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Land Surface Model Representation of the Mutual Information Context between Multi-Layer Soil Moisture and Evapotranspiration

Jianxiu Qiu[1,2], Wade T. Crow[3], Jianzhi Dong[3], Grey S. Nearing[4]

[1]Guangdong Provincial Key Laboratory of Urbanization and Geo-simulation, School of Geography and Planning, Sun Yat-sen University, Guangzhou, 510275, China

[2]Southern Laboratory of Ocean Science and Engineering (Guangdong, Zhuhai), Zhuhai, 519000, China

[3]USDA ARS Hydrology and Remote Sensing Laboratory, Beltsville, MD 20705, USA

[4]Department of Geological Sciences, University of Alabama, AL 35487, USA

Correspondence to: Jianxiu Qiu (qiujianxiu@mail.sysu.edu.cn)

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Abstract. Soil moisture (θ) impacts the climate system by regulating incoming energy into outgoing evapotranspiration (ET) and sensible heat flux components. Therefore, investigating the coupling strength between θ and ET is important for the study of land surface/atmosphere interactions. Here, we use in-situ AmeriFlux observations to evaluate θ/ET coupling strength estimates acquired from multiple land surface models (LSMs). For maximum robustness, coupling strength is represented using the sampled normalized mutual information (NMI) between θ estimates acquired at various vertical depths and surface flux represented by fraction of potential evapotranspiration (fPET, the ratio of ET to potential ET). Results indicate that LSMs are generally in agreement with AmeriFlux measurements in that surface soil moisture (θ_S) contains slightly more NMI with fPET than vertically integrated soil moisture (θ_V). Overall, LSMs adequately capture variations in NMI between fPET and θ estimates acquired at various vertical depths. However, one model – the Global Land Evaporation Amsterdam Model (GLEAM) – significantly overestimates the NMI between θ and ET and the relative contribution of θ_S to total ET. This bias appears attributable to differences in GLEAM's ET estimation scheme relative to the other two LSMs considered here (i.e., the Noah with Multi–parameterization option and the Catchment Land Surface Model). These results provide insight into improved LSM model structure and parameter optimization for land surface-atmosphere coupling analyses.

Keywords. Land surface/atmosphere interaction, soil moisture, surface evapotranspiration

1 Introduction

Soil moisture (θ) modulates water and energy feedbacks between the land surface and the lower atmosphere by partitioning incoming energy into evapotranspiration (ET) and sensible heat (H) surface flux components (Seneviratne et al., 2010, 2013). In water-limited regimes, θ exhibits a dominant control on ET and, therefore, commonly exerts significant terrestrial control on the earth's water, energy and biochemical cycles. Accurately representing θ/ET coupling in land surface models (LSMs) is therefore expected to improve our ability to project the future frequency of extreme climates (Seneviratne et al., 2013).

A key question is how the constraint of θ on ET and H varies as θ is vertically integrated over deeper vertical soil depths. Given the tendency for the time scales of θ dynamics to vary strongly with depth, the degree to which the ET is coupled with vertical variations in θ determines the temporal scale at which θ variations are propagated into the atmosphere. Therefore, in order to represent θ/ET coupling, and thus land/atmosphere interactions in general, LSMs must accurately capture the relationship between vertically varying θ values and ET. Unfortunately, their abilities to do so remains an open question.

Recently, land surface/atmosphere coupling strength has been investigated by sampling mutual information proxies (e.g., correlation coefficient or other coupling indices) between time series of θ and ET (or air temperature proxies for ET). Results suggest that, even when confined to very limited vertical support (e.g., within the top 5 cm of the soil column), surface θ estimates retain significant information for examining θ controls on local climate (Ford and Quiring, 2014b; Qiu et al., 2014; Dong and Crow, 2018; Dong and Crow, 2019). These findings are in contrast with the common

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perceptions that ET is dominated by θ values at deeper soil layers (Hirschi et al., 2014). Hence, it is necessary to examine whether LSMs can realistically reflect observed variations of θ/ET coupling strength in the vertical soil profiles.

Previous studies examining the θ/ET relationship have generally been based on Pearson product-moment correlation (Basara and Crawford, 2002; Ford et al., 2014a), which captures only the strength of a linear relationship between two variables. However, the coupling between θ and ET is generally nonlinear. Therefore, non-parametric mutual information measures are generally more appropriate. Nearing et al. (2018) used information theory metrics (transfer entropy, in particular) to measure the strengths of directed couplings between different surface variables, including soil moisture, and surface energy fluxes at short timescales in several LSMs. They found that the LSMs were generally biased as compared with strengths of couplings in observation data, and that these biases differed across different study sites. However, they did not look at the effect of vertical moisture profiles or of subsurface soil moisture on partitioning surface energy fluxes.

Here we apply the information theory-based methodology of Qiu et al. (2016) to examine the relationship between the vertical support of θ estimates and their mutual information (MI) with respect to ET. Our approach is based on analyzing the MI content between ET and θ time series - acquired from both LSMs and AmeriFlux in-situ observations. MI values are then normalized by corresponding ET entropy to remove the effect of inter-site variation and generate estimates of Normalized Mutual Information (NMI) between θ and ET. Examined θ time series have two different vertical supports: surface soil moisture (θ_S) and vertically integrated soil moisture (θ_V). AmeriFlux NMI results are compared with analogous NMI results obtained from LSM-based θ and ET time series.

Further details on our methodology are presented in Sect. 2. Results are presented in Sect. 3 and discussed/summarized in Sect. 4.

2 Data and Methods

The AmeriFlux network provides temporally continuous measurements of θ, surface energy fluxes and related environmental variables for sites located in a variety of North American ecosystem types, e.g., forests, grasslands, croplands, shrublands and savannas (Boden, et al., 2013). To minimize sampling errors, AmeriFlux sites lacking a complete 3-year summer months (June, July and August) daily time series between the years of 2003 and 2015 (i.e., $3 \times 92 = 276$ daily observations in total) of θ_S, θ_V and latent heat flux (LE) were excluded here - resulting in the 34 eligible AmeriFlux sites listed in Table 1. These sites cover a variety of climate zones within the contiguous United States (CONUS). Table 1 gives background information on these 34 sites including local land cover information. Hydro-climatic conditions in each site were characterized using the aridity index (AI) – calculated using CRU (Climate Research Unit, v4.02) monthly precipitation and potential evaporation (PET) datasets.

