Received: 28 April 2023 | Accepted: 31 October 2023

DOI: 10.1002/vzj2.20298

Vadose Zone Journal

ORIGINAL ARTICLE

The value of soil temperature data versus soil moisture data for state, parameter, and flux estimation in unsaturated flow model

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Assigned to Associate Editor Venkat Lakshmi.

Abstract

This synthetic study explores the value of near-surface soil moisture and soil temperature measurements for the estimation of soil moisture and soil temperature profiles, soil hydraulic and thermal parameters, and latent heat and sensible heat fluxes using data assimilation (ensemble Kalman filter) in combination with unsaturated zone flow modeling (HYDRUS-1D), for 12 United States Department of Agriculture soil textures in a homogeneous and bare soil scenario. The soil moisture profile is estimated with a root mean square error (RMSE) of 0.04 cm^3/cm^3 for univariate soil temperature assimilation and 0.01 cm^3/cm^3 for univariate soil moisture assimilation. Soil temperature assimilation performs better for soils with higher clay content compared to soils with higher sand content. The latent and sensible heat fluxes are estimated with smaller RMSE for univariate soil temperature assimilation compared to univariate soil moisture assimilation for 8 out of 12 soil types. As the climate condition changes from hot semi-arid to sub-humid climate, the soil moisture assimilation performs better for high permeable soil but worse for low permeable soil. In summary, the findings suggest that for most soil texture classes, assimilating soil temperature in vadose zone models is skillful to improve latent heat flux, soil moisture profile, and soil hydraulic parameters. Joint assimilation with soil moisture can further enhance the accuracy of the model outputs for all range of soil texture and climate conditions.

Abbreviations: CZO, Critical Zone Observatory; DREAM, Differential Evolution Adaptive Metropolis; EnKF, ensemble Kalman filter; ET, evapotranspiration; H, sensible heat flux; LAI, Leaf area index; LE, latent heat flux; NDVI, normalized difference vegetation index; OL, open loop; P, precipitation; PET, potential evapotranspiration; RMSE, root mean square error; SHP, soil hydraulic parameter; SM0, SM5, SM10, SM30, and SM50, soil moisture assimilation at 0, 5, 10, 30, and 50 cm, respectively; SM550, Soil moisture assimilation at 5 and 50 cm; SMT5, soil moisture and temperature assimilation at 5 cm; SMT550, Soil moisture and temperature assimilation at 5 and 50 cm; ST0, ST5, ST10, ST30, and ST50, Soil temperature assimilation at 0, 5, 10, 30, and 50 cm, respectively; ST550, Soil temperature assimilation at 5 and 50 cm; STP, Soil thermal parameter.

1 | INTRODUCTION

Soil moisture plays an important role in both the water cycle (partitioning of rainfall into infiltration and runoff) and the energy cycle (partitioning of net radiation into latent heat and sensible heat) (Seneviratne et al., 2010). Knowledge of root zone soil moisture is important in agriculture for optimizing irrigation scheduling and crop growth (Vereecken et al., 2008). In situ soil moisture is measured using different types of accurate point sensors (Babaeian et al., 2019; Walker et al., 2004a). In recent years, advances have been made to estimate soil moisture at larger scales (e.g., 10 to 100 m) through ground-based sensors using cosmic ray and gamma ray approaches (Bogena et al., 2013; Morrison et al., 2016). Although such in situ measurements provide accurate estimates of the soil moisture profile, they are inadequate to characterize the spatial variation of soil moisture at regional or landscape scale. Many studies analyzed the retrieval of surface soil moisture using microwave satellite platforms (Karthikeyan et al., 2017; Tomer et al., 2016). However, these retrievals have limitations with regard to the spatial and temporal resolutions. Moreover, retrievals using satellite remote sensing do not have the ability to infer deeper horizon soil moisture. Land surface models have a capability to simulate the vertical soil moisture profile at the required spatiotemporal resolutions using meteorological forcings, soil information, and land surface parameters as inputs (Fisher & Koven, 2020; Kumar et al., 2017). However, the soil moisture simulated by these models is often affected by uncertainties in model parameters, model structure, and forcing data. These limitations can be reduced by the use of data assimilation techniques.

Several studies (e.g., Gebler et al., 2019; Lannoy & Reichle., 2016) have reported the use of data assimilation methods in models which encompass the vadose zone and assimilate in situ or remotely sensed surface soil moisture measurements. Other studies use data assimilation to jointly estimate states and parameters of models which encompass the vadose zone. Montzka et al. (2011) noted that joint estimation of states and parameters results in a better estimate of the soil moisture profile compared to only state estimation. Hung et al. (2022) assimilated both soil moisture and groundwater level data in the integrated land surface-subsurface model CLM-Parflow using the localized ensemble Kalman filter (EnKF) and analyzed the impact on the characterization of soil moisture, evapotranspiration, river discharge, and groundwater level. Although soil moisture and groundwater level characterization could be improved substantially, only a very small improvement was observed for the estimation of evapotranspiration.

In addition, studies discussed errors in the estimates of states and parameters with data assimilation approaches (Liu et al., 2012; Reichle et al., 2008). It was found that errors in the soil moisture profile and soil hydraulic parameter (SHP) estimation varied as function of the soil type, the accuracy of surface soil moisture observations, and the assimilation frequency. Montzka et al. (2011) found that estimation of soil moisture profile is better for silt and loamy sand compared to clay and loam. Li and Ren (2011) studied the estimation of van Genuchten–Mualem hydraulic functions using matric potential observations. They reported larger errors in the estimation of parameters for soils with higher sand content. Bandara et al. (2013) also noted that the SHPs are better identified for a soil column with a higher clay content compared to a soil with higher sand content.

Studies were also conducted on the estimation of soil moisture from soil temperature measurements. The water and energy balance equations at the land surface are coupled via the land surface temperature which affects the latent and sensible heat fluxes (Lakshmi, 2000). Lu et al. (2009) proposed a method where thermal inertia was first calculated using daily maximum and minimum soil temperature observations and then soil moisture content was inversely estimated using models based on thermal inertia–soil moisture characteristics. Dunne et al. (2010) pointed out that the dependence of soil thermal properties on soil moisture allows the estimation of soil moisture from soil temperature data. In their approach they determined thermal diffusivity first using soil temperature data and then soil moisture was estimated from thermal diffusivity. Given the non-uniqueness in the estimation of soil moisture from thermal diffusivity, it was suggested that using data assimilation methods is better than inverse methods. Dong et al. (2015a, 2015b) showed in a series of synthetic experiments how the soil moisture profile is estimated from soil temperature measurements with help of data assimilation techniques like the EnKF, particle filter, and particle batch smoother. They suggested that the use of soil temperature measurements at two depths is sufficient to estimate the soil

Core Ideas

- Soil moisture can be estimated with good accuracy using soil temperature assimilation.
- Soil temperature data assimilation is superior for estimating soil hydraulic parameters in clayey soils.
- Heat flux is better estimated by soil temperature assimilation than soil moisture assimilation.
- Assimilating both soil moisture and soil temperature improved estimation of state, parameter and heat fluxes.
- Soil moisture assimilation performs better for high (low) permeable soil in humid (arid) climate.

moisture profile and also showed that particle batch smoothing significantly reduced the root mean square error (RMSE) for the estimation of the soil moisture profile compared to the particle filter. Further, Dong et al. (2016) attempted estimation of soil moisture along with soil hydraulic properties and noted that joint estimation of soil states and parameters improved the accuracy in the estimates of the soil moisture profile.

Previous studies also compared joint assimilation of soil moisture (in situ or remotely sensed) and soil temperature or land surface temperature versus univariate assimilation. Steenpass et al. (2010) examined the estimation of soil hydraulic properties using (i) only infrared-measured surface soil temperature and (ii) both surface soil temperature and water content at different depths using the Differential Evolution Adaptive Metropolis (DREAM) algorithm for a silty loam soil. They observed that with the help of land surface temperature measurements alone the estimation of soil hydraulic properties could be improved and that additional conditioning to water content data further reduced the uncertainty in the estimation of soil hydraulic properties. Ridler et al. (2012) studied the calibration of the MIKE-SHE model, an integrated hydrological modeling system for simultaneous surface water and groundwater flow, for a sandy soil using both in situ measurements and satellite retrievals of land surface temperature and surface soil moisture to improve the estimates of latent and sensible heat fluxes. They found that the joint use of land surface temperature and soil moisture outperforms the use of only land surface temperature or soil moisture in the estimation of fluxes. They also found that in situ measurements of surface soil temperature and soil moisture gave improved results compared to satellite-based observations. Han et al. (2013) studied joint assimilation of land surface temperature and brightness temperature observations versus univariate assimilation of these observations for the estimation of soil moisture and soil temperature profiles and latent and sensible heat fluxes. Only for dry periods, joint assimilation performed marginally better than univariate assimilation with an additional RMSE reduction of 0.1 K for the characterization of soil temperature and 1.5 W/m^2 for the characterization of latent heat flux.

Most of the studies discussed above focused on one or a few selected soil textural classes. There is no reported study evaluating systematically the effect of soil textural class (e.g., according the United States Department of Agriculture [USDA] with 12 soil texture classes) on the estimation of soil states and parameters using soil moisture and/or soil temperature observations. In addition, there is a need to understand how the value of surface soil moisture and soil temperature measurements varies for different soil types, and for which type of soils the complementary nature of soil moisture and soil temperature measurements is more enhanced. In this study, we exhaustively investigate the relative significance of soil moisture and soil temperature measurements for the estimation of soil states and parameters for all 12 USDA soil textural classes. We focus also especially on the performance of soil moisture and soil temperature assimilation for simulating latent heat and sensible heat fluxes. It is found in several studies that univariate soil moisture assimilation does not improve the simulation of the latent heat flux (e.g., Gebler et al., 2019; Hung et al, 2022; Pipunic et al., 2008, 2013). The potential of soil temperature assimilation for better simulating latent heat flux is evaluated here and compared with soil moisture assimilation. Results will be discussed in this paper comparing univariate soil moisture or soil temperature assimilation versus joint assimilation of soil moisture and temperature. We also study the influence of observation depth on the estimation of soil states, parameters, and fluxes. Finally, we compare the worth of soil temperature data to estimate the soil moisture, hydraulic parameters, and heat flux for different soil types considering different climate conditions, that is, hot semi-arid, semi-arid, and sub-humid.

