep layers (see WCEnKF-Inf-Loc in Figure 5a).

515 Comparing to traditional EnKF without inflation and localization, although  
516 mainly the soil moisture contents of layers above the threshold layer (usually the 5<sup>th</sup> or  
517 6<sup>th</sup> layer) were updated at each time step during the assimilation process when the  
518 WCEnKF-Inf-Loc was used, Figure 5a shows that the soil moisture contents of the  
519 layers below the threshold layer, especially the 6<sup>th</sup> and 7<sup>th</sup> layers, are also improved.  
520 This may be because the model propagates changes in the shallow layers downward,  
521 adjusting the soil moisture contents of the deep layers. Because the soil moisture  
522 content of layers above the threshold layer was improved during the previous time  
523 step, this process results in better predictions of the soil moisture contents of layers  
524 below the threshold layer, and therefore, reduces the analysis error in layers below the  
525 threshold layer.

526

## 527 7.2 Bias correction

528 Geophysical models are never perfect and usually produce estimates with biases  
529 that vary in time and in space (Reichle 2008). Therefore bias correction is important  
530 for assimilating data into models. The model bias can be removed when all model  
531 variables are observed, such as the case studied by Yilmaz et al (2011). However in  
532 this study only soil moisture in shallow layers can be observed (in order to mimic the  
533 satellite observation). There is no observation available to correct the bias of soil  
534 moistures in deeper layers. If only remove the bias in shallow layers, it would  
535 introduce error in model dynamics. Therefore in this study, we still use traditional  
536 (bias-blind) data assimilation framework.

537 However in the present study, the analysis error variance was decomposed to a



538 short-lived component (Figures 5b-7b) and a bias component (Figures 5c-7c) for the  
539 synthetic experiment and the two real data experiments, respectively. It shows that for  
540 our proposed bias-blind data assimilation scheme (WCEnKF-Inf-Loc), both  
541 short-lived errors and biases reduce in the layers close to observation, while maintain  
542 the similar levels for the deeper layers. The covariance inflation can play an important  
543 role in bias reduction. Bias can only be seen during whole assimilation period. At an  
544 instant time, bias and error are mixed. For the traditional EnKF, the forecast error  
545 covariance matrix obtained from the ensemble of their anomalies (Eq. (2)) mainly  
546 represents short-lived error, so it has to be inflated to include error related to bias.

547 There are other bias estimation approaches in data assimilation. For example,  
548 treating bias as model variables and estimate in assimilation (De Lannoy et al. 2007;  
549 Dee and Da Silva 1997; Dee and Da Silva 1998), adjusting the state variable of the  
550 forecast model not only their covariance matrix in each forecast step (Zhang et al.  
551 2015; Zhang et al. 2014), addressing the biases in the model and observations by  
552 rescaling their cumulative distribution functions (Koster et al. 2009; Reichle and  
553 Koster 2004). The scheme proposed here can provide a base line to validate the  
554 efficacy of these approaches and could be further improved after these bias  
555 corrections.

556

## 557 **8. Conclusions**

558 In this study, observations of the soil moisture content at a depth of 3 cm were  
559 assimilated using an ensemble Kalman filter with three improvements. Firstly, an  
560 adaptive forecast error inflation based on maximum-likelihood estimation was  
561 adopted to reduce the analysis error. This study supports the idea that the proper form  
562 of the forecast error covariance matrix is crucial for reducing the analysis error near



563 the layers in which observations are made. Secondly, an adequate vertical localization  
564 for the ensemble-based filter was proposed associated with the forecast error  
565 covariance inflation, to avoid misestimates of the soil moisture contents of deep layers.  
566 Lastly, a constraint on the water balance was used in this study to reduce the water  
567 budget residual substantially without significantly changing the assimilation accuracy.  
568 The experiment results of synthetic study and real data show that the  
569 WCEnKF-Inf-Loc assimilation scheme can reduce both the short-lived analysis error  
570 and the analysis bias in the shallow layers, which also lead to a rational water budget  
571 residual.

572 The work presented in this paper may have some limitations. For example, the  
573 iterations involved in the optimization process reduce the computational efficiency,  
574 and the study area was homogeneous grassland without a compound type of land  
575 cover. Because the accuracy of the microwave soil moisture content is significantly  
576 affected by the land cover type (Dorigo et al. 2010), it is necessary to perform more  
577 experiments using other regions.

