

**Bridging Past and Future Climate Across Paleoclimatic Reconstructions,  
Observations, and Models: A Hydroclimate Case Study**

JASON E. SMERDON\*

*Lamont-Doherty Earth Observatory of Columbia University, New York, USA*

BENJAMIN I. COOK

*NASA Goddard Institute for Space Studies, New York, USA*

*Lamont-Doherty Earth Observatory of Columbia University, New York, USA*

EDWARD R. COOK

*Lamont-Doherty Earth Observatory of Columbia University, New York, USA*

RICHARD SEAGER

*Lamont-Doherty Earth Observatory of Columbia University, New York, USA*

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\*Corresponding author address: Jason E. Smerdon, Lamont-Doherty Earth Observatory of  
Columbia University, 61 Route 9W, P.O. Box 1000, Palisades, NY 10964.

E-mail: jsmerdon@ldeo.columbia.edu

1 **Abstract.** Potential biases in tree-ring reconstructed Palmer Drought Severity Index (PDSI) are  
2 evaluated herein using Thornthwaite (TH), Penman-Montieth (PM), and Self-Calibrating  
3 Penman-Montieth (SC) PDSI in three diverse regions of the United States and tree-ring  
4 chronologies from the North American Drought Atlas (NADA). Minimal differences are found  
5 between the three PDSI reconstructions and all compare favorably to independently  
6 reconstructed Thornthwaite-based PDSI from the NADA. Reconstructions are bridged with  
7 model-derived PDSI\_TH and PDSI\_PM, both of which closely track modeled soil moisture  
8 (near-surface and full column) during the 20<sup>th</sup> century. Differences between modeled moisture-  
9 balance metrics only emerge in 21<sup>st</sup>-century projections. These differences confirm the tendency  
10 of PDSI\_TH to overestimate drying when temperatures exceed the range of the normalization  
11 interval; the more physical accounting of PDSI\_PM compares well with modeled soil moisture  
12 in the projection interval. Remaining regional differences in the secular behavior of projected  
13 soil moisture and PDSI\_PM are interpreted in terms of underlying physical processes and  
14 temporal sampling. Results demonstrate the continued utility of PDSI as a metric of surface  
15 moisture balance, while additionally providing two recommendations for future work: 1)  
16 PDSI\_PM (or similar moisture-balance metrics) compare well to modeled soil moisture and are  
17 an appropriate means of representing soil-moisture balance in model simulations; and 2)  
18 although PDSI\_PM is more physically appropriate than PDSI\_TH, the latter metric does not bias  
19 tree-ring reconstructions of past hydroclimate variability, and as such, reconstructions targeting  
20 PDSI\_TH can be used with confidence in data-model comparisons. These recommendations and  
21 the collective results of our study thus provide a framework for comparing hydroclimate  
22 variability within paleoclimatic, observational, and modeled data.

23

24 **1. Introduction.**

25 The increasing availability of forced-transient simulations over the last millennium (e.g.,  
26 *Fernández-Donado et al. 2012; Masson-Delmotte et al. 2013*) from fully-coupled General  
27 Circulation Models (GCMs) has drastically improved our ability to compare paleoclimate  
28 reconstructions with model output and to investigate multidecadal to centennial-scale climate  
29 dynamics (*Schmidt et al. 2014*). Among the currently available collection of simulations, the  
30 Coupled and Paleo Modeling Intercomparison Projects Phases 5 and 3 (CMIP5/PMIP3) have for  
31 the first time produced multiple last-millennium, historical, and future simulations using the  
32 same model configurations and resolutions (*Taylor et al. 2012*). This important development  
33 makes comparisons between paleoclimatic data and last-millennium simulations directly  
34 applicable to historical simulations and future projections. Coincident with these advances in  
35 modeling efforts, the number of gridded or regional mean proxy reconstructions of multiple  
36 climatic variables is also increasing (e.g., *Mann et al. 2009; Cook et al. 2010; PAGES2k 2013;*  
37 *Wahl and Smerdon 2012; Neukom et al. 2010a,b; Trouet et al. 2009*), as is our understanding of  
38 the methods used to perform these reconstructions (e.g. *Jones et al. 2009; Smerdon 2012;*  
39 *Tingley et al. 2012*), expanding the detail and accuracy with which the actual climate of the last  
40 several millennia is characterized. This collective progress opens the possibility that  
41 comparisons between paleoclimatic reconstructions and model simulations can be used to  
42 improve understanding of decadal to centennial climate dynamics and to constrain model  
43 projections of 21<sup>st</sup>-century climate change in truly direct and quantitative ways (e.g. *Schmidt*  
44 *2010; Ault et al. 2014*).

45 Many paleoclimate data-model comparison studies are emerging that both interpret  
46 comparison results and work to refine the methods by which the comparisons are made (e.g.

47 *Phipps et al.* 2013; *Schmidt et al.* 2014; *Hind et al.* 2012, 2013; *Coats et al.* 2013a,b, 2014;  
48 *Anchukaitis et al.* 2010; *Seager et al.* 2008; *Fernández-Donado et al.* 2012; *Ault et al.* 2013a,b;  
49 *Lehner et al.* 2012; *Goosse et al.* 2010, 2012; *Sundberg et al.* 2012). This collection of studies,  
50 *inter alia*, has highlighted numerous considerations for how comparisons should accommodate  
51 the unique strengths, weaknesses and uncertainties of paleoclimatic reconstructions and model  
52 simulations. Each new comparison requires attention to the type of proxies used, the climatic  
53 variables considered, the means by which different models and model experiments are  
54 incorporated, and ultimately how to statistically characterize an ensemble of comparison results.

55       Among the collection of studies, paleoclimate data-model comparisons of hydroclimatic  
56 variability over the last millennium (e.g. *Seager et al.* 2008; *Coats et al.* 2013, 2014; *Ault et al.*  
57 2013b; *Tierney et al.* 2013) is one emerging and important area of focus, given the critical social  
58 and ecological implications of hydroclimate variability and change (e.g. *Allen and Ingram* 2002;  
59 *Hoerling et al.* 2012a, 2014; *Ding et al.* 2011; *Headey* 2011; *Li et al.* 2011; *Lobell et al.* 2011;  
60 *Peng et al.* 2011; *Seager et al.* 2013). Robust, high-resolution, and gridded drought atlas  
61 reconstructions that span most, if not all, of the last millennium and part of the first millennium  
62 CE are one critical tool for efforts on these time scales (*Cook et al.* 2007; *Cook et al.* 2010; *Cook*  
63 *et al.* 2014). Comparisons between models and drought atlases are nevertheless complicated by  
64 the fact that the reconstructions have targeted the Palmer Drought Severity Index (PDSI; *Palmer*  
65 1965), an integrated estimate of soil moisture balance that is not a simulated state variable in  
66 model integrations. In addition to the fact that model data must therefore be used in offline  
67 calculations that estimate PDSI for comparison to hydroclimate reconstructions (emerging  
68 capabilities using process-based tree-growth models (e.g. *Anchukaitis et al.* 2006; *Evans et al.*  
69 2006) may provide an alternative approach in which model data are used to directly estimate tree