2 | MATERIALS AND METHODS

2.1 | Forward model

In this study, HYDRUS-1D is used as the forward model. It can simulate coupled water, vapor, and heat movement in one-dimensional unsaturated media (Šimůnek et al., 2013). HYDRUS is a numerical model, which solves Richards' equation for unsaturated flow and the advection–dispersion equation for heat transport. The governing equation for water and vapor transport in HYDRUS is described by a modified form of the Richards' equation as follows:

$$\frac{\partial \theta_T(h)}{\partial t} = \frac{\partial}{\partial z}\left[\left(K + K_{vh}\right)\left(\frac{\partial h}{\partial z} + 1\right) + \left(K_{LT} + K_{vT}\right)\frac{\partial T}{\partial z}\right] - S, \tag{1}$$

where θ_T is the sum of volumetric soil water content (θ) and vapor content (θ_v) (cm^3/cm^3), t (s) and z (cm) (positive upward) are time and space coordinates, h is pressure head in the soil column (cm), T is temperature (K), K and K_{vh} are isothermal hydraulic conductivity of liquid phase and vapor phase (cm/s), respectively, K_{LT} and K_{vT} are thermal hydraulic conductivity of the liquid phase and vapor phase (cm^2/K/s), respectively, and S is the sink term to account for root water uptake (cm^3/cm^3/s). In HYDRUS-1D, one can choose from five different analytical models (Brooks & Corey, 1964; Durner, 1994; Kosugi, 1996; van Genuchten, 1980; Vogel & Cislerova, 1988) for the soil water retention, $\theta(h)$, and relative permeability, $K(h)$, functions. In this study, the soil hydraulic functions according van Genuchten were used:

$$\theta\ (h) = \begin{cases} \theta_r + \frac{\theta_s-\theta_r}{[1+|\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases}, \tag{2}$$

$$K\ (h) = K_s\ S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2, \tag{3}$$

where, $m = 1 - 1/n$ and effective saturation $S_e = \frac{\theta-\theta_r}{\theta_s-\theta_r}$.

The van Genuchten equation consists of five independent parameters: θ_r (residual water content) (cm^3/cm^3), θ_s (saturated water content) (cm^3/cm^3), K_s (saturated hydraulic conductivity) (cm/s), and α (1/cm), and n (-) are van Genuchten empirical fitting/shape parameters (also called unsaturated flow parameters). For this study K_s, θ_r, θ_s, α, and n vary with the soil types but l is kept as a constant with a value of 0.5 for all soil types.

The governing equation for heat transport in HYDRUS-1D is as follows:

$$C_p(\theta)\frac{\partial T}{\partial t} + L_0\frac{\partial \theta_v}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\frac{\partial T}{\partial z}\right]$$
$$-C_w q\frac{\partial T}{\partial z} - C_v\frac{\partial q_v T}{\partial z} - L_0\frac{\partial q_v}{\partial z}, \tag{4}$$

where $\lambda(\theta)$ is the coefficient of apparent thermal conductivity of the soil (W/m/K), and C_p, C_w, and C_v are the volumetric heat capacities (J/K/m^3) of the soil medium, liquid phase, and vapor phase, respectively, q and q_v are water and vapor flux density (cm/s), and L_0 is volumetric latent heat of vaporization of liquid water (J/m^3). The heat capacity of composite soil is expressed as:

$$C_p\ (\theta) = \left(1.92 f_{\text{solid}} + 2.51 f_{\text{organic}} + 4.18\theta\right) 10^6. \tag{5}$$

Here, f_{solid} and f_{organic} refer to volumetric fractions (cm^3/cm^3) of solid phase and organic matter, respectively. Since, in this study it is assumed that there is no organic matter in the soil, $f_{\text{solid}} = 1 - \theta_s$. For the composite soil medium, $\lambda(\theta)$ is given by:

$$\lambda\ (\theta) = \lambda_0\ (\theta) + \beta_t C_w |q|, \tag{6}$$

where β_t is thermal dispersivity (cm). Two models are available in HYDRUS-1D for the estimation of thermal conductivity (λ_0). One is the Chung and Horton model (Chung & Horton, 1987), which provides thermal conductivity for three soil classes, that is, clay, loam, and sand. The other is the Campbell model (Campbell, 1985), which requires soil textural information (sand fraction [f_{sand}], clay fraction [f_{clay}], and silt fraction [$f_{\text{silt}} = f_{\text{solid}} - f_{\text{sand}} - f_{\text{clay}}$]) to estimate thermal conductivity. In this study, the Campbell model is used to generate ensembles of thermal conductivities corresponding to soil moisture and soil texture values:

$$\lambda_0\ (\theta) = A + B\theta - (A - D)\exp\left[-(C\theta)^E\right], \tag{7}$$

$$A = \frac{0.57 + 1.73 f_{\text{sand}} + 0.93 f_{\text{silt}}}{1 - 0.74 f_{\text{sand}} - 0.49 f_{\text{silt}}} - 2.8 f_{\text{solid}}\left(1 - f_{\text{solid}}\right), \tag{7a}$$

$$B = 2.8 f_{\text{solid}}, \tag{7b}$$

$$C = 1 + 2.6 f_{\text{clay}}^{-1/2}, \tag{7c}$$

$$D = 0.03 + 0.7 f_{\text{solid}}^2, \tag{7d}$$

$$E = 4.$$

Thermal dispersivity (β_t) is kept constant with a value of 5 cm for all soil types.

2.2 | Sequential data assimilation

This section provides a brief description of the EnKF and its usage in the study. Further details on the EnKF can be found in Burgers et al. (1998), Evensen (2003), Moradkhani et al. (2005), and Chaudhuri et al. (2018a, 2018b). SHPs ($\log(\alpha)$, $\log(n)$, $\log(K_s)$), soil thermal parameters (STPs, f_{sand} and f_{clay}) and soil states (θ and T) are estimated simultaneously by assimilating soil moisture and/or soil temperature observations. The EnKF consists of a forecast and analysis step. The forecast is given by:

$$x_{\tau+1}^{i,f} = M\left(x_\tau^{i,a}, p_\tau^{i,a}, u_\tau^i\right), \tag{8}$$

where i refers to the ensemble realization, a and f denote analysis and forecast, respectively, τ is model time step, M represents the physical model for 1D moisture and heat transport according Equations (1)–(7), used for propagating soil states forward in time ($x_{i,f}^{\tau+1}$), given soil states ($x_\tau^{i,a}$), soil parameters ($p_\tau^{i,a}$), and forcings (u_τ^i) at the current time step.

The analysis is given by:

$$\pi_{t+1}^{i,a} = \pi_{t+1}^{i,f} + \delta K_{t+1}\left(y_{t+1}^i - H x_{t+1}^{i,f}\right), \tag{9}$$

where, t is time of assimilation, $\pi_{t+1}^i = \binom{x_i^{t+1}}{p_i^{t+1}}$ is the vector with states and parameters, δ is the damping factor that takes a value between 0 and 1, y_{t+1}^i is a vector containing the perturbed observations, H is a linear operator that maps model states to observations, in this study it is composed of 0's and 1's, and K_{t+1} is Kalman gain. The damping factor (δ) is applied only for parameter updates and not for state updates.

The Kalman gain (K_{t+1}) is given by:

$$K_{t+1} = P^f_{t+1} H^T \left(H P^f_{t+1} H^T + R_{t+1} \right)^{-1}, \quad (10)$$

where R_{t+1} is the observation error covariance matrix and P^f_{t+1} the model error covariance matrix. P^f_{t+1} is estimated from the ensemble of forecasted results as follows:

$$P^f_{t+1} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\pi^{i,f}_{t+1} - \bar{\pi}^f_{t+1} \right) (\pi^{i,f}_{t+1} - \bar{\pi}^f_{t+1})^T, \quad (11a)$$

$$\bar{\pi}^f_{t+1} = \frac{1}{N} \sum_{i=1}^{N} \pi^{i,f}_{t+1}, \quad (11b)$$

where N is the number of ensemble members.

2.3 | Simulation set-up and experiments

Synthetic experiments are conducted to evaluate the effect of soil texture, observation depth, and climate on the estimation of soil moisture and temperature profile, soil hydraulic and thermal parameters, and latent and sensible heat fluxes. The impact of soil texture is studied using 12 different soil types according to USDA classification and the impact of observation depth is studied using soil moisture and soil temperature observations at five different depths from the surface. To compare the impact of different climates on the estimation of soil states, parameters, and fluxes we have used data of three meteorological stations, one situated in the Berambadi catchment, a second one in the Mulehole catchment (both are experimental watersheds and are part of Kabini CZO), and a third meteorological station is situated in Kalaburagi district, state of Karnataka in India. The Kabini CZO is situated in the southern part of India and provides time series of different climatic, hydrological, and geochemical variables to better understand the hydrological and biogeochemical cycles of the Kabini basin (Riotte et al., 2021; Sekhar et al., 2016). Berambadi, Kalaburagi, and Mulehole represent three different climate zones, that is, semi-arid, hot semi-arid, and sub-humid, respectively. Figure 1 shows the cumulative potential evapotranspiration (PET) and precipitation (P) for all three different regions. The PET/P ratios are 0.8, 1.5, and 2.2 for Mulehole, Berambadi, and Kalaburagi, respectively. Weather inputs (precipitation, wind speed, relative humidity, air temperature, and solar radiation) are obtained from all three meteorological stations. Figure 2 shows the time series of weather inputs of Berambadi.

2.3.1 | Reference runs

True (synthetic) soil moisture and soil temperature profiles are generated using the HYDRUS-1D forward model with weather data and soil parameters as inputs. Mean values of SHPs (saturated hydraulic conductivity and van Genuchten parameters) and STPs (sand fraction and clay fraction) of 12 different soil types are taken from Carsel and Parrish (1988) and used as true parameters as given in Table 1. The depth of the soil profile is 2 m and discretized into layers of 1 cm in HYDRUS. Initial soil moisture content is 0.30 cm^3/cm^3 and initial soil temperature 20°C, uniform along the soil column. The upper boundary condition for soil moisture transport is given by the atmospheric boundary condition including surface runoff. The actual water flux across the upper boundary is controlled by both atmospheric and existing soil moisture conditions. The lower boundary condition for soil moisture transport is free drainage. Free drainage is chosen as the lower boundary condition since the groundwater level in the study region ranges between 10 and 50 m depth, which is well below the simulated soil column here. The upper boundary condition for heat transport is the heat flux estimated from the soil surface energy balance and the lower boundary condition is zero gradient. Figures 3 and 4 show the variation of soil moisture and soil temperature with time and depth for the reference simulations for the 12 different soil types, using the meteorological inputs from the weather station installed in the Berambadi watershed as shown in Figure 2 and the mean soil hydraulic and thermal parameters given in Table 1. It is important to note that unless otherwise specified, results are obtained using meteorological data from the weather station installed at the Berambadi watershed.

