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Surface heat flux estimation with the ensemble Kalman smoother: Joint estimation of state and parameters

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The estimation of surface heat fluxes based on the assimilation of land surface temperature (LST) has been achieved within a variational data assimilation (VDA) framework. Variational approaches require the development of an adjoint model, which is difficult to derive and code in the presence of thresholds and discontinuities. Also, it is computationally expensive to obtain the background error covariance for the variational approaches. Moreover, the variational schemes cannot directly provide statistical information on the accuracy of their estimates. To overcome these shortcomings, we develop an alternative data assimilation (DA) procedure based on ensemble Kalman smoother (EnKS) with the state augmentation method. The unknowns of the assimilation scheme are neutral turbulent heat transfer coefficient (that scales the sum of turbulent heat fluxes) and evaporative fraction, EF (that represents partitioning among the turbulent fluxes). The new methodology is illustrated with an application to the First International Satellite Land Surface Climatology Project Field Experiment (FIFE) that includes areal average hydrometeorological forcings and flux observations. The results indicate that the EnKS model not only provides reasonably accurate estimates of EF and turbulent heat fluxes but also enables us to determine the uncertainty of estimations under various land surface hydrological conditions. The results of the EnKS model are also compared with those of an optimal smoother (a dynamic variational model). It is found that the EnKS model estimates are less than optimal. However, the degree of suboptimality is small, and its outcomes are roughly comparable to those of an optimal smoother. Overall, the results from this test indicate that EnKS is an efficient and flexible data assimilation procedure that is able to extract useful information on the partitioning of available surface energy from LST measurements and eventually provides reliable estimates of turbulent heat fluxes.


1. Introduction

Surface sensible and latent heat fluxes interact with the overlying atmosphere and influence the characteristics of the planetary boundary layer (temperature, water vapor content, and height), ultimately influencing the presence and growth of low level clouds and rainfall [Pal and Eltahir, 2001; Lewellen and Lewellen, 2002; Maxwell et al., 2007; Ma et al., 2010]. Thus, the accurate estimation of surface turbulent heat fluxes plays an important role in many fields such as meteorology, hydrology, and agronomy [Pitman, 2003].

In situ measurement of surface energy balance components is difficult and expensive. Therefore, a number of models have been developed to estimate surface heat fluxes. In general, there are three major grouping of literature on estimating surface heat fluxes. The first group of studies focuses on obtaining information about the energy and water status of land surface through the empirical relation between remotely sensed land surface temperature (LST) and vegetation indices, VI (e.g., the normalized difference vegetation index, NDVI). Land surface temperature and NDVI in combination can provide information on vegetation, moisture conditions, and partitioning of surface energy budget components [Moran et al., 1994; Carlson et al., 1995; Gillies et al., 1997; Sandholt et al., 2002; Carlson, 2007; Tang et al., 2010].

The second group of studies is typically diagnostic and uses instantaneous observations of LST to solve the surface energy balance and retrieve surface heat fluxes [Bastiaanssen et al., 1998a, 1998b; Jiang and Islam, 2001; Su, 2002; Kalma et al., 2008; Cammalleri et al., 2010]. Because both the land surface temperature (T) and its time derivative (dT/dt) appear in surface energy balance equation, often closure assumptions need to be imposed. The most commonly used closure assumption is to empirically take ground heat flux (G) as a fraction of net radiation (Rn) [Jiang and Islam, 2001; Su, 2002; Santanello and Friedl, 2003].

In a departure from the empirical and diagnostic models, a number of studies [e.g., Caparrini et al., 2003, 2004a, 2004b; Qin et al., 2007; S. Bateni et al., Variational...
assimilation of land surface temperature and the estimation of surface energy balance components, submitted to Journal of Hydrology, 2012) have shown that variational data assimilation (VDA) provides an effective way to retrieve surface heat fluxes through combining land surface models and LST observations. Crow and Kustas [2005] showed that the VDA model of Caparrini et al. [2003] is promising for flux retrievals at dry and lightly vegetated sites but its performance degrades for wet and/or heavily vegetated land surfaces. Sini et al. [2008] used daily precipitation as forcing input to improve energy flux estimation over wet soil and densely vegetated areas.

The VDA models are advantageous over empirical and diagnostic models since they neither use empirical LST-VI-flux relations nor empirically relate ground heat flux to net radiation. Despite the superiority of the VDA models over the empirical and diagnostic approaches, they suffer from several shortcomings. The VDA models require the development of a model adjoint, which is difficult and time consuming in terms of both derivation and coding. Also, the variational schemes produce a single deterministic solution, and extra computations are required to determine the uncertainty of their retrievals. Moreover, a significant computational effort is required to obtain the background error covariance in the variational schemes, and therefore all of the VDA estimation heat flux models [e.g., Caparrini et al., 2003, 2004a, 2004b; Crow and Kustas, 2005; Qin et al., 2007; Sini et al., 2008; Bateni et al., submitted manuscript, 2012] have assumed a static background error covariance.

Monte Carlo or ensemble-based approaches to estimating uncertainties can be used in data assimilation. The best-known forms of ensemble-based DA are the ensemble Kalman filter (EnKF) and ensemble Kalman smoother (EnKS) [Zhang and Snyder, 2007]. In recent years, EnKF and EnKS have drawn considerable attention as an alternative DA technique to the variational methods, especially in the atmospheric science and hydrology community [Dunne and Entekhabi, 2006; Moradkhani, 2008; Reichle, 2008; Reichle et al., 2008; Meng and Zhang, 2011]. These approaches do not suffer from the VDA models deficiencies and have some unique characteristics: (1) they are much easier to formulate and employ compared to the variational techniques, (2) they directly provide statistical information on the accuracy of its estimates, (3) they can easily generate and utilize flow-dependent background error covariance, (4) they are robust even if the land surface model and measurement equations include nonlinearities, and (5) they are able to account for a wide range of possible model and measurement errors [Margulis et al., 2002; Reichle et al., 2002; Kalnay et al., 2007; Whitaker et al., 2009].