As described above, θ/ET coupling assessments made using AmeriFlux observations were compared with comparable assessments based on output from state-of-the-art LSMs including Noah with Multi–parameterization option

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(NOAHMP), Catchment Land Surface Model (CLSM), and Global Land Evaporation Amsterdam Model (GLEAM). See below for more model details. To avoid any spurious correlations between θ and ET due to seasonality, all NMI analyses were performed on θ and ET time series anomalies acquired during the period 2003–2015. The θ and ET anomalies were calculated by removing the seasonal cycle – defined as 31-day window averages centered on each day-of-year sampled across all years of the 2003–2015 historical data record – from the raw θ and ET time series data. The analysis was limited to the CONUS during summer months (June, July and August) when θ/ET coupling was expected to be maximized.

Table 1 Attributes of selected AmeriFlux sites

AmeriFlux sites	Land cover	Elevation [m]	Top-layer depth [cm]	Bottom-layer depth [cm]
ARM SGP Main	Cropland	314	10[a]	20[b]
ARM USDA UNL OSU Woodward Switchgrass 1	Grassland	611	10	30
Audubon Research Ranch	Grassland	1469	10	20
Bondville	Cropland	219	10[c]	20
Brookings	Grassland	510	10	20
Chimney Park	Evergreen needleleaf forest	2750	0-15	15-45
Duke Forest Hardwoods	Deciduous broadleaf forest	168	10	25
Duke Forest Open Field	Grassland	168	10	25
Fermi Agricultural	Cropland	225	2.5	10
Fermi Prairie	Grassland	226	2.5	10
Flagstaff Managed Forest	Evergreen needleleaf forest	2160	2	10
Flagstaff Unmanaged Forest	Woody savannas	2180	2	10
Flagstaff Wildfire	Grassland	2270	2	10
Fort Peck	Grassland	634	5[d]	20
Freeman Ranch Woodland	Woody savannas	232	10	20
Glacier Lakes Ecosystem Experiments Site	Evergreen needleleaf forest	3190	5	10
Howland Forest Main	Mixed forest	60	NA	NA
Lucky Hills Shrubland	Open shrubland	1372	5	15
Marys River Fir Site	Evergreen needleleaf forest	263	10	20
Metolius Intermediate Pine	Evergreen needleleaf forest	1253	0-30	NA
Missouri Ozark	Deciduous broadleaf forest	219	10	100
Nebraska SandHills Dry Valley	Grassland	1081	10	25
Quebec Boreal Cutover Site	Evergreen needleleaf forest	400	5	20
Quebec Mature Boreal Forest Site	Evergreen needleleaf forest	400	5	10
Santa Rita Creosote	Open shrubland	991	2.5	12.5
Santa Rita Mesquite	Woody savannas	1116	2.5-5	5-10
Sherman Island	Grassland	-5	10	20
Sylvania Wilderness	Mixed forest	540	5	10
Tonzi Ranch	Woody savannas	169	0	20

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University of Michigan Biological Station	Deciduous broadleaf forest	234	0-30	NA
Vaira Ranch	Grassland	129	0	10
Walker Branch	Deciduous broadleaf forest	343	5	10
Willow Creek	Deciduous broadleaf forest	515	5	10
Wind River Field Station	Evergreen needleleaf forest	371	30[e]	50[f]

[a] Was 5 cm prior to 4/13/2005
[b] Was 25 cm prior to 4/13/2005
[c] Was 5 cm prior to 1/1/2006
[d] Was 10 cm (2003-2008)
[e] Was 0-30 cm prior to 2007
[f] Was NaN prior to 2007

2.1 Ground-based AmeriFlux measurements

The Level 2 (L2) AmeriFlux LE and sensible heat (H) flux observations are based on high-frequency (typically > 10 Hz) eddy covariance measurements processed into half-hourly averages by individual AmeriFlux investigators. LE and θ observations at a half-hour time step and without gap-filling procedures were collected from the AmeriFlux Site and Data Exploration System (see http://ameriflux.ornl.gov/). The LE and θ observations were further aggregated into daily (0 to 24 UTC) values, and daily LE was converted into daily ET using the latent heat of vaporization. Daily ET values based on less than 30% half-hourly coverage (i.e., < 15 half-hourly observations per day) were considered not representative at a daily time scale and therefore excluded.

Soil moisture measurements are generally available at two discrete depths that vary between the AmeriFlux sites (Table 1). Here, the top (i.e., closest to the surface) soil moisture observation was always used to represent surface soil moisture (θ_S). Since the depth of this top layer measurement varies between 0 and 15 cm (see Table 1), we consider the surface-layer measurement θ_S to be roughly representative of 0–10 cm (vertically integrated) θ.

Given variations in the depth of the lower AmeriFlux θ observations (see Table 1), we applied a variety of approaches for estimating vertically integrated soil moisture (θ_V). Our first approach, hereinafter referred to as Case I, was based on the application of an exponential filter (Wagner et al., 1999; Albergel et al., 2008) to extrapolate θ_S to a consistent 40 cm bottom layer depth. Therefore, only θ_S was used to derive θ_V and the bottom-layer AmeriFlux θ measurement was neglected in this case. The application of the exponential filter requires a single time-scale parameter T. Since θ measurements from United States Department of Agriculture's Soil Climate Analysis Network (SCAN) are taken at fixed soil depth, we utilized this dataset to determine the most appropriate parameter T at AmeriFlux sites. Following Qiu et al. (2014), first, we estimated the optimal parameter T (Topt) for the extrapolation of θ measurements from 10 cm to 40 cm depth and established a global relationship between Topt and site-based NDVI (MOD13Q1 v006, 250m, 16-day) (Topt = 2.098 × exp(–1.895 × (NDVI + 0.6271)) + 2.766). Then, this global relationship (Goodness of Fit R^2: 0.85) was applied to AmeriFlux sites to extrapolate 0–10 cm θ_S times series into 0–40 cm θ_V.