Figure 5 shows soil moisture versus soil temperature for different soils averaged over depth and time. From Figures 3–5 it is observed that for the same meteorological inputs, sandy soil has a lower soil moisture content compared to clayey soil, which leads to higher soil temperatures for sandy soil compared to clayey soil. The mean soil moisture varies from 0.1 cm^3/cm^3 (sand) to 0.37 cm^3/cm^3 (silty clay loam) and mean soil temperature varies from 26°C (sand) to 23°C (silty clay loam). Figure 3 shows that in sandy soils infiltration fronts advance quickly during precipitation events from the surface to the bottom of the soil column as compared to soils with a higher clay content, implying that any addition of water at the surface will be reflected in the whole soil column faster in sandy soils compared to clayey soils. The color in Figure 3 indicates that the higher soil moisture content and the streaks are relatively more slanted for soil types with lower hydraulic conductivity. For clayey soil the moisture content below 50 cm soil depth is uniform. It is because the drainage of soil moisture in clayey soil by gravity is less but the moisture diffusion is more. For heat transfer, the streaks in the temperature plot

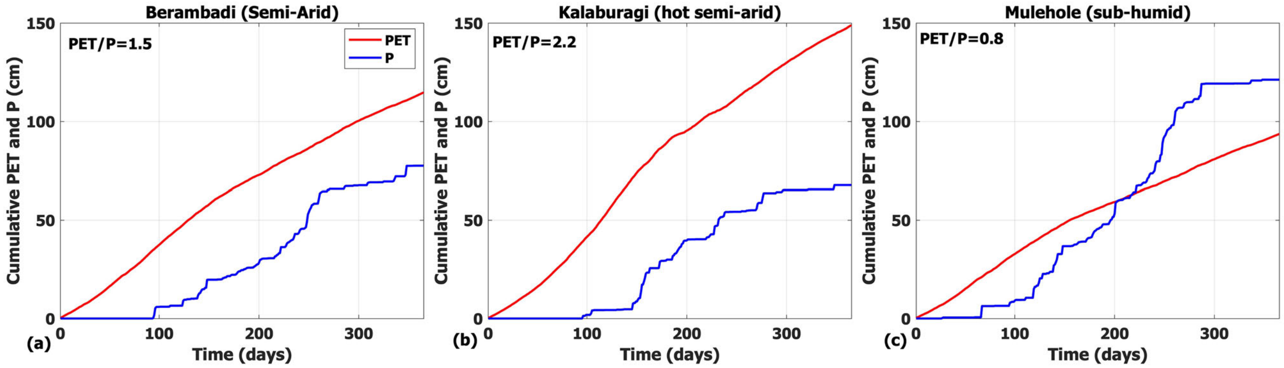

FIGURE 1 Cumulative potential evapotranspiration (PET) and cumulative precipitation (P) of three different places in South India, that is, (a) Berambadi, (b) Kalaburagi, and (c) Mulehole representing different climate zones, that is, semi-arid, hot semi-arid, and sub-humid, respectively.

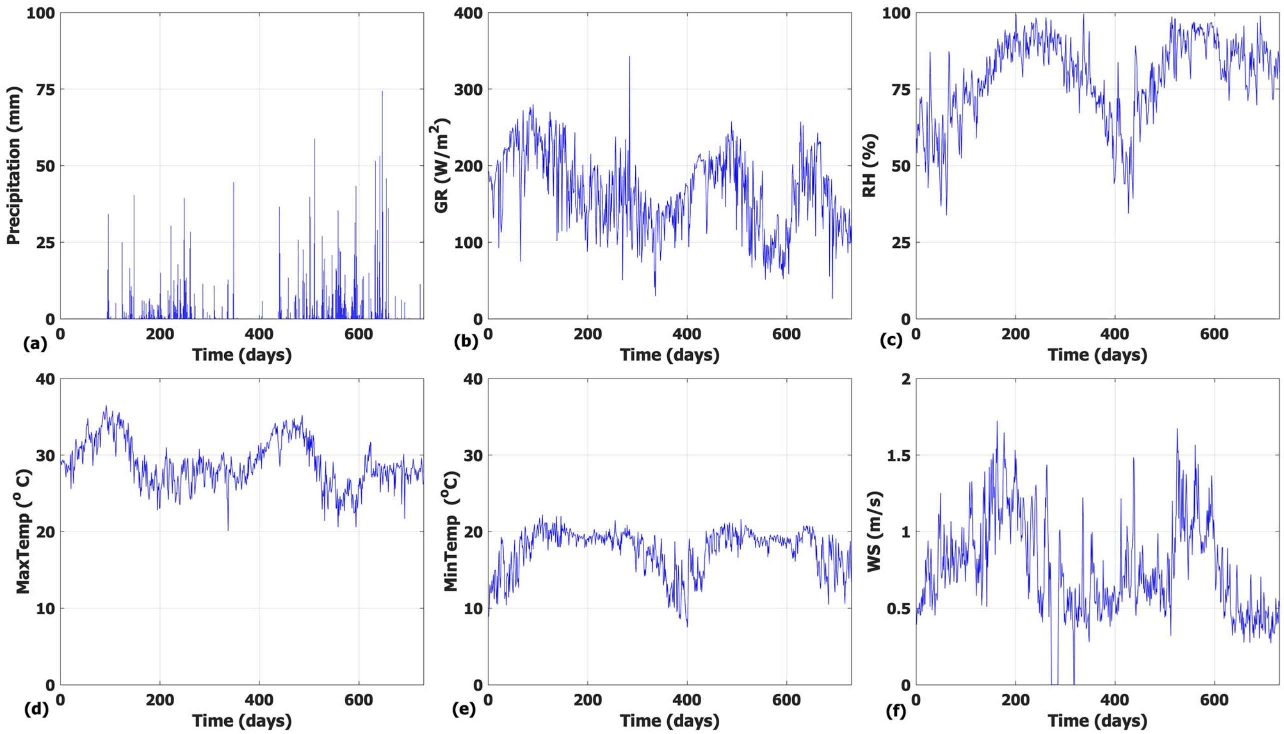

FIGURE 2 Time series of daily meteorological inputs: (a) precipitation, (b) global radiation, (c) relative humidity, (d) maximum temperature, (e) minimum temperature, and (f) wind speed, for the year 2017–2018 obtained from the weather station installed at Berambadi, Kabini CZO.

are more slanted for soil with more clayey soil because of less convective heat transfer.

2.3.2 | Ensemble runs

For estimation of states (soil moisture and soil temperature), parameters (soil hydraulic and STPs), and fluxes (latent heat and sensible heat) from soil moisture and/or soil temperature assimilation, an ensemble of soil parameters is generated considering SHPs (K_s, α, and n) to be lognormally distributed, STPs (f_{sand} and f_{clay}) to be normally distributed, and θ_r and θ_s deterministic. In this paper, SHPs are independently perturbed and estimated, and no pedotransfer function is used for them. Hundred realizations are used in this study and each experiment is repeated 10 times to compare robustly the accuracy of the estimated soil parameters for different assimilation settings and different soil textures. The 100 realizations of soil parameters for each repetition are sampled from a normal distribution with mean of the parameters ranging from $\mu + 2\sigma$ to $\mu - 2\sigma$, where μ is the true mean value of a parameter and σ is the standard deviation (see Table 1).

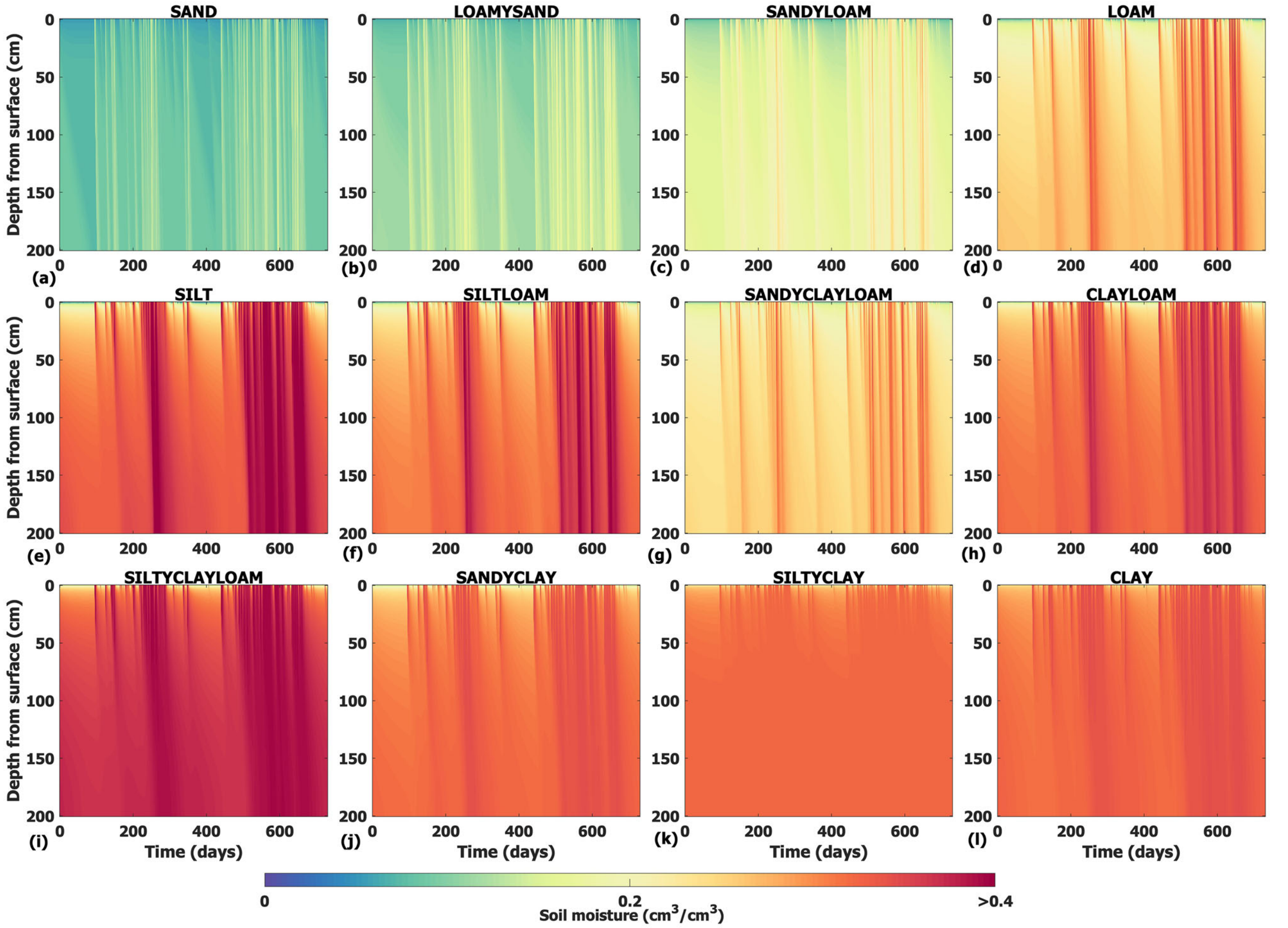

FIGURE 3 Time series of true soil moisture profiles (synthetic) over 2 years for 12 different soils simulated using meteorological inputs of Berambadi watershed as shown in Figure 2 and mean soil hydraulic and thermal properties given in Table 1.

Errors in the estimation of soil moisture and soil temperature are majorly due to uncertainties in forcings, initial conditions, and soil parameters. Model forcings are perturbed as indicated in Table 2. Ensembles of soil moisture and soil temperature observations are generated by perturbing true observations following a normal distribution with zero mean and standard deviation of 0.03 cm^3/cm^3 and 0.2 K, respectively and the perturbations are uncorrelated and also not correlated in time. Observations of soil moisture and soil temperature are assimilated daily at 00:00 h (midnight). The observation error of soil moisture and soil temperature are the same as the perturbation of the observations, that is, 0.03 cm^3/cm^3 and 0.2 K, respectively.

A damping factor of 0.1 is applied to counteract filter divergence (Franssen & Kinzelbach, 2008; Keller et al., 2018). Damping reduces spurious updates of parameters and stabilizes the parameter estimation with EnKF. To further stabilize the estimation of parameters, they are not updated when the intensity of precipitation is greater than 30 mm/day (Bauser et al., 2016). A spin up period of 2 years is chosen in this study, as it is long enough to reach equilibrium soil moisture and soil temperature conditions. Weather inputs for the period 2017–2018 are considered for both spin up and simulation.