578 In the near future, we plan to validate the major conclusions under different soil  
579 conditions and land cover types. Vertical localization, which uses adjacent  
580 observations, should also be tested in future work. More detailed analyses of the bias  
581 correction for assimilating remote sensing retrievals should be performed. The  
582 response of the analytic soil moisture content to weather predictions also needs to be  
583 investigated. Completing these studies should improve the state of research into  
584 land-atmosphere interactions.

585



586 **Data availability** The soil moisture observation and hourly measurements of forcing  
587 data are available at <http://www.ceop.net>. The ERA-interim forcing data used in the  
588 synthetic experiments is obtained from <https://apps.ecmwf.int/datasets>. The  
589 downward shortwave and longwave radiation data used in the realistic experiments  
590 are provided by the Japanese Meteorological Agency at <https://www.jma.go.jp/en>.

591

592 **Author Contributions** BD performed the simulations and assimilations. XZ designed  
593 the research. GW analyzed the results. TL collected and preprocessed the data. GW  
594 and XZ prepared the manuscript with contributions from all co-authors.

595

596 **Conflicts of Interest** The authors declare that they have no conflict of interest.

597

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604

#### 605 **Appendix A. Proof of Eq. (18)**

606 For a location and vertical soil layer, the analysis error variance in the synthetic  
607 experiment is defined as



$$\begin{aligned}
 v_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h})^2 \\
 608 \quad &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h} - b_a + b_a)^2 \quad (A1) \\
 &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h} - b_a)^2 + b_a^2 + \frac{2b_a}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (x_{t,h}^f - x_{t,h} - b_a)
 \end{aligned}$$

609 From the definition of analysis bias (Eq. (17)), the last term on the right hand side of  
 610 is zero, so Eq. (18) is proved.

611

## 612 Appendix B. Proof of Eqs. (20)-(21)

613 Since

$$\begin{aligned}
 B_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - o_{t,h}) \\
 614 \quad &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - \mathbf{h}\mathbf{x}_{t,h} - \varepsilon_{t,h}) \quad (B1) \\
 &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h})) - \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} \varepsilon_{t,h}
 \end{aligned}$$

615 The second term of the right-hand side of Eq. (B1) is approximate zero, because the  
 616 observation error  $\varepsilon_{t,h}$  has zero mean. Therefore Eq. (20) holds.

617 Since

$$\begin{aligned}
 V_a &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - o_{t,h})^2 \\
 &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}\mathbf{x}_{t,h}^f - (\mathbf{h}\mathbf{x}_{t,h} + \varepsilon_{t,h}) - B_a + B_a)^2 \\
 618 \quad &= \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h}) - B_a)^2 + B_a^2 + \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} \varepsilon_{t,h}^2 \quad (B2) \\
 &\quad + \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} (\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h}) - B_a) B_a \\
 &\quad + \frac{1}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} [\mathbf{h}(\mathbf{x}_{t,h}^f - \mathbf{x}_{t,h}) - B_a] \varepsilon_{t,h} + \frac{B_a}{23a_{ts}} \sum_{t=1}^{a_{ts}} \sum_{h=7}^{29} \varepsilon_{t,h}
 \end{aligned}$$



619 The third term of the right-hand side Eq. (B2) is denoted as  $C$ , it is determined by all  
620 the true values and observations, but not related to any prediction scheme. By the  
621 definition of analysis bias  $B_a$  (Eq. 20), the fourth term of the right-hand side Eq. (B1)  
622 is approximate zero; since the observation error  $\varepsilon_{t,h}$  has zero mean and is  
623 statistically independent of the forecast error  $\mathbf{h}(\mathbf{x}_{t,h}^f - x_{t,h})$ , the fifth and sixth terms  
624 of the right-hand side Eq. (B1) are approximate zero too. Therefore, Eq. (21) holds.  
625



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872



873 **Figure captions**

874 Figure 1. The topography and river distribution (left plot) and the geographical  
875 location of the synthetic study area and the two application stations, the DGS and the  
876 BTS (right plot).

877

878 Figure 2. The assimilation procedure and localization scale factor estimation in the  
879 experiments. All of the equations are in accordance with that described in the text.

880

881 Figure 3. The areal average of the model's bias (a) and error (b) for one step in the soil  
882 moisture content between the CoLM and the CLM 4.0. The horizontal axis represents  
883 the layer depth.

884

885 Figure 4. The threshold layers and analysis error for each pixel in the synthetic  
886 experiment. Graph (a) illustrates the optimal and WCEnKF-Inf-Loc threshold layers  
887 of each pixel. Graph (b) shows the column RSME of each pixel in different schemes  
888 with water balance constraint (Optimal, WCEnKF-Inf-Loc, WCEnKF-Inf and  
889 WCEnKF). The horizontal axes of (a) and (b) represent the 40 pixels in the study  
890 domain.

