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A land surface soil moisture data assimilation framework in consideration of the model subgrid-scale heterogeneity and soil water thawing and freezing

TIAN XiangJun† & XIE ZhengHui

Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029, China

The Ensemble Kalman Filter (EnKF) is well known and widely used in land data assimilation for its high precision and simple operation. The land surface models used as the forecast operator in a land data assimilation system are usually designed to consider the model subgrid-heterogeneity and soil water thawing and freezing. To neglect their effects could lead to some errors in soil moisture assimilation. The dual EnKF method is employed in soil moisture data assimilation to build a soil moisture data assimilation framework based on the NCAR Community Land Model version 2.0 (CLM 2.0) in consideration of the effects of the model subgrid-heterogeneity and soil water thawing and freezing: Liquid volumetric soil moisture content in a given fraction is assimilated through the state filter process, while solid volumetric soil moisture content in the same fraction and solid/liquid volumetric soil moisture in the other fractions are optimized by the parameter filter. Preliminary experiments show that this dual EnKF-based assimilation framework can assimilate soil moisture more effectively and precisely than the usual EnKF-based assimilation framework without considering the model subgrid-scale heterogeneity and soil water thawing and freezing. With the improvement of soil moisture simulation, the soil temperature-simulated precision can be also improved to some extent.

dual EnKF, NCAR/CLM, soil moisture assimilation framework, subgrid-heterogeneity, soil water thawing and freezing

Soil moisture is an important component in the interactions between the atmosphere and land surface. It is a crucial variable for many hydrologic and climate studies: soil moisture content affects surface evaporation, runoff, albedo, emissivity, and portioning of sensible and latent heat fluxes. Some studies[1] show that the effect of soil moisture on the atmosphere is secondary only to that of sea surface temperature (SST) on a global scale and even exceeds SST's over land surface. According to Chahine[2], more than 65% of the precipitation over land comes from continental evaporation, which is strongly affected by soil moisture content. Accurate knowledge of spatial and temporal variations of soil moisture is needed for numerous weather predictions and other applications.

To improve our knowledge of soil moisture variability, great efforts have been made to create estimates of soil moisture fields using land surface models forced with realistic precipitation and other atmospheric data[3,4]. However, because these efforts currently do not assimilate observational soil moisture data, they are not the data assimilation systems in a conventional sense.

Data assimilation, which originated from atmospheric and oceanographic sciences, is defined as a method to produce as accurate as possible a description of the system state under observations by using all the available information and by taking account of the observational

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†Corresponding author (email: tianxj@mail.iap.ac.cn)
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and model errors. Compared with data assimilation in atmospheric and oceanographic sciences, data assimilation in the fields of land surface and hydrological sciences was not well established as a distinct field until the mid 1990s. Since then, land surface data assimilation has been becoming an increasingly active field and some pioneering studies were carried out[5−10]. Assimilating the microwave remote sensing data with the "off-line" land surface models has become the prominent characteristic of land data assimilation. On the basis of the hypotheses that the land modeling, observation techniques and analysis methods are advanced enough, one can produce as accurate as possible a description of the land surface state and fluxes by assimilating the remote sensing data or *in situ* observation in such land data assimilation framework. In 1998, North American (NLDAS) and global (GLDAS) land data assimilation systems were initiated by NASA GSFC/DAO and some other institutes in order to provide a global or regional assimilated land surface dataset. The European Land Data Assimilation System (ELDAS) to predict floods and droughts was also launched on December 1, 2001, which was supported by the European Union. ELDAS was designed to develop a general data assimilation infrastructure for estimating soil moisture fields on the regional (continental) scale, and to assess the added value of these fields for the prediction of the land surface hydrology in models used for Numerical Weather Prediction (NWP) and climate studies. In China, Li et al. (http://ldas.westgis.ac.cn) have built a preliminary China Land Assimilation Systembased on the Common Land Model (CoLM)[11,12] and the Ensemble Kalman Filter (EnKF) method and have assimilated the passive microwave remote sensing data practically. Being pushed by these studies aforementioned, land data assimilation has become a more and more active research filed[13−24]. In soil moisture data assimilation, Kalman filter methods, such as the Extended Kalman Filter[5] and Ensemble Kalman Filter[25], are the most frequently used optimization algorithms. In the Extended Kalman Filter, the state variables can only propagate through the first-order linearization of the nonlinear system, which can introduce large errors in variable estimation, especially for some highly nonlinear systems like the soil water hydrodynamic equation. These errors could result in sub-optimal performance and sometimes divergence of the filter. The Ensemble Kalman Filter is well known and widely employed for its high precision and simple operation.

