

Supplementary Information and Discussion for “The increasing importance of atmospheric demand for ecosystem water and carbon fluxes”

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Section S1: Ameriflux Data Quality Control and filtering: Ameriflux Study Sites are described in Table S1:

Table S1: The Ameriflux synthesis sites. 'h' indicates canopy height. The 'DOY start' and 'DOY end' dates indicate the start and end of the site-specific analysis period, which is assumed to be the period of time during which leaf area index is relatively constant. DI_PM indicates the dryness index (= mean annual potential evapotranspiration/precipitation) determined using the Penman-Monteith model for potential evapotranspiration. 'MAP' is mean annual precipitation derived from the FLUXNET database. Sites that are included in the analysis of future climate effects are indicated with a 'Y.'

SITE NAME	CODE	LAT	LONG	STATE	TYPE	h (m)	Years used	DOY Start	DOY End	DI_PM	MAP (mm)	Future analysis?	Reference
ARM - MAIN	US-ARM	36.61	-97.49	OK	CRO	0.5	2003-2012	141	239	1.52	843	Y	1
Bartlett Experimental Forest	US-BAR	44.06	-71.29	NH	DBF	19	2005-2011	169	225	0.76	1246		2
Black Hills	US-BLK	44.16	-103.65	SD	ENF	12	2004-2008	169	225	2.4	574		
Blogett	US-BLO	38.9	-120.63	CA	ENF	7	2001-2007	170	250	1.08	1226		3
Bondville Main	US-BO1	40.01	-88.29	IL	CRO	3	2001-2008	210	270	1.02	991	Y	4
Brooks Field 11	US-BR3	41.97	-93.69	IA	CRO	1	2005-2011 (odd)	200	250	0.67	847		5
Duke Forest hardwood	US-DK2	35.97	-79.09	NC	DBF	27	2001-2008	141	239	1.24	1170	Y	6,7
Duke Forest loblolly pine	US-DK3	35.98	-79.09	NC	ENF	16.5	2001-2008	127	253	1.37	1170	Y	6,7
Duke Forest open field	US-DK1	35.97	-79.1	NC	GRA	1	2001-2008	141	239	1.18	1170	Y	6,7
Fermi Agriculture	US-IB1	41.86	-88.22	IL	CRO	0.3	2005-2011 (odd)	200	250	0.56	929		8
Fermi Prairie	US-IB2	41.84	-88.24	IL	GRA	0.3	2005-2011	155	225	0.918	930		8
Flagstaff Managed Forest	US-FMF	35.09	-111.763	AZ	ENF	18	2006-2010	169	239	4.02	546		9
Flagstaff Unmanaged Forest	US-FUF	35.09	-111.76	AZ	ENF	18	2006-2010	169	267	3.38	562		9
Freeman Ranch	US-FR2	29.95	-98	TX	SAV	4	2005-2008	113	281	2.15	864		10
GLEES	US-GLE	41.36	-106.24	WY	ENF	12.1	2005-2012	210	240	0.93	525		11
Kansas Field Station	US-KFS	39.06	-95.19	KS	GRA	0.5	2008-2012	140	253	1.02	1014		12
Kendall Grassland	US-WKG	31.74	-109.94	AZ	GRA	0.1	2005-2012	113	281	4.36	407		13
KennedyScrub Oak	US-KS2	28.61	-80.67	FL	SRB	1.5	2000-2006	29	337	0.8	1310		
Konza Prairie	US-KON	39.08	-96.56	KS	GRA	0.4	2007-2012	141	239	1.4	867		12
Lucky Hills Shrubland	US-WHS	31.75	-110.05	AZ	SRB	1	2008-2012	113	281	7.89	320	Y	13
Mary's River Fir	US-MRF	44.65	-123.55	OR	ENF	34	2006-2011	141	253	0.45	1820		14
Mead Irrigated	US-NE1	41.17	-96.48	NE	CRO	1	2001-2012	200	250	0.862	790		15
Mead Rainfed	US-NE3	41.18	-96.44	NE	CRO	1	2001-2011 (odd)	200	250	0.429	784		15
Metolius Intermediate Pine	US-ME2	44.45	-121.56	OR	ENF	22	2002-2012	169	225	2.55	523	Y	16
Metolius Second Young Pine	US-ME3	44.5	-121.62	OR	ENF	3	2004-2007	155	220	1.41	719		17
Missouri Ozark Site	US-MOZ	38.74	-92.2	MO	DBH	24.2	2004-2010	141	239	1.89	986	Y	18,19

Table S1 continued

SITE NAME	CODE	LAT	LONG	STATE	TYPE	<i>h</i> (m)	Years used	PGS Start	PGS End	DI_PM	MAP (mm)	Future analysis?	Reference
Morgan-Monroe State Forest	US-MMS	39.32	-86.41	IN	DBF	27	2000-2012	141	239	1.43	1032	Y	20
NC loblolly pine	US-NC2	35.8	-76.67	NC	ENF	14.1	2005-2010	113	267	1.24	1320		21
Niwot Ridge	US-NR1	40.03	-105.55	CO	ENF	11.5	2000-2012	160	230	1.76	800	Y	22
Oak Openings	US-OHO	41.55	-83.84	OH	DBF	24	2004-2012	160	239	1.2	849	Y	23
Santa Rita Creosote	US-SRC	31.91	-110.84	AZ	SRB	1.7	2008-2012	57	281	5.56	294*		24
Santa Rita Grassland	US-SRG	31.79	-110.83	AZ	GRA	0.5	2008-2014	85	267	5.85	420		
Santa Rita Mesquite	US-SRM	31.82	-110.87	AZ	SAV	2.5	2004-2012	71	281	8.06	380	Y	13
Sylvania	US-SYV	46.24	-89.35	MI	ENF	22	2001-2008	169	239	0.8	380	Y	25
Tonzi Ranch	US-TON	38.43	-120.97	CA	SAV	9	2001-2012	100	170	3.48	559	Y	26
U. of MI Biological Station	US-UMB	45.56	-84.71	MI	DBF	21	2007-2012	169	239	1.347	803		27
Vaira Ranch	US-VAR	38.41	-120.95	CA	GRA	0.55	2000-2012	100	170	2.28	559	Y	26
Walker Branch	US-WBW	35.96	-84.29	TN	DBH	25	1998-2006	141	253	0.8	1372	Y	28
Willow Creek	UW-WCR	45.81	-90.08	WI	DBF	24.2	2000-2012	183	225	0.59	787		25

* Mean annual precipitation data were not reported to FLUXDATA.org for this site; MAP is therefore that reported in reference 24

Half-hourly or hourly records of eddy-covariance derived ET and ancillary meteorological data were obtained from 38 Ameriflux sites in the continental U.S. Sites were chosen for inclusion in the study if at least four years of data, including soil moisture data, were available and generally free of large gaps, though most flux records were much longer (see Table S1).

Hourly data quality control: The ET data were subjected to a standardized quality control procedure whereby data were first filtered to remove missing data and ET measurements greater than 2 mm/hour or less than 0.6 mm/hour. Meteorological data were also screened for obvious outliers (i.e. air temperature less than -30°C or greater than 50°C , $\text{VPD} < 0$, net radiation less than -500 W m^{-2} or greater than 1500 W m^{-2}). Data were not gapfilled; rather, all analysis relied only on screened observations. Most of the analysis was limited to daytime periods ($R_n > 50 \text{ W m}^{-2}$) when wind speed exceeded 1 m s^{-1} and $\text{VPD} > 0.6 \text{ kPa}$ (to minimize stability effects).

Filtering data to periods of relatively stationary leaf area index: Our analysis includes sites that span a wide range of leaf area index and canopy height, which are variables known to affect vegetative hydraulic functioning^{29, 30}. Within a site, temporal variation in leaf area or other aspects of canopy architecture were not explicitly considered, though they may also have affected the temporal dynamics of ET. To minimize the influence of those effects, we filtered our data to exclude periods when leaf area was expected to be low or highly dynamic. In evergreen forests, the analysis period was defined to start two weeks after the average date of the last sub-zero hourly air temperature observation, and was defined to end one week before the average date of the first sub-zero hourly air temperature observation in the fall/winter. In deciduous forests and temperate grasslands, the analysis period was defined to start three weeks after the average date of the last sub-zero hourly air temperature observation, and was defined to end two weeks before the average date of the first sub-zero hourly air temperature observation in the fall/winter. In croplands, semi-arid grassland and shrublands, and Mediterranean ecosystems (i.e. US-TON, US-VAR), the analysis period was defined based on previously published site-specific estimates of leaf area or communication from site data providers. The start and end of the analysis period at each site are given in Table S1.

Limiting the analysis to exclude low VPD: When parameterizing the model of Eq. 1 in the main text, we limited the data to those collected when $\text{VPD} > 1.0 \text{ kPa}$. This approach is consistent with other work³¹, and recognizes that estimates of conductances become unreliable when they are derived by dividing measured water fluxes by near-zero VPD. Furthermore, at low VPD when atmospheric conditions are often stable, boundary layer conductances may become an important constraint on observations of ET. These challenges are exacerbated by the fact that, at low VPD, ET fluxes are also low and of a magnitude comparable to the uncertainty in the observations themselves.

When using the soil-moisture-specific parameterizations of Eq. 1 to determine the total growing season limitations to G_s and ET, we assume that VPD is not limiting when it is less than 0.6 kPa. To an extent, this assumption is one of convenience, since the model of Eq. 1 can produce large errors when VPD is close to zero (and $\ln(\text{VPD})$ is approaching infinity). We note, however, that the difference between PET and ET is typically near zero or negative when $\text{VPD} < 0.6 \text{ kPa}$ (Figure S1). Specifically, across all sites, a linear model for PET-ET as a function of VPD tends to cross zero at $\text{VPD} = 0.6 \text{ kPa}$ on average (std.dev = 0.3 kPa), indicating that at low VPD, ET is not limited from its potential rate.

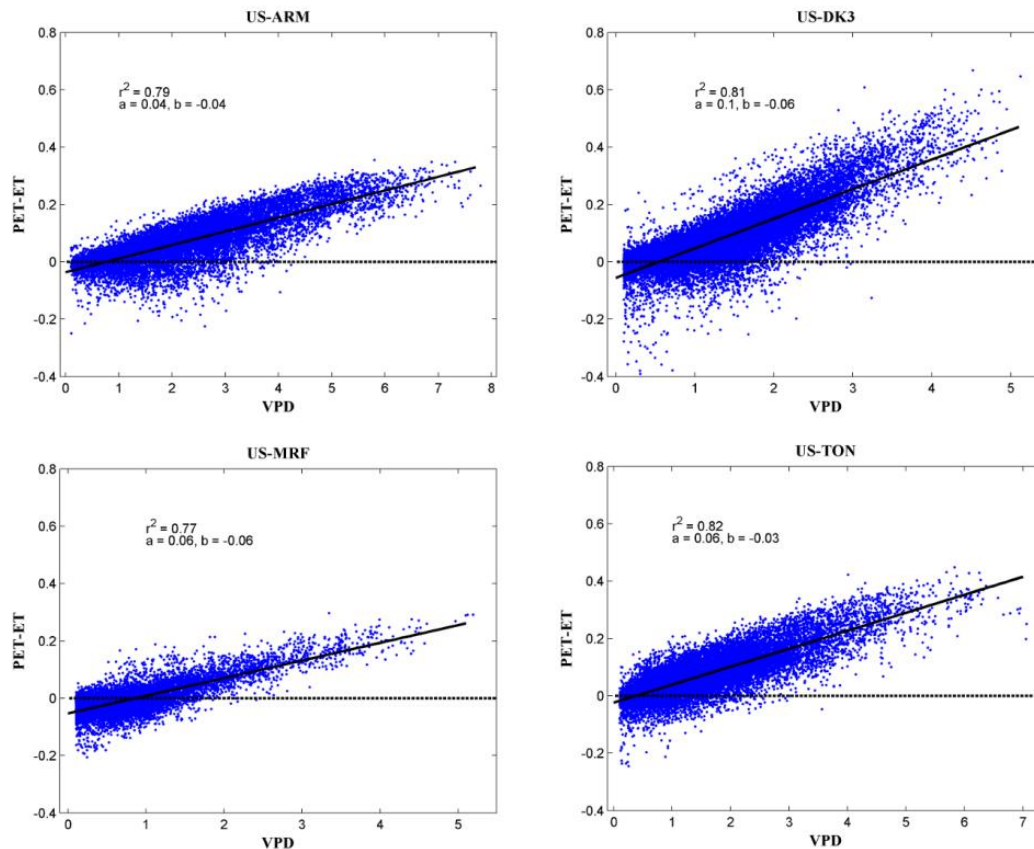


Figure S1: The relationship between PET-ET (i.e. the difference between potential and observed ET) as a function of VPD for four representative sites. The slope (a) and intercept (b) of the derived linear relationship are also shown, together with the coefficient of correlation (r^2)