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Previous research has suggested that such a filtering approach does not significantly squander ET information present in actual measurements of θ_V (Qiu et al., 2014; Qiu et al., 2016). Nevertheless, since the quality of θ_V estimates is important in our analysis, we also calculated two addition cases where 0–40 cm θ_V was estimated using: 1) the bottom-layer soil moisture measurement acquired at each AmeriFlux site (hereinafter, Case II) and 2) linear interpolation of θ_S and the bottom-layer AmeriFlux soil moisture measurement (hereinafter, Case III). The sensitivity of key results to these various cases is discussed below.

2.2 LSM-based simulations

LSM output was acquired from NOAHMP (Niu et al., 2011) and CLSM (Koster et al., 2000) simulations embedded within the NASA Land Information System (LIS, Kumar et al., 2006) and a satellite-observation-based model GLEAM (Miralles et al., 2011). Both NOAHMP and CLSM were set-up to simulate 0.125 °θ profiles at a 15-minute time step using North America Land Data Assimilation System, Phase 2 (NLDAS-2) forcing data. A 10-year model spin-up period (1992 to 2002) was applied for NOAHMP and CLSM.

NOAHMP numerically solves the one-dimensional Richards equation within four soil layers of thicknesses of 10, 30, 60, and 100 cm. Major parameterization options relevant to θ simulation include: 1) options for canopy stomatal resistance; 2) options for θ factor for stomatal resistance (the β factor). Here we employed the Ball-Berry-type stomatal resistance scheme and Noah-type soil moisture factor controlling the β factor. The specific expressions are as follows:

$$\beta = \sum_{i=1}^{N_{\text{root}}} \frac{\Delta Z_i}{Z_{root}} \min\left(1.0, \frac{\theta_i - \theta_{\text{wilt}}}{\theta_{\text{ref}} - \theta_{\text{wilt}}}\right) \quad (1)$$

where θ_{wilt} and θ_{ref} are respectively soil moisture at witling point ($m^3\ m^{-3}$) and reference soil moisture ($m^3\ m^{-3}$), which is close to field capacity. θ_i and Δz_i are soil moisture ($m^3\ m^{-3}$) and soil depth (cm) at ith layer, N_{root} and z_{root} are total number of soil layers with roots and total depth (cm) of root zone, respectively.

Following the Ball-Berry stomatal resistance scheme, the θ-controlled β factor and other multiplicative factors including temperature, foliage nitrogen simultaneously determine the maximum carboxylation rate V_{max} as follows:

$$V_{\text{max}} = V_{\text{max25}}\, \alpha_{\text{vmax}}^{\frac{T_V - 25}{10}}\, f(N) f(T_v)\, \beta \quad (2)$$

where V_{max25} is maximum carboxylation rate at 25 ℃ (μmol CO_2 m^{-2} s^{-1}); α_{vmax} is a parameter sensitive to vegetation canopy surface temperature T_v; $f(N)$ is a factor representing foliage nitrogen and $f(T_v)$ is a function that mimics thermal breakdown of metabolic processes. Based on V_{max}, carboxylase-limited (Rubisco limited) and export-limited (for C3 plants) photosynthesis rates per unit LAI (A_C and A_S respectively) are calculated, and the minimum of A_C, A_S and light-limited photosynthesis rates determine stomatal conductance r_s, and, consequently, the ET over vegetated areas. For the complete NOAHMP configuration, please see Table S1 in the supplementary material.

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CLSM simulates the 0–2 and 0–100 cm soil moisture and evaporative stress as a function of simulated θ and environmental variables. ET is then estimated based on the estimated evaporative stress and land-atmosphere humidity gradients. Energy and water flux estimates are iterated with soil state estimates (e.g., θ and soil temperature) to ensure closure of surface energy and water balances. For the detailed explanation of CLSM, please refer to Koster et al. (2000).

GLEAM is a set of algorithms dedicated to the estimation of terrestrial ET and root-zone θ from satellite data. In this study, the latest version of this model (v3.2a) is employed. In GLEAM, the configuration of soil layers varies as a function of the land-cover type. Soil stratification is based on three soil layers for tall vegetation (0–10, 10–100, and 100–250 cm), two layers for low vegetation (0–10, 10–100 cm) and only one layer for bare soil (0–10 cm) (Martens et al., 2017).

The cover-dependent PET (mm day^{-1}) of GLEAM is calculated using the Priestley and Taylor (1972) equation based on observed air temperature and net radiation. Following this, estimates of PET were converted into actual transpiration or bare soil evaporation (depending on the land-cover type, ET (mm day^{-1})), using a cover-dependent, multiplicative stress factor S (–), which is calculated as a function of microwave vegetation optical depth (VOD) and root-zone θ (Miralles et al., 2011). The related expressions are as follows:

$$\mathrm{ET} = \mathrm{PET} \times S + E_\mathrm{i} \tag{3}$$

$$S = \sqrt{\frac{\mathrm{VOD}}{\mathrm{VOD_{max}}}}\left(1 - \left(\frac{\theta_\mathrm{c} - \theta\omega}{\theta_\mathrm{c} - \theta_\mathrm{wilt}}\right)^2\right) \tag{4}$$

where E_i is rainfall interception (mm); S essentially represents the fPET (see Sect. 2.3) estimated by GLEAM; θ_c (m^3 m^{-3}) is the critical soil moisture and θ_ω (m^3 m^{-3}) is the soil moisture content of the wettest layer, assuming that plants withdraw water from the layer that is most accessible. Based on (4), GLEAM S (or fPET) tend to become more sensitive to θ in areas of low VOD seasonality (i.e., low differences between VOD and $\mathrm{VOD_{max}}$). As for bare soil conditions, S is linearly related to surface soil moisture (θ_1):

$$S = 1 - \frac{\theta_\mathrm{c} - \theta_1}{\theta_\mathrm{c} - \theta_\mathrm{wilt}}. \tag{5}$$

To resolve variations in the vertical discretization of θ applied by each model, we linearly interpolated NOAHMP, CLSM and GLEAM outputs into daily 0–10 and 0–40 cm soil moisture values using depth-weighted averaging.