The commonly used land surface models, such as the NCAR/Community Land Model[26] version 2.0 (CLM2.0), usually are designed to consider the model subgrid-heterogeneity and soil water thawing and freezing: soil moisture of different fractions in one model grid could have large difference because of the model subgrid-heterogeneity. The soil moisture content calculation is portioned into two steps in CLM2.0 in order to consider the process of the soil water thawing and freezing. Liquid soil moisture content is firstly calculated, and liquid/solid soil moisture content is adjusted again based on the soil energy change by the soil temperature modeling. Both solid soil moisture and liquid soil moisture are the model state (prognostic) variables, whose physics characteristics are considerably different, however total soil moisture is only a model diagnostic variable.

As far as soil moisture data assimilation concerned, it could lead to some inaccurate results if neglecting the effects of the model subgrid-heterogeneity and soil water thawing and freezing, which is mainly due to the following facts: The observations are usually based on a whole model grid and are the mean state of this grid. To confuse the mean state of the model grid with that of any fraction in the model grid directly would destroy the fundamental framework of the model subgrid-heterogeneity; on the other hand, the processing of the soil water thawing and freezing makes it difficult to add the assimilation effects to the model state and definitely results in some errors if taking total soil moisture content (only a model diagnostic variable) as the model forecast (state) variable. The modeling of soil ice in CLM2.0 also increases the difficulty to operate soil moisture assimilation.

In this paper, we employ the dual EnKF method to consider the land surface subgrid-scale heterogeneity and soil water thawing and freezing and implement it in the Natioanl Center for Atmosphere Research (NCAR) Community Land Model Version 2.0 (CLM2.0) to build a soil moisture data assimilation framework: Liquid volumetric soil moisture content in a given fraction in one model grid is assimilated through the state filter process, while solid volumetric soil moisture content in the same fraction and solid/liquid volumetric soil moisture content in the other fractions are optimized by the parameter filter. To our knowledge, there have been few studies on land surface subgrid-scale heterogeneity and soil water thawing and freezing in data assimilation up to date. Preliminary assimilation simulations show that the dual EnKF-based assimilation framework can assimilate soil moisture more effectively and precisely than the usual EnKF-based assimilation framework without considering the model subgrid-scale heterogeneity and soil water thawing and freezing. Assimilated soil moisture can be improved greatly not only in the layers where observed soil moisture is assimilated directly, but also, to some extent, in the layers where no observation is available. With the improvement of soil moisture simulation, the soil temperature-simulated precision can be also improved to some extent.

1 Model and methods

1.1 The Community Land Model

We used the land model CLM2.0[26] in this study. The CLM2.0, an NCAR version of the Common Land Model[11,12], is a comprehensive, global land surface model used as the land component of the Community Climate System Model (CCSM) and is developed based on several commonly used land surface models, such as LSM[27], BATS[28] and IAP94[29]. Although the CLM2.0 is a point or grid model, it considers the subgrid-scale heterogeneity by subdividing each grid into a number of fractions. Each fraction contains a single land cover type. By default, each grid box is divided into up to five fractions for a dominant vegetation type, a secondary vegetation type, a fraction with bare soil, a wetland fraction, and an inland water fraction. Energy and water balance calculations are performed over each fraction at every time step and each fraction maintains its own prognostic variables. The fractions within a grid cell respond to the mean conditions from the overlying atmospheric grid box, and this grid box, in turn, responds to the area-weighted mean fluxes of heat and moisture from the fractions. The fractions within a grid cell do not interact with each other directly. The CLM 2.0 has one vegetation layer, 10 unevenly spaced vertical soil layers, and up to 5 snow layers (depending on the total snow depth). It computes soil temperature and soil water content in the 10 soil layers to a depth of 3.43 m in every fraction within one grid cell.