Estimating the dryness index: The estimates of the dryness index ($DI = PET/P$), which rely on annual estimate of PET and P, are sensitive to missing meteorological data, and in particular missing precipitation data. As evidence, when the mean annual precipitation was determined from the hourly Level 2 Ameriflux data, the ratio of observed ET to observed precipitation (i.e. the evaporative fraction) exceeded 1.0 for about 30% of sites. A multi-year evaporative fraction greater than 1.0 is physically possible if a site experiences significant run-on soil moisture or groundwater convergence; however, in Ameriflux sites that tend to be biased to flat locations, significant run-on is not likely in most sites. Therefore, we calculated the DI using the long-term mean annual precipitation reported by each site to the Fluxnet Database (<http://fluxnet.ornl.gov/>) instead of calculating mean annual precipitation from the Level 2 Ameriflux data. There may be some discrepancies between the DI estimated this way and the true DI for each site's study period if the mean annual precipitation during the study period is much different than the longer-term reported average. However, because the site-specific study periods are generally long and are not limited to the same years (see Table S1), systematic biases across sites (for example due to the occurrence of a large regional drought event) should be minimal.

Section S2: Selecting the model for potential evapotranspiration (PET)

In this study, the potential evapotranspiration rate (PET) is used to calculate the dryness index, and also to quantify limitations to ET imposed by soil moisture and VPD. In many previous studies focused on understanding ecosystem hydrologic processes, the PET has been calculated using the Priestley-Taylor equation³², which may be represented as:

$$PET_{PT} = a_{PT} \frac{S \cdot R_n}{S + \gamma} \cdot \frac{1}{\lambda_v} \quad (S1)$$

where $a_{PT} = 1.26$ is the Priestley-Taylor coefficient, S is the temperature-dependent slope of the saturation-vapor pressure curve, γ is the temperature-dependent psychrometric constant, and λ_v is the temperature-dependent latent heat of vaporization. In this study, which is strongly focused on atmospheric limitations to ET, we estimate PET using the Penman-Monteith^{33, 34} approach, which in addition to accounting for energy constraints to ET, also accounts for aerodynamic and atmospheric constraints. The Penman-Monteith equation for PET may be expressed as:

$$PET_{PM} = \frac{S \cdot R_n + c_p \rho_a g_a VPD}{\lambda_v \left[S + \gamma \left(1 + \frac{g_a}{G_s} \right) \right]} \quad (S2)$$

where S is the temperature-dependent slope of the saturation-vapor pressure curve, R_n is net radiation, ρ_a is the density of dry air, γ is the temperature-dependent psychrometric constant, λ_v is the temperature-dependent latent heat of vaporization, g_a is the aerodynamic conductance, and c_p is the specific heat capacity for dry air.

The formal definition of the Penman-Monteith equation for canopy evapotranspiration relies on a big-leaf assumption, and in many applications G_s is equated to the canopy-level stomatal conductance³⁵. However, ecosystem evapotranspiration includes a significant contribution from soil evaporation (typically on the order of 15-30% for a range of biomes^{36, 37, 38, 39, 40}). In modeling studies, this problem is often met with a two-source (i.e. canopy and soil) modeling procedure where both canopy and soil evaporation are independently simulated from Penman-Monteith type equations. However, in data driven applications like this one, when surface conductance is derived by inverting the Penman-Monteith equation from measured ecosystem scale ET observations, the derived G_s is influenced by soil evaporation, and should not be assumed to be representative of canopy stomatal conductance alone^{35, 41, 42, 43, 44}. Because soil evaporation increases linearly with VPD, a greater ratio of soil evaporation to total evapotranspiration will tend to reduce the magnitude of the VPD sensitivity parameter m .

The aerodynamic conductance (g_a) is formulated as a function of wind speed and canopy height after Campbell & Norman (1998)⁴⁵ as:

$$g_a = \frac{U \cdot k^2}{\left[\ln \left(\frac{z_m - z_d}{z_o} \right) \right]^2} \quad (S3)$$

Where U is the measured wind speed (m/s), k is the Von Karman Constant, z_m is the measurement height, z_d is the zero plane displacement, and z_o is the momentum roughness length. The z_d and z_o were taken as $0.67h$ and $0.1h$, respectively, where h is canopy height, as is common practice in the absence of other information about these parameters^{45, 46}. In some applications, it is common to incorporate a correction for stability effects on g_a via the modification:

$$g_a = \frac{U \cdot k^2}{\left[\ln \left(\frac{z_m - z_d}{z_o} \right) + \Psi_H \right]^2} \quad (S4)$$

where the diabatic correction factor Ψ_H can be specified as a function of the ratio of convective to mechanical production of turbulence as described in Campbell & Norman (1998)⁴⁵.

Filtering the data to remove observations collected when VPD < 0.6 kPa and wind speed < 1 m s⁻¹ should minimize the influence of stability effects on the derived surface conductance. To be sure, we repeated the analysis in a subset of sites spanning the range of dryness index for three scenarios: 1) no stability corrections to g_a (i.e. using Eq. S3) and no wind speed filter, 2) no stability corrections to g_a (i.e. using Eq. S3) with the wind speed filter, and 3) stability corrections to g_a using Eq. S4 with the wind speed filter. In US-DK3, the relationship between g_a and VPD was similar in all scenarios. In the other sites, the relationship between g_a and VPD was similar for scenario 1 & 2, but scenario 3 resulted in higher g_a at high VPD.

Importantly, however, regardless of which scenario was used, the relationship between G_s and VPD was similar in all sites, and nearly indistinguishable in most. Thus, we elected not to correct g_a for stability effects in order to minimize additional uncertainties associated with the parameterization of the stability correction itself.

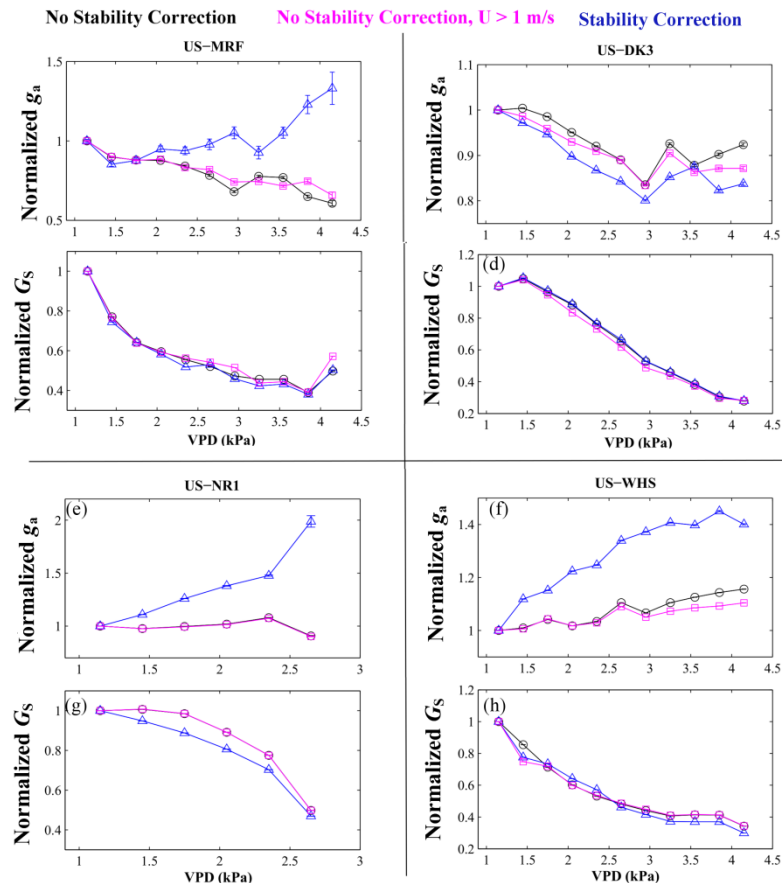


Figure S2: The relationship between aerodynamic conductance and VPD (panels a, c, e, g), and surface conductance (G_s) and VPD (panels b, d, f, and h), showing results from the three stability correction scenarios.

When calculating PET_{PM} for use in determining the site dryness index, we elected to set G_s in Eq. S2 equal to .0148 m/s. This represents the highest value of the reference, well-watered surface conductance rate (i.e. $G_{S,ref,ww}$) observed across the study domain. This approach of using a finite G_s to determine PET is conceptually consistent with the use of the Priestly-Taylor equation, since the parameter a_{PT} is set to approximate well-watered evapotranspiration rates from terrestrial ecosystems, and not, for example, open water (over which G_s is infinite).

The agreement between the dryness index calculated using PET_{PT} and PET_{PM} is shown for reference in Figure S3. The dryness index values tend to be higher when calculated using the Penman-Monteith equation, but overall the two estimates of PET are strongly correlated.

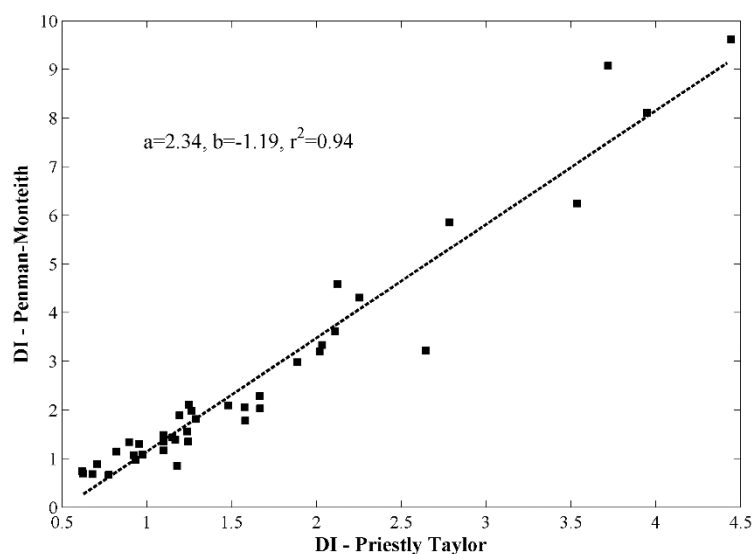


Figure S3: The relationship between dryness index estimated using the Penman-Monteith and Priestly-Taylor Models for PET.

