Characterizing the Relationship between Temperature and Soil Moisture Extremes and Their Role in the Exacerbation of Heat Waves over the Contiguous United States

DAVID O. BENSON[a] AND PAUL A. DIRMEYER[a,b]

[a] George Mason University, Fairfax, Virginia
[b] Center for Ocean-Land-Atmosphere Studies, George Mason University, Fairfax, Virginia

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ABSTRACT: Increased heat-wave frequency across the United States has led to the need for improved predictability of heat-wave events. A detailed understanding of land–atmosphere interactions and the relationship between soil moisture and temperature extremes could provide useful information for prediction. This study identifies, for many locations, a threshold of soil moisture below which there is an increase in the sensitivity of atmospheric temperature to declining soil moisture. This shift to a hypersensitive regime causes the atmosphere to be more susceptible to atmospherically driven heat-wave conditions. The soil moisture breakpoint where the regime shift occurs is estimated using segmented regression applied to observations and reanalysis data. It is shown that as the soil gets drier, there is a concomitant change in the rate of decrease in latent heat flux and increase in sensible heat flux leading to a strong positive feedback of increased air temperature near the surface, which further dries out the soil. Central, southwestern, and southeastern parts of the United States seem to have regions of clear regime shifts, while the eastern part of the United States generally does not get dry enough to reveal significant breakpoints. Sensible heat flux is seen to be a primary driver of this increased temperature sensitivity aided by the drop in latent heat flux. An investigation of flux tower sites verifies the breakpoint–flux relationships found in reanalysis data. Accurate estimation of these breakpoints can contribute to improved heat-wave prediction.

KEYWORDS: Extreme events; Atmosphere-land interaction; Soil moisture; Surface fluxes; Temperature; Reanalysis data

1. Introduction

The frequency and intensity of heat waves have been increasing (Perkins et al. 2012; Sheridan and Lee 2018; Founda et al. 2019; Yu et al. 2020). Over the past 60 years, there has been a significant rise in contemporaneous heat-wave and drought events across a majority of the United States (Mazdiyasni and AghaKouchak 2015). Heat waves have severe ramifications for ecology, land management, and regional hydrology (Zaitchik et al. 2006). A continuous increase in the duration, intensity, and frequency of heat-wave events is anticipated as a response to anthropogenic climate forcings (Jia et al. 2019). Consequently, it is important to be able to predict these events in order to mitigate the harmful impacts on health and sustainability. As the importance of accurate prediction cannot be understated, it is imperative that the nature of heat waves and the mechanisms that drive them are fully understood for there to be adequate representation of the phenomenon in forecast models.

The conventional wisdom regarding heat-wave formation has been that it is an atmospherically driven phenomenon (Della-Marta et al. 2007), originating from high-frequency vertically propagating baroclinic waves that generate high pressure blocking systems, which in turn thermodynamically maintain hot dry air at the surface through subsidence (Cassou et al. 2005). However, studies have shown that land–atmosphere feedbacks can be important contributing factors to the magnitude and persistence of heat waves (e.g., Seneviratne et al. 2006b; Miralles et al. 2019). Dry soil leads to stronger sensible heat and reduced latent heat flux, which leads to a deeper boundary layer that enhances the feedback loop and leads to heat-wave persistence (Dirmeyer et al. 2014). Upwind drought conditions have also been shown to lead to advection of sensible heat thereby prompting rises in air temperature (Schumacher et al. 2019). Land surface moisture deficits and land–atmosphere (L-A) feedbacks have been connected to the onset and maintenance of heat waves in many regions (e.g., Mueller and Seneviratne 2012; Hirsch et al. 2014; Ford and Schoof 2017). It has been shown that a reduction in soil moisture would lead to an increase in 2 m air temperature caused by the redistribution of the surface fluxes by the soil layer (Liu and Pu 2019). The slow variation of soil moisture is believed to provide memory and predictability on subseasonal time scales (Seneviratne et al. 2006a; Dirmeyer et al. 2018). When considering the role of land–atmosphere feedbacks in the persistence of heat waves, certain questions arise. Can we improve upon our current understanding of the relationships between soil moisture and temperature? How do these relationships behave over the continental United States?

Hence, this study seeks to provide a detailed analysis of the characteristics of heat waves over the United States, focusing specifically on evidence of land–atmosphere interactions in their persistence and intensification. The role of soil moisture deficits in enhancing the magnitude and duration of heat waves via their effect on surface heat and moisture fluxes is of particular importance in this study. This objective is approached starting from the accepted notion that drier soil conditions lead to a higher incidence of heat waves. It is postulated here that this relationship may not be simply linear, with features such as changes in temperature sensitivity across the range of soil moisture that are not captured by simple statistics like

Corresponding author: David O. Benson, dbenson3@gmu.edu

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TABLE 1. Overview of data products. The SCAN and FLUXNET2015 in situ observations were used to verify the ERA5 data.

Data product	Variables	Data type	Time step
SCAN	Soil moisture, 2 m air temperature	In situ observations (sensors)	Daily
FLUXNET2015	Soil moisture, 2 m air temperature, latent heat flux, sensible heat flux	In situ observations (sensors)	Daily
ERA5	Soil moisture, 2 m air temperature, latent heat flux, sensible heat flux	Reanalysis	Daily

correlation. Hence, more sophisticated tests that go beyond simple linear relationships may be able to better capture the behavior of hot extremes and provide additional information beyond that from linear relationships already explored (Ford et al. 2018; Miralles et al. 2012; Cai et al. 2009).

In this paper, the data used for this study and the framework for analysis are described in section 2. Section 3 details results from the experiment, bringing to bear in situ measurements and reanalysis data in the characterization of soil moisture and temperature relationships. The main findings are discussed in section 5 and conclusions are drawn in section 6.

2. Data and methods

Ideally, collocated measurements of soil moisture, surface heat fluxes and 2 m temperature spanning many years encompassing multiple heat-wave events, periods without extreme heat, and covering a wide range of soil moisture values would be available in a self-consistent network representing a large number of locations across the study area: the portion of North America bounded by 24°–50°N, 75°–125°W; referred to hereafter as CONUS. In fact, only a few such sites exist in the region that have adequate, consistent measurements. If we confine the requirements to just soil moisture and temperature, nearly a tenfold increase can be had from any single self-consistent network, but spatial and temporal coverage is inevitably uneven and incomplete in all observational networks.

Reanalyses provide complete coverage in space and time (for many decades), but while temperatures are well constrained and validated by observations, other quantities are not. Surface fluxes in particular are largely a function of the physical parameterizations of the reanalysis model (Kalnay et al. 1996) and are not assured to resemble observations. Because no single dataset provides ideal coverage in terms of space, time, quality, and coverage of the variables that illuminate the processes linking soil moisture to extremes in 2 m air temperature, we examine a combination of datasets. A summary of the datasets described below is given in Table 1.

a. In situ measurements

Products from two observational networks are used in this analysis. The first is the Soil Climate Analysis Network (SCAN) data product from the National Resources and Conservation Service (NRCS) and National Water and Climate Center of the U.S. Department of Agriculture (USDA; Schaefer et al. 2007). This network is comprised of 221 stations across the United States and is focused mainly in agricultural areas. Although only soil moisture and temperature data were used for this analysis, SCAN stations produce automated records of several other meteorological variables and soil temperature. However, the sites do not measure surface sensible and latent heat fluxes. The shallowest soil moisture measurements, at 5 cm depth generally indicative of soil moisture between 0 and 7.5 cm, are used for this analysis.