2.3 Variable indicating soil moisture and surface flux coupling

Soil moisture – ET coupling can be diagnosed using a variety of different variables derived from ET, e.g. the fraction of PET (fPET, the ratio of ET and PET) or the evaporative fraction (EF, the ratio of LE and the sum of LE and sensible heat). Since ET is strongly tied to net radiation (Rn) (Koster et al., 2009), both fPET and EF are advantageous in that

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they normalize ET and removing the impact of non-soil moisture influences on ET (e.g., net radiation, wind speed and soil heat flux (G)). However, since sensible heat flux is not provided in the GLEAM dataset, we are restricted here to using fPET.

It should be noted that the applied meteorological forcing data for NOAHMP and CLSM were somewhat different from those used for GLEAM. Therefore, to minimize the impact of this difference, NOAHMP and CLSM fPET were computed from North American Regional Reanalysis (NARR) using the modified Penman scheme of Mahrt and Ek (1984) while GLEAM fPET was calculated using its own internal PET estimates. To examine the impact of PET source, AmeriFlux fPET calculations were calculated using both GLEAM- and NARR-based PET values.

2.4 Information measures

Mutual information (MI) (Cover and Thomas, 1991) is a nonparametric measure of correlation between two random variables. MI and the related Shannon-type entropy (Shannon, 1948) are calculated as follows. Entropy about a random variable ζ is a measure of uncertainty according to its distribution p_ζ and is estimated as the expected amount of information from p_ζ sample:

$$\mathrm{H}(p_\zeta) = \mathrm{E}_\zeta[-\ln(p_\zeta(\zeta))]. \quad (6)$$

Likewise, MI between ζ and another variable ψ can be thought of as the expected amount of information about variable ζ contained in a realization of ψ and is measured by the expected Kullback-Leibler (KL) divergence (Kullback and Leibler, 1951) between the conditional and marginal distributions over ζ:

$$\mathrm{MI}(\zeta;\psi) = \mathrm{E}_\psi[D(p_{\zeta|\psi} \parallel p_\zeta)]. \quad (7)$$

In this context, the generic random variables ζ and ψ represent fPET and θ (soil moisture) respectively. The observation space of the target random variable fPET was discretized using a fixed bin width. As bin width decreases, entropy increases but mutual information asymptotes to a constant value. On the other hand, increased bin width requires more sample size, which cannot always be satisfied. The trick is choosing a bin width where the NMI values stabilize with sample size. After careful sensitivity analysis, we choose a fixed bin width of 0.25 [-] for fPET and make sure that each AmeriFlux site have enough samples to accurately estimate the NMI, and change of this constant bin width from 0.1–0.5 [-] will not significantly alter our conclusions. Following Nearing et al. (2016), a bin width of 0.01 $m^3\ m^{-3}$ (1% volumetric water content) for θ was applied. Integrations required for MI calculation in Eq. (7) are then approximated as summations over the empirical probability distribution function bins (Paninski, 2003).

By definition, the MI between two variables represents the amount of entropy (uncertainty) in either of the two variables that can be reduced by knowing the other. Therefore, the MI normalized by the entropy of the AmeriFlux-based fPET measurements represents the fraction of uncertainty in fPET that is resolvable given knowledge of the soil moisture state (Nearing et al., 2013). Unlike Pearson's correlation coefficient, MI is insensitive to the impact of

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nonlinear variable transformations. Therefore, it is well suited to describe the strength of the (potentially non-linear) relationship between θ and fPET.

Here, we applied this approach to calculate the MI content between soil moisture representing different vertical depths (as reflected by θ_S and θ_V) and fPET at each AmeriFlux site. All estimated site-specific MI were normalized by the entropy of the corresponding AmeriFlux-based fPET measurements to remove the effect of inter-site entropy variations on the magnitude of NMI differences. The resulting normalized MI calculations between both θ_S and θ_V and fPET are denoted as NMI(θ_S, fPET) and NMI(θ_V, fPET) respectively.

The underestimation of observed θ/ET coupling via the impact of mutually-independent θ and ET errors in AmeriFlux observations (Crow et al. 2015) was minimized by focusing on the ratio between NMI(θ_S, fPET) and NMI (θ_V, fPET). To quantify the standard error of NMI differences between various soil moisture products, we applied a nonparametric, 500-member bootstrapping approach, and calculated pooled average of sampling errors across all sites assuming spatially independent sampling error.

Finally, we also examined the impact of potential nonlinearity in the θ/ET relationship by comparing non-parametric NMI results with comparable inferences based on a conventional Pearson's correlation calculation. The correlation-based coupling strength between θ_S and fPET was denoted as R(θ_S, fPET) and between θ_V and fPET as R(θ_V, fPET).

3 Results

3.1 Comparison of NMI(θ_S, fPET) and NMI(θ_V, fPET)

Figure 1 contains boxplots of modelled and observed NMI(θ_S, fPET) and NMI(θ_V, fPET), i.e., the relative magnitude of fPET information contained in surface soil moisture and vertically-integrated (0–40 cm) soil moisture, sampled across all the AmeriFlux locations listed in Table 1. According to the AmeriFlux ground measurements, median values of NMI(θ_S, fPET) and NMI(θ_V, fPET) (across all sites) are near 0.3 [-]. This suggests that approximately 30% of the uncertainty (i.e., entropy at this particular bin width of 0.25 [-]) in fPET can be eliminated given knowledge of either surface or vertically integrated soil moisture state. This is consistent with earlier results in Qiu et al., (2016) who used similar variables to evaluate θ/EF (evaporative fraction) coupling strength. The sampled medians of NMI(θ_S, fPET) and NMI(θ_V, fPET) estimated by the NOAHMP and CLSM models are similar to these (observation-based) AmeriFlux values. With the single exception that CLSM predicts much larger site-to-site variation in NMI(θ_S, fPET).

In contrast, NMI(θ_S, fPET) and NMI(θ_V, fPET) values sampled from GLEAM θ and fPET estimates are biased high (with median NMI(θ_S, fPET) and NMI(θ_V, fPET) values of about 0.5 and 0.4 [-], respectively) with respect to all other estimates.