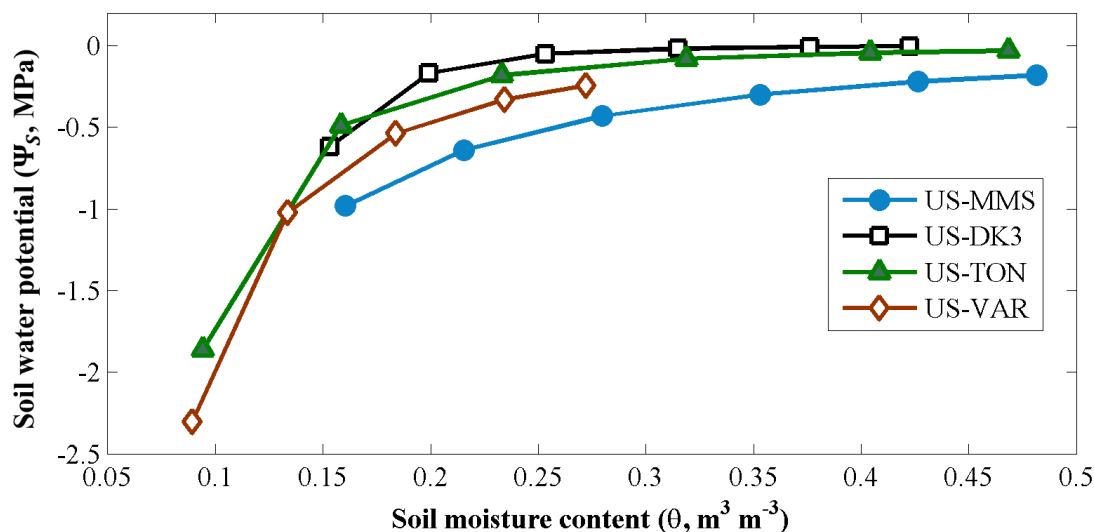
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143 Section S3: The use of soil moisture content as an indicator of plant water 144 availability

145 We elected to use the total volumetric soil moisture (θ) in the top 30 cm as the primary proxy for plant
146 water availability. Most Ameriflux sites rely on time-domain reflectometry (TDR) measurements for θ ,
147 which often require a site-specific calibration. Details of these site-specific calibrations are not available
148 in the Ameriflux database, and thus cross-site comparisons of soil moisture content should be approached
149 with caution. In other studies, the relative extractable water (REW, which represents soil moisture content
150 scaled by the minimum and maximum observed values) is used instead to facilitate cross-site comparisons
151 of ecosystem water use^{47, 48}.

152 It could be argued that soil water potential (Ψ_s) is a more appropriate measure of soil water availability
153 than either θ or REW, since water tension in the soil is an important physical driver of water movement
154 through soil matrices and plants^{49, 50}. Unfortunately, soil water potential is rarely measured in the field.
155 Occasionally, laboratory-based dry down experiments are used to derive an empirical relationship
156 between θ and Ψ_s . This relationship is not linear⁴⁹, though it is monotonically increasing. As illustrated in
157 Figure S4, in sites for which estimates of Ψ_s are available, Ψ_s increases more rapidly with increasing θ
158 when the latter is low; consequently, the results of this study associated with the drier soil moisture bins
159 will likely reflect the response to a relatively wider range of Ψ_s conditions.

160 It is important to note that the choice of the soil moisture variable (i.e. θ vs. REW vs. Ψ_s) has no effect on
161 our primary results concerning the relative importance of soil moisture versus VPD limitations to surface
162 conductance and ET (e.g. the results presented in Figures 2, 3 & 4 in the main text). This is because the
163 analytical approach relies on binning the data into quantiles defined by the 0-15th, 15th-30th, 30th-50th, 50th-
164 70th, 70th-90th, and 90th-100th percentiles of θ , and then parameterizing Eq. 1 within each bin. Because the
165 relationships between θ and REW and Ψ_s are all monotonically increasing, the same data will fall into the
166 same bins regardless of which soil moisture metric is used.



167

168 Figure S4: The relationship between soil water potential (Ψ_s) and soil moisture content (θ) in four study sites for
169 which site-specific relationships between θ and Ψ_s were available (see references Wayson et al. 2016 for US-MMS,
170 Hacke et al. 2000 for US-DK3, and Baldocchi et al. 2004 for US-TON and US-VAR.

S4. Determining the well-watered reference surface conductance (i.e. $G_{S,ref,ww}$).

The limitations to G_S imposed by soil moisture and VPD were estimated by comparing hourly estimates of G_S to the well-watered reference value of surface conductance (i.e. $G_{S,ref,ww}$). This parameter represents the surface conductance when soil moisture content exceeds the 90th percentile in each site, and $0.9 < VPD < 1.1$ kPa. Choosing the reference VPD of 1.0 kPa is consistent with previous work³¹. The approach recognizes the fact that surface conductance estimates at low VPD are sensitive to biases introduced by low boundary layer conductance and instabilities in the determination of G_S from ET when VPD is low.

The magnitude of $G_{S,ref,ww}$ tends to be low in sites with a high dryness index, and variable but generally higher in more mesic sites (Figure S5). The low $G_{S,ref,ww}$ in the driest sites is expected, as canopy stomatal conductance – an important component of G_S – is driven by leaf area⁵¹, which is very low in semi-arid ecosystems. The variability in $G_{S,ref,ww}$ in more mesic sites may be explained, to an extent, by variation in leaf area as well as variation in canopy height, which introduces another important structural control on canopy stomatal conductance^{30, 52}. While these sources of variability in well-watered G_S are an important long-term constraint on ecosystem carbon and water cycling, they are not the focus of this present study. We point readers elsewhere³² for a more thorough treatment of the topic.

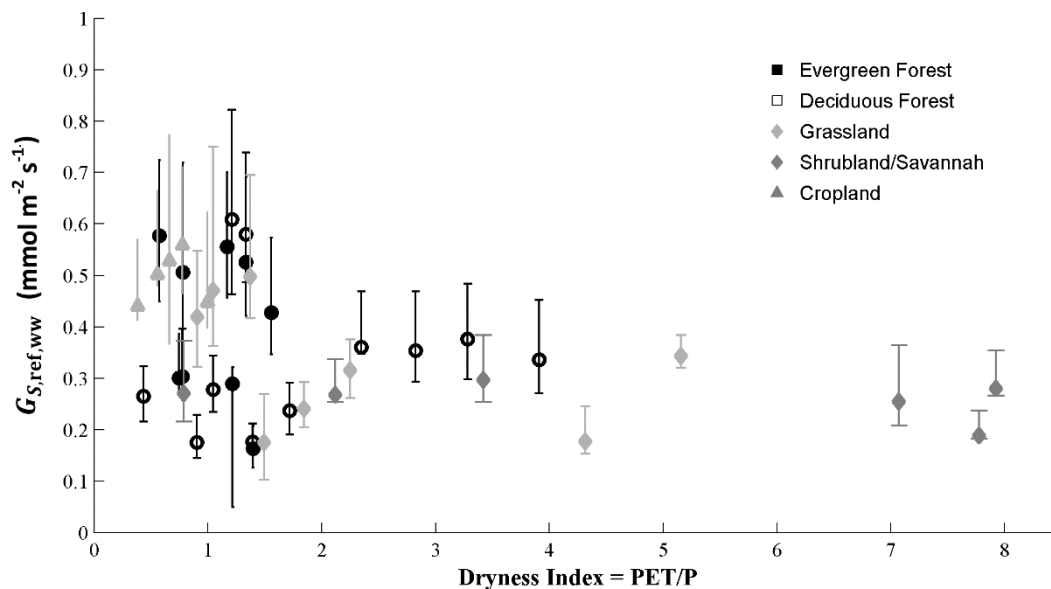


Figure S5: The relationship between the well-watered reference surface conductance ($G_{S,ref,ww}$) and dryness index. Error bars indicates the 50% confidence interval on the estimate of $G_{S,ref,ww}$ as derived from a non-parametric bootstrap.

Section S5: The relationship between VPD and θ at various timescales

Our analysis leverages the fact that while VPD and θ are moderately to strongly correlated at long time-scales (i.e. monthly to annual), they are relatively weakly coupled at the hourly and daily timescales over which Ameriflux data is gathered. In Figure 1 of the main text, we present a summary of the correlation between θ and VPD averaged across all study sites for varying averaging periods (i.e. seasonal, monthly, weekly, daily, and hourly). For illustrative purpose, we show the data that inform that summary presentation for one representative site in Figure S6, and present the statistics of the linear regressions between the two variables over the various timescales in Table S2.

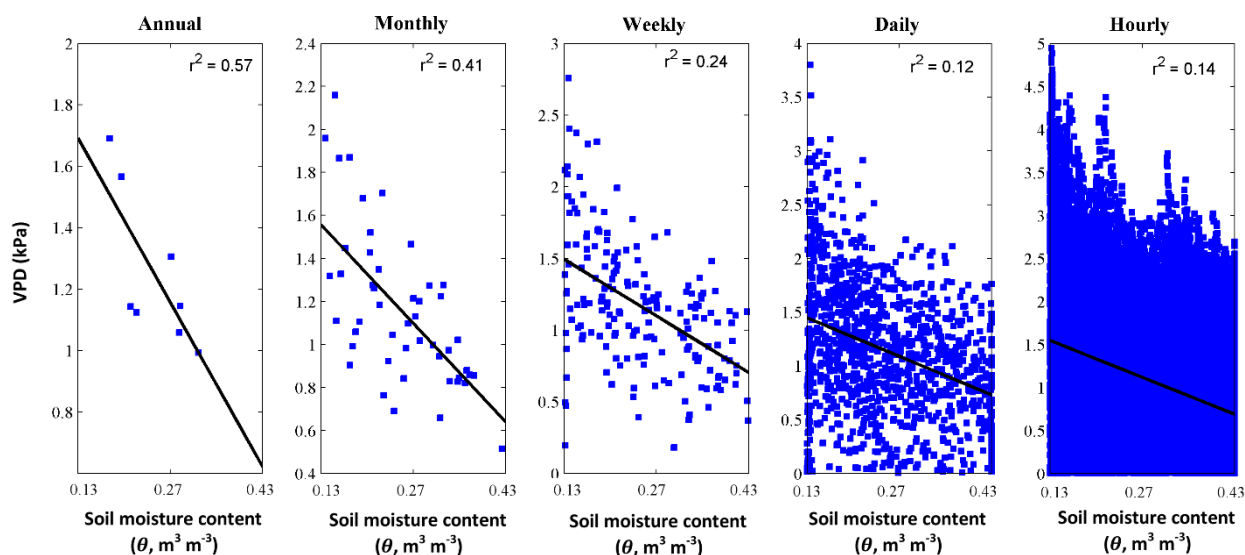


Figure S6: The relationship between vapor pressure deficit (VPD) and soil moisture content (θ) when both are averaged over various timescales. Data are from the US-DK3 (Duke Pine Forest).

Table S2: The slope, intercept, and correlation coefficient of the relationship between vapor pressure deficit (VPD) as a linear function of soil moisture content (θ) inferred by averaging the data over various timescales. In general, the slope and intercept parameters are relatively stationary across timescales, but the two variables become increasingly decoupled (i.e. r^2 is lower) at shorter timescales.