Daily collocated observations of soil moisture, near-surface meteorology and surface fluxes are obtained from the 2015 flux network (FLUXNET2015) station dataset (Pastorello et al. 2017). FLUXNET data may be considered the best representation of ''ground truth'' for environmental variables linking the near-surface atmosphere to the land surface (Baldocchi et al. 2001). There are 28 available FLUXNET2015 tier 1 sites with soil moisture and surface fluxes across the United States and southern Canada. The length of available data ranges from 1 to 22 years. To provide continuous observations at the station sites, FLUXNET2015 has produced gap-filled uninterrupted time series for meteorological, energy and water budget variables from the FLUXNET dataset, using continuous globally available ERA-Interim (ERA-I) data to account for missing data (Vuichard and Papale 2015). In situ soil moisture (shallowest sensors are typically 5 or 10 cm below the surface depending on the site), 2 m air temperature, and latent and sensible heat flux (eddy covariance measurements) data are obtained from the sites. A comparable set of variables are also available from the Atmospheric Radiation Measurement observatories combining best estimates of soil moisture, near-surface meteorology, and mainly energy balance Bowen ratio flux estimates (Xie et al. 2010), but as these measurements are concentrated in a relatively small fraction of the study area, we do not use them in this study.

b. Reanalysis data

The ERA5 from the European Centre for Medium-Range Weather Forecasts (ECMWF) is used in this study. We have used data covering the 40-yr period 1979–2018. ERA5 data have a 31 km resolution on a reduced N320 Gaussian grid (Hersbach et al. 2020), which have been regridded with nearest-neighbor interpolation to a regular latitude–longitude grid, effectively repopulating the full Gaussian grid. Daily fields are used in this analysis, including daily maximum 2 m air temperature, soil moisture (top layer: 0–0.07 m), and daily mean surface fluxes (latent heat, sensible heat, and evaporative fraction).

c. Methodology

Inconsistencies in the definition or classification of heat waves, and varying degrees of intensity and duration of events,

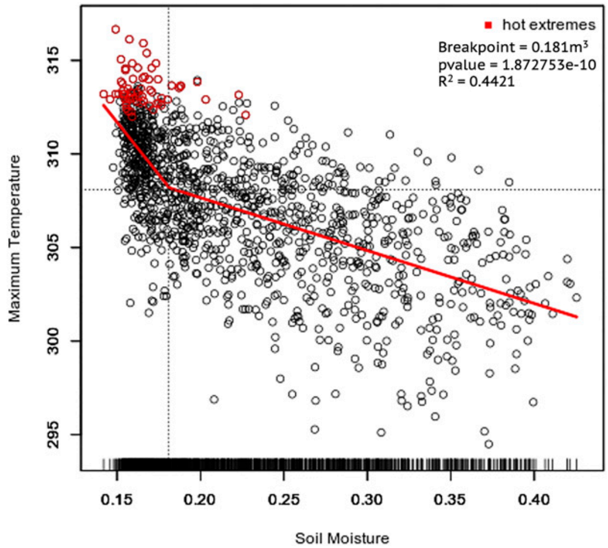

FIG. 1. Scatterplot showing the estimated breakpoint for volumetric soil moisture ($0.1814\,m^3$) as a driver of maximum temperature extremes at 36.1124°N, 97.875°W (a location in Oklahoma) for August 1979–2018 with extreme hot days (warmest 5%) are shown in red. Obtained using the ERA5 dataset.

have hindered an integration of results across studies (Anderson and Bell 2011). However, for this study, a heat-wave day will simply be defined as any day when temperature anomaly exceeds the upper 95th percentile of the local probability density function based on the 40-yr (1979–2018) climatology (Stéfanon et al. 2012). Duration is not a factor in this study. This definition provides the opportunity to investigate the role of L-A interactions in heat-wave exacerbation from a purely physical standpoint, regardless of the social and human factors that are oftentimes associated with the definition of heat waves.

Many studies have investigated the coupling of the land and atmosphere using linear statistics to quantify the relationship between soil moisture and temperature (Lakshmi et al. 2003; Miralles et al. 2012; Stéfanon et al. 2012; Hirsch et al. 2019). As we will show, in extremely hot and dry conditions, the relationship of maximum temperature to soil moisture can change, with maximum temperatures increasing even more rapidly as soil moisture declines. As such, the relationship appears to shift from one roughly linear regime to another (i.e., regressions with differing slopes). An example is shown in Fig. 1. At this location, an optimal piecewise linear regression, described below, indicates a sharp transition where the sensitivity of maximum temperatures to drying soil increases significantly. A linear fit across all data would miss this transition. Dirmeyer et al. (2021) have found such transitions to be emerging across much of Europe. However, it needs to be shown whether this is a widespread feature in soil moisture–temperature relationships for CONUS. If it is, then furthermore it must be determined whether it can generally be well characterized as a piecewise linear function, and finally whether process linkages can be determined that indicate a causal connection from soil moisture to high temperatures that would serve as an aid to improved predictability of such extreme events.

Koster et al. (2009) addressed the behavior of droughts and extreme temperature response to soil moisture conditions by emphasizing two distinct evaporative regimes: moisture-limited and energy-limited. A region is said to be moisture-limited when there is an ample amount of net radiative energy at the surface but a deficit in soil moisture to supply evaporation near the potential rate. This leads to the variations in soil moisture becoming the regulating component for the variations in evapotranspiration. On the other hand, when soil moisture is abundant but there is insufficient net radiation available for evapotranspiration, the region is energy limited and evapotranspiration is not controlled by soil moisture availability (Dirmeyer 2011). If these distinct evaporative regimes are evident between soil moisture and surface fluxes, and if they also align with the piecewise linear relationship for temperature transitioning at the same critical soil moisture value, new insight could be gained.

To determine this threshold for soil moisture, segmented regression analysis is employed (Muggeo 2008). At each station/grid cell, a segmented regression with one breakpoint is generated. This is done in Python using the SciPy method ''optimize.curve_fit'' and the model function ''piecewise-linear'' with reasonable bounds and first-guess values. A piecewise-linear function is defined with a single intersection point (having a value for soil moisture and its predictand, e.g., temperature) and two slopes, one on either side of the intersection; that is, four parameters are predicted. The function iterates and optimizes the best fit for these parameters based on minimization of total mean square error across the linear regressions of both segments and returns the best choices for values of the breakpoint and the slopes, along with confidence statistics. The soil moisture value at the intersection, below which the land surface is primed for strong feedback to atmospherically driven events, is referred to as the breakpoint.