70 growth chronologies that are not calibrated on PDSI or other climate variables), a growing  
71 debate has emerged around the efficacy of PDSI as a metric of soil moisture balance in  
72 observations and model simulations (e.g. *Guttman 1998; Vicente-Serrano et al. 2010; Burke et*  
73 *al. 2006, 2008, 2011; Dai 2011a,b, 2013; van der Schrier et al. 2011, 2013; Seneviratne 2012;*  
74 *Hoerling et al. 2012b; Sheffield et al. 2012; Trenberth et al. 2014; Cook et al. 2014).*

75         Much of the discussion and criticism of PDSI has hinged on its different formulations and  
76 more specifically on the means by which potential evapotranspiration (PET) is estimated within  
77 the PDSI calculation. A common method for estimating PET, the Thornthwaite formulation  
78 (*Thornthwaite 1948*), scales PET as a function of temperature and latitude only, and associated  
79 Thornthwaite-based PDSI estimates (hereinafter PDSI\_TH) can consequently overestimate  
80 drying when temperatures exceed the range of variability spanned by the PDSI normalization  
81 interval (*Hoerling et al. 2012b; Sheffield et al. 2012; Dai 2013*). This effect has been shown to  
82 be significant for PDSI\_TH estimates at the end of the 20<sup>th</sup> century in observational records  
83 (*Sheffield et al. 2012*) and in the use of PDSI\_TH as a moisture balance metric in 21<sup>st</sup>-century  
84 model projections (*Hoerling et al. 2012b; Dai 2013; Schmidt et al. 2013*). PDSI estimates that  
85 use the Penman-Monteith formulation (hereinafter PDSI\_PM) for PET alternatively have been  
86 proposed as more physically appropriate (e.g. *van der Schrier et al. 2011*), along with additional  
87 modifications using self-calibrating PDSI (hereinafter PDSI\_SC) that employ both the Penman-  
88 Monteith PET formulation and regionally estimated soil and vegetation properties (*Wells and*  
89 *Goddard 2004, van der Schrier et al. 2013*). Additional metrics, such as the Standardized  
90 Precipitation-Evaporation Index, which can incorporate Penman-Monteith estimated PET, also  
91 have been developed (e.g. *Vincent-Serrano et al. 2009; Hernandez and Uddameri 2014*) and  
92 compare well with PDSI\_PM in model projections (*Cook et al. 2014*).

93           Despite the above discussions, PDSI remains a useful metric of soil moisture balance for  
94 several reasons. While soil moisture is ultimately the applicable state variable for evaluating  
95 model-simulated changes in hydroclimate and drought, the land-surface models in coupled  
96 GCMs vary widely in their sophistication (e.g., soil depth, number of layers, etc.), tunings, and  
97 parameterizations (e.g., soil texture, rooting depths, vegetation types, etc.), thus complicating the  
98 meaningful comparison of direct soil moisture variables across models. Offline metrics like  
99 PDSI therefore serve to homogenize accounting of soil moisture balance and rely principally on  
100 atmospheric variables in their computation. Well-distributed records of observed soil moisture  
101 also are not widely available over many decades, making soil moisture a difficult quantity on  
102 which to validate simulated hydroclimate variability over the 20<sup>th</sup> century. Recent work  
103 additionally has demonstrated the benefit of separating PET or PDSI into the constituent  
104 influences on these variables (*Scheff and Frierson 2013; Cook et al. 2014*). The separation of  
105 such influences in coupled GCMs is not easily accomplished for model-simulated soil moisture  
106 in which variables such as temperature or precipitation cannot be held constant independent of  
107 other coupled variables. With regard to paleoclimatic data-model comparisons specifically, the  
108 currently available collection of drought atlases also have used PDSI as the reconstructed target  
109 variable, making it necessary to use model-derived PDSI for comparisons between simulations  
110 and reconstructions.

111           Concerns about paleoclimatic drought atlases nevertheless have been raised because tree-  
112 ring derived products have traditionally targeted PDSI\_TH (e.g. *Cook et al. 2007, 2010*).  
113 *Sheffield et al. (2012)* most recently note that: “*Palaeoclimate reconstructions of drought may be*  
114 *particularly susceptible because they are often developed by scaling tree-ring data to match the*  
115 *calculated [PDSI] for their overlap period.*” The authors go on to surmise that such

116 reconstructions may overestimate past changes, while underestimating “*recent trends in the*  
117 *context of the past.*” Such concerns are indeed serious, given the degree to which tree-ring  
118 derived drought atlases have been used to characterize previous droughts and pluvials (e.g. *Cook*  
119 *et al.* 2007; *Cook et al.* 2010) and the extent to which such information has helped define  
120 potential multidecadal risk factors associated with hydroclimatic variability and change.

121         Herein we evaluate the dependence of regional reconstructions targeting different PDSI  
122 formulations using the same dendroclimatic chronologies used in the North American Drought  
123 Atlas (NADA) and observationally estimated PDSI\_TH, PDSI\_PM and PDSI\_SC. We derive  
124 new reconstructions in three diverse regions of the United States for each of these PDSI  
125 formulations, analyze their respective similarities and differences, and compare them to previous  
126 NADA estimates of PDSI\_TH over the same regions, the latter of which are derived using a  
127 different reconstruction method, different predictor processing steps and a spatially-explicit  
128 PDSI\_TH target on a 0.5°x0.5° latitude-longitude grid (in contrast to the regional indices that are  
129 targeted herein). We subsequently turn to bridging paleoclimatic estimates of hydroclimate  
130 variability with modeled 20<sup>th</sup>-century climate simulations and 21<sup>st</sup>-century climate projections.  
131 This challenge is addressed by analyzing model-derived estimates of PDSI\_TH, PDSI\_PM and  
132 two soil moisture estimates from the CanESM2 and CCSM4 GCMs, both of which are available  
133 through the CMIP5 data archive. In addition to comparing simulations and reconstructions, we  
134 characterize where and how the simulated PDSI and soil moisture estimates agree within each  
135 model simulation. It is critically noted that the parameterized impacts of simulated CO<sub>2</sub>  
136 fertilization have implications for secular soil moisture trends and may be an important source of  
137 uncertainty in comparisons between multiple PDSI and soil moisture variables in 21<sup>st</sup>-century  
138 climate projections. Our investigation culminates with guidance on how to interpret our results

139 as a framework for comparing hydroclimate variability across overlapping observational and  
140 modeling intervals and to ultimately use this framework to place future hydroclimate projections  
141 into a longer paleoclimatic context.