In the EnKF, the estimate at time $t$ is based on all observations available prior to and at time $t$. While, in the EnKS, all observations in the interval $[0, \tau]$ are used to estimate the state at some time $t$ where $0 \leq t \leq \tau$. The existing VDA studies [e.g., Caparrini et al., 2003, 2004a, 2004b; Crow and Kustas, 2005; Qin et al., 2007; Sini et al., 2008; Bateni et al., submitted manuscript, 2012] show that surface flux estimation at any time $t$ has been performed by assimilating all LST observations within the assimilation window, and consequently the EnKS is a more appropriate approach than the EnKF for estimating surface heat fluxes.

This study focuses on estimating two key parameters that characterize land influence on surface heat fluxes: neutral heat transfer coefficient ($C_{D\theta}$) and evaporative fraction (EF). $C_{D\theta}$ scales the sum of turbulent heat fluxes and mainly depends on the geometry of the surface. EF scales partitioning between the turbulent heat fluxes, and characterizes the fraction of turbulent heat fluxes ($H + LE$) that is dissipated through latent heat flux. Although the EnKS has generally been used for retrieving states, it can easily estimate parameters within the same framework, by the means of state augmentation [Annan and Hargreaves, 2004]. The state augmentation method, which append parameters to the model state vector is often used to estimate the unknown model parameters [Annan and Hargreaves, 2004; Zapanski and Zapanski, 2006; Kondrashov et al., 2008; Koyama and Watanabe, 2010].

The primary objective of this study is to develop and test a state-augmented EnKS model for estimating surface heat fluxes. It is hypothesized that an EnKS approach, utilizing sequences of LST observations, will allow for the retrieval of heat fluxes. The secondary objective is to study the behavior of the model and the uncertainty of its retrievals under various land surface hydrological conditions. Also, we use an ensemble open loop (EnOL) in which an ensemble of realizations is propagated forward without assimilating any LST observations. The resulting ensemble can be compared to the EnKS to see how the ensemble statistics evolve in the absence of LST assimilation. Finally, as a benchmark for the EnKS, its performance is compared to the VDA approach developed by Bateni et al. (submitted manuscript, 2012).

2. System Model

The core of the model is based on the surface energy balance equation:

$$R_n = H + LE + G$$

where

$$R_n = (1 - \alpha)R^s_d + R^s_i - R^r_i$$

Here $\alpha$ is the surface albedo. $R^s_d$ is the incoming solar radiation, and $R^s_i$ is the downwelling thermal radiation and is given by $\varepsilon_a \sigma T^4_a$. $T_a$ is the air temperature, $\sigma$ is the Stefan-Boltzmann constant, and $\varepsilon_a$ is the atmospheric emissivity which is obtained from the Idso [1981] formulation. The upwelling longwave radiation ($R^l_i$) is given by $\varepsilon_g \sigma T^4$ and is estimated using gray body emissivity $\varepsilon_g = 0.98$ and model LST.

Sensible and latent heat fluxes can be represented based on the gradients in temperature ($T$) and humidity ($q$) between the land surface and the air (subscript $a$) above it:

$$H = \rho c_p C_{sh} U (T - T_a)$$

$$LE = \rho L C_g U (q - q_a)$$

where $c_p$ is the specific heat of air, $\rho$ is the density of air, $L$ is the latent heat of vaporization, and $U$ is the reference height
wind speed. \( C_H \) and \( C_L \) are the bulk heat transfer coefficients for heat and moisture and usually are assumed to be equal.

[13] The bulk heat transfer coefficient for heat \( (C_H) \) primarily depends on the characteristics of the landscape and atmospheric stability. The influence of atmospheric stability on \( C_H \) can be taken into account by the available stability correction functions, which mainly depend on the Richardson number \( (R_i) \). \( R_i \) is an indicator of the atmospheric stability, and can be estimated as

\[
R_i = \frac{g}{\theta} \frac{\Delta \theta}{\Delta z} \left( \frac{\Delta U}{\Delta z} \right)^2
\]

where \( \Delta U \) and \( \Delta \theta \) are wind and potential temperature gradients, respectively, across height difference \( \Delta z \) and \( g \) is gravitational acceleration. For unstable atmospheric conditions, the gradient of potential temperature is positive, which yields \( R_i < 0 \). In contrast, under stable conditions the gradient of the potential temperature is positive, and therefore \( R_i > 0 \). Finally, when the gradient of potential temperature is zero, \( R_i = 0 \) and atmosphere is in a neutral condition.

[14] As mentioned above, the stability correction functions can be used to relate \( C_H \) to \( R_i \) in order to specify the effect of atmospheric stability on \( C_H \). These functions are mainly empirical and site-specific, and thus cannot be used at different sites readily. Moreover, these functions need information on the surface roughness lengths for heat and momentum, which typically are not available \([Byun, 1990; Launainen, 1995; Van den Hurk and Holtslag, 1997; King et al., 2001; Li et al., 2010]\). Therefore, such empirical functions are not used in this study. Instead, we employed the stability correction function introduced by Caparrini et al. [2003]. Their stability correction function is not empirical and does not need information on the momentum and heat roughness lengths. Moreover, it has performed satisfactorily in several studies of estimating surface heat fluxes at different sites \([e.g., Caparrini et al., 2003, 2004a, 2004b; Crow and Kustas, 2005; Sini et al., 2008; Bateni et al., submitted manuscript, 2012]\). The stability correction function proposed by Caparrini et al. [2003] is given by

\[
\frac{C_H}{C_{HN}} = f(R_i) = 1 + 2(1 - e^{10 R_i})
\]

The bulk heat transfer coefficient under neutral atmospheric condition \( (C_{HN}) \) represents the influence of the land surface characteristics on air turbulent conductivity. It depends on the geometry of the surface, varies on the scale of changing vegetation phenology (monthly) \([Caparrini et al., 2003; 2004a, 2004b; Crow and Kustas, 2005; Sini et al., 2008]\), and constitutes the first unknown parameter required for retrieving turbulent heat fluxes.