Results are calculated month by month and monthly statistics are averaged into traditional seasons. To estimate breakpoint statistics across multiple years of data, daily values from the target month of each year are catenated into a single time series covering all years. This introduces discontinuities where the data are stitched together, but they do not affect estimates of the breakpoints as the data are sorted based on soil moisture values before segmented regression is performed. Where catenation does have an effect is on the estimation of significance. We calculate the soil moisture time scale τ from one-day lagged autocorrelations of the soil moisture time series at each location (Dirmeyer et al. 2016). Degrees of freedom (DOF) are estimated by dividing the sample size by ($\tau + 1$). The DOF is rounded to the nearest integer and used to estimate significance of fit and error magnitudes for the regressions. Catenation of monthly time series into multiyear series introduces a small amount of spurious noise that could lead to an underestimation of τ and an overestimation of DOF, so we choose strict p values of 0.01 for all significance testing.

Heat-wave days (calculated using the definition of temperature anomalies for the date exceeding the 95th percentile) are

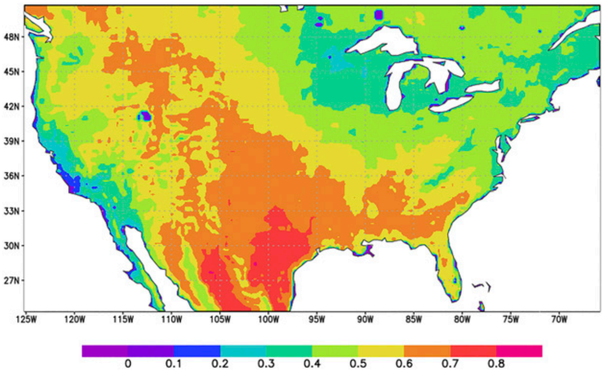

FIG. 2. Seasonal average (JJA) correlation of daily values of soil moisture and maximum temperature, times −1, for the period August 1979–2018.

highlighted in red in Fig. 1. It is clear that almost all of those days occur at very low soil moistures—to the left of the breakpoint. The statistical model endeavors to find the best piecewise linear fit to the data without any knowledge of the underlying physics governing the land–atmosphere interaction, that is, we do not stipulate limitations such as the valid ranges of the breakpoint or slopes. As such, they can take various configurations depending on the data provided. For instance, soil moisture is negatively correlated with air temperature when L-A feedbacks may be in force (Liu and Pu 2019), but positive slopes sometimes result from the regression. Thus, the following screens were enforced after calculation to ensure that parameters representative of potential L-A interactions are retained: the slopes on the dry side of the breakpoint must be negative, the slope to the left of the breakpoint (drier soils) must be more negative than the one on the right—to be consistent with the physical understanding of intensified sensitivity—and there must be more than 10 points on each side of the breakpoint. The last screen is essential to ensure that outliers do not determine the sensitivity of the slopes. Locations passing all screens are candidates for enhancement of heat waves from L-A feedbacks.

While a physical connection can be made between extreme hot days and soil moisture deficit, it is important to note that other mechanisms like large-scale subsidence and horizontal advection of heat can also be causes, which may explain those hot extreme days that fall to the right of the breakpoint in Fig. 1. The hypothesis is that the likelihood of such hot days occurring and potentially intensifying is increased when the soil moisture is extremely low, namely in regions where strong land–atmosphere coupling is possible. Dry soils lead to a decrease in evapotranspiration and concurrently an increase in sensible heating, which could cause the atmosphere near the surface to heat up more severely (Seneviratne et al. 2010; Schumacher et al. 2019). Next, we examine this prospect in the context of breakpoint analyses.

3. Results

As a starting point, we show the relationship between soil moisture and maximum 2 m air temperature in the basic linear framework. Pearson product-moment correlation coefficients calculated month by month using ERA5 data indicate that the linear relationship between soil moisture and maximum temperature grows strongest in the summer months of June–August (JJA), shown in Fig. 2. The Great Plains and areas to the west of it show strong correlations between soil moisture and temperature. Soil moisture, when correlated with mean and maximum temperatures, tends to show these relationships strongly, but correlations using minimum temperature (not shown) are weaker. This is consistent with previous studies of soil moisture–air temperature relationships (Alfaro et al. 2006). There is lower correlation in the Northeast United States. This can be explained by the fact that the northeastern regions are consistently wetter, and evaporation is typically not moisture limited. The Pacific coast shows very low correlation between soil moisture and maximum air temperature. Air temperatures in this region are largely influenced by Pacific sea surface temperatures (SSTs) and predominantly onshore flow. This result has been found in other similar studies (Alfaro et al. 2006; Durre et al. 2000; Huang et al. 1996). This effect is evident in other coastal regions dominated by onshore sea-breeze flow during the day, such as along the Gulf Coast and Atlantic coast, where correlations increase inland from the shore. Soil moisture is negatively correlated with 2 m maximum air temperature but note that Fig. 2 was plotted as the negative of the correlation.

The results from the example correlation field in Fig. 2 provide no information about variations in sensitivity with dryness, the severity of extremes, where they occur, or at what soil moisture values sensitivities increase. While the linear statistics do a good job of explaining a portion of the relationship (mean and variance), it is not a complete tool for understanding the nature of extremes, as pointed out earlier. Hence, this research posits an approach of separating the soil moisture–temperature relationship into regimes that brings to light the nature of extremes and further improves an understanding of this relationship that cannot be discerned solely from statistics as in Fig. 2.

a. Soil moisture relationship with maximum temperature

Observations from the SCAN product were used to investigate the presence of distinct soil moisture–temperature regimes at many locations across CONUS. Although the SCAN dataset consists of 221 stations (Fig. 3), the screens mentioned in section 2, when applied to the dataset, reduce the number of stations in the sample. The numbers in red at the bottom-right corner of Figs. 3 and 4 indicate the number of stations that passed all screens, while the gray crosses (+) represent stations that were omitted after the screens. Additional screens have been applied to remove extreme values and breakpoint values larger than 0.45. This is done to eliminate stations situated over wetlands (i.e., shallow water table), and irrigated locations. As a result, there are differences in the total number of stations in each plot. These station data, though sparse, can provide some information regarding the relationship between extreme soil moisture and extreme temperature across CONUS.