891

892 Figure 5. The assimilation results in each layer for an ensemble Kalman filter with  
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897 traditional assimilation (EnKF) and an open-loop simulation. Graphic (a) is for spatial



898 averaged analysis error of the soil moisture content, (b) is for the short-lived error and  
899 (c) is for the analysis bias.

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901 Figure 6. The assimilation results in each observation layer for an ensemble Kalman  
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908 short-lived error and (c) is for the analysis bias.

909

910 Figure 7. Same as Figure 6, but for BTS station.

911

912 Figure 8. The box plot of the water balance residual in all 40 pixels for the  
913 EnKF-Inf-Loc, WCEnKF-Inf-Loc, WCEnKF-Inf, WCEnKF and EnKF assimilation  
914 schemes.

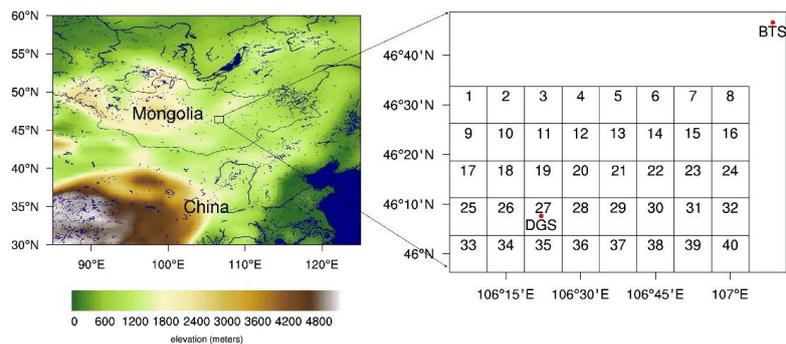
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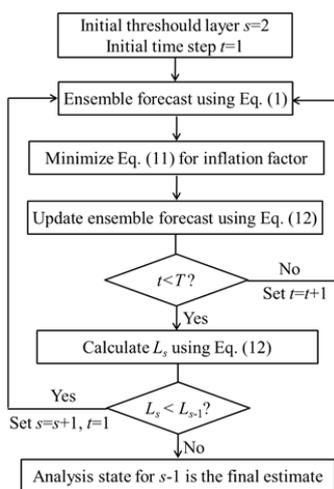
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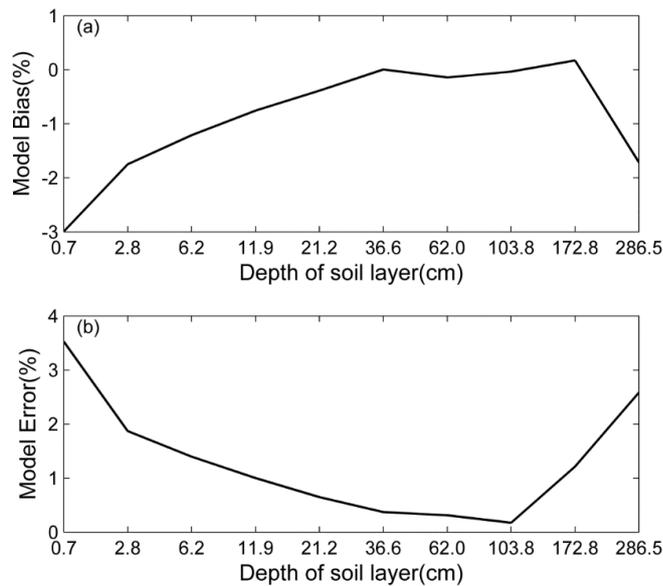
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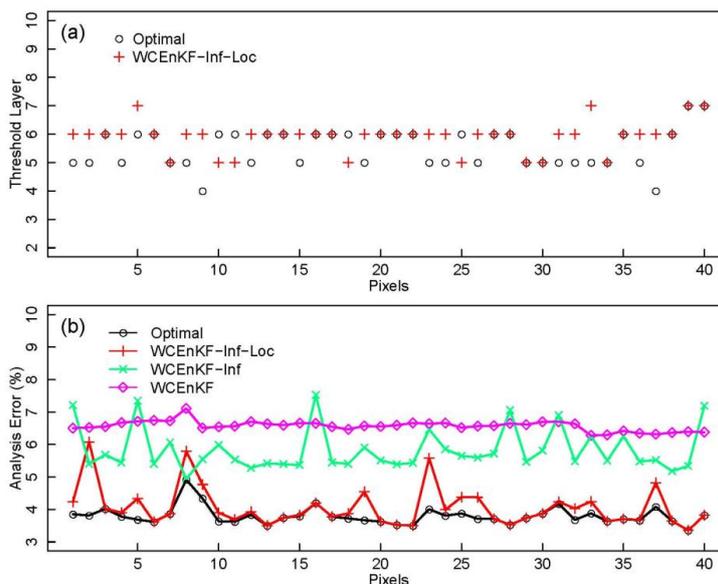