	Slope					Intercept					correlation coefficient (r^2)				
	year	month	week	day	hour	year	month	week	day	hour	year	month	week	day	hour
ARM	-0.91	-1.10	-1.28	-1.36	-0.98	2.54	2.54	2.70	2.76	1.96	0.38	0.12	0.15	0.14	0.06
BAR	-0.46	-0.13	-0.24	-0.24	-0.37	1.15	0.97	1.00	0.98	0.94	0.55	0.02	0.04	0.02	0.03
BLK	-0.65	-0.32	-0.47	-0.60	-0.19	1.73	1.50	1.63	1.67	1.06	0.40	0.04	0.07	0.04	0.01
BLO	0.18	-0.81	-0.39	-0.21	-1.16	1.80	1.95	1.90	1.89	2.08	0.08	0.20	0.04	0.01	0.32
BO1	-0.41	-0.44	-0.63	-0.48	-0.29	1.30	1.36	1.45	1.28	1.01	0.26	0.22	0.24	0.10	0.01
BR3	0.73	0.27	-0.31	-0.50	0.13	0.62	0.94	1.22	1.28	0.88	0.65	0.10	0.09	0.15	0.00
DK1	-1.40	-0.96	-1.04	-0.96	-0.82	1.83	1.60	1.66	1.60	1.53	0.67	0.40	0.31	0.19	0.13
DK2	-1.79	-0.94	-1.08	-1.01	-0.78	1.97	1.57	1.65	1.61	1.53	0.81	0.36	0.31	0.21	0.13
DK3	-1.07	-0.92	-0.79	-0.72	-0.86	1.69	1.56	1.49	1.45	1.55	0.57	0.42	0.25	0.12	0.15
FMF	0.10	-0.56	-0.65	-1.09	-0.88	1.55	1.82	1.94	2.25	1.79	0.01	0.07	0.09	0.12	0.08
FR2	-1.70	-0.92	-1.50	-1.30	-1.13	2.42	1.98	2.34	2.21	2.00	0.98	0.18	0.55	0.33	0.14
FUF	-1.25	-1.20	-1.32	-1.43	-0.91	2.18	2.09	2.20	2.25	1.66	0.95	0.64	0.57	0.40	0.16
GLE	0.06	0.03	0.13	0.14	0.61	0.96	0.93	0.91	0.90	0.20	0.03	0.01	0.04	0.01	0.16
IB1	-0.64	-0.56	-0.65	-0.79	-1.10	1.52	1.45	1.51	1.57	1.62	0.56	0.30	0.42	0.29	0.16
IB2	-0.45	-0.53	-0.44	-0.61	-0.84	1.40	1.39	1.36	1.46	1.39	0.24	0.23	0.12	0.10	0.10
KFS	-2.75	-1.60	-1.66	-1.52	-1.67	2.74	2.02	2.16	2.16	2.17	0.99	0.34	0.36	0.25	0.28
KON	-0.68	-1.42	-1.41	-1.21	-1.23	2.05	2.41	2.49	2.34	2.10	0.49	0.32	0.28	0.18	0.14
KSO	0.25	0.10	-0.09	-0.20	-0.22	1.10	1.11	1.20	1.22	1.25	0.03	0.00	0.00	0.01	0.01
ME2	-0.48	-0.68	-0.38	-0.61	-1.27	1.63	1.53	1.51	1.64	1.78	0.11	0.07	0.02	0.04	0.32
ME3	0.62	-0.48	-0.37	-0.63	-1.38	1.79	2.00	2.03	2.17	2.11	0.06	0.08	0.02	0.04	0.28
MMS	-0.96	-0.42	-0.29	-0.33	-0.78	1.52	1.18	1.09	1.12	1.32	0.43	0.13	0.05	0.04	0.11
MOZ	-0.67	-0.82	-0.93	-1.02	-1.09	1.71	1.75	1.84	1.89	1.69	0.28	0.26	0.27	0.19	0.15
MRF	0.66	-0.76	-0.66	-0.59	-0.72	0.50	0.94	0.93	0.89	0.99	0.09	0.52	0.27	0.10	0.17
NC2	-0.24	-0.27	-0.21	-0.27	-0.45	1.34	1.30	1.28	1.30	1.29	0.48	0.12	0.04	0.03	0.04
NE1	-0.96	-0.98	-0.80	-1.03	-0.20	1.77	1.77	1.66	1.80	1.15	0.30	0.33	0.21	0.18	0.00
NE3	-1.52	-0.84	-0.58	-0.73	-0.57	1.97	1.69	1.58	1.65	1.42	0.56	0.32	0.18	0.15	0.04
NR1	-0.31	-0.25	-0.38	-0.38	-0.05	1.07	1.03	1.07	1.08	0.66	0.27	0.17	0.16	0.06	0.00
OHO	-1.58	-0.86	-0.63	-0.57	-0.86	1.79	1.42	1.34	1.31	1.33	0.47	0.35	0.19	0.11	0.15
SRC	0.82	-1.09	-1.08	-1.11	-1.18	2.25	2.98	3.03	3.02	2.92	0.27	0.10	0.10	0.09	0.07
SRG	-1.17	-1.90	-1.73	-1.73	-1.95	2.90	3.13	3.07	3.09	3.14	0.64	0.45	0.34	0.24	0.33
SRM	-1.61	-0.80	-1.22	-1.38	-1.72	3.04	2.74	2.93	2.99	2.85	0.17	0.07	0.20	0.20	0.22
SYV	0.04	-0.16	-0.13	-0.08	-0.51	1.00	1.03	1.06	1.04	1.11	0.00	0.02	0.01	0.00	0.04
TON	-0.33	-0.27	-0.45	-0.51	-0.64	0.88	0.83	0.90	0.91	1.06	0.47	0.05	0.12	0.11	0.08
UMB	0.09	-0.95	-0.69	-0.68	-0.80	0.88	1.25	1.15	1.13	1.20	0.03	0.54	0.30	0.18	0.17
VAR	-0.32	-0.57	-0.51	-0.56	-0.56	0.87	0.98	0.93	0.95	0.98	0.17	0.27	0.18	0.13	0.09
WBW	-0.83	-0.22	-0.30	-0.41	-0.59	1.52	1.12	1.18	1.23	1.32	0.13	0.03	0.05	0.06	0.07
WCR	0.12	0.04	-0.06	-0.16	0.02	0.47	0.49	0.56	0.60	0.41	0.05	0.00	0.00	0.01	0.00
WHS	-2.49	-0.69	-1.38	-1.49	-0.95	3.65	2.76	3.17	3.24	2.61	0.51	0.03	0.16	0.17	0.05
WKG	-0.03	-1.05	-1.09	-1.16	-0.99	2.38	2.63	2.77	2.82	2.41	0.00	0.12	0.15	0.13	0.06
Mean	-0.62	-0.67	-0.71	-0.76	-0.77	1.68	1.63	1.69	1.71	1.55	0.36	0.20	0.18	0.13	0.12
Std	0.84	0.47	0.48	0.46	0.52	0.71	0.65	0.69	0.70	0.66	0.29	0.17	0.14	0.09	0.09

Section S6: Determining soil moisture as compared to VPD constraints to G_s and ET: The growing season ET and meteorological data were sorted into bins representing the 0-15th, 15th-30th, 30th-50th, 50th-70th, 70th-90th, and 90th-100th percentiles of θ , spanning a gradient of dry to wet conditions in each site. Within each soil moisture bin, we further sorted the data on the basis of VPD; the VPD bins had a width of 0.2 kPa, and there were $j = 1, 2, \dots, N_i$ VPD bins in each soil moisture bin, where N_i varies as a function of the maximum VPD observed at each site. The mean G_s in each bin was determined provided there were more than 10 data points in any given (i, j) bin.

The binned averages were used to derive site- and soil-moisture-specific parameterizations for Eq. 1 in the main text, which were leveraged to quantify the total growing season average supply and demand limitations to G_s and ET. Briefly, θ constraints were inferred from changes in the intercept parameter ($G_{s,ref}$), and VPD constraints were inferred from the sensitivity parameter m . Estimates of hourly G_s reflecting either θ or VPD control for all daytime periods were then subtracted from the $G_{s,ref,ww}$ to quantify the magnitude of limitations to G_s attributable to each driver. These estimates of hourly G_s were then used in Eq. S2 to generate estimates of ET that reflect either θ or VPD constraints to G_s . Limitations to ET were then defined as the difference between hourly PET and ET, where the PET is generated using Eq. S2 forced with the site-specific $G_{s,ref,ww}$. In most sites, the reported θ corresponds to integrated observations over the top 30 cm of the soil. The soil moisture dynamics in the top 30 cm may not always be well coupled to soil moisture at depth, which represents a potential source of bias in sites with deeper roots.

In Figure 2 of the main text, we show representative results from four sites. Here are analogous figures for all study sites. The fitted lines, which show the model of Eq. 1 within each soil moisture bin, do not extend below VPD < 1.0 kPa, as those data were not used to drive the regressions due again to instabilities in the observations at low VPD.

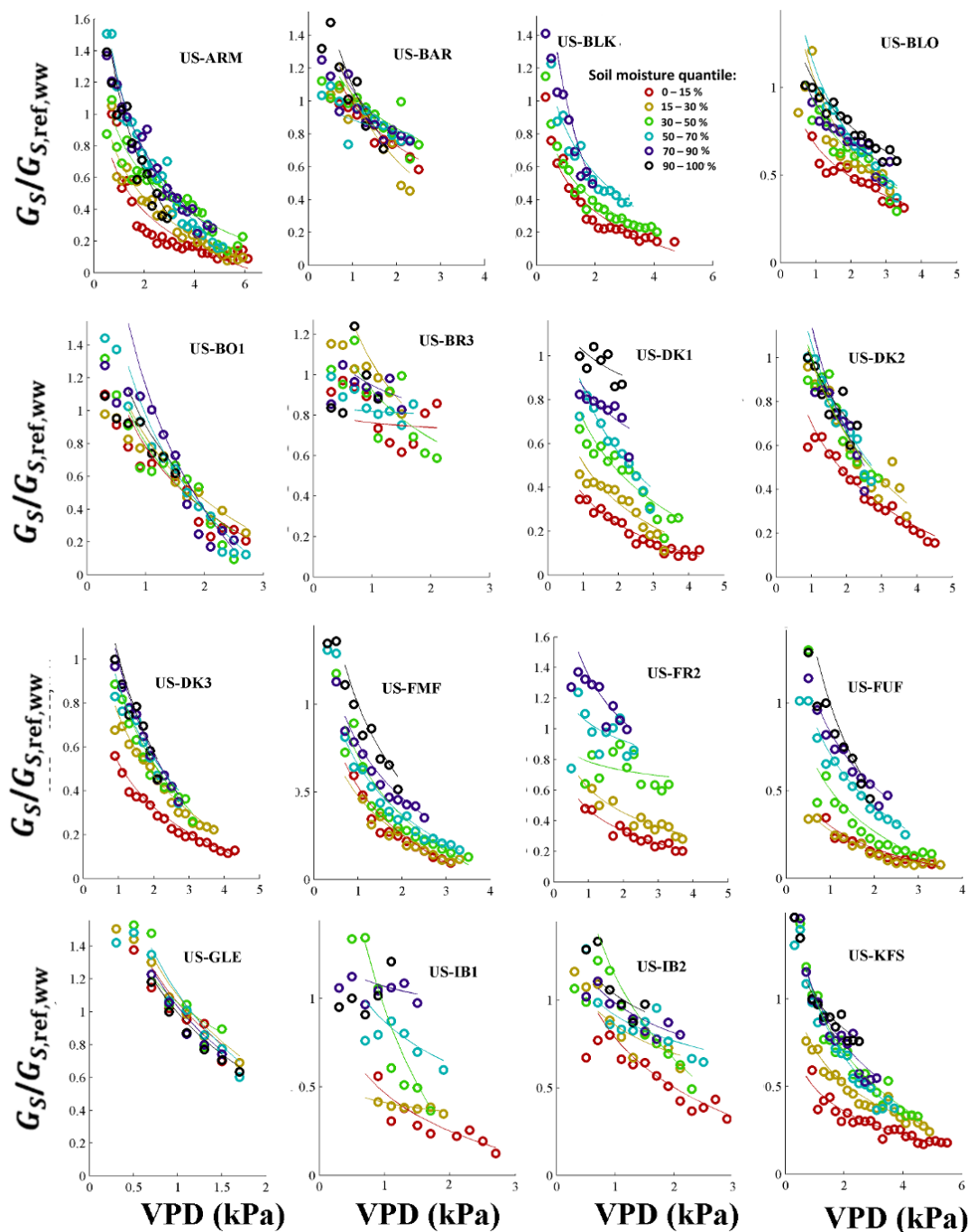


Figure S7. Same as Figure 2a-d in the main text, but for the first sixteen study sites (in alphabetical order).