2.4 | Sensitivity analysis

A global sensitivity analysis is carried out using the VARS-TOOL (https://github.com/vars-tool/vars-tool) (Razavi & Gupta, 2019; Razavi et al., 2019) to compare the sensitivity of soil moisture and soil temperature at different depths to the soil hydraulic [log(K_s), log(α), and log(n)] and soil thermal (f_{sand} and f_{clay}) parameters for different soil types. We have adopted a variance-based sensitivity analysis considering Sobol total-effect index (Sobol, 2001) where the sensitivity index of output variable $Y = f(X_1, X_2, .., X_n)$ to any input/system parameters X_i is given as,

$$S_{Ti} = 1 - \frac{Var\left[E\left[Y|X_{\sim i}\right]\right]}{Var\left[Y\right]}. \tag{12}$$

Here $Var[]$ and $E[]$ represent the calculation of the variance and expectation of random variable and $X_{\sim i}$ corresponds

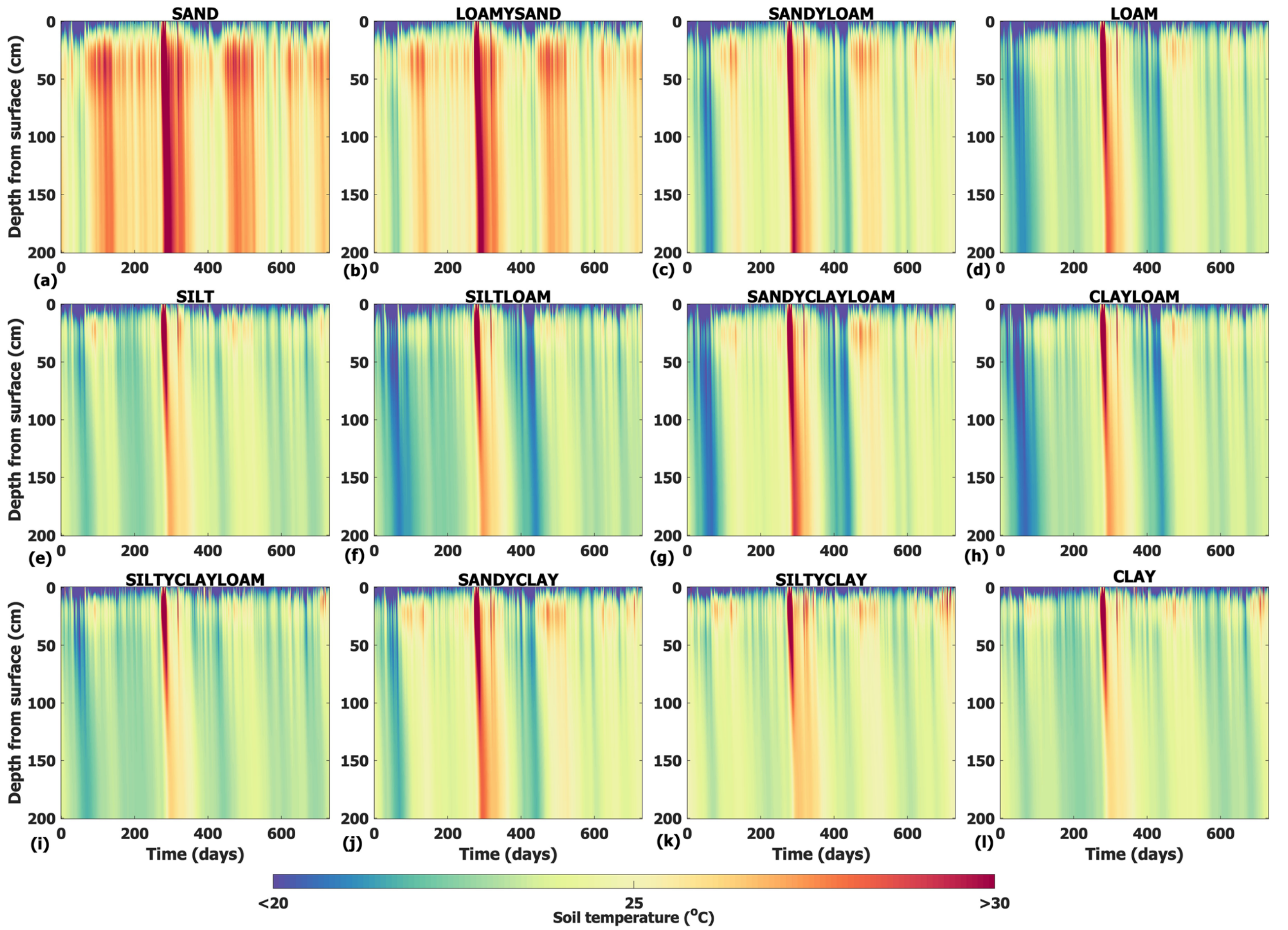

FIGURE 4 Time series of true soil temperature profiles (synthetic) over 2 years for 12 different soils simulated using meteorological inputs of Berambadi watershed as shown in Figure 2 and mean soil hydraulic and thermal properties given in Table 1.

to the vector of all variables except X_i. In this study, Y can be the soil moisture and soil temperature while X_i (for $i = 1, \ldots, 5$) are five soil properties [$\log(K_s)$, $\log(\alpha)$, $\log(n)$, f_{sand}, and f_{clay}]. To perform the sensitivity analysis using the VARS-TOOL for each of the 12 soil types considered in this study, 1000 realizations of the parameter sets [$\log(K_s)$, $\log(\alpha)$, and $\log(n)$, f_{sand}, and f_{clay}] are generated and time series of soil moisture and soil temperature for the period of 365 days (year 2017) are obtained using HYDRUS-1D keeping the meteorological data constant for different runs.

Time aggregated sensitivities of simulated soil moisture and soil temperature at different depths to soil hydraulic and thermal parameters are shown in Figure 6. From Figure 6 it is evident that both soil moisture and soil temperature are more sensitive to $\log(K_s)$ compared to other soil parameters for the majority of soil types. The sensitivity of soil moisture to $\log(K_s)$ is higher in the middle region of the soil texture triangle, that is, loamy soils, whereas the sensitivity of soil temperature to $\log(K_s)$ is higher for soils with higher clay content. In general soil moisture is more sensitive to $\log(K_s)$ compared to soil temperature. Figure 6b1,b2 indicates that the sensitivities of both soil moisture and soil temperature to $\log(\alpha)$ are much smaller for soils with high sand content. However, compared to soil moisture, soil temperature is more sensitive to $\log(\alpha)$ for all soil types (except for soil moisture at surface which is most sensitive to α and n). Figure 6c1 shows that for soils with high clay content such as silty clay and clay soil, moisture is highly sensitive to $\log(n)$ compared to other SHPs. It is evident from Figure 6d1,e1 that soil moisture is insensitive to STPs, that is, f_{sand} and f_{clay}. Interestingly, the sensitivity of soil temperature to f_{sand} is generally less for soils with higher sand content except for pure sand. On the contrary, the sensitivity of soil temperature to f_{clay} is higher for soils with higher sand content. Comparing the sensitivity of soil moisture at different soil depths to $\log(K_s)$, it is clear that the near surface soil moisture is less sensitive to $\log(K_s)$ than deeper soil moisture, for all soil types. The unsaturated flow parameters α and n affect soil moisture at 0 cm more than the deeper soil moisture. Soil temperature at 5 cm is the most sensitive to $\log(K_s)$ and the sensitivity of soil temperature to $\log(K_s)$ decreases for greater depths. The sensitivity of soil temperature to the other SHPs decreases also with depth.

TABLE 1 Mean and standard deviation of soil hydraulic and thermal properties for different soil types taken from Carsel and Parrish (1988).

Soil type	θ_r (cm^3/cm^3)	θ_s (cm^3/cm^3)	log(α) (α in 1/cm)		log(n)		log(K_s) (K_s in cm/d)		f_{sand} (%)		f_{clay} (%)	
			μ	σ	μ	σ	μ	σ	μ	σ	μ	σ
Sand (S)	0.045	0.43	−1.95	0.20	0.98	0.11	6.45	0.49	92.7	3.7	2.9	2
Loamy sand (LS)	0.057	0.41	−2.14	0.34	0.82	0.12	5.62	0.69	80.9	3.8	6.4	3.2
Sandy loam (SL)	0.065	0.41	−2.70	0.47	0.63	0.09	4.18	0.98	63.4	7.9	11.1	4.8
Loam (L)	0.078	0.43	−3.47	0.54	0.44	0.07	2.52	1.18	40	6.5	19.7	5.2
Silt (Si)	0.034	0.46	−4.22	0.42	0.31	0.04	1.29	1.00	5.8	4.5	9.5	2.7
Silt loam (SiL)	0.067	0.45	−4.07	0.55	0.34	0.09	1.31	1.46	16.6	11.7	18.5	5.9
Sandy clay loam (SCL)	0.1	0.39	−3.00	0.59	0.39	0.09	2.61	1.30	54.3	7.3	27.4	4
Clay loam (CL)	0.095	0.41	−4.21	0.70	0.27	0.07	0.78	1.45	29.8	5.9	32.6	3.7
Silty clay loam (SiCL)	0.089	0.43	−4.76	0.55	0.21	0.05	−0.54	1.46	7.6	5.3	33.2	3.7
Sandy clay (SC)	0.1	0.38	−3.78	0.58	0.20	0.08	0.13	1.37	47.5	3.9	41	4.5
Silty clay (SiC)	0.07	0.36	−5.64	0.83	0.08	0.06	−2.46	1.86	6.1	4.5	46.3	4.9
Clay (C)	0.068	0.38	−5.42	1.09	0.08	0.08	0.72	1.30	14.9	10.7	55.2	10.9

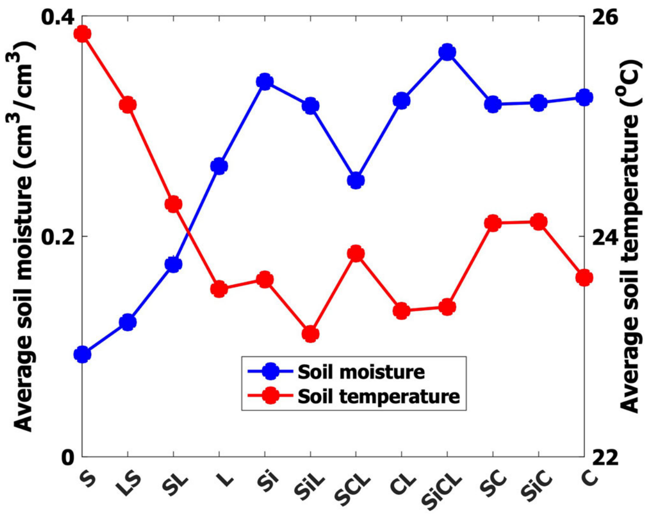

FIGURE 5 Comparison of soil moisture and soil temperature averaged over soil column of 2 m and 2 years for 12 different soil types.

TABLE 2 Perturbation of forcings for the generation of weather inputs for ensemble members.