142

## 143 **2. Data and Methods.**

### 144 *a. PDSI Calculations*

145 We focus on three areas of the United States that are representative of diverse hydroclimatic and  
146 vegetation regimes: the Four Corners (4C), North Plains (NP) and Southeast (SE) regions as  
147 indicated in Figure 1. These areas also contain well-documented and abundant tree-ring  
148 chronologies that will be used to derive regional reconstructions. Three different formulations of  
149 observational PDSI over the three regions are used: PDSI\_TH, PDSI\_PM and PDSI\_SC. The  
150 first two have been calculated using standard formulations (*Thornthwaite 1948; Penman 1948;*  
151 *Xu and Singh 2002*), while the third is taken from the self-calibrating PDSI dataset of *van der*  
152 *Schrier et al. (2013)*. PET in PDSI\_TH has the advantage of only requiring temperature and  
153 latitude data, but is effectively a rescaling of these variables as an estimate of PET (see, for  
154 example, the discussion in *van der Schrier et al. (2011)*):

$$155 \quad PET = 16 \left( \frac{10T}{I} \right)^a, \quad (1)$$

156 where  $PET$  is in  $\text{mm month}^{-1}$ ,  $T$  is the monthly mean of daily averaged temperature ( $^{\circ}\text{C}$ ),  $I$  is the  
157 heat index and  $a$  is a third-order polynomial of the heat index (*Thornthwaite 1948*). This  
158 expression is scaled in the Thornthwaite calculation of PDSI to account for latitudinal variations  
159 in the length of months and days as,

$$160 \quad PET_{TH} = PET(\theta/30)(h/12), \quad (2)$$

161 where  $\theta$  is the length of the month (in days) and  $h$  is the duration of daylight (in hours) on the

162 fifteenth day of the month (e.g. *van der Schrier et al.* 2011; *Willmott et al.* 1985). The  
 163 dependence of PET on  $T$  in Equation 1 is thus the origin of the excessive drying estimated by  
 164 PDSI\_TH when temperatures are significantly outside the range of variability defined by the  
 165 baseline normalization period.

166 The Penman-Monteith PDSI formulation (*Penman* 1948; *Xu and Singh* 2002) has been  
 167 suggested as a physically appropriate alternative method for calculating PET in 21<sup>st</sup>-century  
 168 projections (*Dai* 2013; *Hoerling et al.* 2012; *van der Schrier et al.* 2013; *Sheffield et al.* 2012;  
 169 *Cook et al.* 2014). The Penman-Monteith formulation is based on surface moisture and energy  
 170 balance considerations (*Xu and Singh* 2002) and a commonly used formulation is defined by the  
 171 Food and Agricultural Organization (FAO) of the United Nations (*Allen et al.* 1998). In the FAO  
 172 formulation  $PET$  in  $\text{mm day}^{-1}$  is given by:

$$173 \quad PET = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T_a + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)}, \quad (3)$$

174 where  $\Delta$  is the slope of the vapor pressure curve ( $\text{kPa } ^\circ\text{C}^{-1}$ ),  $R_n$  is the surface net radiation ( $\text{MJ m}^{-2}$   
 175  $\text{day}^{-1}$ ),  $G$  is the soil heat flux density ( $\text{MJ m}^{-2} \text{day}^{-1}$ ),  $\gamma$  is the psychrometric constant ( $\text{kPa } ^\circ\text{C}^{-1}$ ),  
 176  $T_a$  is the air temperature at 2 m ( $^\circ\text{C}$ ),  $u_2$  is the wind speed at 2 m ( $\text{m s}^{-1}$ ),  $e_s$  is the saturation vapor  
 177 pressure (kPa), and  $e_a$  is the actual vapor pressure (kPa). Although there have been some  
 178 suggestions that PDSI\_PM also may be susceptible to overestimated drying trends (*Hoerling et*  
 179 *al.* 2012b), this has not been widely observed in multiple studies (e.g. *Sheffield et al.* 2012; *van*  
 180 *der Schrier et al.* 2011; *Cook et al.* 2014) and reported differences in observationally-based  
 181 PDSI\_PM estimates are more likely related to differences in the precipitation datasets used as  
 182 inputs for various observational PDSI\_PM calculations (*Trenberth et al.* 2014).

183 For both PDSI\_TH and PDSI\_PM calculations presented herein, the normalization

184 interval is 1901-2012 CE. Soil moisture capacities for the top and bottom soil layers are set to  
185 the standard values of 25.4 mm (1 in.) and 127 mm (5 in.). Our observational PSDI\_PM  
186 calculations use the estimate of PET from the updated version (3.21) of the latest CRU TS  
187 dataset, which has been derived using the FAO formulation of PET (*Harris et al.* 2013) given in  
188 Equation 3. The *Harris et al.* (2013) CRU TS dataset is similarly the source for all other input  
189 variables used to calculate PDSI\_TH and PDSI\_PM. The PDSI\_SC dataset of *van der Schrier et*  
190 *al.* (2012) also uses the FAO PET formulation and differs from our calculated version of  
191 PDSI\_PM only in its incorporation of regionally specific soil and vegetation properties and a  
192 snow model (*van der Schrier et al.* 2012); similar to PDSI\_PM, the PDSI\_SC estimates use  
193 climate data from the updated version (3.21) of the latest CRU TS dataset for observational  
194 forcing variables (*Harris et al.* 2013).

195 Area-weighted regional indices were calculated from the 0.5°x0.5° gridded datasets of  
196 PDSI\_TH, PDSI\_PM and PDSI\_SC during the summer season (JJA) over the 4C, NP and SE  
197 regions; all of the regional PDSI series begin in the year 1901 CE and extend to 2012 CE. These  
198 regional series thus comprise the JJA PDSI calibration targets for the reconstructions discussed  
199 in the following subsections.

200 For calculations of PDSI\_TH and PDSI\_PM from the model simulations over the  
201 historical and projection intervals we use the same conventions described above, with several  
202 additional applied choices. Modeled PET in the Penman-Monteith formulation is again  
203 calculated using the FAO version. Relative to changes in energy availability and the vapor  
204 pressure deficit, Penman-Monteith PET is relatively insensitive to near-surface wind speed  
205 (*Scheff and Frierson* 2013; *Cook et al.* 2014), which we set equal to a constant  $1 \text{ m s}^{-1}$  in the  
206 PDSI\_PM model calculations. Ground heat fluxes similarly are only a small fraction of the total

207 surface energy budget, typically totaling about 10-15% (*Betts et al. 1996; Sellers et al. 1997*).  
208 We therefore set the ground heat flux equal to  $0 \text{ W m}^{-2}$  in the model-derived estimates of  
209 PDSI\_PM, a choice that has been found to yield little impact (*Cook et al. 2014*).

210 We do not calculate model-derived estimates of PDSI\_SC. Although the PDSI\_SC  
211 calculation can be done in principle, it additionally includes a snow model and regionally  
212 varying vegetation and soil parameters. These considerations further remove the PDSI  
213 calculation from model-derived quantities (in the case of the snow model) and involve poorly  
214 constrained or unavailable model fields (vegetation and soil properties). In light of these factors  
215 and the good agreement that is later shown for PDSI\_PM and PDSI\_SC, we do not additionally  
216 calculate PDSI\_SC fields for the models.

#### 217 *b. Tree-Ring Chronologies and the NADA*

218 We use tree-ring width chronologies from the regional collection of states shown in Figure 1.  
219 These chronologies are taken from the same network used in the NADA database to derive  
220 version 2a of the drought atlas (*Cook et al. 2007*). A total of 283, 36, and 26 chronologies are  
221 employed in the 4C, NP and SE regions, respectively. The start and end dates vary across the  
222 collection of chronologies in each region, several of which extend to the first century of the first  
223 millennium CE, while many only begin in the 18<sup>th</sup> or 19<sup>th</sup> centuries. For our purposes herein, we  
224 only employ chronologies back to the year 1000 CE; all chronologies extend to at least 1979 CE.  
225 These constraints define calibration interval selections and the nesting procedure for the  
226 reconstruction method detailed in Section 2c.