In these observations, we see results similar to Fig. 1, where there are often two clear regimes: a high soil moisture regime

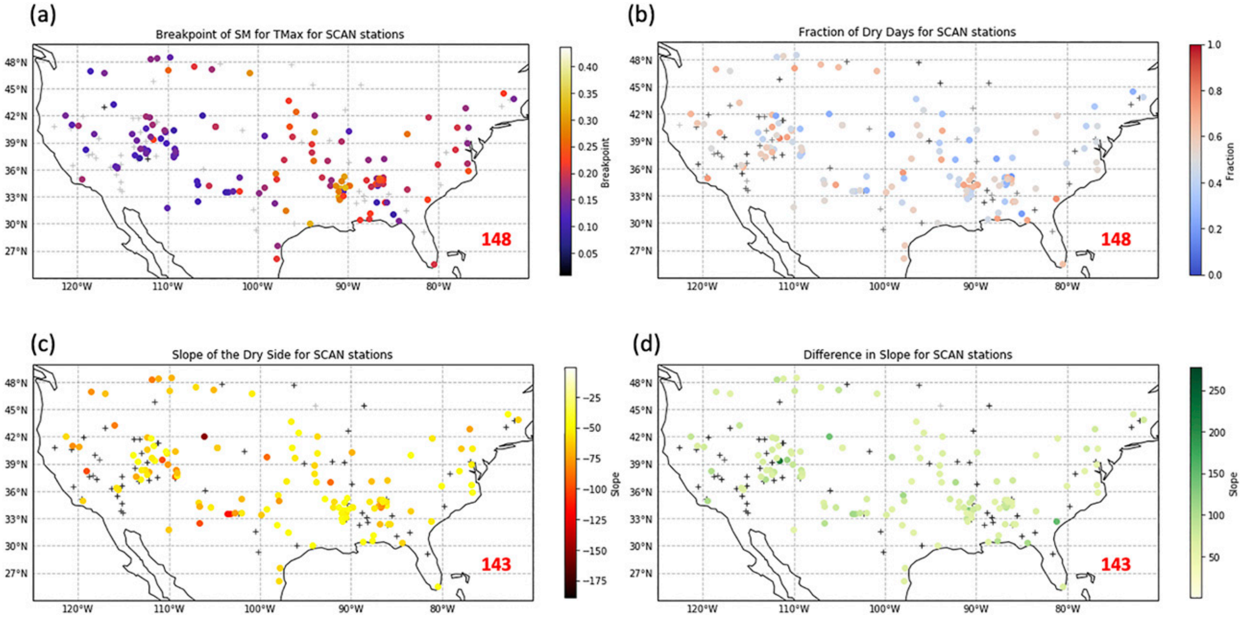

FIG. 3. Breakpoint statistics at SCAN sites for JJA: (a) breakpoints of soil moisture for maximum 2 m temperature; (b) the fraction of days on the dry side of breakpoint; (c) the slope of the best-fit regression through data on the dry side of the breakpoint; (d) dry side slope minus wet side slope.

where there is still typically a negative slope in the regression of maximum surface temperature against soil moisture, and an increase in sensitivity when soil moisture values are in extreme deficit, indicating a hypersensitive regime in which the local atmosphere is primed to exacerbated heat. Stations in the western United States (e.g., Arizona) have most values in the hypersensitive regime due to the limited evapotranspiration caused by the extreme soil moisture deficits that are typical of that region. Locations in the desert have soil moisture values mostly in the dry end of the distribution; it can be assumed that such regions are already ''activated'' to enhanced feedbacks of soil moisture on temperature, conditions necessary for the exacerbation of heat waves. For stations in the eastern United States, the relationship fails to find many significant

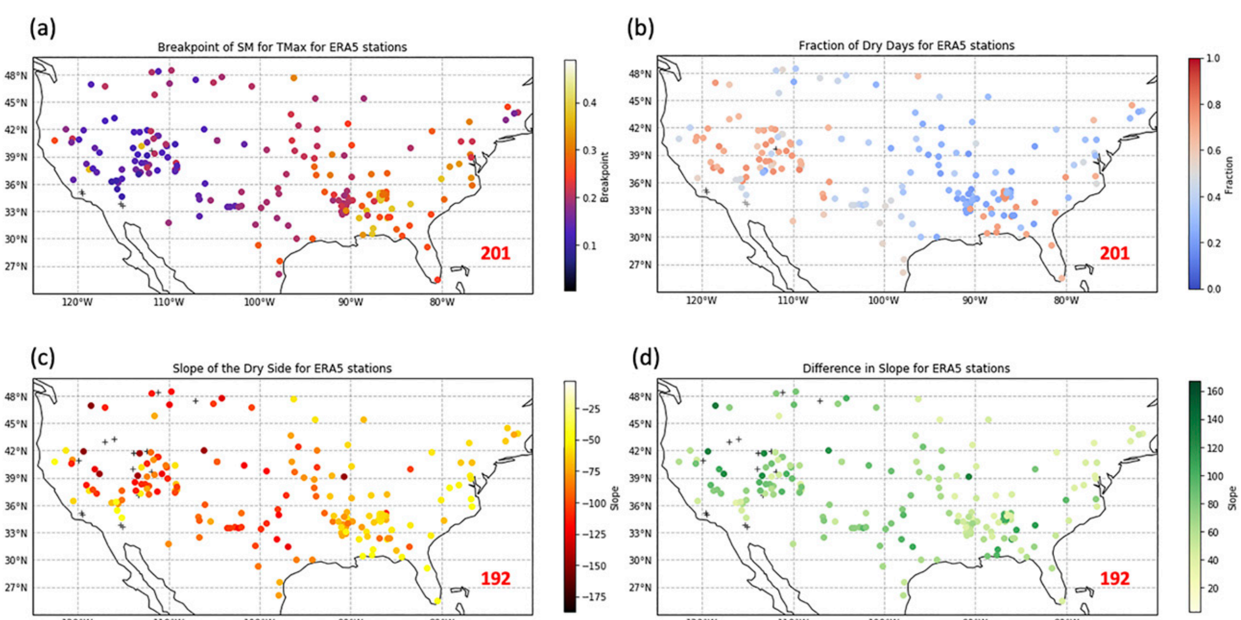

FIG. 4. As in Fig. 3, but for ERA5 grid cells where SCAN sites are located.

breakpoints, and in other cases, the slope relating maximum temperature to soil moisture is small in all months, indicative of a wet region that rarely gets dry enough to cross below the local breakpoint threshold.

In the SCAN product (Fig. 3), there is seen to be a great deal of local and regional variability. Points in the western United States tend to have drier breakpoint values yet are commonly on the dry side of the breakpoint (Fig. 3b) as are southern stations, indicating that these regions are more often in the hypersensitive regime for most of the summer. The locations in the East are usually on the wet side of the breakpoint, while those points in the central United States have more tendency to shift from one regime to the other depending on the amount of moisture in the soil. The fraction of days on the dry side of the breakpoint gives an insight to the frequency of occurrence of these shifts, or likelihood for the region to be in the hypersensitive regime. Figure 3 reveals that most regions in the western United States are most often in the hypersensitive regime during the warm months and as such, are more vulnerable to triggering positive land–atmosphere feedbacks on heat waves. The slope of the best-fit regression of maximum surface temperature on soil moisture to the dry side of the breakpoint and the difference in slopes between the linear fits on the dry versus wet side of the breakpoint (Figs. 3c,d) indicate, respectively, the degree of hypersensitivity of temperatures in dry conditions and the degree of change of sensitivity when crossing the breakpoint, that is, the distinctness of the two regimes.