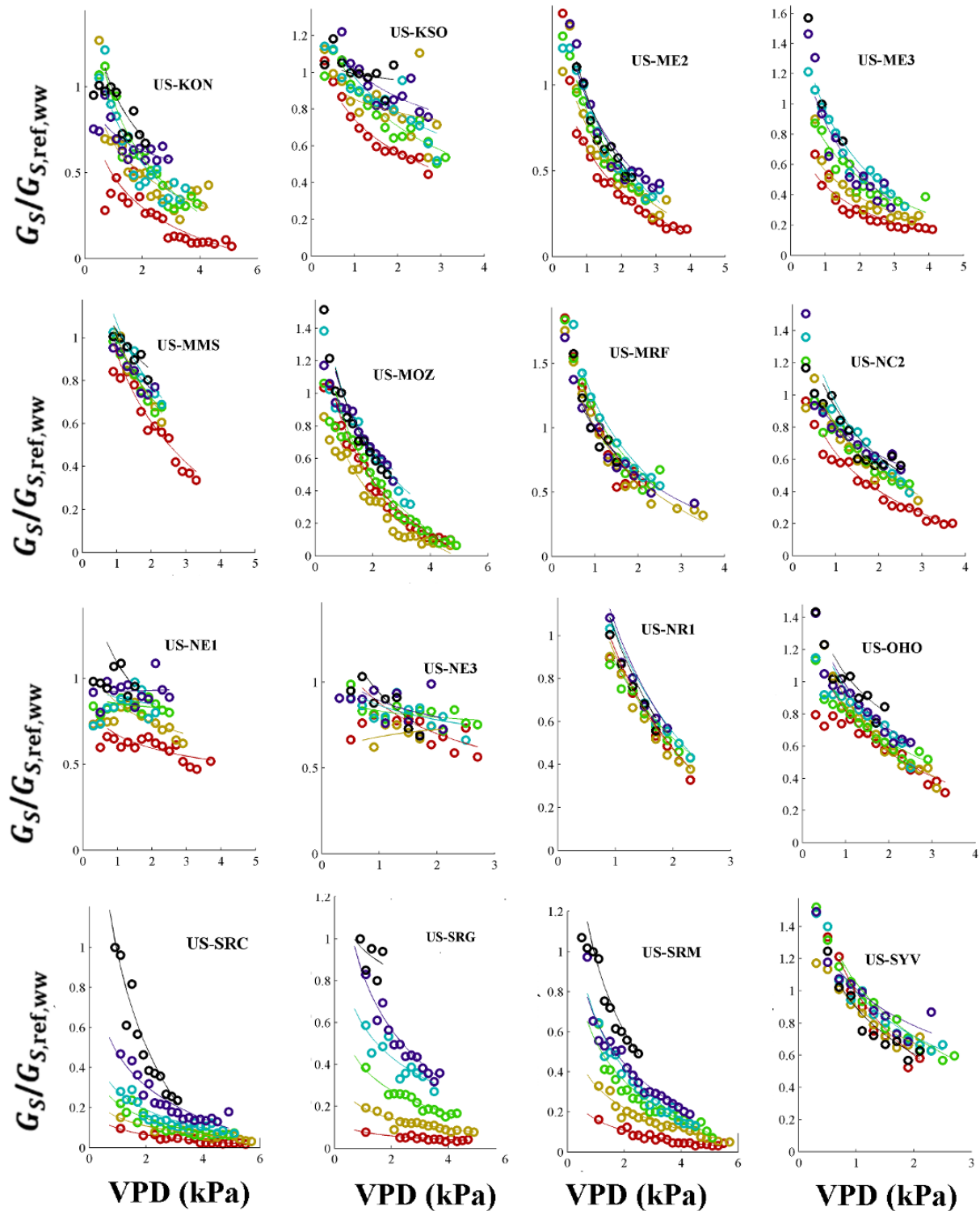


Figure S8. Same as Figure 2a-d in the main text, but for the second sixteen study sites (in alphabetical order).

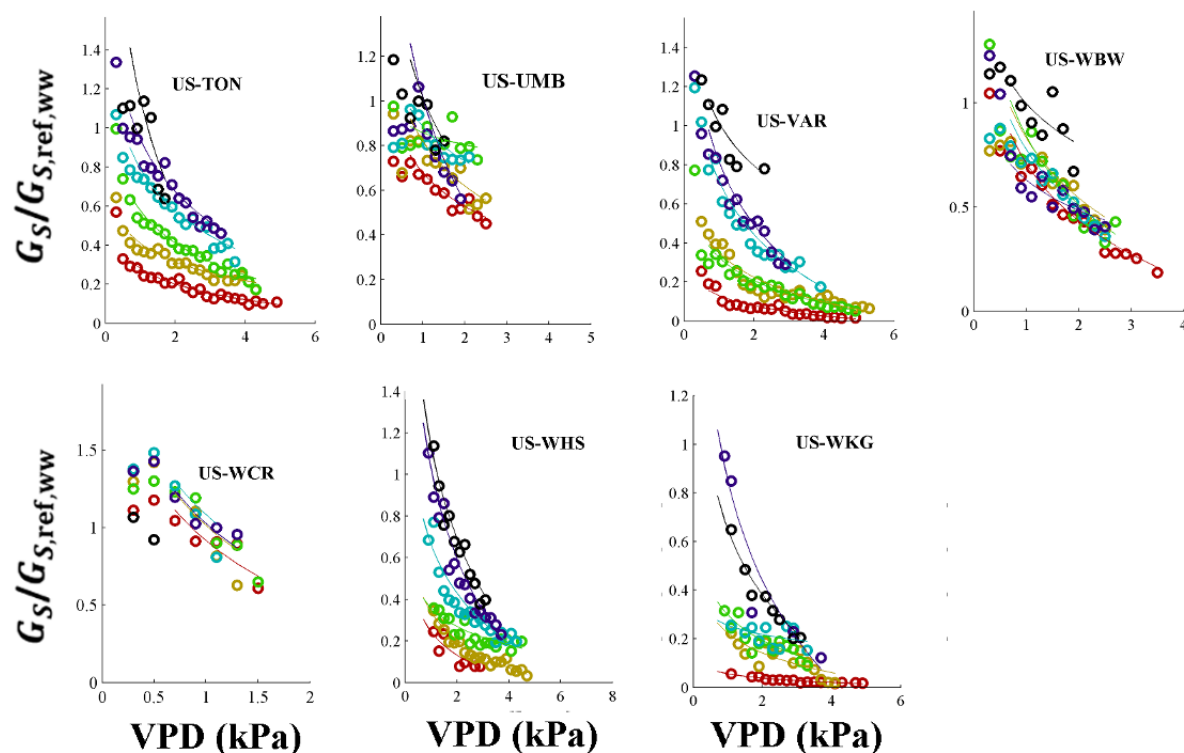


Figure S9. Same as Figure 2a-d in the main text, but for the last seven study sites (in alphabetical order).

Section S7: Effects of other meteorological drivers on $G_{S,ref}$

Other work has demonstrated that the reference surface or stomatal conductance may be sensitive to variations in photosynthetically active radiation (PAR) and air temperature (T_a)^{51, 53}. In this study, variations in $G_{S,ref}$ with PAR or T_a were not explicitly considered, due primarily to the fact that accounting for them (for example, by introducing additional dimensions to the data binning matrix) often results in an insufficient amount of data within each soil moisture bin to properly parameterize Eq. 1. This is particularly true in sites with a short active season, which include both the hottest and coolest sites in the dataset.

In all sites, VPD is directly correlated with temperature (reflecting the fact that the saturation vapor pressure depends exponentially on T_a), and also directly correlated with PAR (since T_a tends to be highest when radiation loads are high, see Figure S10). Soil moisture tends to be inversely correlated with T_a in most sites, and only weakly related to PAR (again, see Figure S10).

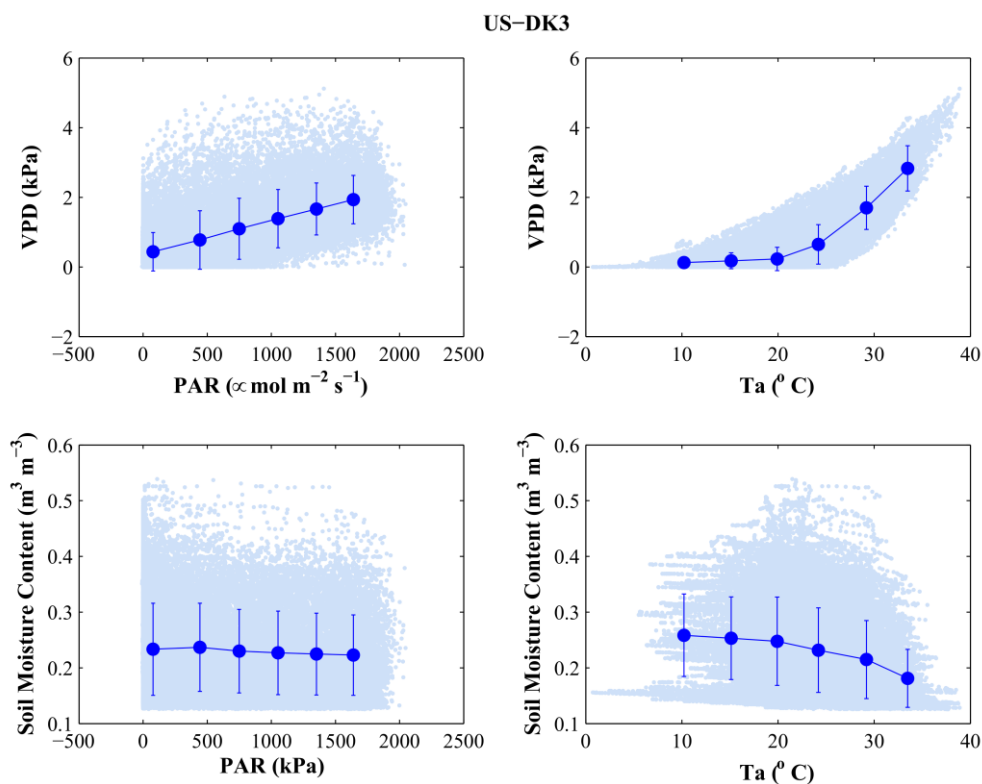


Figure S10: The relationship between vapor pressure deficit (VPD), photosynthetically active radiation (PAR) and air temperature (T_a) at the Duke Forest pine plantation (US-DK3). Light blue dots show all data, and blue circles show binned averages. Error bars show one standard deviation.

It is possible that high T_a may limit G_s and ET through biochemical limitations to leaf-level gas exchange⁵⁴ that occur independent of limitations to G_s imposed by high VPD. In that case, failure to resolve temperature effects on G_s could lead us to overestimate the VPD limitations and underestimate the soil moisture limitations. On the other hand, because canopy stomatal conductance is known to be

monotonically related to PAR^{51,55}, failure to account for independent PAR effects could lead us to underestimate VPD limitations and overestimate soil moisture limitations.

To explore the extent to which these biases are significant, in each site, we attempted separate parameterizations for Eq. 1 when PAR was limited to high values ($\text{PAR} > 1500 \mu\text{mol m}^{-2} \text{s}^{-1}$) and when T_a was limited to a relatively narrow range of 5 °C. In both cases, data were binned according to soil moisture content as described in the methods of the main text. The range of temperature depended on the mean growing season T_a at each site but was usually between 20 and 25 °C. Enough growing season data were available to support this effort in 23 of the sites. In general, the $G_{s,\text{ref},j}$ (i.e. $G_{s,\text{ref}}$ for each of the $j=6$ soil moisture bins) were similar regardless of whether the full or filtered datasets were used (see Fig S11 for results from representative sites). Specifically, across all sites, the slope of the relationship between the $G_{s,\text{ref}}$ values obtained from the full dataset as compared to the dataset filtered to a narrow temperature range was 0.97 on average (st. dev. = 0.44), and the average correlation coefficient was 0.75. Similarly, the slope of the relationship between the $G_{s,\text{ref}}$ values obtained from the full dataset as compared to the dataset filtered to a PAR range was 1.02 on average (std dev. = 0.40), and the average correlation coefficient was 0.80. Thus, the decision not to account for PAR and T_a effects on $G_{s,\text{ref}}$ does not introduce systematic biases across the sites.