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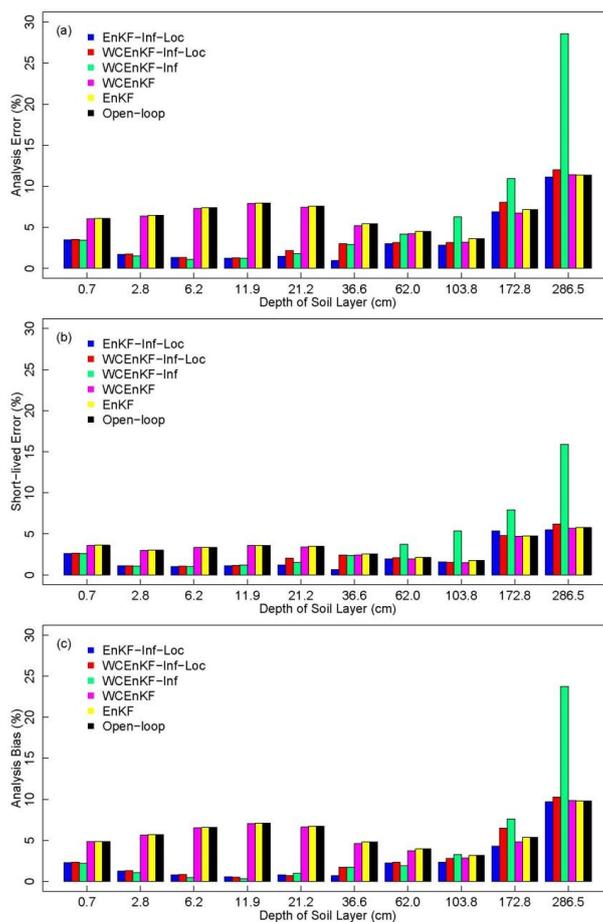
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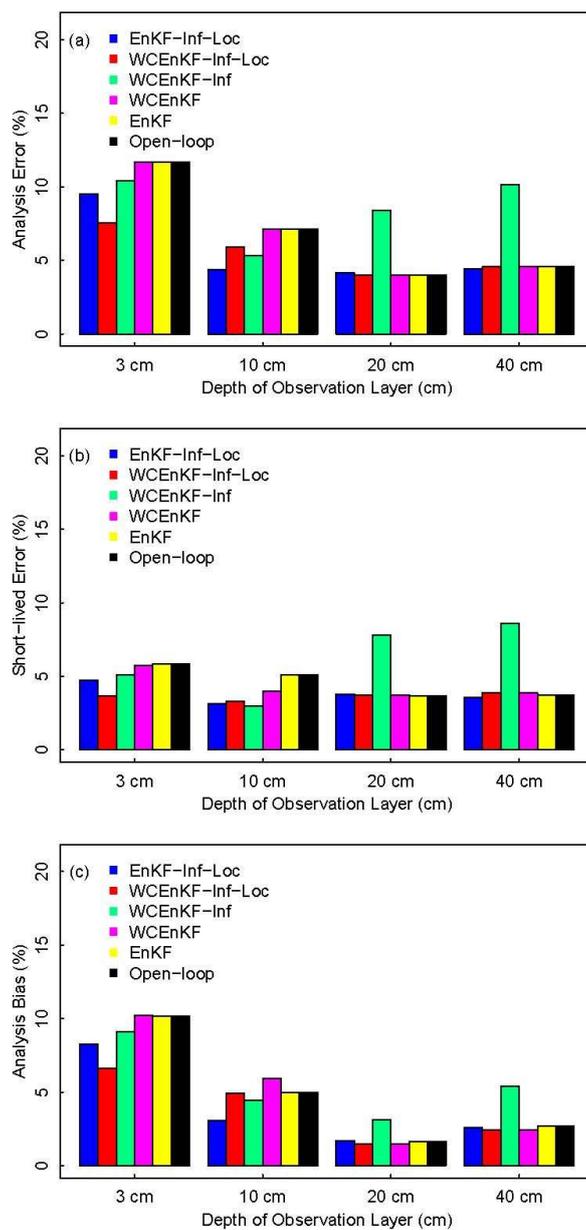
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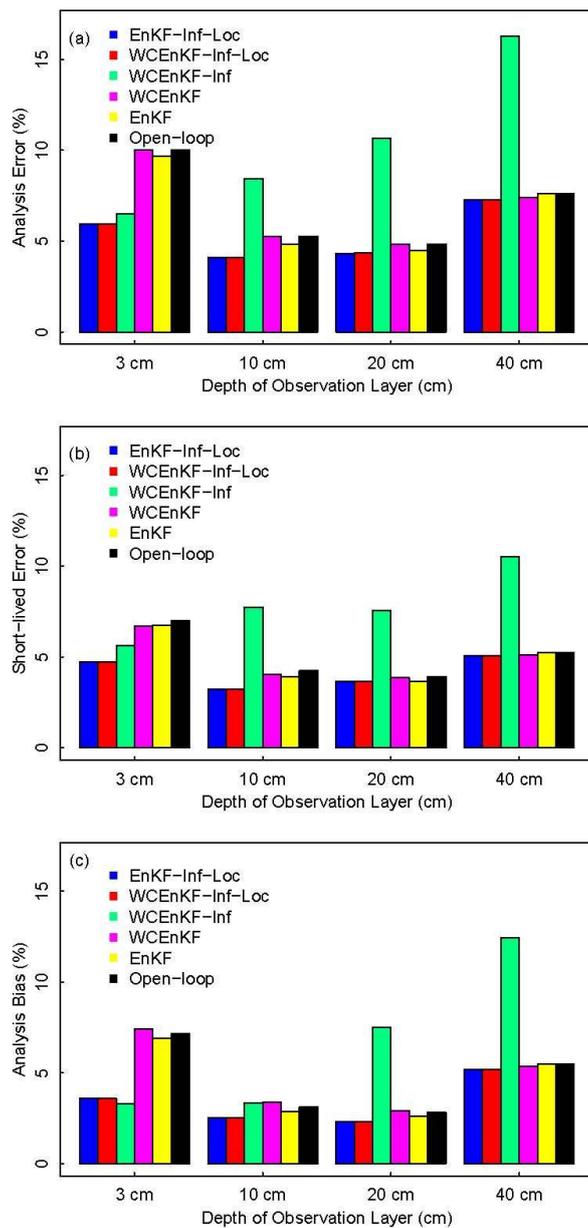