The presence of noise in the observations, for example, random measurement error, variations caused by local differences in soils, vegetation, terrain slope, and other physiographic features, makes it difficult to identify distinct continental-scale patterns, although it can be argued that western and southeastern parts of the United States show the strongest soil moisture–temperature relationships and stronger regime shifts. From these observations, it is suggested that these regions are the most susceptible to L-A feedbacks in heat-wave activity in CONUS.

The ERA5 grid cells at the SCAN sites show more clearly than the station observations a west-to-east gradient in the breakpoint values with lower values in the west and higher values in the east (Fig. 4a). ERA5 also shows a more distinct zonal gradient in the number of days in each regime (Fig. 4b). This is consistent with the understanding of L-A coupling where the western United States is usually moisture limited and drier than the eastern part of the United States, which is wetter and more likely energy limited. The dry-side slope values in the western United States indicate more hypersensitivity than in the East (Fig. 4c). The first-order relationship in ERA5, however, is very similar to that of the station observations. In the reanalysis, although the southeastern region seems to have stations that are generally in the dry regime, they seem to have high breakpoint values and weaker sensitivity of maximum temperature to soil moisture variations.

The very high values of breakpoints seen in parts of CONUS are more likely to be an artifact of the statistical algorithm finding shifts in the data that are unrepresentative of the underlying physical process in nature. The probability distribution of soil moisture in wetter areas may not be sampling the true moisture-limited regime nor including the corresponding breakpoint. It is also possible that some of the breakpoints seen in the eastern part of the United States are indicators of a shift from a barely coupled regime to one that has become sensitive. Koster et al. (2019) has shown that soil moisture can still play a role in L-A feedbacks in regions that are known to be primarily energy limited. This could be an indicator that soil moisture still has the potential to regulate the atmosphere above it even in regions that do not often get extremely dry. Furthermore, it comes as no surprise that more stations pass the screens in the reanalysis dataset, as reanalysis data tend to be less noisy.

Continuous maps of these statistics for the CONUS region from all ERA5 data are shown in Fig. 5. The soil moisture thresholds are very low ($<0.1\,\mathrm{m}^3\,\mathrm{m}^{-3}$) in the Southwest indicating that in those regions, when the topmost layer of soil moisture is almost depleted, the region is susceptible to heat-wave events (Fig. 5a). During heat waves, however, it is expected that the temperatures increase even more rapidly as the soil gets drier on the dry side of the breakpoint (Ford and Quiring 2014). The Southeast also appears to have some lower thresholds as well, especially over Florida, but also some very high estimated breakpoints across the rest of the region. Inasmuch as these regions have higher breakpoints than the western United States, they are generally wetter. Figure 5b shows that majority of the East is noticeably wetter than the West and spends more summer days in that wet state. Considering that these regions are much wetter, a significant amount of drying must take place for the regime shift to occur. Breakpoint values in the Northeast may be unreliable as this region is typically energy limited.

The white portions of Fig. 5 indicate open water or those regions that do not meet the 95% confidence regarding change in slope. Regions in the West around 43°N appear to be the most sensitive to the influence of soil desiccation on the atmosphere (Fig. 5c), and as a response, make the largest shifts from the sensitive to hypersensitive regime (Fig. 5d). This finding reveals these regions as the most susceptible to the exacerbation of heat-wave activities owing to the influence of L-A interactions via soil drying.

It is also important to note that some of the finescale spatial structure seen in Fig. 5 is similar to the structure of soil types and to a lesser extent vegetation and topography as specified in ERA5 (not shown). Results not shown indicate significant correlation ($r = 0.43$) between the map of wilting points and maps of breakpoints across the United States; $r = 0.67$ when total column soil moisture is used to estimate breakpoints. Hence, the wilting points, which are directly a function of soil type, are linked to the spatial variation of the breakpoints.

b. *Surface flux influence on breakpoint determination*

Understanding the role of the surface fluxes in the partitioning of energy is essential to knowledge of the underlying physical processes behind the transition of regimes. Breakpoints of sensible and latent heat flux are estimated to determine which energy flux is the main conduit of hypersensitivity seen in the soil moisture–temperature relationship. The

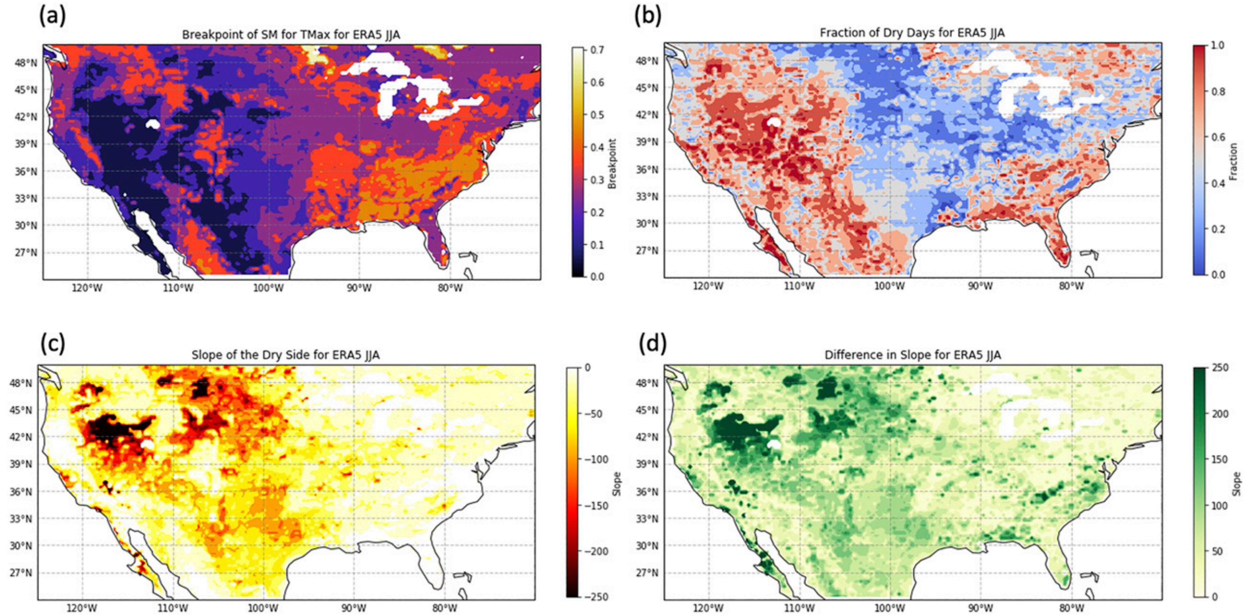

FIG. 5. Breakpoint statistics from ERA5 for JJA: (a) breakpoints of soil moisture for maximum 2 m temperature; (b) the fraction of days on the dry side of breakpoint; (c) the slope of the best-fit regression through data on the dry side of the breakpoint; (d) dry side slope minus wet side slope.