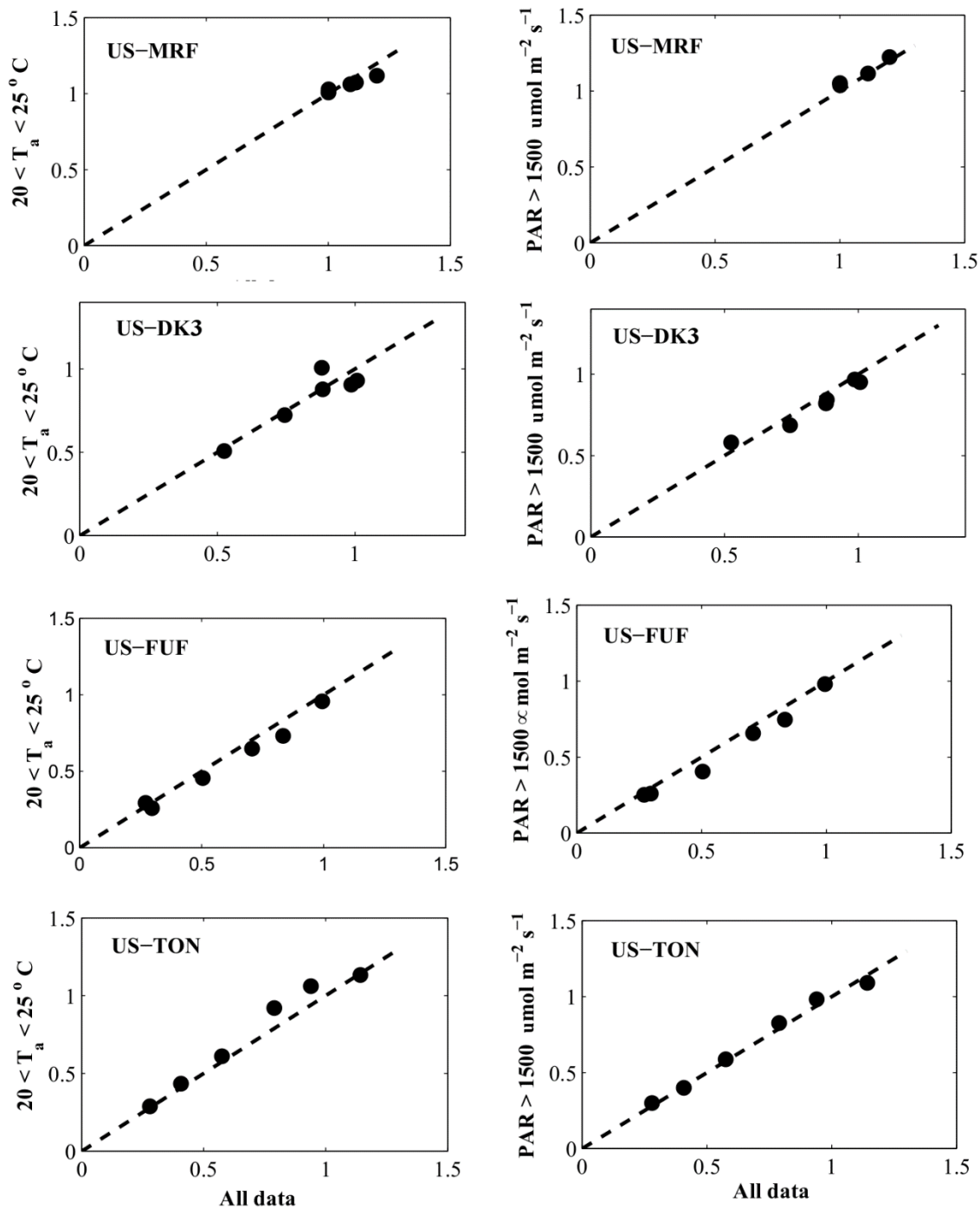


Figure S11: The relationship between the reference G_s within each soil moisture bin (i.e. $G_{s,\text{ref},j}$) as derived from all growing season data (subject to the filtering constraints described in Section S1), and data subjected to an additional temperature filter (left hand column) or PAR filter (right hand column). The sites shown here span a range of dryness index (see Table S1).

Section S8: Future projections – model estimates and downscaling

Projections for future meteorological variables, including R_n , VPD, air temperature, and precipitation were obtained from ten general circulation models for the period from 2071–2080, chosen as the transition point between the mid- and late-21st century. Modeled data were downscaled in space using parametric approaches, and downscaled in time using representative diurnal patterns measured at each study site. Future soil moisture was estimated from a marginal distribution sampling approach based on short- and long-term dynamics of VPD and precipitation that reproduced observed soil moisture dynamics with little bias. The future VPD and soil moisture limitations to G_s and ET were then determined in a manner analogous to the approach for present day conditions.

Obtaining projections of future meteorological drivers: Estimates of the key drivers of the Penman-Monteith model were obtained from the Multivariate Adaptive Constructed Analogs (MACA⁵⁶) data warehouse (<http://maca.northwestknowledge.net/>) for a representative selection of twelve Ameriflux sites that include long-running towers and that span a wide gradient in climate (See Table S1). Specifically, we obtained daily time series of net radiation, air temperature, specific humidity, and wind speed projected from 10 General Circulation Models from the Coupled Model Intercomparison Project – Phase 5 (CMIP5) archive driven by representative concentration pathway 8.5 (highest greenhouse gas emission scenario) were downloaded for the period 1950–2099. The ten models are listed in Table S3.

Table S3: The models used to obtain estimates of future meteorological drivers

Model Name	Model Country	Model Agency
CanESM2	Canada	Canadian Centre for Climate Modeling and Analysis
CNRM-CM5	France	National Centre of Meteorological Research, France
CSIRO-Mk3-6-0	Australia	Commonwealth Scientific and Industrial Research Organization/Queensland Climate Change Centre of Excellence, Australia
GFDL-ESM2G	USA	NOAA Geophysical Fluid Dynamics Laboratory, USA
HadGEM2-ES	United Kingdom	Met Office Hadley Center, UK
inmcm4	Russia	Institute for Numerical Mathematics, Russia
IPSL-CM5A-LR	France	Institut Pierre Simon Laplace, France
MIROC-ESM-CHEM	Japan	Japan Agency for Marine-Earth Science and Technology, Atmosphere and Ocean Research Institute (The University of Tokyo), and National Institute for Environmental Studies
MIROC5	Japan	Atmosphere and Ocean Research Institute (The University of Tokyo), National Institute for Environmental Studies, and Japan Agency for Marine-Earth Science and Technology

Spatial downscaling of the model data: While the MACA CMIP data have already been downscaled with respect to the climate models, the spatial resolution of these data (4 km x 4 km) still exceeds the size of a typical flux footprint (typically <1 square km during the daytime). Furthermore, significant biases were observed between the CMIP and observed meteorological drivers. Thus, the meteorological data were further downscaled using a parametric approach driven by the site-level observations.

Specifically, for air temperature, VPD, R_n , and wind speed, histograms of the downscaled GCM data for the period coincident with the study period at each site were compared to histograms of the measured data after the latter was aggregated to daily averages to match the temporal resolution of the modeled data. Biases were removed by first log-transforming both datasets, and then determining the mean and standard deviation of the resulting log-normal distributions. The modeled time series were then further transformed to a standard log-normal variable that was then scaled using the mean and standard deviation of the log-transformed measured time series, and exponentiated (hereafter the “modeled_{present,scaled}” data). This downscaling was performed separately for each model.

Next, the modeled meteorological time series for the period 2071–2080 were extracted as representative of the mid-to-late 21st century. The shift in the mean of each modeled variable between the measurement (“present”) time period and the future was determined from the unscaled daily projections according to:

$$\mu_{\text{factor}} = \left(\frac{\text{mean}[\ln(\text{modeled}_{2071-2080})]}{\text{mean}[\ln(\text{modeled}_{\text{present}})]} \right) \quad (\text{S4})$$

$$\sigma_{\text{factor}} = \left(\frac{\text{stdev}[\ln(\text{modeled}_{2071-2080})]}{\text{stdev}[\ln(\text{modeled}_{\text{present}})]} \right) \quad (\text{S5})$$

The time series for the period 2071–2080 was then transformed into a standard normal variable that was scaled using the mean and standard deviation of the modeled_{present,scaled} distributions after correcting those moments by μ -factor and σ -factor, respectively. This approach preserves the projected relative changes in the mean and variance of the modeled time series between the present and future conditions, but retains the spatial downscaling to the site level.

Projecting future relative extractable soil water: Projections of downscaled soil moisture were not available from the MACA data warehouse. Thus, future soil moisture (at a daily time step) was estimated using a site-specific marginal distribution sampling approach (i.e. a look-up table), similar to the approaches frequently used to gapfill missing eddy covariance data⁵⁷. Accordingly, measured θ data were binned according to the following classification scheme, which depends on the total time since a significant rain event (>20 mm), among other hydrologic variables:

1) If the time since a significant (>20 mm) rain event is less than two days, then soil moisture is the mean of measured values when:

- The total precipitation within the last 7 days agrees to within 10 mm
- The day-of-year agrees to within 10 days;

else, 2) If the time since a significant (>20 mm) rain event is between 2 and 3 days, then soil moisture is the mean of measured values when:

- The total precipitation within the last 30 days agrees to 20 mm
- The total precipitation within the last 7 days agrees to 10 mm
- The mean VPD within the last 30 days agrees to within 0.15 kPa
- The day-of-year agrees to within 10 days;

else, 3) If the time since a significant (>20 mm) rain event is greater than three days, then soil moisture is the mean of measured values when:

- The time since a significant rain event agrees to within 5 days
- The total precipitation within the last 30 days agrees to 20 mm
- The total precipitation within the last 7 days agrees to 10 mm
- The mean VPD within the last 30 days agrees to within 0.15 kPa
- The day-of-year agrees to within 10 days

Most of the data fall into category three. We found that it was sometimes necessary to iteratively relax the search criteria in order to obtain at least two observations of soil moisture that match the criteria for every hourly or half-hour observation in the record. Specifically, for category three data, the criteria were loosened as follows:

ITERATION 2:

- *The time since a significant rain event agrees to within 8 days*
- *The total precipitation within the last 30 days agrees to 30 mm*
- *The total precipitation within the last 7 days agrees to 20 mm*
- *The mean VPD within the last 30 days agrees to within .25 kPa*
- *The Julian day of year agrees to within 20 days*

ITERATION 3:

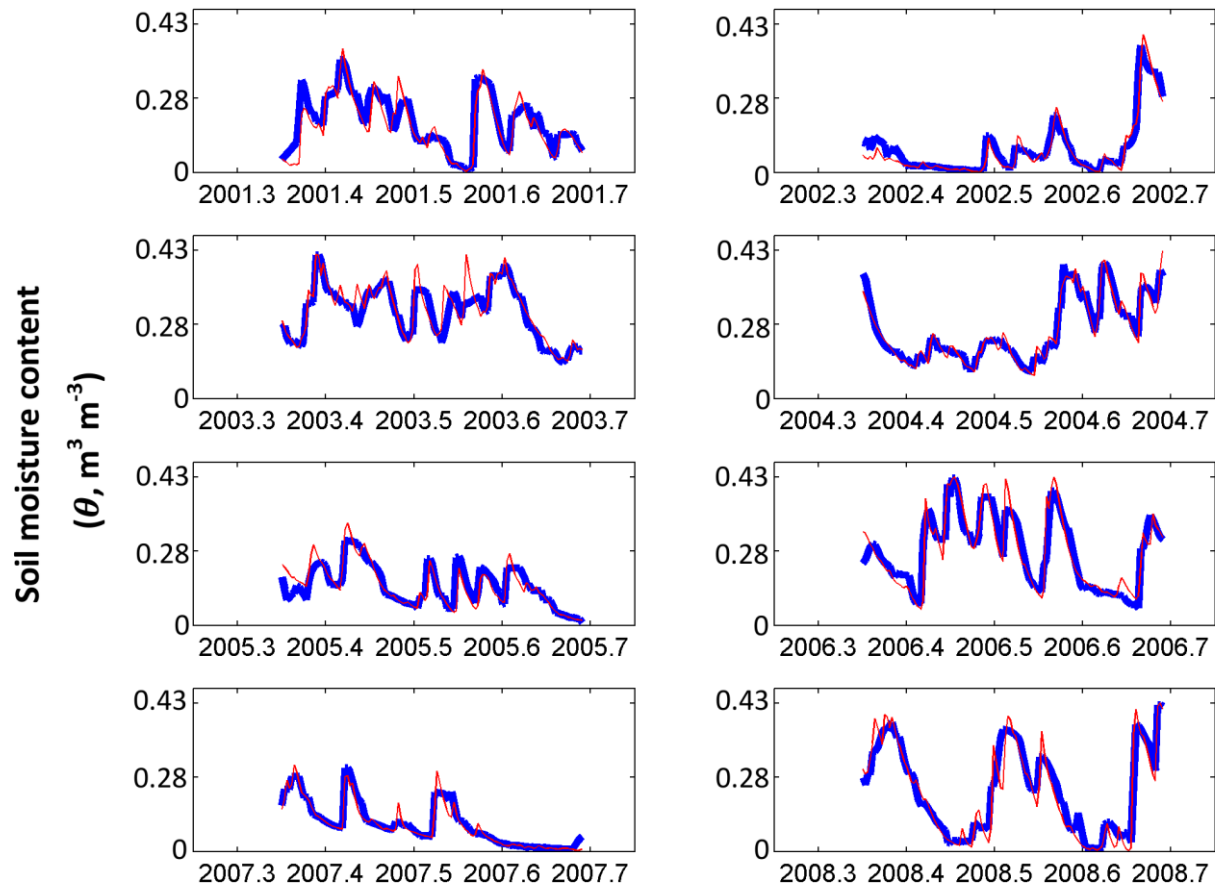
- *The time since a significant rain event agrees to within 10 days*
- *The total precipitation within the last 30 days agrees to 40 mm*
- *The total precipitation within the last 7 days agrees to 30 mm*
- *The mean VPD within the last 30 days agrees to within 0.4 kPa*
- *The day-of-year agrees to within 180 days*

ITERATION 4:

- *The mean VPD within the last 30 days agrees to within 0.4 kPa*

Any remaining gaps in the modeled θ record were linearly interpreted.