[15] The second unknown parameter required for estimating turbulent heat fluxes is \( EF \). It represents partitioning among the turbulent heat fluxes, and is defined as the ratio of latent heat flux to the sum of turbulent heat fluxes,

\[
EF = \frac{LE}{LE + H}
\]

Shuttleworth et al. [1989], Nichols and Cuenca [1993], Crago [1996], Crago and Brutsaert [1996], Lhomme and Elguero [1999], and Gentine et al. [2007] have shown that \( EF \) changes from day to day, but it is almost constant for near-peak radiation hours on days without precipitation.

3. State-Augmented Ensemble Kalman Smoother

[16] As mentioned in section 1, in this study we develop a new methodology for estimating surface heat fluxes based on EnKS with the state augmentation method. The state augmentation technique treats the model parameters as additional model state and update the model parameters as part of the DA process \([Fertig et al., 2009]\). To estimate the unknown model parameters \((i.e., C_{HN} \text{ and } EF)\) via the state augmentation method, the state vector \( (\text{LST and EF}) \) is augmented by the EF, and the state-augmented EnKS model is run for a number of reasonable \( C_{HN} \) values to estimate the augmented state \((\text{LST and EF}) \). Finally, the \( C_{HN} \) value which leads to a minimum misfit between the observed and estimated LST and the corresponding retrieved EF values are chosen as optimum parameters. Each run is conducted over a monthly time period in which \( C_{HN} \) can be assumed to be constant. It is worth mentioning that in the first try the system state \((\text{LST}) \) was augmented by both of the unknown parameters. It was observed that the model performs poorly because it allows both the EF and \( C_{HN} \) to vary on the same timescale. To overcome this problem, the system state is augmented only by EF.

[17] The state-augmented EnKS technique applies in turn a forecast step and an update step. The forecast step advances the soil state dynamics in time via integrating the heat diffusion equation \((\text{explained in section 3.1})\). In the update step, the augmented state \((\text{LST and EF}) \) is updated by assimilating LST observations into the dynamic augmented state estimates \((\text{described in section 3.2})\).

3.1. State and Parameter Propagation Models (Forecast Step)

[18] In the forecast step, the EnKS propagates an ensemble of ground temperature, \( T(z, t) \), via integrating the heat diffusion equation in a one-dimensional vertical soil column, forward in time. The heat diffusion equation produces dynamics of land temperature in response to atmospheric forcing and is given by

\[
\frac{c \partial T(z, t)}{\partial t} = p \frac{\partial^2 T(z, t)}{\partial z^2} + \omega
\]

where \( T(z, t) \) is the ground temperature at depth \( z \) and time \( t \) (for brevity ground temperature at the surface, \( T(z = 0, t) \), is shown by \( T(t) \) in this study), \( p \) is the soil thermal conductivity, \( c \) is the soil volumetric heat capacity, and \( \omega \) is the model error. Uncertainty in model forcing data and deficiencies in the model formulation are summarized in the model error \((\omega)\).

[19] In order to characterize the model error term, normally distributed random numbers \((\text{with zero mean and specified variance})\) were generated. The random numbers were used to create error within physically reasonable ranges for perturbing uncertain inputs when creating ensembles. These random errors are chosen to reflect uncertainties in measurements and propagated states. The uncertain inputs for this application are initial soil temperature in the soil column, heat diffusion coefficient \((D = p/c)\), air temperature,
wind speed, incoming solar radiation, and augmented state vector variables (LST and EF).

[20] The unknown true initial soil temperature will vary from the nominal, sometimes significantly. In order to account for this, a normally distributed random fluctuation with a mean of zero and a standard deviation of 2 K is added to the initial profile of soil temperature. Uncertainties in the heat diffusion coefficient control the upper and lower limits on heat diffusivity through the soil slab. Heat diffusivity is assigned a standard deviation equal to 0.1 m$^2$ s$^{-1}$. Standard deviation for the perturbation of incoming solar radiation is set to 30 W m$^{-2}$. Air temperature and wind speed variables are perturbed with the standard deviation of 1 K and 0.1 m s$^{-1}$, respectively. These numbers are based on simple order of magnitude considerations. The magnitudes of the standard deviation for perturbing the augmented state variables (i.e., LST and EF) are calibrated to achieve the best possible performance of the EnKS. It is found that the standard deviations of 3 K and 0.05 for LST and EF, respectively, yield the best possible performance of the EnKS.

[21] The forward model (heat diffusion equation) is initialized by introducing an ensemble of $N_c$ model errors into initial condition $T(z, \tau_0)$ and generating an ensemble of initial conditions $T_j(z, \tau_0)$, $(j = 1, \ldots, N_c)$, where $j$ represents the $j$th ensemble member, and $t = \tau_0$ is the initial time. The ensemble of generated initial condition is integrated forward in time using the heat diffusion equation to obtain the prior estimate of the state (LST) or the so-called open loop LST estimates.

[22] Applying equation (8) requires specification of boundary conditions at the top and bottom of the soil column. According to Hu and Islam [1995] and Hirota et al. [2002], soil temperature at a sufficiently deep depth, 0.3–0.5 m, is almost constant. Therefore, at the lower boundary ($z = 0.5$ m), a Neumann boundary condition is implemented:

$$\frac{\partial T(z, 0.5 \text{ m}, t)}{\partial z} = 0 \quad (9)$$

[23] The upper boundary condition at the top of the soil column, $T(z = 0, t)$, is obtained from the surface boundary forcing equation, $p\theta T(0, t)/\partial z = -G(t)$. In order to solve the heat diffusion equation and retrieve the system state (LST), the heat diffusion is discretized by dividing the soil into different layers and expressing the spatial derivatives as finite differences. In this study, a 0.5 m soil column is modeled with 50 layers with the grid interval size of 0.01 m. Given the half-hourly temporal resolution of meteorological forcing data, the heat diffusion equation is integrated at half-hourly time steps for each day within the assimilation period from $\tau_0 = 0900$ till $\tau_1 = 16:00$ LT when EF can assumed to be constant.