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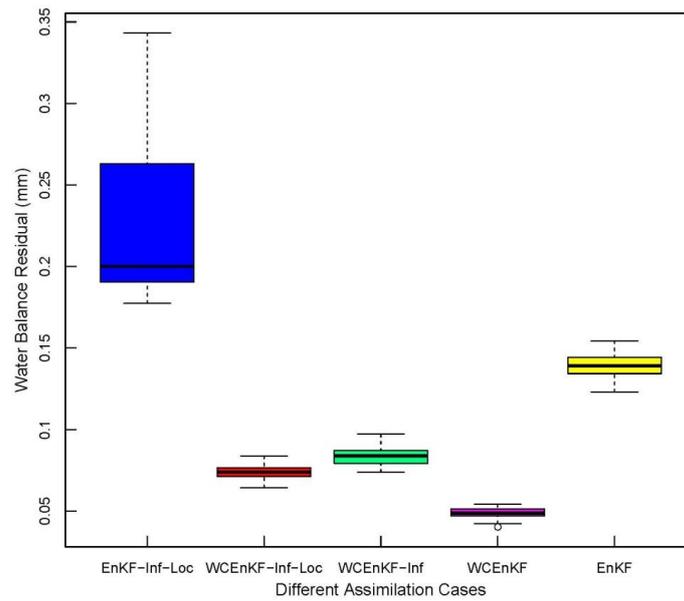
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967



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969 EnKF-Inf-Loc, WCEnKF-Inf-Loc, WCEnKF-Inf, WCEnKF and EnKF assimilation  
970 schemes.  
971



972 Table 1. The node depths (cm) of the 10 soil layers in the CoLM model.

973

Layer	1	2	3	4	5	6	7	8	9	10
Depth (cm)	0.7	2.8	6.2	11.9	21.2	36.6	62.0	103.8	172.8	286.5

974

975

976

977 Table 2. Estimated localization scale factor for different cases.

Layer	2	3	4	5	6	7	8	9	10
$\mu_s$	0.2824	0.1256	0.0587	0.0300	0.0163	0.0093	0.0053	0.0025	0.0001

978