In general, the marginal distribution sampling approach reproduced measured θ time series very well. A representative case is shown in Figure S10 and S11 for US-DK3, the Duke Pine Forest Site. Figure S12 shows the slope and correlation coefficient (r^2) between the measured and modeled θ for all sites used in this portion of the analysis. Biases in the slope were less than 5% in most sites, and correlation was generally between 0.8 and 1.0.



430
431

432 *Figure S10: The measured (red) and modeled (blue line) trends in growing season, daily-averaged soil*
433 *moisture content (θ) for the eight site-years of data available from the Duke Pine Forest Site (US-DK3).*

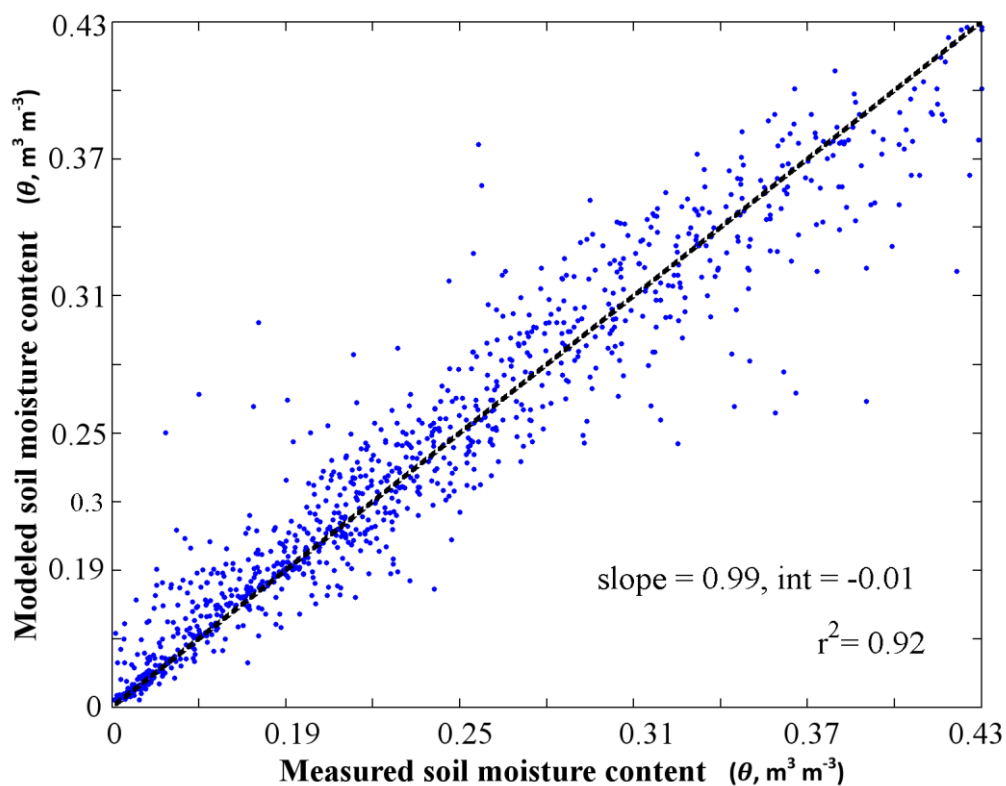


Figure S11: The 1:1 comparison between modeled and measured daily soil moisture content in the Duke Forest Pine Site (US-DK 3).

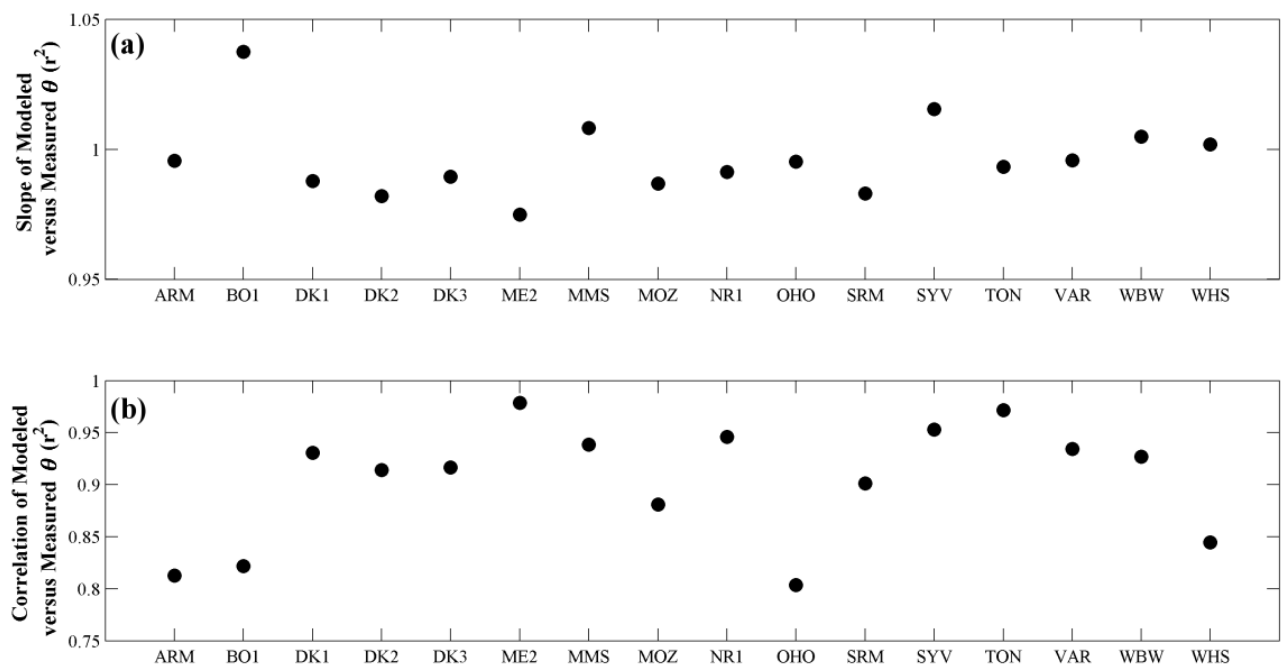
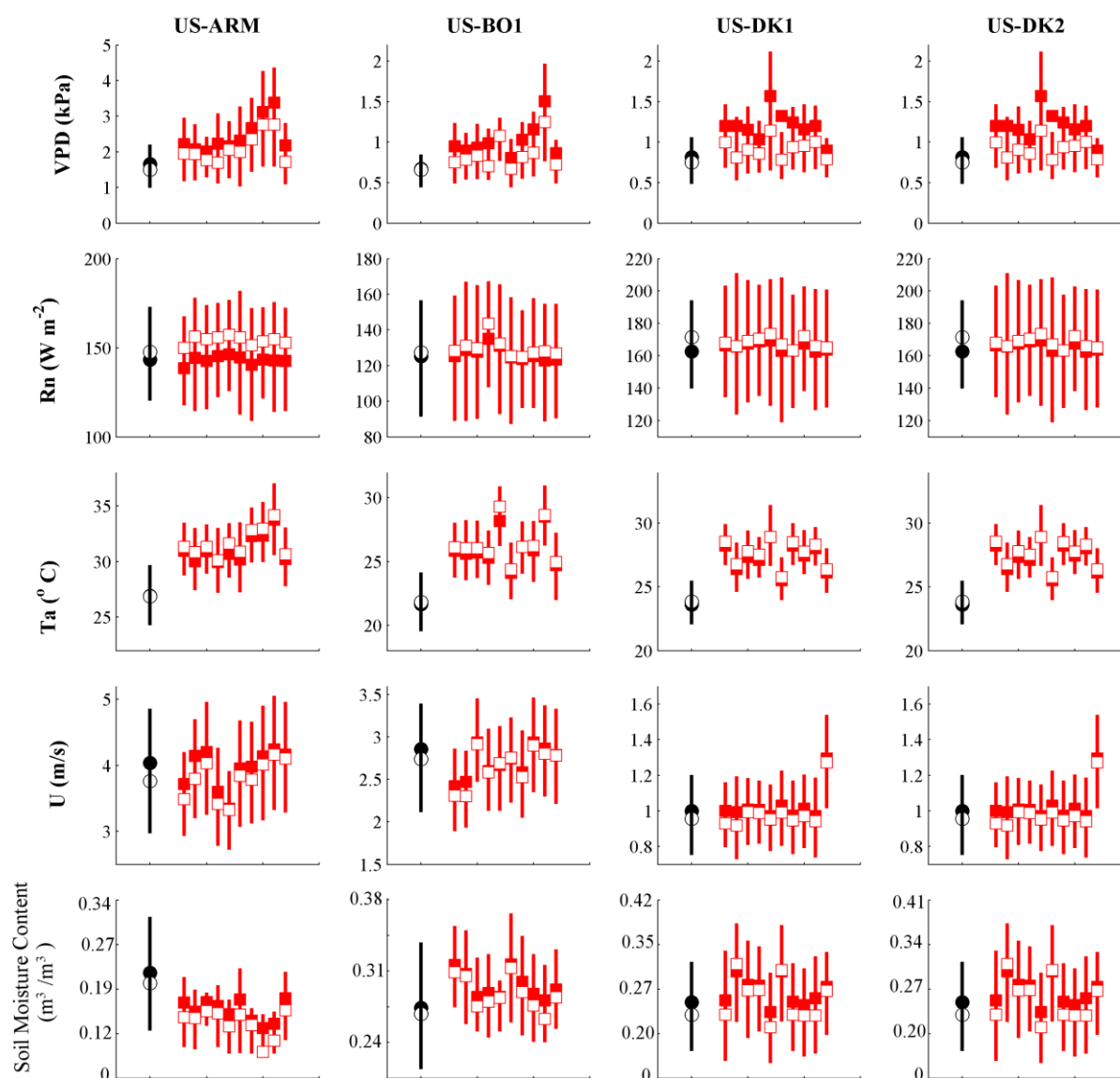


Figure S12: The slope (top panel) and correlation coefficient (bottom panel) between modeled and measured soil moisture content across all of the sites included in the analysis of future limitations to surface conductance and ET.

Future changes in key meteorological drivers: The following figures (Figure S13-16) show the present and projected future means for the key drivers of the Penman-Monteith equation. In every site, nearly all models project increases in future VPD relative to present, occurring concurrently with projected increases in air temperature (T_a). Projected changes in net radiation (R_n) and wind speed (U) are relatively small. Models tend to agree on the change in θ at each site, although across sites no clear trends emerged (i.e., it increases in some, but decreases in others).

Because it is important to preserve the coupling between precipitation and VPD when determining how soil moisture and VPD limit ET, the models were not ensemble averaged. Rather, each of the ten models was used to quantify the limitation to future ET from soil moisture and VPD, and these limitations were then ensemble averaged across the model runs.