227 The NADA version 2a is also used for comparison to the new regional reconstructions.  
228 Version 2a of the NADA is a gridded reconstruction on a  $0.5^\circ \times 0.5^\circ$  latitude-longitude grid of JJA  
229 average PDSI\_TH values over much of North America. The grid has been reconstructed using a

230 point-by-point regression scheme that employs a principal component ordinary least-squares  
231 regression method, although multiple steps of predictor processing and ensemble estimation have  
232 been included (see *Cook et al. (2007)* and references therein for further details).

### 233 *c. Reconstruction Method*

234 The new regional reconstructions are derived using a nested ‘composite-plus-scale’ (CPS)  
235 method (e.g. *Jones et al. 2009*) with an ensemble correlation-weighting scheme (*PAGES2k*  
236 2013). 50-year nests were used in each regional reconstruction that employed all chronologies  
237 available back to the beginning of each nest period. A CPS reconstruction was computed for  
238 each nest by standardizing (normalizing and centering) the available tree-ring chronologies over  
239 the calibration interval, and subsequently calculating a weighted composite in which the relative  
240 weight of each chronology was determined by the strength of the correlation with the target  
241 index. Each composite was finally centered and scaled to have the same mean and variance as  
242 the target index during the calibration interval.

243 The CPS methodology was implemented using a resampling scheme for validation and  
244 calibration that uses 50 and 29-year blocks for calibration and validation, respectively (the last  
245 year of uniformly available predictor series is 1979 CE, providing 79 years of overlap with the  
246 target indices that all start in 1901). The initial calibration period extends from 1901-1950 CE  
247 and was incremented by one year until reaching the final period of 1930-1979 CE, yielding a  
248 total of 29 reconstructions for each nest. Within each calibration step, the 29 years excluded  
249 from calibration were used for cross validation. For each nest, the final CPS reconstruction was  
250 taken as the median reconstructed value in each year within the 29-member reconstruction  
251 ensemble. Uncertainties were estimated from the mean variance of the residuals across all of the  
252 validation intervals; 1.96 times the square root of the estimated mean variance was added to the

253 median ensemble values in each year to derive the 95% confidence intervals. The final nested  
254 reconstruction was combined by splicing the median reconstruction and estimated uncertainties  
255 of each nest such that every reconstructed year was derived from the nest with the maximum  
256 number of chronologies.

#### 257 *d. Model Data*

258 We use publicly available GCM output from the CMIP5 archive, the suite of model experiments  
259 organized and contributed in support of Assessment Report Five (AR5) of the Intergovernmental  
260 Panel on Climate Change (IPCC). Output from the historical and RCP8.5 21<sup>st</sup>-century projection  
261 experiments is used, the latter of which is the high-emission, business-as-usual scenario that has  
262 been justified in many studies by the current lack of international action to limit greenhouse gas  
263 emissions. Our analyses are nevertheless not dependent on the employed emissions scenario  
264 beyond the fact that the RCP8.5 simulations represent the most extreme warming scenario and  
265 therefore embody the maximum impact of temperature changes on PDSI comparisons.  
266 Historical CMIP5 experiments are run for the years 1850-2005 CE and are forced with  
267 observations of transient climate forcings (e.g. solar variability, land use change, greenhouse gas  
268 (GHG) concentrations, etc.). These experiments are initialized in 1850 CE using output from  
269 long, unforced control runs with fixed pre-industrial boundary conditions. The RCP8.5  
270 projection scenario is one of a suite of future GHG forcing scenarios spanning the 2006-2099 CE  
271 period; RCP8.5 is designed so that the top of the atmosphere radiative imbalance will equal  
272 approximately  $+8.5 \text{ Wm}^{-2}$  by the end of the 21<sup>st</sup> century, relative to pre-industrial conditions. The  
273 RCP8.5 projections are initialized using the end of the historical runs. Our analysis is restricted  
274 to two models (CanESM2 and CCSM4) that have available five continuous ensemble members  
275 spanning the historical through projection time intervals. These models and associated ensemble

276 members also have been selected based on the availability of their layered soil moisture output  
277 which extends to ~4 m and ~43 m over 3 and 15 layers in the CanESM2 and CCSM4 models,  
278 respectively. For both models, we employ a near surface JJA soil moisture estimate that is taken  
279 from approximately the first 30 cm in each model and full-column soil moisture taken over the  
280 total depth of each modeled soil column. For comparison to PDSI, both soil moisture variables  
281 spanning the historical to projection interval are centered and scaled to match the corresponding  
282 PDSI<sub>PM</sub> variance from 1901-2005 CE, the same normalization window used to calculate the  
283 PDSI variables.

284

### 285 **3. Analyses of Target Series and Reconstructions**

#### 286 *a. Observational Estimates of PDSI*

287 The area-weighted regional time series for the three observational PDSI estimates are shown for  
288 the 4C, NP and SE regions in Figure 1; all time series are centered to have a mean of zero over  
289 the reconstruction calibration/validation window (1901-1979 CE). The square of Pearson's  
290 correlation coefficient calculated between the series in each region is 0.83 or higher. The largest  
291 shared variances ( $r^2$ ) occur over the SE region (0.96, 0.86, 0.90), while the NP (0.88, 0.85, 0.90)  
292 and 4C (0.85, 0.83, 0.92) regions rank in descending order for pairings of PDSI<sub>TH</sub> vs.  
293 PDSI<sub>PM</sub>, PDSI<sub>TH</sub> vs. PDSI<sub>SC</sub> and PDSI<sub>PM</sub> vs. PDSI<sub>SC</sub>, respectively. These relative  
294 comparisons are qualitatively consistent with the correlations between the Thornthwaite and  
295 Penman-Monteith versions of PDSI<sub>SC</sub> reported by *van der Schrier et al.* (2011) for similar  
296 regions in North America.

297 The standard deviations of the observational PDSI series indicate regionally dependent  
298 differences in the variability of the PDSI estimates in the 4C (TH: 1.65, PM: 1.13, SC: 1.07), NP

309 (TH: 1.84, PM: 1.73, SC: 1.27) and SE (TH: 1.38, PM: 1.50, SC: 1.27) regions. These estimates  
300 are consistent with previously reported comparisons between Thornthwaite and Penman-  
301 Monteith derived PDSI estimates (e.g. *Sheffield et al.* 2012, *van der Schrier et al.* 2011) in which  
302 PDSI\_TH displays larger variance relative to the PDSI\_PM formulation because of its greater  
303 sensitivity to temperature variations. Nevertheless, the results also indicate that in some regions,  
304 such as the SE, PDSI\_PM has a larger variance than PDSI\_TH and therefore all areas do not  
305 follow the generally described behavior.