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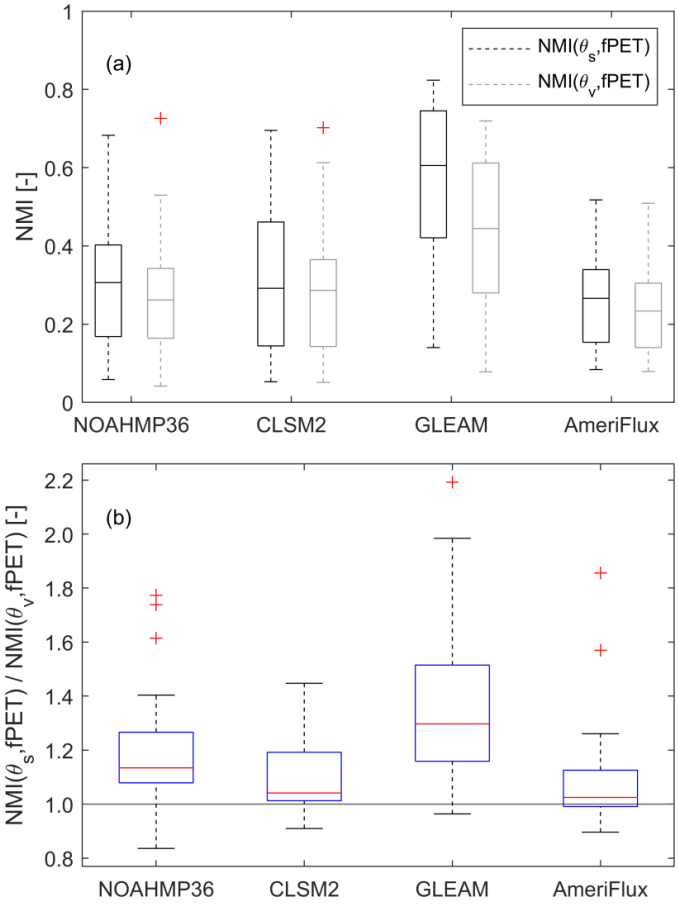

Fig.1 The θ/ET coupling strengths for summertime anomaly time series acquired from various LSMs and AmeriFlux measurements: (a) NMI(θ_S, fPET) and NMI(θ_V, fPET) individually and (b) NMI(θ_S, fPET) normalized by NMI(θ_V, fPET).

All three LSMs overall exhibit significantly (at $p = 0.05$ [-] confidence, using the 34 AmeriFlux site-collocated samples pixels for pair t-test) higher NMI(θ_S, fPET) compared to NMI(θ_V, fPET) – implying the surface soil moisture observation contain more fPET information than vertically-integrated soil moisture. However, the difference between NMI(θ_S, fPET) and NMI(θ_V, fPET) is less discernible in AmeriFlux measurements (Fig. 1(a)).

Here, AmeriFlux observations are used as a baseline for LSM evaluation. However, it should be stressed that random observation errors in θ and fPET will introduce a low bias into AmeriFlux-based estimates of both NMI(θ_S, fPET) and NMI(θ_V, fPET) (Crow et al., 2015) and thus their difference as well. To address this concern, Fig. 1(b) plot the ratio of NMI(θ_S, fPET) and NMI(θ_V, fPET), which normalizes and minimizes such observation error impacts. Ratio results illustrate the general tendency for NMI(θ_S, fPET) > NMI(θ_V, fPET) discussed above. They also highlight the tendency for GLEAM to overvalue θ_S (relative to θ_V) when estimating fPET. A second approach for reducing the random error of θ and fPET measurement errors is the Triple Collocation (TC)-based correction applied in Crow et al. (2015).

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247 However, this approach is currently restricted to linear correlation and cannot be applied to NMI. Future work will
248 examine extending the information-based TC approach of Nearing et al. (2017), to the examination of NMI.

249 **3.2 Sensitivity of AmeriFlux-based NMI(θ_S, fPET)/NMI(θ_V, fPET)**

250 As mentioned in Sect. 2.1, an important concern is the impact of interpolation errors used to estimate 0–40 cm θ_V from
251 AmeriFlux θ_S observations acquired at non-uniform depths. To ensure that different methods for calculating
252 AmeriFlux θ_V values do not affect the main conclusion of this study, we configured three cases for θ_V calculation, and
253 compared their NMI(θ_S, fPET)/NMI(θ_V, fPET) results in Fig. 2. Case I reflects the baseline use of the exponential
254 filter described in Sect. 2.1. However, slight changes to AmeriFlux results are noted if alternative approaches are used.
255 Specifically, AmeriFlux-based NMI(θ_V, fPET) increases and closes the gap with NMI(θ_S, fPET) if the bottom-layer
256 soil moisture measurements are instead directly used as θ_V (Case II) or if 0–40 cm θ_V is based on the linear interpolation
257 of the two AmeriFlux θ observations (Case III), the impact of this modest sensitivity on key results is discussed below.