Many efforts have been devoted to improving the CLM's hydrological simulations[30 – 32], and many of these improvements have been incorporated into the latest version (version 3.5) of the CLM. There is an important change with respect to soil water/heat transport from version 2.0 to 3.5: The mean grid soil moisture is not an area-weighted sum of soil moisture content from the fractions in the CLM3.5 (in fact, there is no “fraction” in the CLM3.5 grid cell framework at all). Here we used the CLM2.0 as the model platform of our data assimilation framework in order to study the influences of the subgrid-scale heterogeneity on the assimilated soil moisture. The assimilation techniques described here can be easily implemented into the updated CLM3.5.

The conservation of liquid water mass for one-dimensional vertical water flow in a soil column in the CLM2.0 is expressed as

$$\frac{\partial \theta_{\mathrm{liq}}}{\partial t} = -\frac{\partial q}{\partial z} - E - R_{\mathrm{fm}}, \tag{1}$$

where θ_{liq} is the volumetric soil moisture content ($\mathrm{m^3/m^3}$), q is the vertical soil water flux ($\mathrm{mm \cdot s^{-1}}$) (note there are no horizontal movements of water within soils in the CLM 2.0), E is the evapotranspiration rate, and R_{fm} is the melting (negative) or freezing (positive) rate, and z is the depth from the soil surface. Both q and z are positive downward.

The soil water flux q is described by Darcy's law:

$$q = -k\frac{\partial(\psi + z)}{\partial z}, \tag{2}$$

where k is the hydraulic conductivity ($\mathrm{mm \cdot s^{-1}}$), and ψ is the soil matric potential (mm). The CLM 2.0 computes liquid volumetric soil moisture content in the 10 soil layers by eqs. (1) and (2) in every cell fraction and then adjusts solid volumetric soil moisture content and liquid volumetric soil moisture content again based on the energy (released from freezing soil water or consumed by melting) modeling in the soil energy sub-models, which is finally followed by updating the whole grid-cell volumetric soil moisture content (including solid volumetric soil moisture content and liquid volumetric soil moisture content) as the sum of area-weighted soil moisture averaged over all the fractions within the grid cell, that is

$$\theta_{\mathrm{g}} = \sum_{j=1}^{M} a_j(\theta_{\mathrm{liq},j} + \theta_{\mathrm{ice},j}), \tag{3}$$

where θ_{g} is the whole grid cell, total volumetric soil moisture content, M is the number of fractions in the grid cell, a_j is the area-based weighting factor, and $\theta_{\mathrm{liq},j}$, $\theta_{\mathrm{ice},j}$ are, respectively, liquid and solid volumetric soil moisture content in the jth fraction of the grid cell.

1.2 The dual Ensemble Kalman Filter

The dual Ensemble Kalman Filter[19,33] can combine the model forecasting with the observational information to optimize the model state and the model parameters simultaneously. The optimization process can be divided into two steps during one time interval: the state variable is firstly optimized through the state filter (suppose the model parameters are constant during this step); then the model parameters can be calibrated and adjusted by the parameter filter.

(1) The state filter. The basic EnKF analysis scheme[25] can be summarized as follows:

(i) The ensemble covariance matrix

(a) The matrix holding the ensemble members can be defined as: $A=(\psi_1,\ \psi_2,\ \cdots \psi_N) \in R^{n\times N}$,

(b) The ensemble perturbation can be defined as:

$$A' = A - \overline{A} = A(I - 1_N), \quad (\overline{A} = A1_N),$$

(c) The ensemble covariance matrix is defined as:

$$P_e = \frac{A'(A')^T}{N-1},$$

where N is the number of ensemble members and n is the size of the model state vector. $1_N \in R^{N\times N}$ is the matrix with each element being equal to $1/N$.