[24] The forecast step also propagates an ensemble of model parameter, which is appended to the model state. Because the hypothesis of constant EF holds during the assimilation window [09:00–16:00 LT], a parameter dynamic equation between successive analysis times may be formulated as

$$EF(t + 1) = EF(t) + \omega' \quad (10)$$

The uncertainty in the EF is given by the parameter error ($\omega'$), which is assumed to be normally distributed. To initialize the parameter dynamic equation, an ensemble of $N_c$ parameter errors ($\omega'$) is introduced into an initial guess of EF at $t = \tau_0$ and producing an ensemble of initial guesses, $EF^j (j = 1, \ldots, N_c)$, at $t = \tau_0$. The ensemble of created EF at $t = \tau_0$ is propagated forward in time using the parameter dynamic equation (equation (10)) to obtain the prior estimate of EF or the so-called forecast EF estimates.

3.2. Joint State-Parameter Update Model (Update Step)

[25] In this section, we describe an approach for estimating (updating) the state (LST) and model unknown parameters (EF and $C_{DIN}$) based on the state-augmented EnKS method. Estimation of EF through the EnKS approach is an indirect procedure, consisting of transforming the parameter estimation problem into a state estimation problem. This is implemented by augmenting the system state vector by artificially treating EF as an additional state variable. The augmented state vector, $T$, is then defined as

$$T(t) = \begin{bmatrix} T_1(t) & T_2(t) & \cdots & T_N(t) \\ EF_1(t) & EF_2(t) & \cdots & EF_{N_c}(t) \end{bmatrix}$$

where each column of $T(t)$ contains a single realization of the relevant variable at time $t$. The elements of $T$ at any time $t$ are obtained by propagating an ensemble of $N_c$ realizations of soil temperature (equation (8)) and EF (equation (10)) forward in time.

[26] At each update time $t$, a LST observation, $T_{obs}(t)$, becomes available. The operator $H$ relates the augmented state vector, $T(t)$, to the measured land surface temperature, $T_{obs}(t)$:

$$T_{obs}(t) = HT(t) + \epsilon \quad (11)$$

where $H = \begin{bmatrix} 1 & 0 \end{bmatrix}$ and $\epsilon$ is additive Gaussian measurement error with zero mean and covariance $R$. The random error $\epsilon$ is synthetically generated and added to LST observations to take into account the contribution of observations error to the posterior covariance and prevent correlation among the ensembles [Burgers et al., 1998]. As mentioned before, the standard deviation for perturbing LST observations is set to 3 K.

[27] Following Evensen [2007], the so-called analysis or update (superscript $a$) is obtained by updating each ensemble member, $T_{ref}$, individually:

$$T_{ref}(r) = T_j(r) + \frac{1}{N_c-1} \tilde{T}(r)^T \left( HC(r)H^T + R \right)^{-1} \left[ T_{obs}(r) + \epsilon - HT_{ref}(r) \right]$$

$$\tilde{T}(r) = \begin{bmatrix} T_1(r) & T_2(r) & \cdots & T_N(r) \\ EF_1(r) & EF_2(r) & \cdots & EF_{N_c}(r) \end{bmatrix}$$

The EnKS merges the forecasts of the LST and EF, which are obtained from equations (8) and (10), respectively, with the LST observations through equation (12). It uses information from the LST observation at update time $t$ to update not only the augmented state estimate at that update time, but also at prior times, $t'$ [Dumne and Entekhabi, 2006]. Therefore, the ensemble at the previous times must be saved and become available to be updated each time a new LST observation is available. Each update with a subsequent set of observations modifies ensemble mean and decreases ensemble variance (spread). $\tilde{T}$ indicates that the ensemble mean has been removed from each column. $C$ represents the error covariance of the forecast model state (LST) and
parameter \((\text{EF})\). The propagated covariance matrix \((\mathbf{C})\) contains not only a state-state covariance term, but also state-parameter cross covariances,

\[
\mathbf{C}(t) = \frac{1}{N_e - 1} \mathbf{T}(t) \mathbf{T}^T(t) = \begin{bmatrix} C_{T,T}(t) & C_{\text{EF},T}(t) \\ C_{\text{EF},T}(t) & C_{\text{EF},\text{EF}}(t) \end{bmatrix}
\]

The components of \(\mathbf{C}(t)\) can be shown as follows:

\[
C_{T,T}(t) = \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (T_j(t) - T(t))^2 
\]

(14a)

\[
C_{\text{EF},T}(t) = \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (\text{EF}_j(t) - \text{EF}(t))^2 
\]

(14b)

\[
C_{T,\text{EF}}(t) = C_{\text{EF},T}(t) = \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (T_j(t) - T(t))(\text{EF}_j(t) - \text{EF}(t))
\]

(14c)

where \(T(t) = \frac{1}{N_e} \sum_{j=1}^{N_e} T_j(t)\) and \(\text{EF}(t) = \frac{1}{N_e} \sum_{j=1}^{N_e} \text{EF}_j(t)\).

[28] The developed EnKS system is run for a number of reasonable \(C_{\text{HN}}\) values to retrieve the augmented state \((\text{LST and EF})\). Finally, the \(C_{\text{HN}}\) value for which the misfit between the observed and estimated LST is minimized and the corresponding EF estimates are chosen as optimum parameters. The ensemble size \((N_e)\) should be large enough to ensure that repeated experiments converge on the same result [Dumne and Entekhabi, 2006]. Our tests (Figure 9) indicate that an ensemble of \(N_e = 100\) replicates is sufficiently large to provide accurate estimates of surface heat fluxes, and thus an ensemble size of \(N_e = 100\) is used in this study.

4. FIFE Data Set

[29] The First ISLSCP (International Satellite Land Surface Climatology Project) Field Experiment (FIFE) took place in the tall grass prairies of central Kansas during the summer of 1987 and 1988 [Sellers et al., 1992]. It was designed to study the flows of heat and moisture between the land surface and the atmosphere over a 15 km \(\times\) 15 km region (centered near 39°N, 96°W). Data acquired from FIFE have been widely used to enhance our understanding of land surface processes and to improve the representation of the land surface and boundary layer in atmospheric models.