FLUXNET stations provide observational information on the behavior of surface fluxes and the role they play in determining this relationship between soil moisture and maximum temperature. The FLUXNET data suggest that the breakpoints of soil moisture for sensible heat flux are typically very close to those for maximum temperature, while the breakpoints of soil moisture for latent heat flux tend to be at somewhat higher values of soil moisture (Fig. 6). However, there is little variation in latent heat response to soil moisture from month to month, signaling a consistent local response of latent heat flux to soil moisture (not shown). The consistency of this pattern might be an indicator that latent heat plays some role in determining the breakpoints of soil moisture.

To be clear, this does not mean that the role of sensible heat flux in stimulating the shift in regimes is nonexistent. Figure 6b shows the breakpoints of soil moisture dependent on sensible heat flux. Sensible heat flux appears to be an important controlling factor for the shift in regimes as its breakpoints have the better fit to those of maximum air temperature. As latent heat shuts down below the breakpoint, more energy goes to the sensible heat flux, which in turn raises the temperature at the surface. The transition below the breakpoint can be viewed as a two-phase process initiated by the shutting down of latent heat flux, which then enables the sensible heat to dominate the shift to the hypersensitive regime.

Subsurface soil moisture influences the breakpoints of soil moisture for latent heat flux, while surface soil moisture is more important for the determination of breakpoints for sensible heat flux. This occurs because the process of evaporation involves transpiration by plants, which is strongly connected to the subsurface soil moisture. The influence of the total soil column on latent heat flux can be seen in the difference

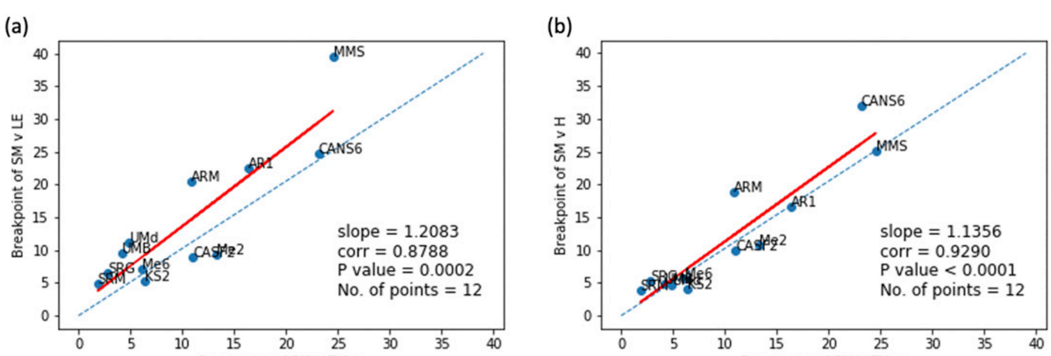

FIG. 6. Breakpoint values of soil moisture for maximum temperature vs breakpoints of soil moisture for (a) latent heat flux and (b) sensible heat flux for JJA at FLUXNET2015 tier 1 stations.

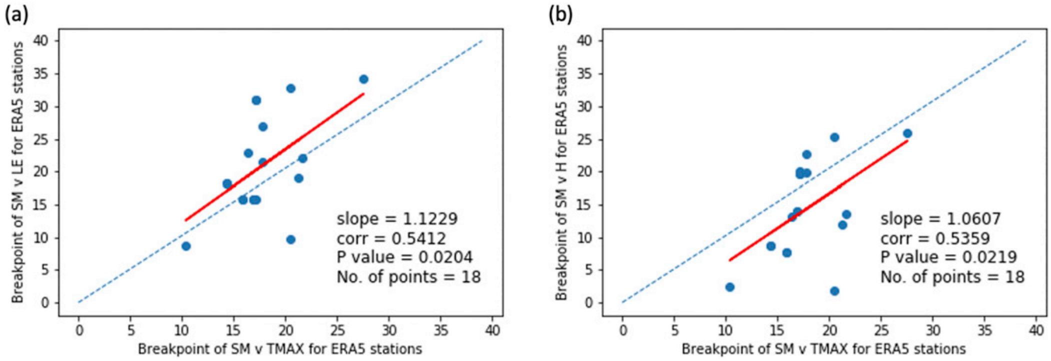

FIG. 7. As in Fig. 6, but for ERA5 grid cells where FLUXNET2015 tier 1 stations are located.

between the breakpoint values of sensible heat and latent heat. Results (not shown) show strong correlations between column soil moisture breakpoints for maximum temperature and column soil moisture breakpoints for latent heat flux. Similarly, strong correlations are also seen between surface soil moisture breakpoints for maximum temperature and surface soil moisture breakpoints for sensible heat flux. However, in regions with coarse soil types and a low wilting point values, rapid drainage results in weak vertical gradients of soil moisture. In such regions, there is negligible difference between the surface and subsurface soil moisture influence on breakpoint values for latent heat flux. Further investigation should be carried out to determine the role of soil types in breakpoint determination.

Other external factors besides the energy fluxes may also have effects on the soil moisture response to atmospheric conditions. The point, however, is to emphasize that the primary driver of soil moisture sensitivity over CONUS appears to be the sensible heat flux, attributable to the changes in latent heat flux. This supports the findings of Koster et al. 2009 regarding the role of evaporation regimes in soil moisture–atmosphere response.

The roles of latent and sensible heat fluxes are also seen in the corresponding grid cells in the reanalysis dataset (Fig. 7). This is generally consistent with Fig. 6, however, the breakpoints of soil moisture for maximum temperature and latent heat flux tend to occur at higher soil moisture values in Fig. 7 when compared to Fig. 6. Even with a very limited number of stations, the ERA5 appears to be consistent with observations as quantified by the *p* values. The behavior at the grid cells containing FLUXNET stations (Fig. 7) is similar to that of the observations but tends to have lower albeit still significant correlations. However, when we increase the number of sampled grid cells by considering instead those where the SCAN stations are located, we can see a more strongly correlated representation of the relationship (Fig. 8). The same soil moisture relationship to the surface fluxes applies and is seen more clearly across the larger sample size. The similarities to the FLUXNET sites, with latent heat flux having higher breakpoints, attests to the robustness of these features across very different datasets at the SCAN sites.

c. Comparison of observations versus reanalysis

Figures 6–8 strongly suggest that analysis of the increase in sensitivity of daily maximum temperatures below a breakpoint threshold of soil moisture, depicted in Fig. 5 for the CONUS area using ERA5 data, is tied to soil moisture's control on surface heat flux partitioning, and is in very good agreement with observational data where it is available. Agreement with reanalysis data allows us to widen the scope of this study beyond just specific locations with soil moisture observations. ERA5's complete and seamless data allow for production of maps of heat-wave sensitivity parameters and makes for easy comparisons with forecast and operational climate models. To have complete confidence in the ERA5-based analyses, there remains the need to investigate the robustness of the reanalysis dataset in capturing the other soil moisture–maximum temperature parameters.