#### 306 *b. Reconstructed Estimates of PDSI*

307 The median PDSI reconstructions and associated uncertainties for each region are compared to  
308 the corresponding observational target series in Figure 2. Each reconstruction compares well  
309 with the targets, although there are some differences among the collection of validation statistics.  
310 The PDSI\_TH reconstructions are generally the most skillful across all regions and nests (Figure  
311 3), while the PDSI\_SC reconstruction is the second-most skillful in the 4C region and the  
312 PDSI\_PM reconstruction is second or first most skillful in the NP and SE regions. In all cases,  
313 the reconstructions yield validation-interval coefficients of determination over all nests that are  
314 skillful above the 99% ( $p < 0.01$ ) significance level. Assuming the traditional threshold of zero  
315 for the reduction of error (RE) coefficient, all regional reconstructions are skillful across all  
316 nests, except for the NP reconstructions, for which the PDSI\_TH, PDSI\_PM, and PDSI\_SC  
317 reconstructions are only skillful back to 1500, 1500 and 1600 CE, respectively. By the more  
318 stringent coefficient of efficiency (CE) statistic, which also uses a skill threshold of zero, the 4C  
319 and SE reconstructions are skillful across all nests, except the PDSI\_SC reconstruction in the SE  
320 region during several nests in the early part of the millennium (Figure 3). In the NP, all of the  
321 reconstructions yield negative CE values prior to 1600 CE and the PDSI\_SC yields an additional

322 negative nest from 1650-1700 CE. Although not all nests in the NP region are skillful back to  
323 1500 CE across all of the validation metrics, the reconstructed time series are truncated at that  
324 year to reflect the bulk validation performance described above.

325 Regional comparisons between each of the three different PDSI reconstructions yield  
326 consistent and very similar results, despite the small differences in the validation statistics  
327 discussed above. All regional pairings of reconstructions indicate shared variances of 0.99 or  
328 higher during the reconstruction intervals (1000-1900 CE for the 4C and SE regions and 1500-  
329 1900 CE for the NP). The only notable, though modest, differences between the reconstructions  
330 are their standard deviations: 4C (TH: 1.45, PM: 1.05, SC: 1.07), NP (TH: 1.64, PM: 1.39, SC:  
331 1.10) and SE (TH: 1.26, PM: 1.39, SC: 1.32). With the exception of the SE, a region in which  
332 the three reconstructions are virtually identical, the PDSI\_TH reconstructions exceed the  
333 standard deviations of the other two reconstructions by 20-50%. These variance differences are  
334 further reflected in the right-hand panels of Figure 3, in which the linear relationship between  
335 each combination of the reconstructions deviate from the one-to-one line by varying amounts in  
336 each region. Given the stated differences between the variances of the target indices, these  
337 differences in the standard deviations are expected based on the CPS methodology that matches  
338 variances between the composite reconstruction and target indices during the calibration interval.  
339 In other words, the standard deviations of each reconstruction reflect the relative differences  
340 between the variance of the target time series (although not perfectly so). Importantly, these  
341 differences in variance are merely a scaling of the overall reconstructions and do not reveal  
342 temporal variance dependencies that would bias interpretations of hydroclimate variability  
343 during the 20<sup>th</sup> century relative to the past.

344 *c. Comparisons between NADA and the CPS Reconstructions*

345 It is worth investigating whether the presented CPS reconstructions are representative of the  
346 NADA product, thus making our findings more applicable to interpretations of the latter. In  
347 Figure 4 we compare the derived CPS PDSI\_TH reconstructions to area-weighted regional  
348 averages from the NADA that have been sampled from gridded regions approximating the CPS  
349 reconstruction areas shown in Figure 1 (see Figures 11 and 12 for the specific sample regions  
350 extracted from the NADA grid). We limit the comparisons in Figure 4 to PDSI\_TH, given that  
351 the NADA also has targeted PDSI\_TH. The shared variances between the NADA time series  
352 and the CPS reconstructions of PDSI\_PM (4C: 0.94, NP: 0.65, SE: 0.68) and PDSI\_SC (4C:  
353 0.94, NP: 0.65, SE: 0.68) are nevertheless virtually identical to the shared variances reported for  
354 PDSI\_TH in Figure 4.

355 Comparisons between the NADA regional averages and the CPS PDSI\_TH  
356 reconstructions are consistent, despite the different methods by which the reconstructions were  
357 derived. The CPS reconstructions target a single regional average and use a sliding  
358 calibration/validation scheme to weight chronologies based on correlation. The NADA index is  
359 the regional average of a gridded product that uses principal component regression to target  
360 PDSI values at each grid point on a  $0.5^\circ \times 0.5^\circ$  spatial grid, uses a static calibration/validation  
361 interval, and involves various predictor processing steps not included in the CPS methodology  
362 used herein. The reconstructions therefore have targeted different characteristics of the  
363 instrumental PDSI fields and used contrasting methods to derive the respective reconstructions.  
364 Despite these dissimilarities, the CPS PDSI\_TH and NADA reconstructions compare extremely  
365 well (Figure 4); the reported shared variances for PDSI\_PM and PDSI\_SC similarly support a  
366 strong agreement between the NADA and the two additional sets of regional reconstructions.  
367 These results not only support the idea that analyses of the new CPS reconstructions are relevant

368 to interpretations of the NADA, but they more generally support the robustness and consistency  
369 of the employed methods and derived reconstructions.

370

#### 371 **4. Bridging Paleoclimatic, Observational and Model Data**

372 We now turn specifically to the challenge of bridging PDSI reconstructions with historical model  
373 simulations and future projections. We do not take up the related and important endeavor of  
374 comparing last-millennium PDSI reconstructions with forced-transient model simulations  
375 targeting the same interval. Such comparisons involve additional considerations regarding the  
376 interpretation of internal and forced variability and the realism with which the reconstructed  
377 exogenous forcings are estimated and employed in the last-millennium simulations. Detailed  
378 examples of such work can be found in *Coats et al.* (2013a, 2014, 2015), who specifically  
379 perform paleoclimate data-model comparisons focused on hydroclimate in North America.  
380 Alternative to these specific comparisons of data and models over the last millennium, we  
381 endeavor to address how to bridge PDSI reconstructions with historical and future climate  
382 projections in the context of the noted differences between multiple PDSI formulations. We  
383 analyze four estimates of modeled soil moisture balance: PDSI\_TH, PDSI\_PM, soil moisture in  
384 approximately the first 30 cm of the soil column (30cmSM), and full-column soil moisture  
385 (FCSM), the latter two of which are centered and scaled to match the PDSI\_PM variance during  
386 the 1901-2012 CE interval for comparison.

##### 387 *a. Historical Interval*

388 The four characterizations of modeled soil moisture balance in each region over the historical  
389 interval (1901-2005 CE) are shown in Figure 5 for the CanESM2 and CCSM4 models.  
390 Consistent with the observation-based estimates, these four measures of soil moisture balance

391 yield internally consistent results over the 20<sup>th</sup> century, and both formulations of PDSI reproduce  
392 modeled soil moisture with high fidelity. Agreement between the two PDSI calculations is  
393 expected given that they are both calibrated over the 1901-2012 CE period and therefore any  
394 unrealistic temperature-driven differences in the PDSI\_TH calculation are minimized. PDSI\_TH  
395 and PDSI\_PM in fact reveal a large amount of shared variance over the historical interval,  
396 matching or exceeding  $r^2$  values of 0.9 in all regions over all ensemble members in both models  
397 (Figures 6 and 7).