[30] At the FIFE site, forcing variables and micrometeorological data were acquired from ten Portable Automatic Meteorological (PAM) stations. LST, also referred to as skin temperature, was measured in each station from the thermal emission of the land surface with a downward looking radiometer. Surface flux measurements were collected at 22 and 10 sites in the summers of 1987 and 1988, respectively. Betts and Ball [1998] applied range filters to collected data at each station to eliminate erroneous data and then intercompared the time series of all PAM stations based on mean and standard deviation to exclude physically unrealistic data from each station. Finally, all the station data that passed this test were used by Betts and Ball [1998] to generate a site-averaged time series of forcing variables, LST, and micrometeorological measurements as well as surface flux observations with a 30 min time step.

[31] To validate the developed model with real data, it is applied to the area-averaged observations over the 15 km \(\times\) 15 km FIFE domain [Betts and Ball, 1998]. It is acknowledged that more recent single-point observations from the existing flux tower networks (e.g., Fluxnet, EuroFlux, Ameriflux) could be used to test the model. However, the main purpose is then to extend the data assimilation model to use remote sensing measurements and map land surface energy balance components over large-scale domains with a computational grid size of a few kilometers. Because a grid box in a large-scale domain represents an area average, it is necessary to validate the DA model by area-averaged observations [Chen et al., 1996]. It is obvious from the above reasons that area-averaged measurements over the FIFE site offer a valuable opportunity to validate the DA model at a scale compatible with remotely sensed observations. Through verifying the DA model with FIFE site-averaged measurements, this study provides insights into the ability of the DA scheme to estimate surface heat fluxes over large-scale domains with grid resolutions of a few kilometers from remotely sensed LST observations.

[32] In situ measurements of soil thermal properties \((\text{i.e., } p \text{ and } c)\) are not available at the FIFE site during the period of our modeling. On the other hand, the accurate estimation of these parameters requires a significant amount of detailed information \((\text{e.g., soil water content, porosity, temperature})\) that is often inaccessible. Thus, in this study, \(p\) and \(c\) are assumed to be constant throughout the soil column and during the modeling period. Following Bateni et al. (submitted manuscript, 2012), the soil heat conductivity \((p)\) and volumetric heat capacity \((c)\) are set to 0.65 \((\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1})\) and 2.35 \(\times 10^6\) \((\text{J m}^{-3} \text{K}^{-1})\) in this study. It is apparent that assuming constant values for \(p\) and \(c\) may cause error in the soil temperature predictions and consequently can negatively affect the performance of the data assimilation scheme. However, the results show that this assumption does not significantly influence the model performance and the surface heat fluxes can be retrieved reasonably well as long as the selected values for \(p\) and \(c\) fall within a physically accepted range.

[33] The retrieval model is designed to operate with the data stream provided by observations. The required data are LST, incoming solar radiation, air temperature, and wind speed. For FIFE 87, we start from 28 May (Julian day 148) and integrate the model until 31 August (Julian day 243). The assimilation period for FIFE 88 is from Julian day 160 till 243. The assimilations are performed in 30 day blocks during which landscape characteristics \((\text{e.g., vegetation phenology})\) and consequently \(C_{\text{HN}}\) can be assumed to be constant. The assimilations have a 15 day overlap to ensure that the ensemble scheme has converged to the same result. The daily assimilation window ranges from 0900 to 1600 local time when substantial energy is available for surface turbulent flux and EF is self-preserved, i.e., constant for the day.

5. Results

[34] As mentioned earlier, \(C_{\text{HN}}\) varies on the scale of changing vegetation phenology and can be retrieved monthly. To find the best possible value of \(C_{\text{HN}}\), the developed EnKS model is run for a number of reasonable \(C_{\text{HN}}\) values during
each monthly assimilation period. Finally, the $C_{HN}$ value for which the misfit between observed and estimated LST is minimum is chosen as the optimum value. In this study, $C_{HN}$ is varied from 0.001 to 0.04 for FIFE 87 (0.001 to 0.03 for FIFE 88) by increment of 0.001. Figure 1 displays LST misfit root mean square errors (RMSEs) for the range of tested $C_{HN}$ values in each assimilation time block within FIFE 87 and 88. As indicated for each assimilation time block, the LST misfit RMSE reaches its minimum at a specific $C_{HN}$ value, and therefore it provides a good basis for choosing the best possible $C_{HN}$.

The retrieved $C_{HN}$ values for each time block within FIFE 87 and 88 are shown in Table 1. For comparison, the $C_{HN}$ estimates from the VDA model of Bateni et al. (submitted manuscript, 2012) are also indicated in Table 1. As illustrated, the magnitude of EnKS $C_{HN}$ estimates are comparable to those of the VDA model. Also, the variation of EnKS $C_{HN}$ retrievals among the assimilation time blocks is consistent with those of the VDA scheme. Since the $C_{HN}$ estimation in each time block is obtained by running the EnKS system with a limited number of $C_{HN}$ values by increment of 0.001, it has less numerical precision compared to that of the VDA model. The leaf area index (LAI) value for each assimilation block is also shown.

LAI increases slightly during the summer of 1988. A similar increasing trend is also observed in the estimated $C_{HN}$ values as summer progresses. These results show that the variations in $C_{HN}$ estimates among the time blocks are consistent with the LAI dynamics. This is particularly important because no information on vegetation cover characteristics is used within the EnKS framework, and thus any similarities in the temporal variation of $C_{HN}$ and LAI can be interpreted as a partial test of estimation realism.