(ii) Measurement error covariance matrix

Given a vector of measurement $d \in R^m$, with m being the number of measurements, one can define the N vectors of perturbed observations as

(a) $d_j = d + \varepsilon_j,\ j = 1,\cdots N,$

(b) $D = (d_1, d_2, \cdots, d_N) \in R^{m\times N},$

(c) $E = (\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_N) \in R^{m\times N},$

(d) $R_e = \dfrac{EE^T}{N-1}.$

(iii) Analysis equation

$$A^a = A + P_e H^T (HP_e H^T + R_e)^{-1}(D - HA), \tag{4}$$

where H is the measurement model (observation operator).

In our formulation, the process (forecast) model (denoted by F) is given by eqs. (1) and (2) and their discrete formats and the state variable x_k is liquid volumetric soil moisture content in each fraction of one grid cell, while the measurement model H can be an arbitrary operator (linear or nonlinear, in our experiments, it is simply a real matrix) and the input variable x_k (the sum of liquid and solid volumetric soil moisture) of the measurement model H is usually based on the whole-grid value. That means, in our data assimilation framework, the state variable x_k of the process model is actually different from the input signal of the measurement model: the former is a variable defined on the grid fractions, while the latter is defined on the whole grid cell. This issue is addressed together with the parameter filter in the next subsection.

(2) The parameter filter. The variables of the process model and the measurement model have the following relationship (cf. eq. (3)):

$$\begin{aligned}\theta_g &= \sum_{j=1,j\neq i}^{M} a_j(\theta_{\text{liq},j} + \theta_{ice,j}) + a_i(\theta_{\text{liq},i} + \theta_{\text{ice},i}) \\ &= \sum_{j=1,j\neq i}^{M} a_j(\theta_{\text{liq},j} + \theta_{\text{ice},j}) + a_i\theta_{\text{liq},i} + a_i\theta_{\text{ice},i},\end{aligned} \tag{5}$$

where θ_g is the whole grid cell, total volumetric soil moisture content. For simplicity, the time denotation k is omitted in eq. (5).

The observation operator can be written as

$$\theta_k^{\text{obs}} = H(\theta_{\text{liq},i}, w_k) + \eta_k, \tag{6}$$

where θ_k^{obs} is observational soil moisture based on the model grid cell, k stands for time step. In our study, the observation operator is taken as the left-hand side of eq. (5). For each time step, the CLM 2.0 makes the simulation loop through all the fractions within the simulated grid cell. When the assimilation is being conducted in a given fraction i, it is hard to know whether assimilation is done or not for all the other fractions within the same grid cell. To address this problem, we take solid soil moisture in the same fraction, and liquid/solid soil moisture in the other fractions as parameters that can be optimized during the assimilation procedure. The vector w_k is composed of $\theta_{\text{liq},j}^k, \theta_{\text{ice},j}^k (j = 1,\cdots,M, j \neq i)$ and $\theta_{\text{ice},i}^k$.

The equations for the parameter filter, which is usually coupled with the measurement model in the dual setting usually, are

$$\begin{aligned} w_k &= w_{k-1} + v_{k-1}, \\ y_k &= H(F(\overline{x}_{k-1},\ w_k), w_k) + \eta_k, \end{aligned} \tag{7}$$

where v_k and η_k are the process and measurement noises.

2 Preliminary assimilation experiments

In this section, we use a carefully constructed global forcing dataset[34] for 1948—2004 with 3-hour and T62 (~1.875°) resolution and its update[35] to drive the assimilation framework at a station (Changlin, 44.25°N, 123.97°E) in North China and assimilate observed soil moisture from the station from 1991 to 1992 to examine the applicability of the soil moisture data assimilation framework described above. We chose this station partially because it is located in the seasonally frozen soil zone, which allows us to investigate how the dual EnKF-based assimilation framework in consideration of the subgrid-scale heterogeneity and soil water thawing and freezing performs during the thawing and freezing periods. For comparisons, the usual EnKF-based assimilation framework without considering the model subgrid-scale heterogeneity and the effects of soil water thawing and freezing was also used to carry out the same assimilation experiments. Soil moisture content (m^3/m^3, mean volumetric soil moisture content averaged over the whole depth of each layer) at this station was measured once a day at 11 vertical layers — two 5 cm layers from 0 to 10 cm and nine 10 cm layers from 10 cm to 1 m. Only the top-4 layer-observed soil moisture is assimilated in our experiments. The soil moisture-observed data are provided by China Meteorological Administration (CMA), which is attained through intensive observation and is total volumetric soil moisture (including solid/liquid volumetric soil moisture content).