398 Comparisons between the two PDSI estimates and modeled soil moisture during the  
399 historical interval indicate weaker, but still high levels of shared variance (Figures 6 and 7). In  
400 most cases, PDSI\_TH and PDSI\_PM compare best with 30cmSM. The shared variance is  
401 strongest in CCSM4 for the 4C and SE regions, where  $r^2$  values exceed 0.7 for comparisons  
402 between the two PDSI variables and 30cmSM. These numbers reduce slightly for the NP where  
403 some ensemble members yield values between 0.5 and 0.6. Comparisons weaken in CanESM2,  
404 in which values of shared variance between the two PDSI variables and 30cmSM range between  
405 about 0.5 and 0.75 across all regions. Comparisons between the two PDSI variables and FCSM  
406 generally indicate less shared variance than with 30cmSM because FCSM incorporates longer-  
407 scale variations and time lags that exceed the timescales that PDSI and near-surface soil moisture  
408 more strongly sample. The depth of sampling is not, however, the only factor, as indicated by  
409 the fact that shared variances between PDSI estimates and FCSM are larger than for 30cmSM in  
410 the SE region in the CanESM2 model and for some variable pairings and ensemble members in  
411 both models in the NP. Moreover, FCSM spans a much greater depth in the CCSM4 model than  
412 in CanESM2, but the  $r^2$  values between the PDSI variables and FCSM are comparable or larger  
413 in CCSM4 than in CanESM2. Depth effects are therefore not the only determining factor in the

414 comparison.

415           Comparisons between the two direct soil moisture estimates (30cmSM and FCSM) are  
416 similar or worse within each model than the comparisons between the two PDSI estimates and  
417 either of the soil moisture variables, the one exception being in the CanESM2 model in the SE.  
418 This highlights the fact that it is not straightforward to determine which metric is most  
419 appropriate as a measure of modeled soil moisture variability or even which soil moisture target  
420 is the most appropriate analogue to compare against PDSI. Even within models, the agreement  
421 between direct soil moisture metrics is variable and depends strongly on the selected regions.  
422 The differences among these variables are likely associated with the specific tunings,  
423 parameterizations, and other modeling choices in the land-surface components of the GCMs, and  
424 further highlights the challenges of even direct comparisons between soil moisture variables in  
425 the current generation of coupled GCMs.

426           We finally note that we avoid direct comparisons between the regional PDSI\_TH  
427 reconstructions and the associated model variables beyond the collective plotting of these  
428 variables in Figures 8-10. We have normalized and centered all of the moisture-balance  
429 variables over the common reference interval from 1901-2005 CE, leaving any consistencies in  
430 means and variances of the reconstructed and modeled variables over the reference interval a  
431 product of construction. Furthermore, shared variance between the reconstructed and modeled  
432 moisture-balance metrics should not be expected for the CMIP5 historical model runs, in which  
433 the simulations are initialized from pre-industrial control runs. These initializations do not  
434 constrain modes of internal variability that impact hydroclimate over North America, such as the  
435 El Niño-Southern Oscillation or the Pacific Decadal Oscillation, to be in phase with those that  
436 have dictated the actual climate states represented in the reconstructions. Unless all of the

437 hydroclimate variability in the analyzed regions were forced over the 20<sup>th</sup> century, which is  
438 certainly not the case, the interannual to decadal variance in the reconstructions and the models  
439 will not share consistently common features. These considerations therefore must inform  
440 attempts to compare reconstructions and model simulations directly over the interval of overlap  
441 and require more detailed and specific analyses that are beyond the scope of this investigation.  
442 The bridging approach that we have outlined herein nevertheless demonstrates the use of the 20<sup>th</sup>  
443 century as a common interval for referencing reconstruction and model data in order to compare  
444 earlier paleoclimatic intervals and model projections of the 21<sup>st</sup> century.

445 *b. Projection Interval*

446 Shared variance between the four soil moisture variables during the projection interval (2005-  
447 2099 CE) are given in Figures 6 and 7, while Figures 8-10 provide comparisons between the four  
448 soil moisture metrics for the first ensemble member from both models over the historical through  
449 projection intervals. Shared variances for detrended time series over the projection interval, in  
450 addition to the original time series, are also shown in Figures 6 and 7. The shared variances  
451 among all of the detrended soil moisture metrics in the projection interval in all regions are  
452 generally comparable to those of the historical interval (with some exceptions particularly in the  
453 CCSM4 output). Larger differences are observed between the original time series, in which  
454 differences in 21<sup>st</sup>-century trends reduce the  $r^2$  values among the different soil moisture metrics  
455 (in cases where trends are comparable among variables, the shared variances in original and  
456 detrended time series are similar). Secular drying in PDSI\_TH exceeds that of all other modeled  
457 soil moisture metrics over the 21<sup>st</sup> century in all three regions, a clear demonstration of the  
458 tendency for PDSI\_TH to overestimate drying during the projection interval. There are,  
459 however, regional differences in the relative comparisons among variables, as discussed below.

460 PDSI\_TH includes secular trends in the 4C region that in some cases are larger in  
461 magnitude or opposite in sign relative to the three other metrics in both models (Figure 8),  
462 despite the fact that some of the other metrics compare favorably to PDSI\_TH over the full  
463 century or during specific intervals of time. PDSI\_PM and 30cmSM compare well throughout  
464 the projection interval in the CCSM4 model, while 30cmSM projects enhanced drying, relative  
465 to PDSI\_PM, in the CanESM2 model. FCSM again compares favorably to PDSI\_PM and  
466 30cmSM in the CCSM4 simulation, while it suggests a wetting trend in the CanESM2 simulation  
467 that is not reflected in any of the other estimates. This may again be representative of the  
468 deeper-column soil moisture dynamics in the model (although no such trend is observed for the  
469 CCSM4 model with a much deeper soil column).

470 In the NP, the behavior of PDSI\_TH is again consistent with previously discussed  
471 expectations (Figure 9). The variable estimates drier 21<sup>st</sup>-century mean conditions than any of  
472 the other soil moisture metrics and projects secular drying trends in both models that are either  
473 larger or not present in the other variables. Similar to the 4C region, PDSI\_PM compares  
474 favorably to 30cmSM throughout the projection interval in the CCSM4 model, while 30cmSM  
475 projects slightly enhanced drying, relative to PDSI\_PM, in the CanESM2 model. The FCSM  
476 estimate in CanESM2 contains a pronounced wetting trend and multidecadal variability in the  
477 NP that, in addition to contrasting with PDSI\_PM, is also not present in the 30cmSM output.  
478 The FCSM is similarly wetter in the CCSM4 projection for the NP, but not by nearly as much as  
479 the CanESM2 projection. In the SE, the behavior of PDSI\_TH is the same as discussed for the  
480 other two regions in both models (Figure 10). Comparisons between 30cmSM and FCSM  
481 variables are more consistent in both models in the SE, both of which project wetter conditions  
482 or a wetting trend (CCSM4) in the SE that is not present in the PDSI\_PM estimate.