Table 1. Estimated $C_{HN}$ Values by the EnKS Model and the Bateni et al. (submitted manuscript, 2012) VDA Scheme for FIFE 87 and 88

<table>
<thead>
<tr>
<th>Julian Days</th>
<th>$C_{HN}$</th>
<th>LAI</th>
<th>Julian Days</th>
<th>$C_{HN}$</th>
<th>LAI</th>
</tr>
</thead>
<tbody>
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*LAI value for each assimilation time block is also shown.
Evaporative fraction values from measured heat fluxes are also shown on Figures 2 (top) and 3 (top) as open circles. The retrieved EF values from the EnKS are able to capture the rising/falling pattern of the EF obtained from the measured fluxes (i.e., track the dry down and wetting events), although the EnKS model does not use rainfall or soil moisture as input. As shown in Figures 2 (top) and 3 (top), EF estimates from the EnKS model are much closer to the observations than those of the open loop simulation. This eventually has a significant impact on the quality of the smoother’s sensible and latent heat estimates. The good agreement between the retrieved and observed EF values indicates that the EnKS model is able to use the significant amount of information contained in LST measurements in order to constrain EF estimates and capture the signature of partitioning among the turbulent heat fluxes [Bateni and Entekhabi, 2012]. For EnOL, there is no constraint by the LST observations and EF is not updated. As a result, EnOL performs poorly, especially for the days in which the initial guess for EF is not close to the true value.

Unlike the VDA models that yield a single deterministic solution and require an extra procedure to provide information on the estimates of analysis error, the EnKS scheme directly offers statistical information, which is useful for evaluating the accuracy of its estimates. Ensemble spread is an indicator of uncertainty in the estimates. A suitable and easy way to quantify ensemble spread is via its standard deviation [Dunne and Entekhabi, 2006]. Figures 2 (bottom) and 3 (bottom) show the estimation error standard deviation of EF estimates from the EnKS (solid lines) and EnOL (dashed lines) model for FIFE 87 and 88, respectively.

Unlike open loop, the EnKS model uses information
Figure 4. Statistical box plot of the ensemble distribution of retrieved evaporative fraction for a wetting sample period within FIFE 87 experiment. Thick and thin boxes correspond to the EnOL and EnKS estimates, respectively.

... contained in LST measurements. This additional information causes the uncertainty of EF estimates (the estimation error standard deviation) to reduce considerably. Thus, uncertainty (estimation error standard deviation) is consistently higher in the EnOL estimates since they are not constrained by LST measurements. Note also that the estimation error standard deviation of EF estimates from the EnOL shows only a slight variation during the modeling periods of FIFE 87 and 88. In contrast, the EnKS error standard deviation demonstrates significant fluctuations during the corresponding periods. Our purpose is to find out what these variations physically exhibit.

[39] As shown in Figure 2 (top), in the initial period of FIFE 87 experiment (especially Julian days 158–166), observed EF values (circles) are very close to the potential evaporative fraction, EF_{pot} estimates (crosses). In this period, the assimilation scheme performs weakly and sharp jumps are observed in the EF retrievals since evaporation is at its first stage (i.e., controlled mainly by the atmospheric factors), and the coupling between EF and LST observations is weak. Therefore, estimating EF from the LST measurements becomes more uncertain and consequently we observe higher uncertainty (estimation error standard deviation) in EF estimates. In contrast, during the drydown period (e.g., Julian days 200–215 of FIFE 87) the linkage of EF to LST is more vigorous, and therefore the retrieval of EF from the LST evolution becomes less uncertain. This hypothesis can be easily confirmed since the standard deviation of EF estimates decreases continuously as soil moisture reduces during the aforementioned drydown period. The above analyses enable us to find out the relative dependency of evaporation on the atmospheric factors and/or surface properties under different land surface hydrological conditions.

[40] For very large estimates of EF (close to unity), the standard deviation decreases since most ensemble members of EF reach the upper bound (e.g., Julian days 170–173, 184, and 189 of FIFE 87). To have a better understanding of this behavior, the box plots for the ensemble distribution of retrieved evaporative fraction are shown in Figure 4 for a wetting sample period (Julian days 170–186) within FIFE 87 experiment. The lower and upper edges of the box indicate the first and third quartiles, respectively, in the ensemble distribution, and the median position is marked within the box. Lines extending from the box ends represent the minimum and maximum values in the ensemble. Boxes with the thick and thin boundaries, respectively, correspond to ensemble distribution of EF estimates from the EnOL and EnKS schemes. The ensembles within the EnKS model use the information contained in LST observations and move toward the true solution. As a result, thin boxes are almost always shorter than the thick ones.

[41] This wetting period is chosen specifically to understand more clearly the reason for the decrease in standard deviation of EnKS EF estimates when computed EF values are close to unity (e.g., Julian days 170–173, 184, and 189 of FIFE 87, Figure 2). As indicated, for very high EF estimates most of the ensemble members of EF reach the upper bound of 0.99, and therefore the standard deviation reduces. It is apparent that in this case the decrease of standard deviation does not imply that coupling between EF and LST is strong and occurs only because the ensemble members reach the upper bound of 0.99.

[42] A straightforward way to evaluate the performance of the EnKS model is to explore the fidelity of the ensemble mean of the estimated state (LST) in tracking the LST observations and more importantly, the ability of the EnKS to reduce ensemble spread when compared to the open loop by improving the surface energy balance parameters among the ensemble members. The LST observations are used in...
the EnKS to update the model parameters in the replicates compared to their priors. Thus, in evaluating the EnKS estimates of LST with the corresponding observations, it is expected that the mean of the ensembles tracks the time series of the observations. It is also anticipated that the uncertainty (standard deviation) in the estimated LST from the EnKS is reduced when compared with the uncertainty in the open loop. These expectations occur if the EnKS updates of the model parameters provide an improved estimate of surface energy balance and LST series among the replicates.

Figures 5 (top) and 6 (top) compare the EnKS (solid lines) and EnOL (lines with dots) daily average (0900–16:00 LT) estimates of LST with observations (open circles) for FIFE 87 and 88, respectively. Figures 5 (top) and 6 (top) clearly indicate the improvements in the LST estimates provided by the EnKS scheme. In other words, LST estimates from the EnKS model are almost always closer to ground truth measurements compared to those of the EnOL scheme. The decreased misfit between the observed and EnKS estimates of LST indicates that the EnKS model can successfully constrain the model unknown parameters (i.e., $C_{HN}$ and EF) and derive the signature of partitioning of available energy among the turbulent heat fluxes from the evolution of LST.