458

459 *Figure S13: The mean (filled symbols) and median (open symbols) daytime growing season value for key*
 460 *meteorological drivers for present climate conditions (black symbols, derived from Ameriflux*
 461 *observations) and the future (red symbols, derived from model predictions) for select study sites. Error*
 462 *bars show the 50% range daytime values of each variable, and are expected to overlap as these*
 463 *meteorological drivers experience wide shifts over the course of a day and the course of the growing*
 464 *season. The future data and associated error lines are associated with the ten models of Table S3, in*
 465 *sequential order.*

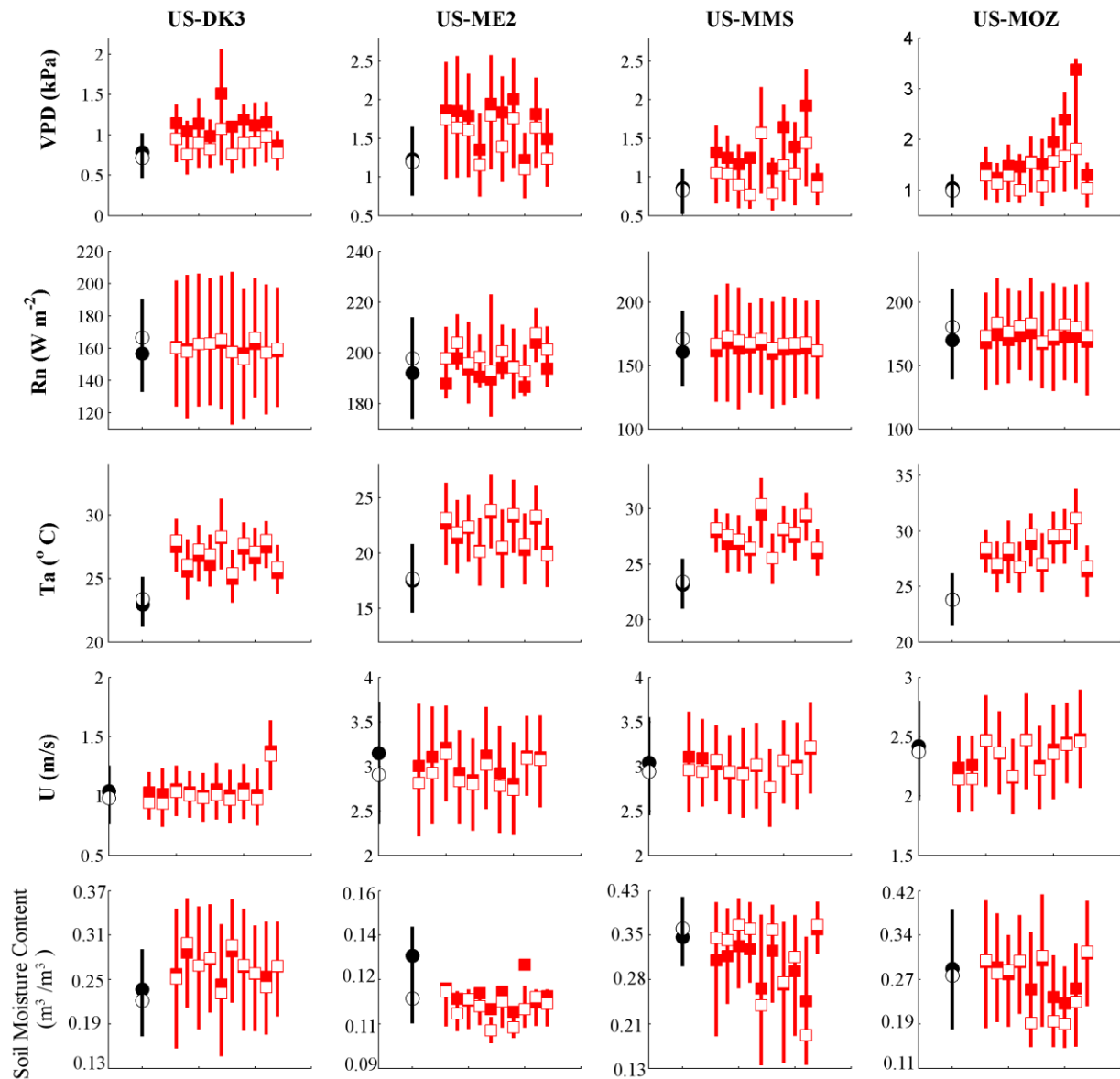


Figure S14: Same as Figure S13, but for additional sites

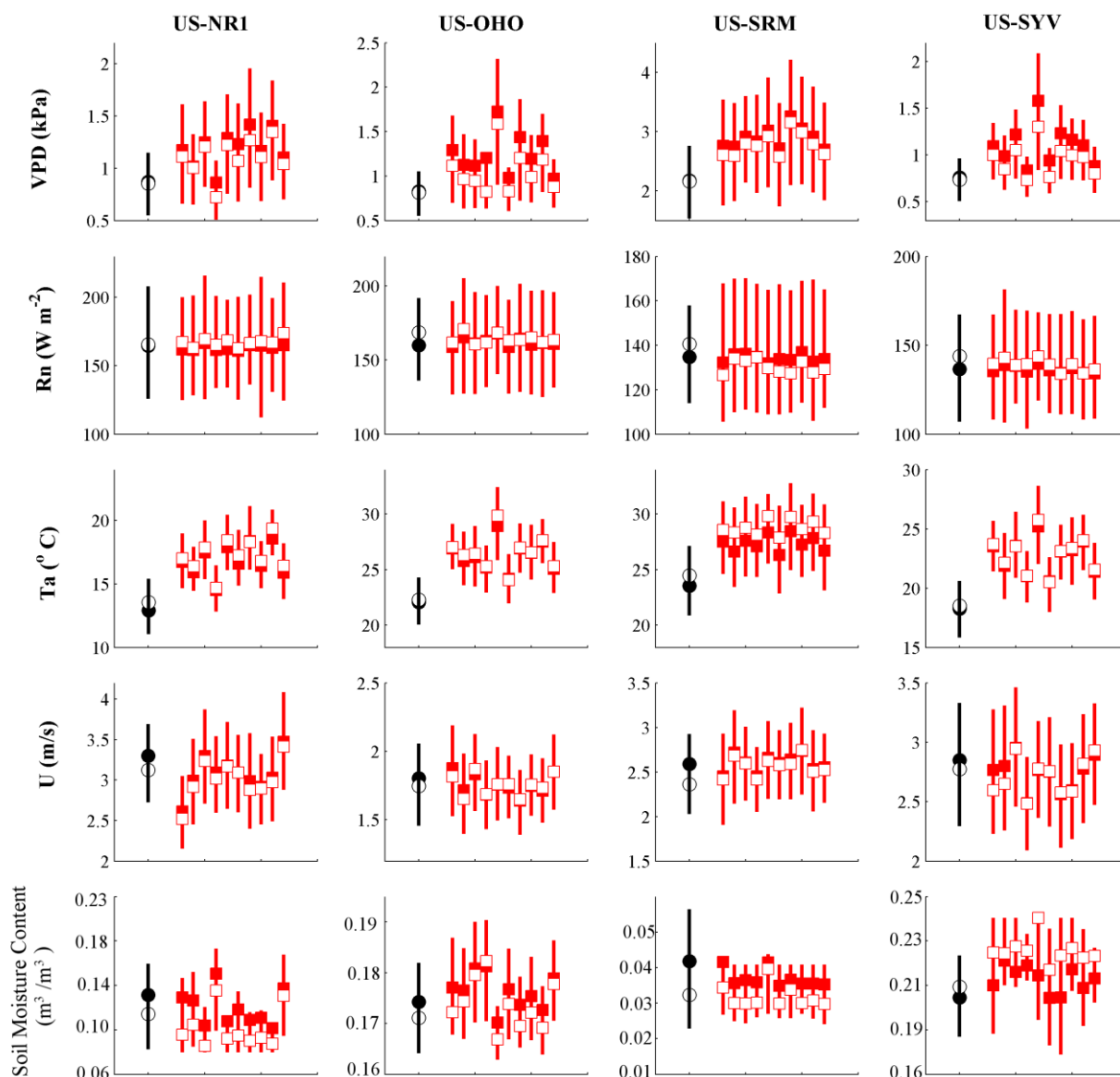


Figure S15: Same as Figure 14, but for additional sites

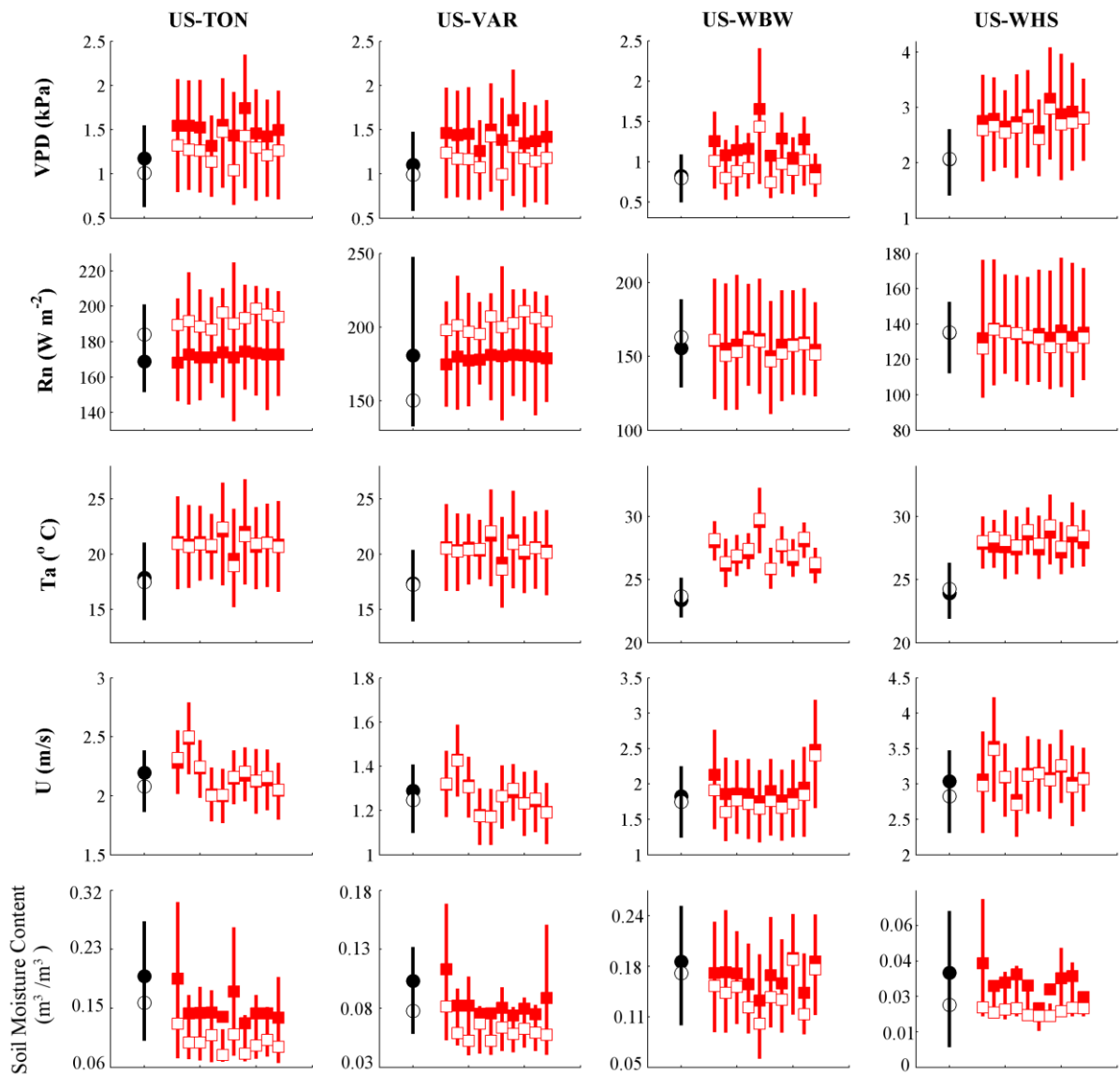


Figure S16: Same as Figure 15, but for additional sites

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