483           Given the three regional analyses presented above, it is evident that all of the soil  
484 moisture metrics compare well over the 20<sup>th</sup> century in both models over all three regions.  
485 Regional differences are evident, however, in comparisons between the variables over the 21<sup>st</sup>-  
486 century, including some large disparities between the two modeled soil moisture metrics  
487 themselves. This is particularly true of the secular trends estimated by the various metrics.  
488 While PDSI\_TH projects varying degrees of exaggerated drying over all regions and models,  
489 PDSI\_PM either matches well 30cmSM, falls between 30cmSM and FCSM, or projects  
490 relatively constant moisture balance conditions when 30cmSM and FCSM indicate wetting  
491 trends. These regional observations are given broader context in Figures 11 and 12 that plot the  
492 projected mean values of PDSI\_PM, 30cmSM and FCSM for the last two decades (2080-2099  
493 CE) of the 21<sup>st</sup>-century using the first ensemble member of the CanESM2 and CCSM4  
494 simulation; the agreement between the three variables in the direction of either wetting or drying  
495 is also plotted. Inspections of Figures 11 and 12 indicate that it is difficult to draw consistent  
496 characterizations of how the variables compare across models or regions. In the CanESM2  
497 simulation, for instance, PDSI\_PM and FCSM project wetting throughout much of western  
498 North America, while 30cmSM projects drying over those regions (note that this wetting  
499 projection is anomalous over the CMIP5 ensemble (*Cook et al.* 2014), but the analyzed models  
500 have been selected based on the availability of their layered soil moisture output and ensemble  
501 members that are continuous across the historical to projection intervals). In contrast to  
502 CanESM2, the PDSI\_PM projection from CCSM4 is almost uniformly toward drying, while a  
503 heterogeneous pattern of wetting emerges in 30cmSM and is further enhanced in FCSM. A full  
504 diagnosis of the physical underpinnings of these differences is beyond the scope of this paper,  
505 but we discuss various explanations for the regional differences in the following section and

506 suggest that parsing the differences between these soil moisture metrics is an important area of  
507 further research.

508

## 509 **5. Discussion**

510 This study has been motivated by two considerations: 1) the growing interest in performing  
511 paleoclimatic model-data comparisons; and 2) the ongoing debate about how to properly  
512 represent hydroclimatic variability and change from a host of possible soil moisture metrics. Our  
513 results demonstrate the robustness of PDSI as a metric of near-surface moisture variability in  
514 observations, reconstructions, and 20<sup>th</sup>-century model simulations. Reconstructions derived for  
515 three diverse regions of the United States compare favorably, regardless of the reconstruction  
516 target (PDSI-TH, PDSI-PM, or PDSI-SC) or technique (CPS vs. the NADA-based approach).  
517 The variances of the derived reconstructions are the principal, though modest, differences among  
518 them, and are consistent with the expected character of PDSI formulations estimated from  
519 observations over the historical interval. Importantly, these results indicate that previous  
520 concerns about biases in tree-ring reconstructions due to the use of PDSI\_TH as a calibration  
521 target (*Sheffield et al.* 2012) are unfounded over North America. Similarly, model estimates of  
522 soil moisture and PDSI are all consistent during the historical interval: PDSI\_TH, PDSI\_PM and  
523 two normalized soil moisture estimates all compare well in the CanESM2 and CCSM4 historical  
524 model simulations. Together, these results support the continued use of PDSI as a valuable tool  
525 for empirical and model-based investigations of drought and hydroclimate.

526 Principal differences emerge only in model-derived estimates of PDSI and soil moisture  
527 during the 21<sup>st</sup>-century projection interval. Specifically, the secular behavior of the various  
528 metrics diverges in the projections, while the interannual variability remains relatively consistent

529 across all variables throughout the 21<sup>st</sup>-century projection interval. In the case of PDSI\_TH,  
530 enhanced secular drying is now a well-understood consequence of unrealistically scaling PET as  
531 a function of temperature when values exceed the range defined by the normalization interval. It  
532 is less clear, however, how and why modeled near-surface and full-column soil moisture would  
533 compare well with the more physically-based PDSI\_PM during the 20<sup>th</sup> century and in the 21<sup>st</sup>-  
534 century on interannual timescales, while their 21<sup>st</sup>-century secular trends would diverge.

535         Several possibilities may explain some of the different secular behavior in the model-  
536 based metrics. The differences may arise, in part, from the difficulty in identifying the most  
537 appropriate modeled soil moisture variable for comparison with the model-derived PDSI. We  
538 have demonstrated various situations in which PDSI most closely reflects near surface soil  
539 moisture, others where PDSI was a better indicator of full column soil moisture, or places where  
540 PDSI resolved both equally well. Importantly, we also illustrated ample instances where even  
541 the two soil moisture metrics diverge, sometimes to quite extreme effect (e.g., the Northern  
542 Plains in CanESM2). Additional differences between PDSI and modeled soil moisture also are  
543 likely to arise through the typically more sophisticated treatment of processes (e.g., vegetation,  
544 soil physics, etc.) in the land-surface components of GCMs. These parameterizations and  
545 tunings vary across models, meaning that any concerns in comparing PDSI and soil moisture  
546 within models must also be extended to comparing soil moisture trends across models.

547         One major issue that is often discussed in the context of future drought projections is the  
548 CO<sub>2</sub> fertilization effect. The direct physiological effect of elevated atmospheric CO<sub>2</sub>  
549 concentrations (eCO<sub>2</sub>) is to reduce water loss during photosynthesis by lowering stomatal  
550 conductance. This effect is typically incorporated into the physics of GCM land-surface and  
551 vegetation models, but not in standard PDSI calculations, including those employed herein. Two

552 expectations are therefore associated with eCO<sub>2</sub>: 1) drought stress on model vegetation will be  
553 reduced, translating into lower rates of evapotranspiration and increases in soil moisture and  
554 runoff; and 2) standard PDSI projections, which do not include the impact of eCO<sub>2</sub>, will not  
555 reflect any associated wetting tied to the effect. This may explain areas in the presented  
556 projections where PDSI indicates drying while model soil moisture indicates wetting or little  
557 change.

558 While the physiological effect of eCO<sub>2</sub> is well understood at the leaf level (*Ainsworth*  
559 *and Rogers* 2007), there are large uncertainties associated with the scaling of this effect on  
560 hydrology at larger scales that may lead to an overestimate of the eCO<sub>2</sub> effect in model  
561 projections. For example, many experiments in which plants are exposed to elevated levels of  
562 CO<sub>2</sub> show only modest and often insignificant changes in transpiration and soil moisture (e.g.,  
563 *Domec et al.* 2009; *Hussain et al.* 2013; *Inauen et al.* 2013; *Naudts et al.* 2013; *Stocker et al.*  
564 1997). Additionally, few eCO<sub>2</sub> studies simultaneously incorporate ambient warming into their  
565 experiments, an accompanying element of climate change that is expected to increase ET and  
566 potentially counteract any moisture gains from eCO<sub>2</sub>. Despite this ambiguity in the empirical  
567 evidence, however, most land surface and vegetation models, including those models typically  
568 incorporated into GCMs, substantially reduce transpiration when exposed to eCO<sub>2</sub> and, in some  
569 cases, dramatically overestimate the transpiration response relative to observations (*De Kauwe et*  
570 *al.* 2013). This suggests that the modeled response to eCO<sub>2</sub> may be oversimplified and the eCO<sub>2</sub>  
571 effect on hydrology overestimated. In fact, this host of uncertainties in both the modeled and  
572 empirical eCO<sub>2</sub> responses led Working Group II of the IPCC to conclude in AR5 (*Scholes et al.*  
573 2014) that the net effect of eCO<sub>2</sub> on runoff and transpiration is still “*poorly constrained*”, and  
574 that “*precipitation and temperature effects are likely to remain the prime influence on global*

575 runoff.” Notably, eCO<sub>2</sub> does not appear to have a strong influence on soil moisture in other  
576 CMIP5 simulations before the rapid increases in the RCP scenarios, as evidenced by the tight  
577 coupling between PDSI and modeled soil moisture in the historical simulations presented herein.