When ERA5 breakpoint estimates are summarily compared to the two observational data products, the breakpoint of soil moisture for maximum temperature appears very dependable (Table 2). It is a clear indication that similar relationships exist in both observations and the reanalysis model. The comparison of breakpoints of soil moisture for latent heat flux and sensible heat flux are also significant (not shown). When comparing the sites in observations to those from reanalysis, only points that pass all predetermined screens mentioned earlier, for both the observations and reanalysis, are included. This is to ensure consistency in the comparisons but greatly limits the number of sites available for comparison, with only 8 out of 28 FLUXNET sites included, and 79 out of 221 SCAN sites. The limited number of samples also leads to limited significance, particularly among the FLUXNET sites, where only the breakpoint statistic has high significance at 97%–98% confidence. Correspondence of ERA5 results with the more numerous SCAN stations is significant with >99% confidence for all metrics except for the difference in slopes across the breakpoint. This result is encouraging and enhances the trustworthiness of the ERA5 for this assessment of heat-wave sensitivity. Note that instead of the slope ratios used throughout this study, the angles corresponding to the slopes (the arctangents of the slopes after renormalization based on the range of values on each axis) at each location are compared to prevent very large slope magnitudes (angles near 90°) from skewing the correlations.

It is also important to note when making comparisons that there is a significant scale difference between the observations and

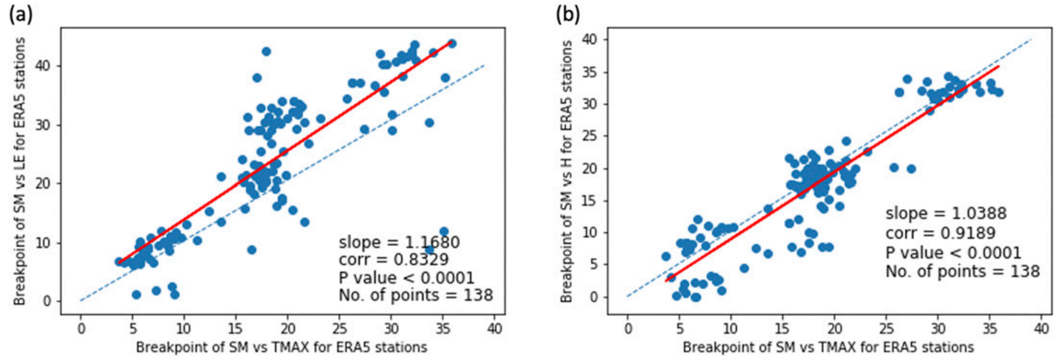

FIG. 8. As in Fig. 6, but for ERA5 grid cells where SCAN stations are located.

reanalysis. The station observations represent an area of less than 1 km^2 for flux tower footprints, much less for the SCAN stations, while the ERA5 grid cells are nearly 1000 km^2 in area. Additionally, the SCAN stations are mainly situated in agricultural areas that may not be representative of the average landscape conditions in the reanalysis grid cell. FLUXNET stations are also sited to represent a single land cover class. Finally, the finescale local soil characteristics affecting the observations often do not match with the parameters used in the global land surface model of ERA5. Despite these many limitations, we find significant relationships emerge, linking observational and reanalysis representations of soil moisture controls on extreme heat.

4. Discussion and conclusions

In an endeavor to characterize the potential role of soil moisture in heat-wave exacerbation, in situ observations from 221 SCAN stations and 28 FLUXNET sites over CONUS, and ERA5 data were analyzed to determine breakpoints of soil moisture below which the atmosphere becomes more susceptible to heat-wave conditions. The breakpoint values are calculated directly from daily soil moisture and maximum temperature data using a statistical approach without consideration of the underlying physics, and the results are interpreted in the context of physical process linkages (Santanello et al. 2018). Breakpoints function as thresholds that signal a shift in the sensitivity of daytime maximum temperatures to declining soil moisture. These breakpoints are seen quite clearly in observational data, and the ERA5 dataset suitably represents the values and spatial distribution of the breakpoints. We conclude ERA5 captures the spatial patterns and essential physical processes linking soil moisture and extreme temperatures.

Breakpoints for soil moisture based on surface heat fluxes corroborate previous findings (e.g., Hirsch et al. 2014; Ford and Schoof 2017; Liu and Pu 2019) while expanding our understanding of the roles played by coupled L-A processes. Sensible heat flux is seen to be the primary avenue of this shift in temperature sensitivity, aided by the change in latent heat flux response to soil moisture, which shuts down as soil moisture is depleted. This prompts additional net radiative energy at the surface to go into sensible heat flux, ultimately inducing intensification of high temperatures at the surface.

The western part of the United States appears to be more likely to find itself in the hypersensitive dry regime. Meanwhile, large parts of the eastern United States do not appear to drop below the critical soil moisture value that would cause a shift into a positive L-A feedback regime during hot extremes. Although there may be periods of extreme temperatures, they seem less likely to break from the simple linear relationship between soil moisture and temperature over that region. This can be explained by the low values for actual thresholds or breakpoints of soil moisture that are rarely reached or sustained, corroborated by the unrealistically high estimated soil moisture breakpoints estimated in the East and the frequent absence of significant breakpoints. In other words, it is an indicator that heat-wave events that occur in areas with high soil moisture values for breakpoints and small changes of sensitivity slopes on either side of the estimated breakpoint are largely independent of soil moisture. This is not true for the southeastern region. While not as dry as the western regions, southeastern CONUS displays significant regime shifts that suggest the influence of soil moisture in heat-wave strength. This could be as a result of atmospherically driven heat-wave conditions that are then intensified by the positive feedback of L-A interactions.

TABLE 2. The p values of the correlations of ERA5 gridcell data to corresponding FLUXNET and SCAN sites. Values in parentheses are the number of stations used in each comparison.

Data	Breakpoint of soil moisture for maximum temperature	Fraction of dry days	Slope of the dry side	Difference in slope
FLUXNET	0.0257 (8)	0.9268 (8)	0.7031 (8)	0.3306 (8)
SCAN	0.0001 (79)	0.0034 (79)	0.0025 (79)	0.2510 (79)