2.1 Soil moisture

Figure 1 shows the time series of daily soil moisture content from 1991 to 1992 at Changlin for the top four layers from corresponding daily observations and CLM 2.0 simulations with or without assimilating the observed soil moisture data. For the time series assimilation, the assimilated (simulated) results display that in all the top four layers, the dual EnKF-based (DEnKF) assimilation framework in consideration of the model subgrid-scale heterogeneity and the effects of soil water thawing and freezing can assimilate the soil moisture much better than the usual EnKF-based assimilation framework compared with observed soil moisture. The correlation coefficients between the daily observed and the corresponding CLM2.0-simulated soil moisture from 1991 to 1992 are listed in Table 1, and the root mean square errors between them are shown in Table 2. The correlation coefficients for the DEnKF are larger than those for the usual EnKF-based assimilation framework. The formers are all greater than 0.95 in the top three layers, but the latters are all less than 0.94. On the contrary, the root mean square errors between the EnKF-based assimilated results and the observations are larger than the DEnKF's. There is no observed soil moisture assimilated directly in the 4th layer in our experiment setup and the observed information can be still transferred from the top three layers to the 4th soil layer (and even deeper layers) through the soil water hydrology dynamics and the covariance information, therefore, we can find that the assimilated soil moisture in the 4th layer is also improved considerably well from Figure 1 though its assimilated effect is not so obvious as the top three layers'. The correlation coefficients between the DEnK/FEnKF-based assimilations and the observations in the 4th layer are 0.76 and 0.62, respectively, while those between the simulations without assimilation and the observations is only 0.06. The root mean square errors between the DEnKF/EnKF-based assimilated results, the simulated ones without assimilation and the observation are 0.08 and 0.10 m^3/m^3. The results display that the assimilated soil moisture can be improved much not only in the layers where there is observed soil moisture assimilated directly but also to some extent in the layers where there is not any observed information available. Six simulation days' soil moisture profiles are shown in Figure 2. It displays that the dual EnKF-based assimilation framework can assimilate soil moisture better than the usual EnKF-based assimilation during the soil water thawing and freezing periods (during such periods, the soil ice existing plays a significant role in the assimilation processes, but the usual EnKF-based assimilation framework can not consider its influence (Figure 2(c) and (f))) and the no ice existing periods (in such periods,

Table 1 Correlation coefficients between the simulated (assimilated) and observed daily soil moisture content at Changlin (44.25°N, 123.97°E) during 1991—1992

	1st layer	2nd layer	3rd layer	4th layer
Simulation	0.13	0.08	0.09	0.06
EnKF	0.94	0.92	0.90	0.62
DEnKF	0.98	0.96	0.95	0.76

Table 2 Root mean square errors (m^3/m^3) between the simulated (assimilated) and observed daily soil moisture content at Changlin (44.25°N, 123.97°E) during 1991—1992

	1st layer	2nd layer	3rd layer	4th layer
Simulation	0.17	0.13	0.06	0.10
EnKF	6.1×10^{-2}	6.3×10^{-2}	6.6×10^{-2}	0.10
DEnKF	2.9×10^{-2}	3.5×10^{-2}	3.9×10^{-2}	0.08