Forcings	Error distribution	Mean	Standard deviation
Precipitation (mm)	Gaussian, multiplicative	1	0.2
Radiation (W/m^2)	Gaussian, multiplicative	1	0.1
Air temperature (°C)	Gaussian, additive	0	0.5
Relative humidity (%)	Gaussian, additive	0	1
Wind speed (m/s)	Gaussian, multiplicative	1	0.2

3 | RESULTS

The synthetic experiments where states (soil moisture and soil temperature), parameters (soil hydraulic and STPs), and fluxes (latent heat and sensible heat) are estimated are conducted for the 12 different soil types. For each soil type the study is done with open loop (OL) and three different assimilation settings. The three assimilation settings are: (i) SM5, where soil moisture alone at 5 cm is assimilated; (ii) ST5, soil temperature alone at 5 cm is assimilated; (iii) SMT5, both soil moisture and soil temperature at 5 cm are assimilated. In addition, to study the effect of measurement depth on the estimation accuracy, soil moisture and soil temperature are assimilated at different depths from the surface, that is, 0 cm (skin surface) (SM0/ST0, soil moisture, or soil temperature at surface), 5 cm (SM5/ST5), 10 cm (SM10/ST10), 30 cm (SM30/ST30), and 50 cm (SM50/ST50). The impact of adding more observations for the estimation of soil states, parameters, and fluxes is also studied. SM550 is assimilation of soil moisture measured at both 5 and 50 cm, ST550 is assimilation of soil temperature measured at both 5 and 50 cm, and SMT550 is assimilation of soil moisture and soil temperature measurements at both 5 and 50 cm.

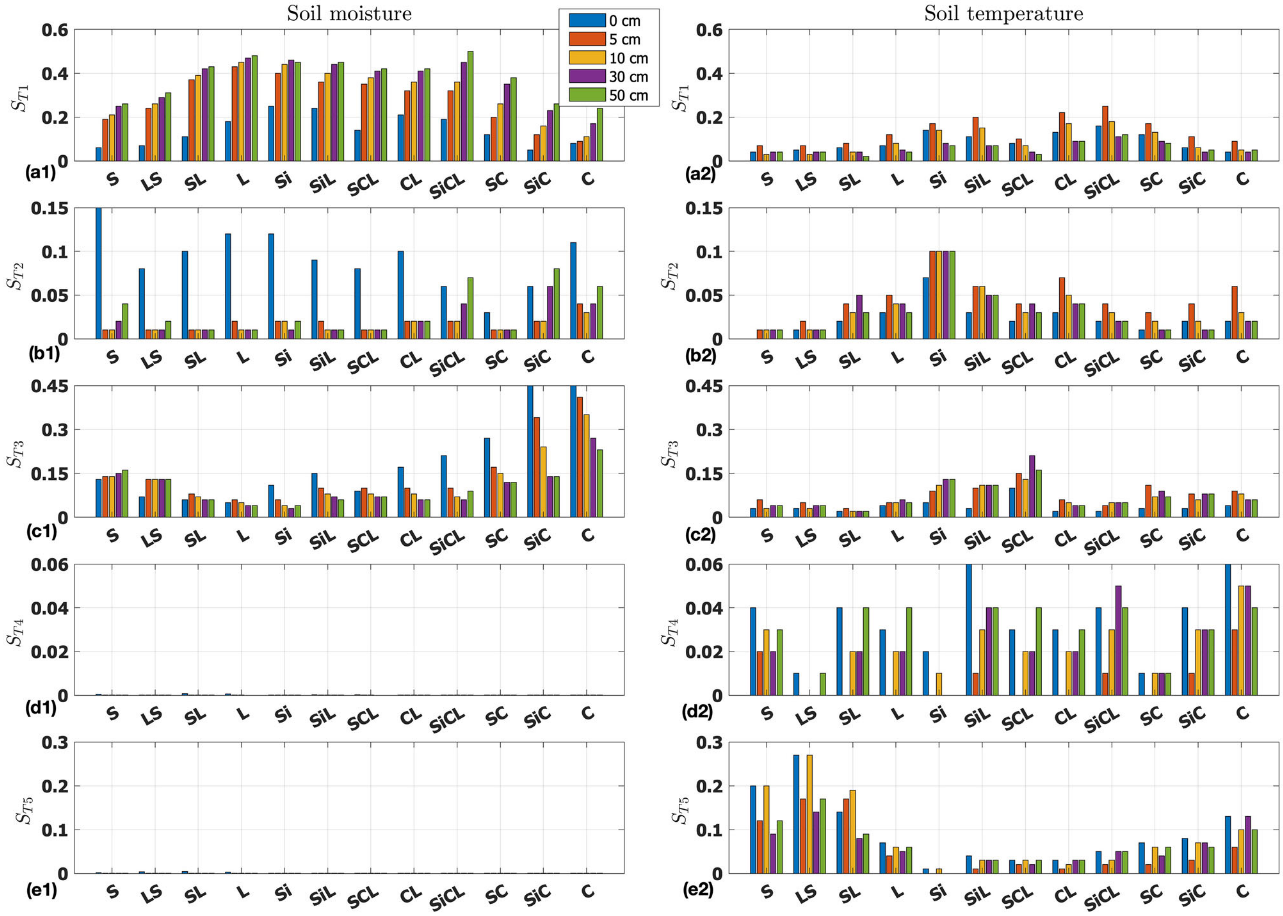

FIGURE 6 Comparison of sensitivity of soil moisture and soil temperature at different depths to soil hydraulic and thermal properties (a1, a2) $\log(K_s)$, (b1,b2) $\log(\alpha)$, (c1,c2) $\log(n)$, (d1,d2) f_{sand}, and (e1,e2) f_{clay}. Soil types: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

3.1 | Effect of soil texture

3.1.1 | Estimation of state variables

Figure 7 shows that the mean RMSE (average over 10 repetitions) for the estimation of the soil moisture profile in the open loop ranges from 0.016 cm^3/cm^3 (silty clay) to as high as 0.066 cm^3/cm^3 (silt loam). The wide range of RMSE in the open loop for different soil textures is due to the high range of uncertainty in the SHPs and the varying sensitivities of soil moisture to SHPs among soil textures. The mean RMSE for the estimation of the soil moisture profile is ≤0.01 cm^3/cm^3 for all soils when soil moisture data at 5 cm depth is assimilated.

Assimilation of soil temperature data at 5 cm improves the estimation of the soil moisture profile compared to the open loop in all 12 soil types. For this case, the mean RMSE for the estimation of the soil moisture profile is ≤0.04 cm^3/cm^3 for all soil types. ST5 shows a better performance for the estimation of the soil moisture profile for soils with a higher clay content compared to soils with a higher sand content. This could be explained by the observed higher correlation between soil moisture and soil temperature in clayey soils compared to sandy soils and also higher sensitivity of soil temperature to SHPs in clayey soils compared to sandy soils.

The RMSE reduction (compared to open loop) for soil types, "S," "SL," "L," "Si," and "SCL," is around 30% when ST5 is assimilated (Table 3). However, reductions higher than 65% are found for soil textures "SiCL," "SiC," and "C." A little additional improvement in the estimation of the soil moisture profile is observed when both soil moisture at 5 cm and soil temperature at 5 cm are assimilated simultaneously (SMT5) as compared to ST5 and SM5 alone, especially in soils with higher clay content. The improvement is very small for scenario SMT5 compared to SM5 as SM5 assimilation already reduced the RMSE to 0.01 cm^3/cm^3. The RMSE reduction averaged over all soil types (always compared with open loop) is 79% for assimilating soil moisture alone and 81% for joint soil moisture and temperature assimilation (SMT5).

Figure 7b compares the estimation of the soil temperature profile using OL, SM5, ST5, and SMT5. A significant RMSE

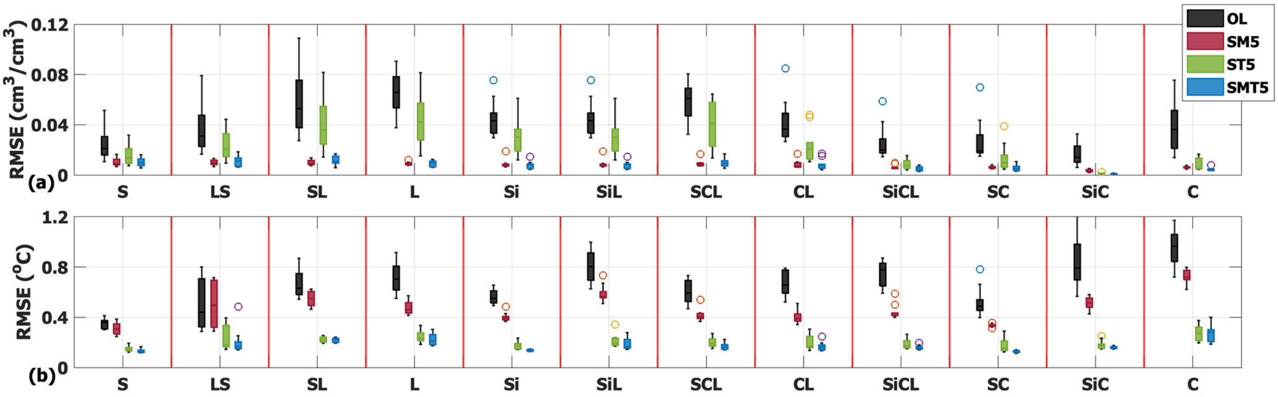

FIGURE 7 Comparison of root mean square error (RMSE) for the estimation of (a) soil moisture profile and (b) soil temperature profile for open loop simulations (OL), univariate assimilation of soil moisture observations from 5 cm depth (SM5), univariate assimilation of soil temperature observations at 5 cm depth (ST5), and joint soil moisture and soil temperature assimilation at 5 cm depth (SMT5). Each box plot represents the results from 10 tests using different initial parameter sets. In the box plot, the middle line denotes the median value, the edges of the box are the interquartile range (IQR), the maximum length of the whiskers is set to be 1.5 times the IQR, and values larger/smaller than the maximum/minimum the whiskers are considered as outliers (hollow circles). Soil types: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

TABLE 3 Root mean square error (RMSE) (average of 10 tests) of the estimated soil moisture profile for 12 soil types compared to open loop (OL) for different data assimilation experiments (soil moisture observations from 5 cm depth [SM5], soil temperature observations at 5 cm depth [ST5], and soil moisture and soil temperature assimilation at 5 cm depth [SMT5]).

RMSE (%)	S	LS	SL	L	Si	SiL	SCL	CL	SiCL	SC	SiC	C
OL	100	100	100	100	100	100	100	100	100	100	100	100
SM5	42	26	17	14	20	18	16	20	24	22	20	16
ST5	67	62	69	68	68	60	69	56	33	49	8	23
SMT5	42	29	20	14	17	16	17	21	19	21	6	12

Abbreviations: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

TABLE 4 Root mean square error (RMSE) (average of 10 tests) of the estimated soil temperature profile for 12 soil types for different data assimilation experiments (soil moisture observations from 5 cm depth [SM5], soil temperature observations at 5 cm depth [ST5], and soil moisture and soil temperature assimilation at 5 cm depth [SMT5]) compared to open loop (OL).

RMSE (%)	S	LS	SL	L	Si	SiL	SCL	CL	SiCL	SC	SiC	C
OL	100	100	100	100	100	100	100	100	100	100	100	100
SM5	89	100	82	67	71	72	69	60	60	64	61	76
ST5	43	46	33	35	32	26	33	30	25	34	22	29
SMT5	38	41	33	31	24	23	28	25	22	25	19	28

Abbreviations: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

reduction in the estimation of the soil temperature profile for all soils is observed when ST5 is assimilated. The RMSE reduction (compared to open loop) for all soil types is between 55% for soils "S" and 80% for "SiC" (see Table 4). Assimilation of soil temperature observation at a particular depth improves the whole profile of soil temperature through correlation with soil temperature at different depths. Joint updating of states and parameters further improves the estimation of the soil temperature profile.