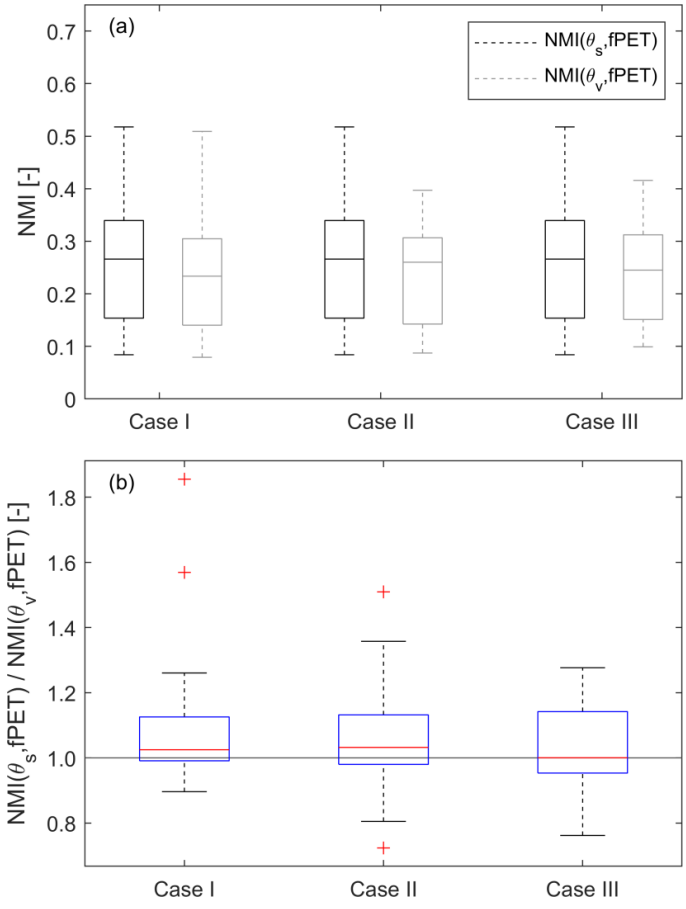

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Fig.2 The θ/ET coupling strengths for summertime anomaly time series from AmeriFlux measurements using three different θ_V calculation methods: (a) NMI(θ_S, fPET) and NMI(θ_V, fPET) individually and (b) NMI(θ_S, fPET) divided by NMI(θ_V, fPET) for multiple θ_V cases. Case I is based on the application of an exponential filter to extrapolate 0–10 cm θ_S to a consistent 0–40 cm bottom layer depth, while Cases II and III refer to the direct use of only the bottom layer measurement and a linear interpolation of both the top and bottom layer, respectively, to calculate θ_V (see Sect. 2.1 for details on each case).

In addition, switching from GLEAM- to NARR-based PET when calculating fPET for AmeriFlux-based NMI(θ_S, fPET) and NMI(θ_V, fPET) does not qualitatively change results and produces only a very slight (~6%) increase in the median NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio.

3.3 Spatial distribution of NMI(θ_S, fPET) and NMI(θ_V, fPET)

Figure 3 plots the spatial distribution of NMI(θ_S, fPET) and NMI(θ_V, fPET) results for each of the individual 34 AmeriFlux sites listed in Table 1. The climatic regime is represented by AI (aridity index) plotted as the background color in Fig. 3. It can be seen in Fig. 3 that NMI(θ_S, fPET) estimates from LSMs are spatially related to hydro-climatic conditions, as NOAHMP and CLSM predict that θ_S is moderately coupled with fPET (NMI(θ_S, fPET) of 0.3–0.5 [-]) in the arid Southwestern US (AI<0.2) and only loosely coupled with fPET in the relatively humid Eastern US. A similar decreasing trend of NMI(θ_S, fPET) from the Southwestern to Eastern US is also captured by GLEAM. However, as noted above, GLEAM generally overestimates NMI(θ_S, fPET) and NMI(θ_V, fPET) compared to NOAHMP, CLSM and AmeriFlux. In contrast, a relatively weaker spatial pattern emerges in AmeriFlux-based NMI(θ_S, fPET) results. In addition, spatial patterns for NMI(θ_S, fPET) are less defined than for NMI(θ_V, fPET) in all four datasets.

Scatterplots in Fig. 4 summarize the spatial relationship between LSM-based NMI(θ_S, fPET) and NMI(θ_V, fPET) results versus AmeriFlux observations. While observed levels of correlation in Fig. 4 are relatively modest, there appears to be a significant level of spatial correspondence between modelled and observed NMI results – motivating the need to better understand processes responsible for spatial variations in NMI results.

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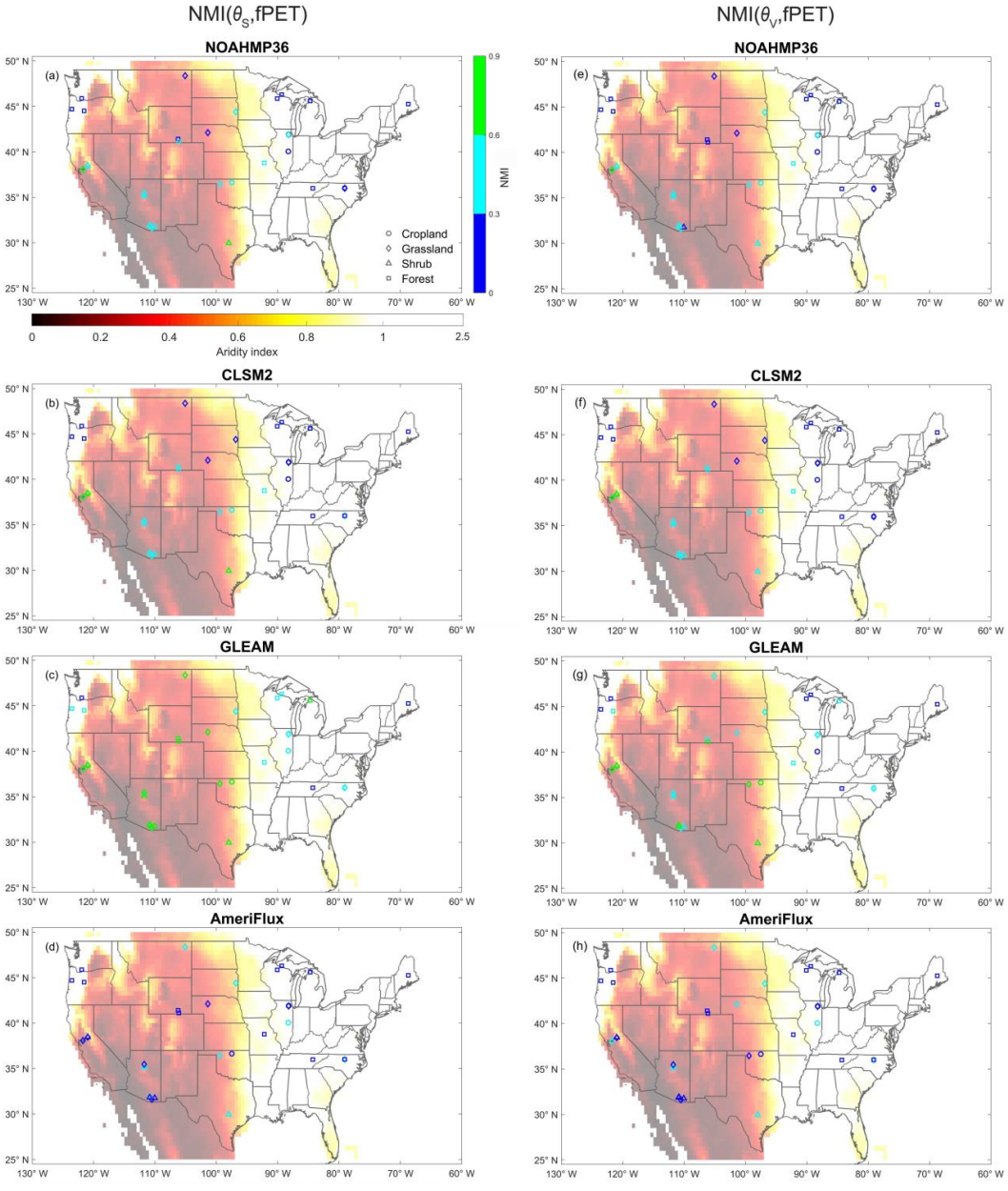