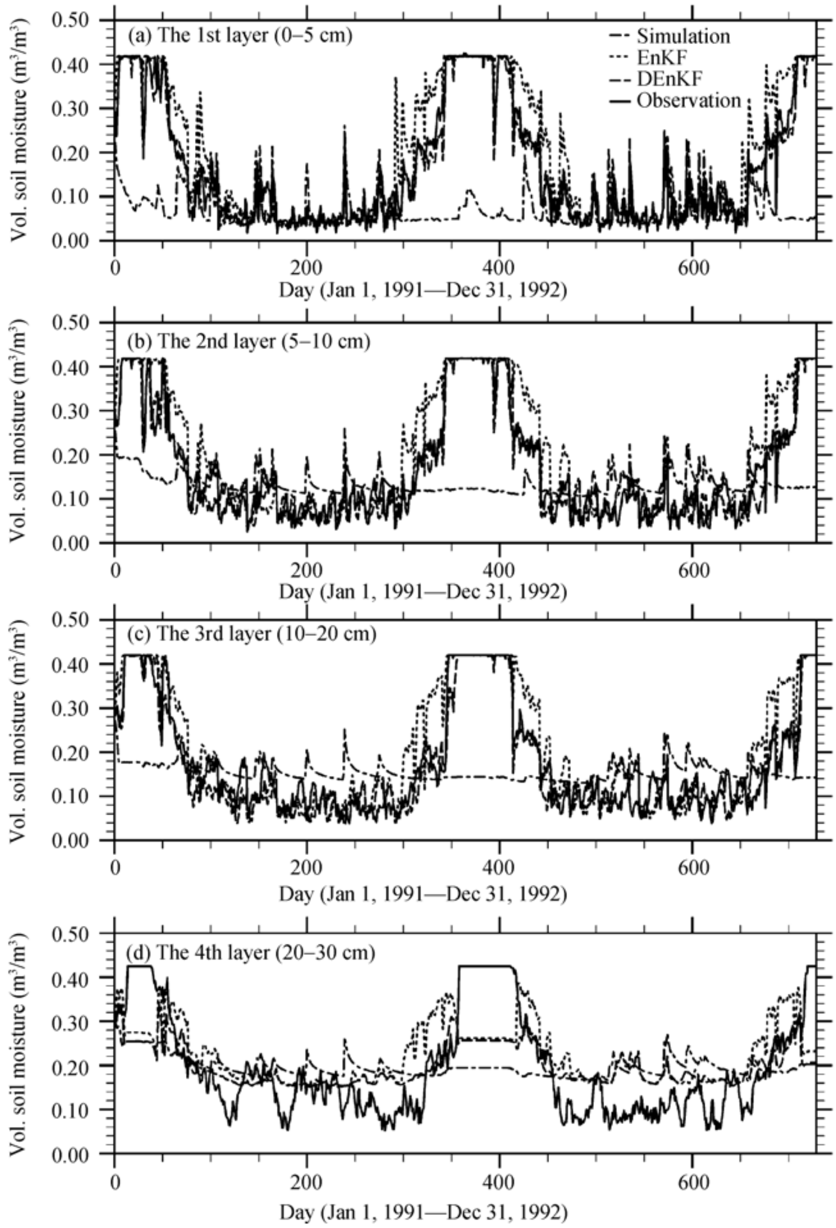

Figure 1 Time series of daily volumetric soil moisture (m^3/m^3) at Changlin (44.25°N, 123.97°E) from 1991 to 1992 for the 1st (0—5 cm depth) (a), 2nd (5—10 cm) (b), 3rd (10—20 cm) (c) and 4th (20—30 cm) (d) soil layers from observations and CLM 2.0 simulations with and without assimilation of observed soil moisture by the usual EnKF-based and the dual EnKF-based assimilation frameworks.

the usual EnKF-based assimilation framework does not suffer from the impact of soil ice any more (Figure 2(a) and (d))).

2.2 Soil temperature

The volumetric heat capacity C_i ($\mathrm{J \cdot m^{-3} \cdot K^{-1}}$) for soil is from De Vries[36] and depends on the heat capacity of the soil solid, liquid water and ice constituents

$$C_i = C_{\mathrm{s},i}(1-\theta_{\mathrm{sat},i}) + \frac{w_{\mathrm{ice},i}}{\Delta z_i} C_{ice} + \frac{w_{\mathrm{liq},i}}{\Delta z_i} C_{\mathrm{liq}}, \tag{8}$$

where i is the soil layer number, $C_{\mathrm{s},i}$ is the heat capacity of soil solids, C_{liq} and C_{ice} are the specific capacity of liquid water and ice, respectively, $\theta_{\mathrm{sat},i}$ is the ith layer-saturated soil moisture, $w_{\mathrm{ice},i}$ and $w_{\mathrm{liq},i}$ are the mass of ice and liquid water ($\mathrm{kg \cdot m^{-2}}$). The one-dimensional soil temperature equation is