It is also observed that assimilation of soil moisture (SM5) can reduce the RMSE of the soil temperature profile compared to the OL. The RMSE for the estimation of the soil temperature profile reduces on average 27% compared to the open loop run for the SM5 assimilation, with

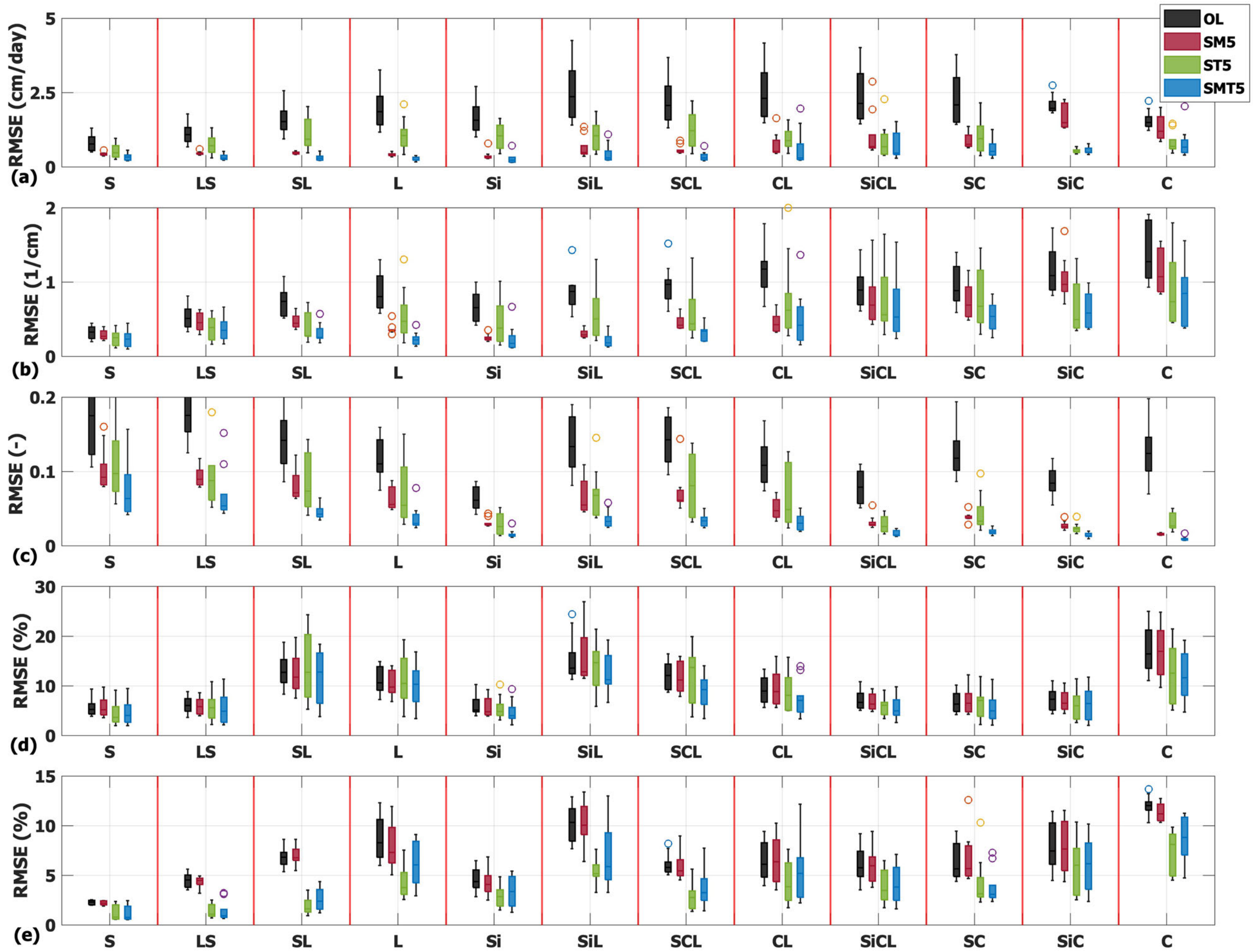

FIGURE 8 Comparison of root mean square error (RMSE) for the estimation of soil hydraulic properties (a) $\log(K_s)$, (b) $\log(\alpha)$, and (c) $\log(n)$ and soil thermal properties (d) f_{sand} and (e) f_{clay} for the data assimilation experiments soil moisture observations from 5 cm depth (SM5), soil temperature observations at 5 cm depth (ST5), and soil moisture and soil temperature assimilation at 5 cm depth (SMT5). Each box plot represents the results from 10 tests using a set of different initial parameters. Soil types: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

higher RMSE reduction for soils with a higher clay content and lower reduction in RMSE for soils with higher sand content. The RMSE of the soil temperature profile reduces by an additional 4%, if soil moisture and soil temperature are jointly assimilated (compared to soil temperature alone).

3.1.2 | Estimation of soil parameters

Figure 8 shows the estimation accuracy of SHPs and STPs for different soil types for the SM5, ST5, and SMT5 assimilation scenarios. Improvement in the estimation of SHP is observed for all three scenarios. In general, error in the estimation of $\log(\alpha)$ is higher than for $\log(K_s)$ and $\log(n)$, which can be explained by the lower sensitivity of soil moisture and soil temperature to $\log(\alpha)$ compared to $\log(K_s)$ and $\log(n)$ as deduced from the sensitivity analysis. It is observed that ST5 performed better for soils with higher clay content compared to sandy soils, especially for $\log(K_s)$. SM5 performed better for soils with higher sand content especially for $\log(K_s)$ which can be explained through sensitivity analysis. Figure 6a1 shows that the sensitivity of soil moisture to $\log(K_s)$ is higher for loamy soils as compared to soils with higher clay content like SiC or C.

Assimilation of SMT5 performed better for all 12 soil types compared to SM5 and ST5 for the estimation of SHPs (see Figure 8). On average (over all 12 soil types) assimilation of SM5 improves the estimation of $\log(K_s)$, $\log(\alpha)$, and $\log(n)$ compared to the open loop by 59%, 35%, and 56%, respectively, and assimilation of ST5 49%, 32%, and 52%, respectively. The joint assimilation of soil moisture and soil temperature (SMT5) gives the largest improvements of 74%, 50%, and 75%, respectively.

Figure 8d,8e shows that there is no improvement over open loop in the estimation of STPs for univariate soil

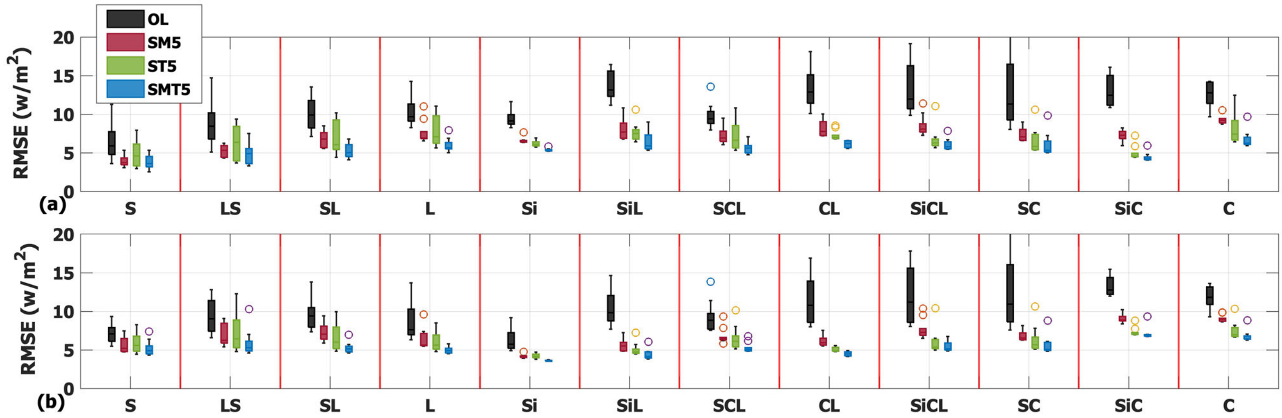

FIGURE 9 Comparison of root mean square error (RMSE) for the estimation of (a) latent heat and (b) sensible heat flux for the data assimilation scenarios soil moisture observations from 5 cm depth (SM5), soil temperature observations at 5 cm depth (ST5), and soil moisture and soil temperature assimilation at 5 cm depth (SMT5). Each box plot represents the results from 10 tests using different initial parameter sets. Soil types: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

moisture assimilation. Soil moisture and soil temperature are one-way coupled, which implies that modifications in soil moisture change soil thermal conductivity, soil heat capacity, surface energy balance, and ultimately soil temperature (Dong et al., 2016). On the other hand, change in soil temperature does not influence SHPs and soil moisture. Assimilation of ST5 improves the estimation of STPs compared to the open loop, and error in the estimation of f_{sand} is higher compared to f_{clay} when ST5 is assimilated. Assimilation of ST5 performed better than SMT5 for the estimation of f_{clay}, whereas SMT5 performed better than ST5 for the estimation of f_{sand}. Assimilation of ST5 improves the estimation of f_{sand} and f_{clay} compared to the open loop by 8% and 45%, respectively, and for SMT5 assimilation the improvement is 18% and 37%, respectively.

3.1.3 | Estimation of latent and sensible heat fluxes

From Figure 9a,b it is observed that assimilation of soil moisture and/or soil temperature (SM5, ST5, and SMT5) also improves the estimation of latent and sensible heat fluxes compared to OL. Estimation of LE and H is better for 8 out of the 12 soil types when ST5 is assimilated as compared to SM5 assimilation. Assimilation of SM5 performs better compared to ST5 for the estimation of LE and H in the soil types with higher sand content such as sand and loamy sand. On average, the assimilation of SM5 improves the estimation of latent heat and sensible heat by 35% and 33%, respectively, compared to the open loop. The assimilation of ST5 improves the estimation of LE and H both by 38%. Tables 5 and 6 show that SMT5 resulted for all soil types in better estimation of both latent heat (LE) and sensible heat (H) fluxes compared to SM5 and ST5. Combined assimilation of soil moisture and soil temperature (SMT5) improves the estimation of LE and H by 49% and 46%, respectively, compared to the open loop. Seneviratne et al. (2010) show that soil moisture and evapotranspiration are strongly coupled in the transition zone, that is, under water limited conditions and the strength of coupling decreases as the regime changes from water limited to energy limited. Due to weak coupling of soil moisture and evapotranspiration under energy limited conditions, improving the soil moisture profile does not impact much the estimation of water and energy fluxes. Assimilation of soil temperature is relatively more important in energy limited conditions for better estimation of latent and sensible heat fluxes.