The behavior of individual ensemble members during the propagation and update steps provides useful insight about the functioning of the ensemble smoother. In the EnKS scheme, at each update the ensemble replicates (and the ensemble mean) move toward the measurement, and the ensemble spread is decreased. Unlike the ensemble smoother, the open loop estimates are not updated and tend to move away from the observations [Margulis et al., 2002]. Therefore, smoothing significantly reduces the uncertainty (the estimation error standard deviation) in the LST estimates (Figures 5, bottom, and 6, bottom) and finally provides better estimates of LST. Unlike the uncertainty of EF estimates that principally depends on the coupling between EF and LST and continuously decreases as soil becomes dry, the temporal variation of estimation error standard deviation of LST estimates depends in a complex way on the evaporative fraction and bulk heat transfer coefficient estimates, incoming solar radiation, and air temperature.

The time sequences of daily average sensible and latent heat flux estimates from the EnKS scheme (solid lines) are compared with the observations (open circles) in Figures 7 and 8 for FIFE 87 and 88, respectively. Gray bands represent the uncertainty of $H$ and LE retrievals. The lower and upper bounds of the gray bands show the lower 15th and upper 85th quartiles (corresponding to minus and plus one standard deviation around the mean). As shown, the EnKS estimates are in good agreement with the observations, which suggest that EnKS is a reliable and effective approach for turbulent heat flux forecasting. Remarkably, the day-to-day variations in the estimated sensible and latent heat fluxes are consistent with those of the observations. Overall, the results show that the assimilation of LST measurements into the EnKS model can successfully constrain the model unknown parameters, and efficiently partition the available energy between the turbulent heat fluxes.

According to equation (3), the uncertainty of the estimated sensible heat flux is mainly dependent on the errors in LST estimates. It was already stated (see Figures 5
and 6) that the uncertainty of LST estimates depends in a complex way on the evaporative fraction and bulk heat transfer coefficient estimates, incoming solar radiation, and air temperature, and therefore it is too difficult to explain its variations. Uncertainty of LE estimates can be investigated by rewriting equation (7) as follows:

\[ LE = \frac{EF}{1 - EF} H \]  

This equation shows that the uncertainty of LE estimates depends not only on the errors in the predicted sensible heat flux but also on the uncertainty of EF retrieval. Broadly speaking, we anticipate the errors in LE estimates decrease as soil becomes dry because it was shown in Figures 2 and 3 that the uncertainty of EF retrieval reduces as soil moisture decreases owing to the more vigorous coupling between EF and LST observations. As expected, Figures 7 and 8 show lower uncertainty (estimation error standard deviation) in LE

**Figure 6.** Same as Figure 5 but for FIFE 88.

**Figure 7.** Time series of daily average (09:00–16:00 LT) (top) sensible and (bottom) latent heat fluxes for FIFE 87: Observed (circles) and EnKS (black lines). Gray bands correspond to estimates of turbulent heat fluxes plus and minus one standard deviation.
estimates during the dry down periods (e.g., Julian days 200–215 of FIFE 87).

[47] Statistically, a larger number of ensemble realizations yields an ensemble mean and covariance that are closer to reality [Pipunic et al., 2008]. The limited number of ensemble members causes sampling error in the measurement and forecast error covariance terms and consequently weakens the performance of the EnKS model. Lorenc [2003] showed that the sampling error of the covariance terms reduces by increasing the ensemble size. The EnKS model converges only when the size of the ensemble is sufficiently large because a small ensemble size causes significant sampling errors in the covariance estimate [Crow and Wood, 2003]. Also, for a small ensemble size, the spread among the ensemble members decreases too rapidly after each update. This yields the ensembles with a very small covariance and finally causes the EnKS divergence [Li, 2008]. On the other hand, by increasing the ensemble size the computational cost increases. Thus, it is desirable to use the minimum number of ensemble members while still obtaining satisfactory results.

[48] An assimilation experiment is undertaken to determine the minimum number of ensemble members required to achieve the best possible results from application of the EnKS. Assimilation over the experiment period was performed separately using six different ensemble sizes: 3, 5, 10, 50, 100, and 150 members. RMSE values were calculated between LST, \( H \), and LE from observations and from assimilation runs performed with each ensemble size. Figure 9 shows the RMSE values of estimation against the number of ensemble members. While the algorithm clearly improves model predictions with increasing ensemble size, very little improvement is seen when increasing ensemble size between 100 and 150. This suggests that, for ensemble sizes >100, alternative error sources (e.g., the assumption of constant daily EF and constant monthly \( C_H \), constant soil thermal conductivity and volumetric heat capacity, etc.) play a larger role than the errors arising from finite ensemble sizes. As the declination in RMSE was minimal for more than 100 ensembles, an ensemble size of 100 members was chosen as adequate in this study.

6. Comparison of EnKS With EnOL and VDA

[49] The daily average turbulent heat flux estimates from the EnKS are compared with those of the EnOL for FIFE 87 in Figure 10. The EnKS algorithm and open loop estimates both rely on the same inputs, which are in all likelihood, imperfect. However, the EnKS algorithm can also benefit from information contained in LST measurements. Improvements in the performance of smoother estimates over open loop results demonstrate (1) the LST variations contain a significant amount of information for the partitioning of available energy among the surface heat fluxes [Bateni and Entekhabi, 2012], and (2) the EnKS can effectively extract and use that information to retrieve surface heat fluxes. The smoother estimates are far superior to the open loop estimates, which continue to underestimate sensible and overestimate latent heat flux. The EnKS estimate of LE has a RMSE of 61.9 W m\(^{-2}\), which is a 31% reduction of the open loop RMSE of 89.7 W m\(^{-2}\) (Figure 10). Similarly, the RMSE of \( H \) estimate decreases from 47.3 W m\(^{-2}\) to 31.4 W m\(^{-2}\). The poor performance of the EnOL shows that the ancillary data alone (air temperature, wind speed, and incoming solar radiation) cannot estimate surface heat fluxes, and the value added by the LST information has a vital role on the model performance. Overall, improvements in the smoother results confirm that LST measurements provide a very useful supplement to the forcing data.