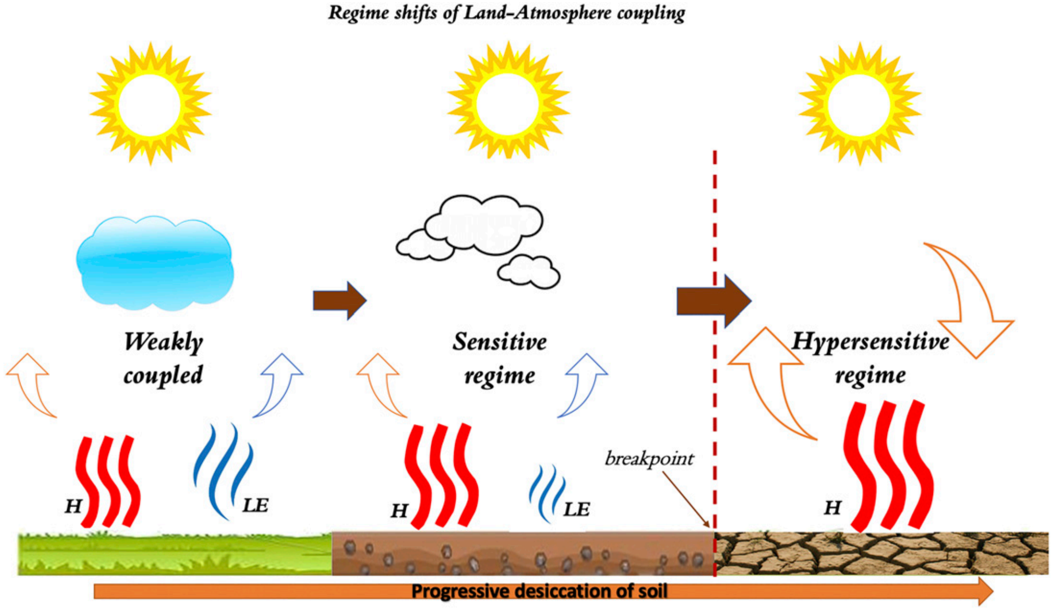

FIG. 9. The link between hypersensitivity of rising temperatures to decreasing soil moisture and the transition to a severely water limited regime, shown in a schematic. Increases in sensible heat flux and decreases in latent heat flux lead to a positive feedback on increasing air temperature at the surface.

Figure 9 illustrates schematically the progressive intensification of L-A coupling and atmospheric sensitivity to the conditions of soil moisture at the surface. This figure summarizes the mechanistic processes these results suggest are at play in the determination of breakpoints and shifts in sensitivity. A region that has sufficient soil moisture sees the net radiative energy at the surface partitioned between sensible heat flux (H) and latent heat flux (LE), with LE the preferred sink. At this stage, the atmosphere is typically considered to be weakly coupled to soil moisture. As desiccation of the soil occurs, there is progressively less moisture available to be evaporated thereby prompting less energy going into latent heat, and more energy into sensible heat. This alteration to the partitioning of the surface energy fluxes generates a gradual shift in atmospheric states, as it is marginally sensitive to soil moisture variations. This accounts for the general positive correlation between soil moisture and temperature but relatively small slopes on the wet side of the breakpoint depicted in Figs. 1, 3d, 4d, and 5d. Progressive drying of soil moisture leads to a threshold that, when exceeded, prompts cessation of latent heat flux and causes nearly all the surface net radiative energy to be in the form of sensible heat generating a strong thermal feedback (Miralles et al. 2014). This threshold has been identified in this study as the breakpoint. Crossing the breakpoint leads to a shift in the soil moisture–temperature relationship from a sensitive regime to a hypersensitive regime. If atmospheric conditions suitable for heat-wave occurrence are met, this state is primed to exacerbate and possibly prolong the heat-wave activity. The term ‘‘cessation’’ is used cautiously to indicate the physical process that occurs as the shift is made from the sensitive to the hypersensitive regime. In reality, this process is more likely to be a gradual transition between regimes due to the uneven nature of reaching specific wilting points across the soil column and latent heat via transpiration across the entire column of soil water, as discussed earlier.

Referring back to Fig. 1, we reiterate that there is no reason to expect heat-wave days to correspond only to the hypersensitive regime. It is acknowledged that there may be other external processes at play in the feedback. Studies have established the role of wind speed and relative humidity in the transition of evaporative regimes, and the effect of an absence of net radiation (Haghighi et al. 2018; Hsu and Dirmeyer 2021). These and vegetation physiology in largely vegetated areas, may constitute additional environmental factors that affect the determination of breakpoint values and ultimately L-A feedback. Furthermore, L-A feedbacks are not solely a factor in the warmest 1% or 5% of days but may be a significant contributor to added warmth on any days lying on the dry side of the local breakpoint of soil moisture. The fraction of summer days lying within the hypersensitive regime varies spatially (Fig. 5b), thus so does the potential of soil moisture conditions to exacerbate heat waves.

While the breakpoint algorithm has performed satisfactorily, there are some caveats to this study that should be acknowledged. In the humid east, the breakpoints found are probably not related to severe moisture stress as they tend to be found at very high values of soil moisture. It is both a strength and weakness of the algorithm that it is unencumbered by physical constraints. There is strength is in the sense that the results are obtained entirely from the data provided without any preexisting expectations. To this point, there is a possibility that the algorithm is revealing physical explanations for the high breakpoint values in the humid east that are outside the scope of this study, such as a transition between unconstrained evaporation at the potential rate and moderately stressed evaporation somewhat constrained by soil moisture (i.e., the transition between energy-limited and water-limited regimes). This point is also a weakness, as a fully statistical algorithm such as this can generate spurious results; thus, we apply a posteriori screens informed by physics. This is where consideration of large data samples, particularly the spatially complete ERA5 data, is a great help.

Other limitations include the scarcity and noisiness (random measurement errors) of observational datasets, the scale differences between the data products used that hamper somewhat the effective comparison between products, and the model compromises and parameter choices in ERA5 that can introduce biases. These limitations hinder greater robustness of the results.

To reiterate, the results found in this study are noteworthy because they are based on a piecewise linear statistical analysis that knows nothing about the physics yet shows physically meaningful outcomes. This supports the hypothesis that breakpoints of soil moisture delineating different regimes of sensitivity of maximum temperatures to soil water content exist in nature. These breakpoints help present a new perspective for improvements in approaches to further heat-wave predictability and prediction, and climate forecast model evaluation. These findings could prove to be very beneficial to the understanding of heat-wave propagation and intensification over CONUS, as they provide geographical distributions of areas where L-A interactions appear to dominate the exacerbation of heat waves, pointing to a need to more carefully monitor soil moisture in those areas. Additionally, these results have potential for improving predictability as these are the regions where antecedent soil moisture could serve as a more nuanced predictor for heat-wave events.

Finally, as we navigate through a changing climate, this study provides some insight into the possible future state of L-A interactions across the United States. Drier conditions could see the Great Plains and other regions become more frequently hypersensitive and readily amenable to L-A interactions, that is, the fractions shown in Fig. 5b could grow with time. Reduced precipitation and progressive drying could see regions shift regimes from uncoupled to sensitive, and from sensitive to hypersensitive. This could consequently lead to more intense and prolonged heat-wave events in those regions. Increased precipitation and soil moisture can also see regions shift regimes in the opposite direction.

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Data availability statement. ERA5 data were accessed directly from the ECMWF data catalogue via the Meteorological Archival and Retrieval System (MARS) but are otherwise openly available from the Copernicus Climate Change Service. FLUXNET2015 Tier 1 data are freely available from https://fluxnet.fluxdata.org/; the following stations were used: US_AR1, US_AR2, US_ARM, US_Blo, US_GLE, US_KS2, US_MMS, US_Me2, US_Me6, US_NR1, US_PFa, US_SRG, US_SRM, US_Syv, US_Ton, US_Tw2, US_Tw3, US_UMB, US_UMd, US_Var, US_WCr, US_Whs, US_Wkg, CA_NS2, CA_NS6, CA_Qfo, CA_SF1, and CASF2. SCAN data are from the archive of the International Soil Moisture Network (https://ismn.geo.tuwien.ac.at/).

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