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283 Fig. 3 NMI(θ_S, fPET) (left column) and NMI(θ_V, fPET) (right column) estimates at AmeriFlux sites for: (a) NOAHMP, (b) CLSM,
284 (c) GLEAM and (d) AmeriFlux. Marker color reflects NMI magnitudes and symbol type reflects local land cover type at each site.
285 Background color shading reflects aridity index (AI) values.

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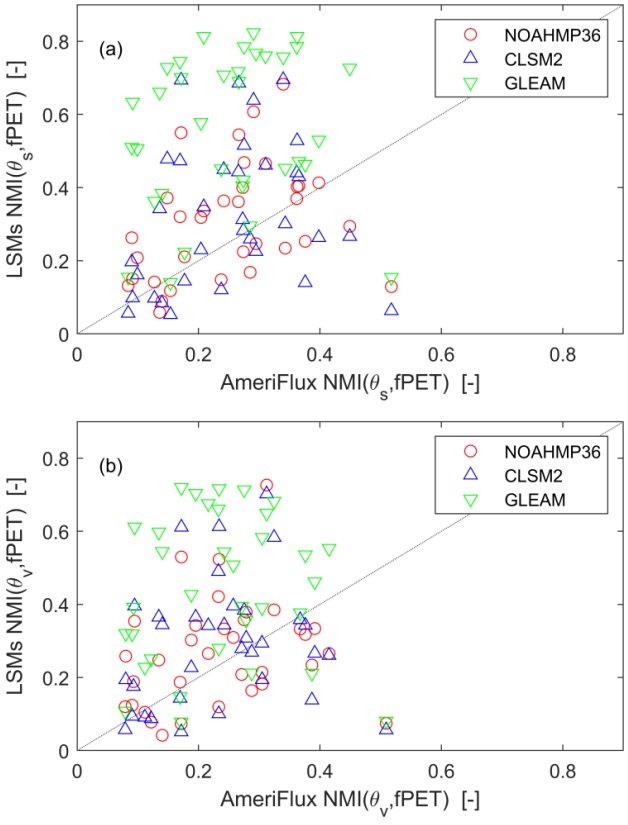

Fig. 4 Scatterplot of LSM-based (a) NMI(θ_S, fPET) and (b) NMI(θ_V, fPET) results versus AmeriFlux observations.

3.4 Sensitivity of NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio to climatic conditions

Figure 5 further summarizes the ratio of NMI(θ_S, fPET) and NMI(θ_V, fPET) as a function of AI for all four products (NOAHMP, CLSM, GLEAM and AmeriFlux). Error bars represent the standard deviation of sampling errors calculated from a 500-member bootstrapping analysis. With increasing AI, there is a decreasing trend in surface and vertically integrated θ/ET coupling within both NOAHMP and CLSM. This decreasing trend is particularly clear when AI is below 1.0 [-]. NOAHMP, CLSM and GLEAM estimates of NMI(θ_S, fPET) are generally higher than NMI(θ_V, fPET) in all climatic conditions. There is relatively lower sensitivity to aridity captured in the AmeriFlux measurements, as the NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio still approximates one under semiarid conditions (i.e., AI < 0.5 [-]).

Connecting these findings to spatial distribution of NMI(θ_S, fPET) and NMI(θ_V, fPET) (Fig. 3), it is confirmed that the relative magnitudes of NMI(θ_S, fPET) and NMI(θ_V, fPET) for all three LSMs are spatially related to hydro-climatic regimes (although in fundamentally different ways). In contrast, this link is weaker in the AmeriFlux measurements which, except for a small fraction of very low AI sites, do not appear to vary as a function of AI. These conclusions

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are not qualitatively impacted by looking at NMI(θ_S, fPET) and NMI(θ_V, fPET) differences, as opposed to their ratio as in Fig. 5, or by looking at R(θ_S, fPET) and R(θ_V, fPET) instead of NMI.