[50] Figure 10 also compares the performance of the EnKS with that of the VDA model of Bateni et al. (submitted manuscript, 2012). The inputs (e.g., air temperature, incoming solar radiation, wind speed, soil thermal conductivity, and volumetric heat capacity) and the assimilation time blocks used in the VDA approach are identical to those used in the EnKS scheme. The conceptual similarities and
differences between the VDA and the EnKS are (1) Both methods use all observations within an assimilation window to update the states and parameters within that window, (2) The EnKS converges only if its ensemble size is sufficiently large, while the performance of the variational model is not affected by sampling considerations, and (3) The estimates from the EnKS are strongly dependent on the observation and model error variances. In contrast, the VDA does not deal with the input error parameters and works only with the nominal values of inputs.

Both the VDA and EnKS schemes estimate $C_{HN}$ (EF) by assimilating all LST observations within the monthly assimilation time blocks (within the daily assimilation window [09:00–16:00 LT]), and thus both VDA and EnKS models use all the available LST information. Also, as shown in Figure 9, the limited number of ensemble members generates sampling error, which consequently weakens the performance of the EnKS. To eliminate this deficiency, the EnKS estimates of heat fluxes are obtained with a sufficiently large ensemble size of 100. Yet, it is observed that the estimates of turbulent heat fluxes from the VDA model are closer to the observations than those of the EnKS scheme (Figure 10). Since the effect of finite ensemble size on the EnKS estimates is reduced by using large sample size, the only major remaining factor for the EnKS is the magnitude of the assigned model and observation error variances.

The model and observation error parameters significantly influence the quality of the assimilation products, and the estimation error rises as the input error parameters depart from their true values [Reichle et al., 2008]. Having this in mind, it is apparent that the main problem in the application of the EnKS to the retrieval of surface heat fluxes is the poorly known uncertainties of the model and observations. As mentioned in section 3.1, the model and observation error parameters in this study are calibrated by running the EnKS model for a limited set of input error parameters and then selecting the parameter set associated with the best possible performance of the EnKS. Since in this study the error parameters are retrieved based on only a few experiments, they may not be the optimum values and therefore yield suboptimal results. However, the degree of sub-optimality is small, and the EnKS outcomes are roughly comparable to those of a dynamic variational model. To provide better estimates of turbulent heat fluxes through an ensemble-based DA approach, we need to develop an adaptive EnKS approach. The adaptive EnKS can adjust the observation and model error parameters on the basis of information from the EnKS internal diagnostics such as the misfit between observations and forecasts, which generally improves the assimilation estimates [Durand and Margulis, 2008; Reichle et al., 2008]. This study focuses on the feasibility of assimilating LST within an EnKS framework in order to estimate the turbulent heat fluxes, and the development of an adaptive EnKS scheme is beyond its scope.

Since we have used a variational approach to benchmark the performance of the EnKS, it is reasonable to ask how the two methods are likely to compare in an operational setting. The EnKS and VDA models each have distinctive features that can be expected to apply over a range of different problems. The EnKS approach is easy to use in forecasting applications because measurements are processed as they become available. Reinitialization of the EnKS algorithm not only at measurement times, but also at previous times is an inherent part of the EnKS and does not require any special treatment. There is no need to compute adjoint models or derivatives. Such flexibility offers many practical advantages and makes it feasible to develop a useful data assimilation algorithm in a relatively short time. The EnKS model is able to easily incorporate different forms of the model and observation errors. Such errors can be additive, multiplicative, or state dependent. The EnKS offers statistical information, which is useful for assessing the accuracy of
Figure 10. Scatterplot of daily average (09:00–16:00 LT assimilation window) modeled versus measured (left) sensible and (right) latent heat fluxes for (top) EnKS, (middle) EnOL and (bottom) the variational scheme developed by Bateni et al. (submitted manuscript, 2012).
its estimates and analyzing the behavior of the model under various land surface hydrological conditions, while such information is not directly available from the variational approach.

7. Conclusions

[54] A new methodology is developed to estimate surface heat fluxes by assimilating the sequences of land surface temperature (LST) within an ensemble Kalman smoother (EnKS) framework. The formulation of the EnKS is based mainly on the discretized diffusion equation of heat transfer through the soil column. The heat diffusion dynamic model produces the soil state estimate forward in time for a time-varying atmospheric boundary condition. LST observations are used as they become available to update the ensemble at prior estimation times in addition to the current forecast ensemble. The unknown parameters that are subjected to control during the estimation procedure include neutral bulk transfer coefficient \( C^{IN} \) and evaporative fraction (EF). \( C^{IN} \) scales the sum of turbulent heat fluxes and EF represents partitioning among the turbulent heat fluxes. To estimate EF, the EnKS state vector (LST) is augmented by EF, and then the augmented EnKS system is run for a number of reasonable \( C^{IN} \) values to estimate both the system state (LST) and parameter (EF). Finally, the \( C^{IN} \) value for which the misfit between estimated and observed LST is minimum and its corresponding estimated EF values are chosen as optimum parameters.

[55] Application of the EnKS model to the FIFE data set shows that the day-to-day variations in the estimated daily evaporative fraction are remarkably consistent with observations, even though no information on the soil moisture dynamics and precipitation events is used within the assimilation model. This demonstrates that the new methodology can effectively extract and use information on the partitioning of available energy from LST measurements. Unlike the VDA models that require an extra procedure to provide information on the estimates of analysis error, the EnKS model directly provides important statistical information for analyzing the behavior of the model under various land surface hydrological conditions, while such information is not directly available from the variational approach. All of these advantages make the EnKS approach an attractive candidate for operational hydrologic data assimilation applications.

References