3.2 | Effect of assimilation depth

Table S1 shows the estimated soil states, fluxes, and parameters for different soil types and assimilation scenarios, including different measurement depths for soil moisture and temperature. Measurements at 0 cm (skin surface), 5, 10, 30, and 50 cm depth are chosen to check the influence of measurement depth on the estimation accuracy. The influence of the measurement depth on the estimation accuracy is in-line with the sensitivity results. The deeper the soil moisture measurement, the better the estimation of the soil moisture profile. On the other hand, the assimilation of soil temperature measurements at 5 cm depth results in the best estimates of soil moisture and temperature profiles, while deeper soil temperature measurements have less value. Latent and sensible heat fluxes are better estimated when the measurement depth is at or near the surface (0 or 5 cm depth) and observations below 5 cm depth have limited value for the estimation of the fluxes. It is important to keep here in mind that simulations are

TABLE 5 Root mean square error (RMSE) (average of 10 tests) of latent heat estimation for 12 soil types for the data assimilation experiments soil moisture observations from 5 cm depth (SM5), soil temperature observations at 5 cm depth (ST5), and soil moisture and soil temperature assimilation at 5 cm depth (SMT5) compared to open loop run.

RMSE (%)	S	LS	SL	L	Si	SiL	SCL	CL	SiCL	SC	SiC	C
OL	100	100	100	100	100	100	100	100	100	100	100	100
SM5	62	60	68	74	70	60	74	61	63	57	55	74
ST5	75	73	70	75	65	56	74	54	50	51	38	64
SMT5	60	56	52	58	57	48	57	46	45	47	34	53

Abbreviations: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

TABLE 6 Root mean square error (RMSE) (average of 10 tests) of sensible heat estimation for 12 soil types for the data assimilation experiments soil moisture observations from 5 cm depth (SM5), soil temperature observations at 5 cm depth (ST5), and soil moisture and soil temperature assimilation at 5 cm depth (SMT5) compared to open loop run.

RMSE (%)	S	LS	SL	L	Si	SiL	SCL	CL	SiCL	SC	SiC	C
OL	100	100	100	100	100	100	100	100	100	100	100	100
SM5	78	73	74	74	66	53	73	53	63	55	69	76
ST5	82	78	67	71	67	48	70	44	49	51	55	63
SMT5	74	63	53	58	57	41	57	39	44	45	54	57

Abbreviations: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

for bare soil conditions. The estimation of K_s is better when soil moisture is measured deeper, but the estimation of shape parameters α and n is better for shallow measurements. The estimation of all three SHP's is better when soil temperature is measured at 0 or 5 cm, compared to deeper layers. Soil temperature measurements at more than 30 cm depth have very low value for the estimation of soil states, parameters, and fluxes. The impact of adding more observations for the estimation of soil states, parameters, and fluxes is also studied for four soil types, that is, loamy sand, loam, silt, and clay. In general, adding more observations further reduces the RMSE and the best estimation accuracy is observed for SMT550, that is, assimilation of soil moisture and soil temperature measurements at both 5 and 50 cm. The RMSE reduction for the soil moisture profile estimation is around 15% for ST550 assimilation (soil temperature at both 5 and 50 cm) compared to ST5 assimilation, except for clay soil where the RMSE reduction is only 6%. The RMSE reduction for the soil moisture profile estimation is only 5% for SM550 assimilation (soil moisture at both 5 and 50 cm) compared to SM5 assimilation. The estimation of latent and sensible heat flux is not much improved when additional observations from deeper layers are assimilated. A small (2%–3%) RMSE reduction is observed in the estimation of SHPs for SM550 compared to SM5 assimilation, whereas 10%–15% RMSE reduction is observed for ST550 compared to ST5.

3.3 | Effect of climate

To investigate the robustness of our study, we have compared the estimation accuracy of states, parameters, and fluxes for three different meteorological forcings from three different places of South India, that is, Berambadi, Kalaburagi, and Mulehole representing three different climate zones, that is, semi-arid, hot semi-arid, and sub-humid, respectively. The simulations for Mulehole and Kalaburagi are done for 1 year and the RMSE for the estimation of states and fluxes is calculated for the last 100 days of the simulation. The RMSE for the parameter estimates is calculated at the end of the simulation period. For the sake of comparing Berambadi results with those of Mulehole and Kalaburagi in this particular section, the RMSE for state variables and fluxes at the Berambadi location were assessed for the final 100 days of the first year of simulation and the RMSE for parameter estimates in Berambadi were determined at the end of the first year. This approach enables a direct comparison of the accuracy of state and flux predictions, as well as parameter estimates, between Berambadi and the other two locations, as in the rest of the paper simulations for Berambadi were analyzed for a period of 2 years.

Table 7 shows that in general soil temperature assimilation resulted in better estimation of soil states, parameters, and fluxes for silt and clay soils than for loamy sand and

TABLE 7 Root mean square error (RMSE) (average of 10 tests) of estimation of soil states, parameters and fluxes for different soil types and meteorological forcings compared to open loop (OL) run.

RMSE (%)			Berambadi (semi-arid) PET/P = 1.5			Kalaburagi (hot semi-arid) PET/P = 2.2			Mulehole (sub-humid) PET/P = 0.8		
		OL	SM5	ST5	SMT5	SM5	ST5	SMT5	SM5	ST5	SMT5
Soil moisture	Loamy sand	100	31	65	33	31	61	34	27	75	28
	Loam	100	16	69	15	23	60	16	15	84	16
	Silt	100	24	75	22	20	60	18	23	74	19
	Clay	100	15	35	12	17	67	15	21	65	14
Soil temperature	Loamy sand	100	98	49	41	93	43	43	83	64	58
	Loam	100	73	44	36	75	31	30	82	68	56
	Silt	100	83	39	33	76	23	16	64	27	24
	Clay	100	78	34	30	84	33	23	93	48	49
Latent heat	Loamy sand	100	57	69	51	58	73	56	54	70	46
	Loam	100	73	81	52	86	85	62	64	71	51
	Silt	100	76	61	52	72	56	50	71	55	45
	Clay	100	79	66	60	64	67	55	83	65	56
Sensible heat	Loamy sand	100	71	73	60	79	84	77	69	78	62
	Loam	100	77	81	59	91	85	67	68	74	56
	Silt	100	71	60	51	67	52	47	71	55	46
	Clay	100	85	69	65	62	74	54	84	71	59
log K_s	Loamy sand	100	48	75	42	49	66	40	44	81	41
	Loam	100	30	65	22	41	56	23	26	78	22
	Silt	100	38	69	28	32	62	28	33	74	24
	Clay	100	82	60	61	79	68	71	84	72	63
log α	Loamy sand	100	93	82	80	90	82	79	90	78	77
	Loam	100	69	80	45	69	91	56	54	77	35
	Silt	100	68	78	58	70	73	51	52	71	38
	Clay	100	84	78	64	90	82	78	80	80	74
log n	Loamy sand	100	54	68	47	59	70	50	54	70	41
	Loam	100	61	71	42	65	75	51	57	79	51
	Silt	100	57	62	37	59	31	23	59	36	29
	Clay	100	19	41	12	14	68	11	18	65	14
f_{sand}	Loamy sand	100	98	97	96	105	102	96	98	84	91
	Loam	100	94	101	92	105	107	102	99	89	91
	Silt	100	96	91	84	99	86	88	95	88	90
	Clay	100	100	85	75	104	102	66	103	85	76
f_{clay}	Loamy sand	100	97	42	41	101	66	69	104	82	83
	Loam	100	92	57	76	101	58	63	98	88	83
	Silt	100	95	74	85	101	83	88	101	90	90
	Clay	100	95	64	76	95	54	82	93	79	86

loam soils, for all three different meteorological forcings. The estimation of latent and sensible heat flux improved more with soil temperature assimilation than with soil moisture assimilation for silt and clay soil types. On the other hand, in loamy sand and loam soils the estimation of latent and sensible heat flux improved more with soil moisture assimilation than with soil temperature assimilation. This was the case for all three sites. Simultaneous assimilation of both soil moisture and temperature consistently performed better for estimating soil states, parameters, and fluxes for all textures and sites compared to univariate assimilation of soil moisture or soil temperature. In general, for soil moisture assimilation the performance increased as we move from hot semi-arid to sub-humid climate regions (sub-humid > semi-arid > hot

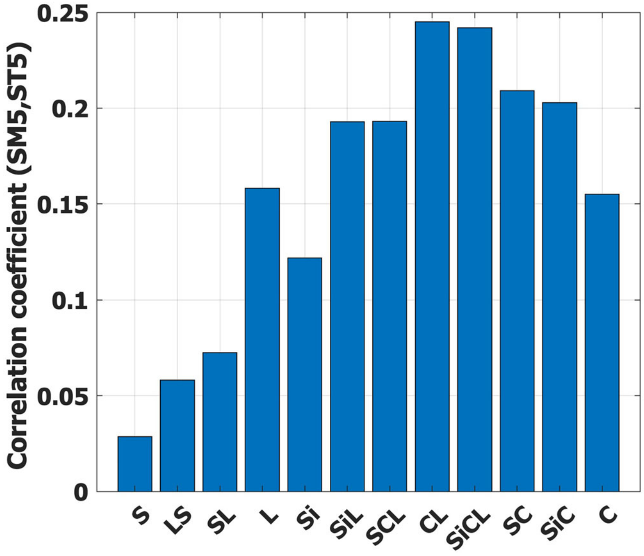

FIGURE 10 Correlation between soil moisture and soil temperature at 5 cm depth for 12 soils. Soil types: S (sand), LS (loamy sand), SL (sandy loam), L (loam), Si (silt), SiL (silt loam), SCL (sandy clay loam), CL (clay loam), SiCL (silty clay loam), SC (sandy clay), SiC (silty clay), C (clay).

semi-arid) and from permeable to less permeable soils (loamy sand and loam > silt and clay). In general, for soil temperature assimilation the estimation of latent and sensible heat fluxes improved more in sub-humid climates (sub-humid > semi-arid > hot semi-arid). The RMSE reduction (compared to open loop) for the estimation of latent heat flux, averaged over four soil types, was 35% for Mulehole (sub-humid), 31% for Berambadi (semi-arid), and 30% for Kalaburagi (hot semi-arid). The RMSE reduction for the estimation of sensible heat flux, averaged over four soil types, was 30% for Mulehole, 29% for Berambadi, and 26% for Kalaburagi.

4 | DISCUSSION

Figure 10 shows the correlation between soil moisture and soil temperature for different soil textures, based on daily data for 10 simulation experiments and 100 ensemble members per simulation experiment. Positive correlation is observed between soil moisture and soil temperature as we have used soil temperature observations at mid-night in our study. Previous studies (Dong et al., 2015b; Kayssi et al., 1990) showed positive correlation when soil temperature at night was considered but negative correlation when soil temperature at day was considered. Thus, the matching trend between our study and previous studies with regard to the correlation between soil moisture and soil temperature confirms the fidelity of our numerical simulation results. With increase in soil moisture content, maximum soil temperature decreases (day-time) and minimum soil temperature (night-time) increases. With increase in soil moisture the soil heat storage capacity increases which leads to reduced difference between day-time soil temperature and night-time soil temperature. The decrease in day-time soil temperature is larger than the increase in night-time soil temperature which leads to lower average soil temperature for soils with higher soil moisture content (Kayssi et al., 1990). Correlations between soil moisture at 5 cm and soil temperature at 5 cm are higher for clayey soils than for sandy soils. Equation (7) shows that thermal conductivity controls the vertical soil temperature distribution, which depends on soil texture and soil moisture. Soils with higher clay content have a higher water retention capacity than soils with higher sand content, which leads to higher soil moisture contents in clayey soils compared to sandy soils. In clayey soils, soil moisture is the major control of soil temperature, whereas in sandy soils it is soil texture. This is the reason for the better estimation of soil moisture using soil temperature measurements in soils with higher clay content compared to soils with higher sand content.