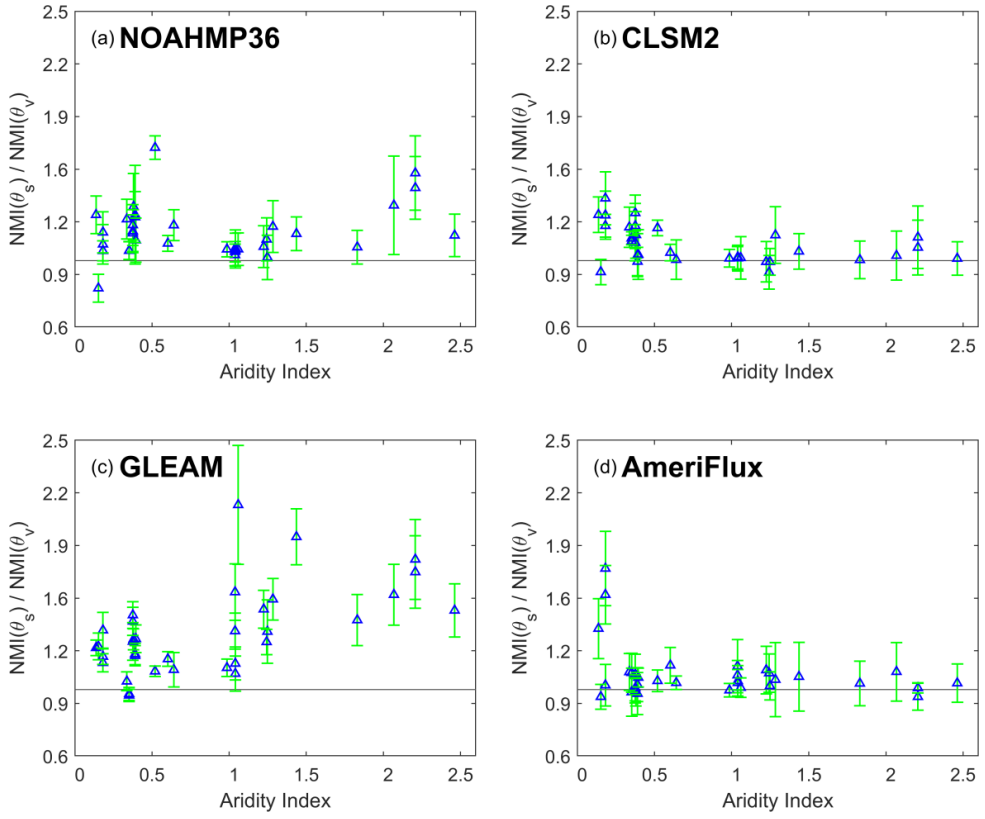

Fig. 5 For a) NOAHMP, (b) CLSM, (c) GLEAM and (d) AmeriFlux estimates, the ratio of NMI(θ_S, fPET) and NMI(θ_V, fPET) as a function of AI across all AmeriFlux sites.

4 Discussion and conclusion

Since transpiration dominates the global ET (Jasechko et al., 2013), deep-layer soil moisture (θ_V) is generally considered to contain more ET information than that of surface soil moisture (θ_S) – given plant transpiration is balanced by root water uptake from deeper soils (Seneviratne et al., 2010). However, this assumption is rarely tested using models and/or observations. Here, we apply normalized mutual information (NMI) to examine how the vertical support of a soil moisture product impacts its relationship with concurrent surface ET.

Specifically, using AmeriFlux ground observations, we examine whether (NMI-based) estimates of LSM θ_S versus ET and θ_V versus ET coupling strength accurately reflect observations acquired at a range of AmeriFlux sites. In general, compared to the baseline case of exponential filter extrapolated 40-cm bottom layer θ_V, LSMs agree with AmeriFlux observations in that the overall fPET information contained in θ_S is slightly higher than that of θ_V (Fig. 1).

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However, the sensitivity analysis showed this difference between NMI(θ_S, fPET) and NMI(θ_V, fPET) diminishes when using different methods for calculating θ_V using AmeriFlux observations (Fig. 2). As a result, this result should be viewed with caution.

While NOAHMP and CLSM derived NMI(θ_S, fPET) and NMI(θ_V, fPET) results are generally consistent with the AmeriFlux observations, GLEAM overestimates NMI(θ_S, fPET), NMI(θ_V, fPET), and the ratio NMI(θ_S, fPET)/NMI(θ_V, fPET) relative to observations. Although both LSMs and GLEAM are based on the same classical two-section (soil moisture-limited and energy-limited) ET regimes framework (Sect. 2.2), they differ in two fundamental aspects. First, the evaporative stress is represented as a more direct and strong function of soil moisture in GLEAM - see Eqs. (4) and (5) - which leads to the overestimation of θ/ET coupling strength. This is consistent with our results that GLEAM generally overestimates NMI(θ_S, fPET) and NMI(θ_V, fPET) consistently across all land covers, compared to AmeriFlux-based estimates.

On the other hand, NOAHMP and CLSM approximate ET in the manner of biophysical models, and expresses biophysical control on ET through the stomatal resistance r_s, which is a function of multiple limiting factors including θ. Therefore, the more complex ET scheme employed by NOAHMP and CLSM would seem to mitigate the overestimation of NMI(θ_S, fPET) and NMI(θ_V, fPET), as other relevant factors besides θ (such as temperature, foliage nitrogen) are also considered in determining maximum carboxylation rate V_{max} and stomatal resistance r_s - and consequently more realistic actual ET. Secondly, the stress factor β in both LSMs considers the cumulative effects of θ conditions along different layers (Eq. (1)), while the corresponding S factor in GLEAM only uses the wettest soil layer condition, which is top layer at most sites. This likely explains the overestimation of the NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio by GLEAM.

Although the median values of NMI(θ_S, fPET) and NMI(θ_V, fPET) predicted by NOAHMP and CLSM are general in line with AmeriFlux observations, they are more spatially related to hydro-climatic conditions (as summarized by AI) than their counter parts acquired from AmeriFlux measurements. Seen from the plot of NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio as a function of AI (Fig. 5), the modelled and observed NMI(θ_S, fPET)/NMI(θ_V, fPET) ratio median decreases with increasing AI, and the decreasing trend is particularly clear when AI is lower than 1.0 [-]. In contrast, there is relatively lower sensitivity to aridity exhibited in the AmeriFlux measurements.

These results provide several key insights into future land-atmosphere coupling analysis and LSM development. First, all the datasets – both model-based and ground-observed – indicates that θ_S contain at least as much ET information as θ_v. Hence, remote-sensing land surface soil moisture datasets are suitable, and should be considered, for analyzing the general interaction between land and atmosphere, e.g., soil moisture – air temperature coupling (Dong and Crow, 2019) and the interplay of soil moisture and precipitation (Yin et al., 2014). Additionally, future generations of GLEAM may consider more sophisticated evaporation stress functions, which may improve its accuracy in representing soil's control on local ET. This may, in turn, improve the accuracy of GLEAM ET product. Finally, our results demonstrate that modeled θ/ET is highly sensitive to hydro-climates, compared to observed relationships.

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Modifying the model structures to reduce such sensitivity might be necessary for accurately representing the interaction of land surface and atmosphere across different climate zone. This may lead to more realistic projections of future drought-induced heatwaves, when coupled with general circulation models.

Data availability

Ground-based soil moisture and surface flux data are available from http://ameriflux.ornl.gov/. GLEAM dataset is available from https://www.gleam.eu/. LSMs simulations of NOAHMP and CLSM used in this study are available by contacting the authors.

Author contributions

Jianxiu Qiu and Wade T. Crow conceptualized the study. Jianzhi Dong helped preparing the LSMs simulation. Grey S. Nearing assisted in the mutual information analysis. Jianxiu Qiu carried out the analysis and wrote the first draft manuscript, and Wade T. Crow refined the work. All authors contributed to the analysis, interpretation and writing.

Competing interests

The authors declare that they have no conflict of interest.

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