$$c\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda \frac{\partial T}{\partial z}\right], \tag{9}$$

where T is soil temperature, and λ is thermal conductive-

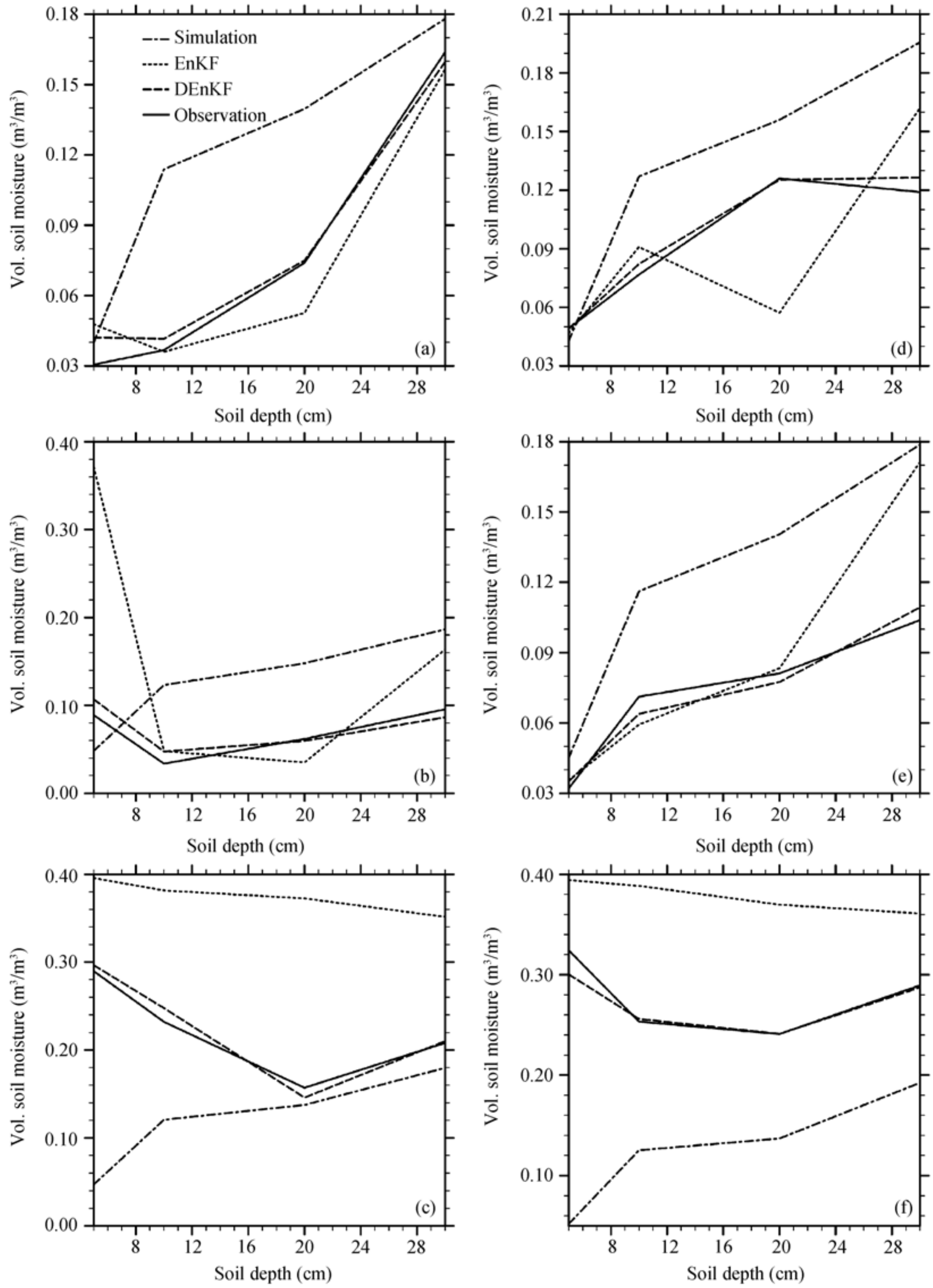

Figure 2 Comparisons between the observed, assimilated, simulated without assimilation top 4 layers' soil moisture profiles in six assimilation days ((a) August 18, 1991; (b) October 18, 1991; (c) December 18, 1991; (d) August 18,1992; (e) October 18, 1992; (f) December 18, 1992) at Changlin (44.25°N, 123.97°E).