Correlation between soil moisture and soil temperature improves the estimation of soil moisture from soil temperature observations and vice versa. Soil hydraulic properties influence the vertical soil moisture distribution, and soil moisture content influences the thermal conductivity and therefore also the soil temperature distribution. Soil thermal properties determine the vertical soil temperature distribution, but soil temperature change hardly influences soil hydraulic properties or soil moisture. This is the reason why soil temperature contains information to estimate both SHPs and STPs while soil moisture only allows to estimate SHPs. The estimation of soil moisture using soil temperature measurements makes use of correlations between soil moisture and soil temperature and improved estimates of SHPs, whereas soil temperature estimation using soil moisture measurements relies exclusively on the correlation between soil moisture and soil temperature. That is why there is a significant difference between the estimation accuracy (averaged over all 12 soils) of the soil moisture profile using soil temperature observation (47% RMSE reduction) and estimation accuracy of the soil temperature profile using soil moisture observations (27% RMSE reduction). In this synthetic study we have assumed that the heat transport model is perfect without any uncertainty, whereas in real field condition the equations (Equations 4–7) that link soil moisture and soil temperature may not be accurate which will lead to lower RMSE reduction compared to a synthetic study.

Compared to the assimilation of observation at one depth, the assimilation of soil moisture or soil temperature observations at two different depths enhances the estimation of the soil moisture and soil temperature profiles. This is because the information on the soil moisture and soil temperature gradients is utilized in case of assimilation of observations at two different depths (Dong et al., 2015b). The improvement

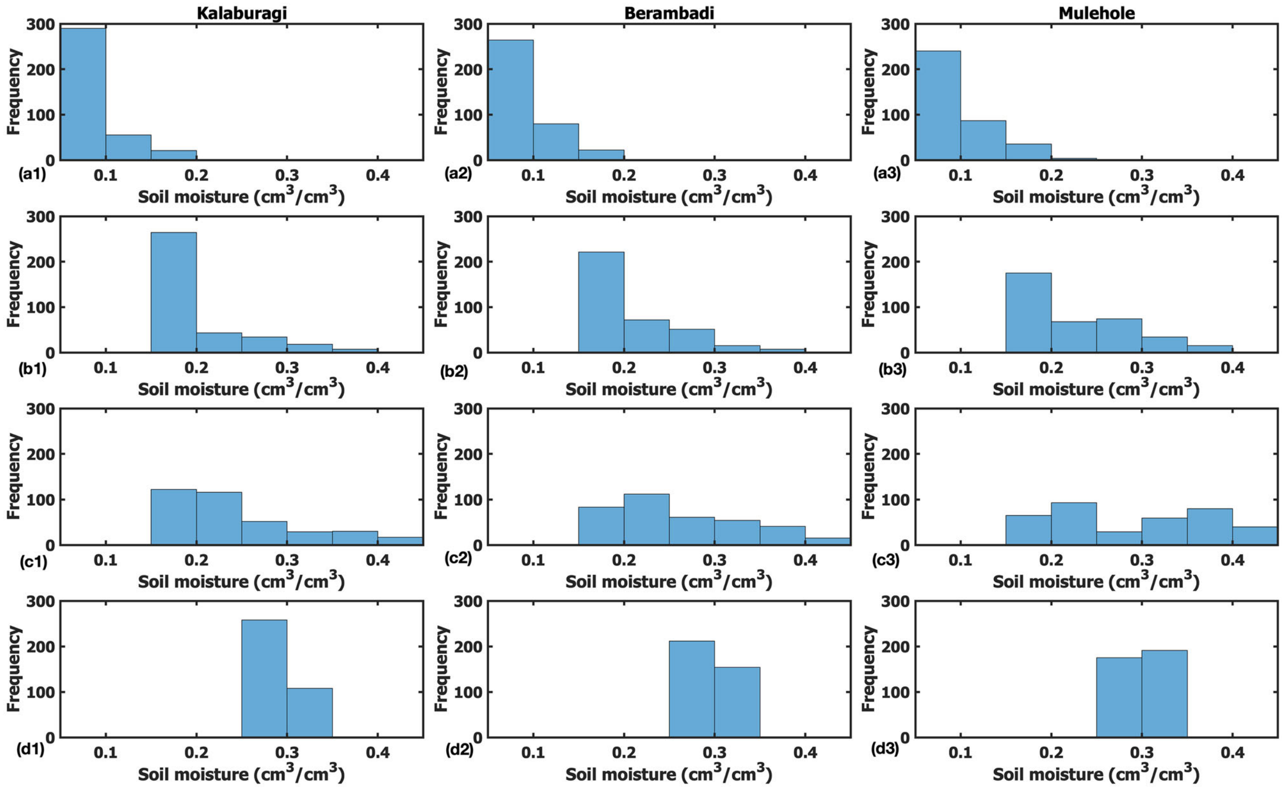

FIGURE 11 Frequency distribution of soil moisture at 5 cm depth for different soil types (a1–a3) Loamy sand, (b1–b3) loam, (c1–c3) silt, and (d1–d3) clay and locations Kalaburagi, Berambadi, and Mulehole.

in the estimation of soil moisture or soil temperature profile when observations at two different depths are assimilated will be more effective for two-layered soils with contrasting soil properties among different layers. In two-layered soils information on the moisture or thermal gradient will provide more information compared to homogeneous soils where the correlation of soil moisture or soil temperature between depths is high and univariate assimilation is already able to improve the characterization of this single-layer soil system.

Figure 11 shows the frequency distribution of the true soil moisture values at 5 cm depth for different soil types and climate regions. The frequency distribution is more skewed toward lower soil moisture values for loamy sand and loam soils in Kalaburagi and Berambadi compared to Mulehole. On the other hand, the frequency distribution is more skewed toward higher soil moisture values for silt and clay soils in Mulehole compared to Kalaburagi and Berambadi. Soil parameters are better retrieved when the soil moisture observations are well distributed and cover the larger range of the soil moisture characteristic curve (Brandhorst et al., 2017). As a consequence, low permeable soils under humid conditions and high permeable soils under dry conditions are worst cases for soil parameter estimation as in the former case observed soil moisture is often near saturation and in the latter case observations are more concentrated around low soil moisture values. Best cases for soil parameter estimation and ultimately state and flux estimation (via soil moisture assimilation) are high permeable soils under humid conditions and low permeable soils under dry conditions. Soil parameters can be better estimated by adding observations which increase the spread of soil moisture contents and using observations from the whole year with alternating drying and wetting cycles. Alternatively, multiple types of observations can be assimilated.

5 | CONCLUSIONS

In this study we have investigated the value of soil moisture and soil temperature measurements at 5 cm depth to estimate soil moisture and temperature profiles, soil hydraulic and thermal parameters, and latent and sensible heat fluxes for 12 different soil textures covering the whole soil texture classification according to USDA, on the basis of synthetic experiments. This has been done using HYDRUS-1D as a software to model water and heat flow in soils, and the EnKF to assimilate soil moisture and/or soil temperature measurements. We found that soil temperature assimilation had different impacts on soil moisture profile characterization depending on the soil type with larger improvements in soil moisture characterization for soils with higher clay content compared to soils with higher sand content. Sensitivity analysis showed that soil temperature in clayey soils is more sensitive to SHPs (mainly $\log(K_s)$) compared to sandy soils. It is also observed that soil temperature is more sensitive to clay fraction than sand fraction. Significant additional RMSE reduction (around 15%) is observed for the estimation of SHPs with joint soil moisture and temperature assimilation, compared to univariate assimilation. For the majority of soil textures (8 out of 12) the RMSE reduction for the estimation of latent and sensible heat fluxes is higher when soil temperature is assimilated instead of soil moisture. The combined assimilation of soil moisture and soil temperature provides again the best results. The results are also compared between hot semi-arid, semi-arid, and sub-humid sites. Results suggest that the performance of soil moisture assimilation is higher in hot semi-arid regions for low permeable soils such as silt and clay and is higher in sub-humid regions for high permeable soils such as loamy sand and loam.

The results show the potential of soil temperature (or land surface temperature) measurements for improving the estimates of land–atmosphere exchange fluxes, especially in clayey soils where soil temperature data show more value for improved evapotranspiration estimation than soil moisture measurements. The simulation experiments also indicate that estimation of SHPs is important for improved estimation of soil states and evapotranspiration. In land surface data assimilation, the estimation of SHPs is still not common, in part because parameter estimation is difficult on the basis of coarse remote sensing information.

Synthetic studies are important to explore in a controlled fashion the value of different measurement types for improving model predictions, or the role of different soil textures. However, it is very important to test the methodology for real field conditions as it can be expected that under real field conditions model structural uncertainty plays a larger role, which is difficult to handle in the data assimilation procedure. In our study we neglected model structural error and considered only errors related to unknown soil parameters and meteorological forcings. Under real world conditions, modeling the heat transport in the soil column is difficult and the relation between soil moisture and soil temperature may not be accurate leading to relatively worse performance compared to a synthetic study. In addition, in the synthetic case presented in this paper we assumed the soil to be homogeneous with vertically constant soil parameters, while in reality soils are vertically heterogeneous with multiple soil layers of different soil characteristics. It is difficult to estimate soil hydraulic and thermal parameters of multi-layered soils using only near-surface measurements. Observations at different depths may be required to better characterize the soil and ultimately estimate soil moisture and temperature at deeper depths. Therefore, it can be expected that the value of near-surface soil moisture and soil temperature measurements in vertically heterogeneous soils will be smaller than for homogeneous soils.

Future research should focus on implementing this approach on layered soils, using remote sensing observations and extending the applications toward vegetated surfaces. This research stresses the importance to consider soil temperature (or land surface temperature) measurements besides soil moisture measurements, to improve evapotranspiration modeling. This exhaustive synthetic study showed that the potential of soil temperature measurements to improve ET characterization is in theory higher than the potential of soil moisture measurements. In addition, research is required to evaluate the value of vegetation variables such as LAI, NDVI along with soil moisture and soil temperature for the estimation of soil moisture and soil temperature profiles, soil parameters, and land surface fluxes in layered soils with crops. The obvious next step is to apply this methodology on real field data.

AUTHOR CONTRIBUTION

Rajsekhar Kandala: Conceptualization; formal analysis; investigation; methodology; software; validation; writing—original draft. **Harrie-Jan Hendricks Franssen**: Conceptualization; formal analysis; methodology; validation; writing—review and editing. **Abhijit Chaudhuri**: Conceptualization; formal analysis; methodology; validation; writing—review and editing. **M. Sekhar**: Conceptualization; formal analysis; project administration; supervision; writing—review and editing.

ACKNOWLEDGMENTS

The financial support provided to the first author from the Karnataka Watershed Development Department is acknowledged. The authors extend their sincere appreciation to the editors and two anonymous reviewers for their invaluable contributions in refining this manuscript. Their constructive feedback and insightful comments greatly improved the clarity and depth of the content, enhancing the overall quality of the article.

CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

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How to cite this article: Kandala, R., Franssen, H.-J. H., Chaudhuri, A., & Sekhar, M. (2024). The value of soil temperature data versus soil moisture data for state, parameter, and flux estimation in unsaturated flow model. *Vadose Zone Journal*, *23*, e20298. https://doi.org/10.1002/vzj2.20298