ity. From the last subsection, we can find that the two assimilation frameworks (the EnKF-based and the DEnKF-based) assimilate the soil moisture much more differently, which consequently makes the volumetric heat capacity C_i different from eq. (8) and results in different soil temperature simulations based on eq. (9). Figure 3 shows the mean monthly skin soil temperature simulated by the two assimilation frameworks and ob-

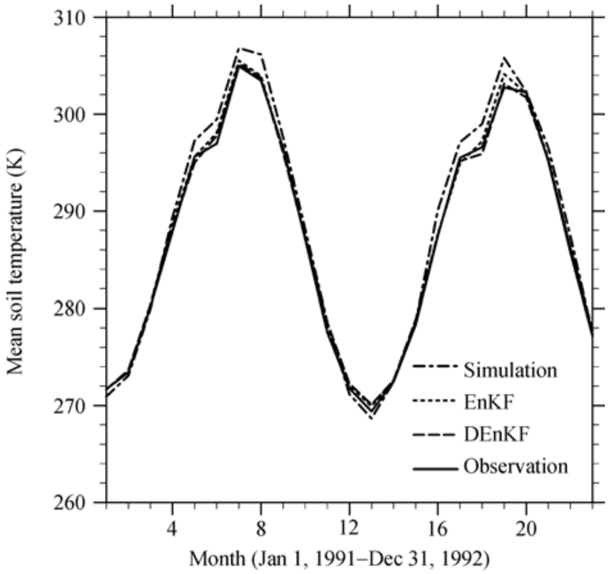

Figure 3 Comparisons between mean monthly skin soil temperature simulated by the two soil moisture assimilation frameworks and observed soil temperature at Changlin (44.25°N, 123.97°E).

served soil temperature from 1991 to 1992. One can find that the soil temperature simulation can be also improved a little with the soil moisture assimilation improving. The correlation coefficients between the mean monthly skin soil temperature simulated by the two assimilation frameworks (the DEnKF-based, and the EnKF-based) and the observed one are 0.996 and 0.907 respectively, and the root mean square errors between them are 0.313 and 0.446 K. All the above shows that the differences between the two assimilation frameworks would result in not only different simulated soil moisture but also different soil temperature. The improvement of the soil moisture assimilation can also enhance the soil temperature simulation precision to some extent. In this paper, the assimilated element is only soil moisture and soil temperature is not assimilated simultaneously. The soil temperature modeling is mainly determined by the land surface energy parameterizations.

3 Summary

In this paper, we employ the dual EnKF method to consider the land surface subgrid-scale heterogeneity and the effects of soil water thawing and freezing and implement it in the NCAR Community Land Model (version 2.0) to build a soil moisture data assimilation framework. Some preliminary assimilation experiments are designed to examine the applicability of this soil moisture data assimilation framework using observation-based forcing data and observed soil moisture. Through analyzing the differences between the usual EnKF-based and the dual EnKF-based assimilated results, we find that the two assimilation frameworks assimilate soil moisture differently to some extent, which consequently results in different volumetric heat capacity and leads to different soil energy transport modeling. This dual EnKF-based assimilation framework has great potential in the land-atmosphere interaction studies. Several issues are under investigation:

(1) The ensemble size is 60 in this study. More discussions about the effects of the ensemble size on the assimilated results and its influence on the computation cost should be held.

(2) Only soil moisture is assimilated in our assimilation framework. How to assimilate soil moisture and soil temperature simultaneously should be taken into account.

(3) We only conducted the soil moisture assimilation at a single station by this dual EnKF-based assimilation framework. How to perform the global assimilation to test its applicability is also an aim to realize.

(4) Only a simple observation operator is adopted in our assimilation framework. How to couple more complex observation operators to assimilate multi-sources observation data is also another question to answer.

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