578 Clearly, there remain significant uncertainties in the interpretation of modeled soil  
579 moisture and PDSI responses in 21<sup>st</sup>-century GCM projections. Further characterizing and  
580 resolving the impact of these modeling choices will be important as a means of resolving  
581 differences between PDSI<sub>PM</sub> and the soil moisture estimates discussed herein, but even more  
582 importantly to constrain the range of realistic soil moisture conditions into the future. In the  
583 context of paleoclimate data-model comparisons, however, it appears that projections using  
584 PDSI<sub>PM</sub> or normalized near-surface soil moisture are the most appropriate variables for  
585 characterizing future projections and for comparing projections to modern and paleoclimatic  
586 observations (e.g. *Dai* 2013; *Cook et al.* 2014).

587

## 588 **6. Conclusions**

589 Given our principal observations, a framework emerges for comparisons between PDSI  
590 reconstructions and model simulations. It is first of all evident that tree-ring based PDSI  
591 reconstructions are robust to the selection of PDSI target variables and the current generation of  
592 PDSI<sub>TH</sub> drought atlases can be confidently used as estimates of hydroclimatic variability over  
593 the last millennium. With regard to comparing these drought atlases to last-millennium  
594 simulations, our results suggests that model-derived PDSI or soil moisture should all estimate  
595 similar hydroclimate histories given that modeled temperature variations over the last  
596 millennium are typically within the range of modeled 20<sup>th</sup>-century climate (e.g. *Fernández-*  
597 *Donado et al.* 2012; *Masson-Delmotte et al.* 2013). Indeed, the similarity between multiple

598 hydroclimate metrics over the last millennium has been demonstrated specifically in the  
599 American Southwest using multiple simulations in the context of assessing the occurrence of  
600 multidecadal drought events in the region (*Coats et al.* 2013, 2014). Similarly, we have shown  
601 that comparisons among observational or modeled soil moisture metrics during the 20<sup>th</sup> century  
602 are largely insensitive to the choice of metric. While it is most consistent to compare the same  
603 metric across reconstructions, observations, and models, such consistency does not appear  
604 essential, and is sometimes not possible, over the last millennium and through the 20<sup>th</sup> century.  
605 In lieu of homogenized products, it therefore is suggested that comparisons simply reference and  
606 scale means and variances of all variables over a common period of overlap.

607 Overall, the current collection of tools can provide robust characterizations of  
608 hydroclimate variability and change during the last millennium, which in turn can be  
609 meaningfully compared to observations and model simulations of 20<sup>th</sup>-century hydroclimate and  
610 model projections of 21<sup>st</sup>-century change. Within these comparisons the most important interval  
611 of consideration is the 21<sup>st</sup> century, in which model projections should be characterized using  
612 either PDSI\_PM (or similarly a Penman-Montieth version of PDSI\_SC or Standardized  
613 Precipitation-Evaporation Index) or a near-surface normalized soil moisture output. In the case  
614 of the latter, however, these results must be carefully interpreted in terms of their applicability  
615 across a collection of model simulations and in terms of the processes that they include. The  
616 impact of CO<sub>2</sub> fertilization on 21<sup>st</sup>-century hydroclimate projections is a particularly important  
617 process to evaluate across models, given the poorly constrained nature of the process on large-  
618 scale vegetation response and because it appears to have potentially important implications for  
619 projected hydroclimatic trends. Although these details complicate comparisons and leave open  
620 important research questions, future model-data comparisons that span the last-millennium

621 through the 21<sup>st</sup>-century projection interval will be vital for assessing and characterizing future  
622 risks associated with hydroclimate variability and change. As we have demonstrated, these  
623 comparisons are possible and appropriate given the current collection of data and tools, all of  
624 which should be used for comparisons within the framework outlined herein.

625

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## Figure Captions

**Figure 1.** Map of the contiguous United States and those states chosen to represent the Four Corners (4C), North Plains (NP) and Southeast (SE) regions (designated with grey shading). The tree-ring sites used in the regional reconstructions are shown as red dots. Plotted time series are the area-weighted mean PDSI estimates for each of the three regions estimated from observational data and three PDSI formulations: PDSI Thornthwaite (PDSI\_TH), PDSI Penman-Monteith (PDSI\_PM) and self-calibrating PDSI with Penman-Monteith (PDSI\_SC).

**Figure 2.** Targeted regional PDSI time series calculated from observational data for the PDSI\_TH, PDSI\_PM and PDSI\_SC formulations and the associated CPS reconstructions and 95% confidence intervals. Reconstructions and observationally-based estimates are shown during their common period of overlap from 1901-1979 CE, which also comprises the calibration/validation interval for the reconstructions.

**Figure 3.** PDSI reconstructions using the CPS method and three regional PDSI target series using the PDSI\_TH, PDSI\_PM and PDSI\_SC formulations (a, c, and e). The 10-yr lowpass time series for each PDSI reconstruction (filtered using a 10-point butterworth filter) are also shown in panels a, c and e, while each panel also plots the annual PDSI\_TH and associated 95% confidence intervals for reference. Panels b, d and f plot resolved variance, RE and CE cross-validation statistics for each of the regional PDSI reconstructions as a function of each 50-yr nest. Figure legends for panels a-f are given in panels c and d. Comparisons between the annually-reconstructed PDSI values are shown in the scatter plots in panels g-i, in which each value of reconstructed PDSI is plotted against the other. Scatter plots do not include the

calibration/validation interval from 1901-1979 and plot a dashed 1:1 line for reference.

**Figure 4.** Comparisons of reconstructed PDSI\_TH from this study using CPS and the regional averages of the gridded NADA product over the targeted CPS reconstruction domains. Time series plot both annual values and the 10-yr lowpass filtered time series using a 10-point butterworth filter. The shared variance ( $r^2$ ) between the annual (filtered) CPS and NADA time series over their periods of overlap are shown within each plot in the left column. Scatter plots for the annual CPS and NADA values are shown in the right column of the figure with one-to-one lines shown for reference.

**Figure 5:** Regional model estimates of PDSI\_TH, PDSI\_PM, normalized 30cmSM and normalized FCSM during the historical interval (1901-2005 CE) in the CanESM2 and CCSM4 models. The first ensemble member of each model is plotted (interannual  $r^2$  estimates across all five ensemble members are shown in Figures 6 and 7). In all cases, PDSI or soil moisture normalizations used the 1901-2005 CE intervals as a baseline, but time series are recentered from 1901-1979 CE to match the calibration/validation interval of the PDSI reconstructions.

**Figure 6:** Regional shared variances ( $r^2$ ) among the collection of soil moisture metrics in the CanESM2 model simulations during the historical (1901-2005 CE) and projection (2006-2099 CE) intervals. Vertical diamond triplets correspond to the maximum, minimum, and median shared variance across the five members of the ensemble. Detrended results have been computed for the projection interval after removing a linear trend over the same period.

**Figure 7:** Same as in Figure 6, but for the CCSM4 model simulations. Maximum, minimum and median results were similarly computed from an ensemble of five simulations.

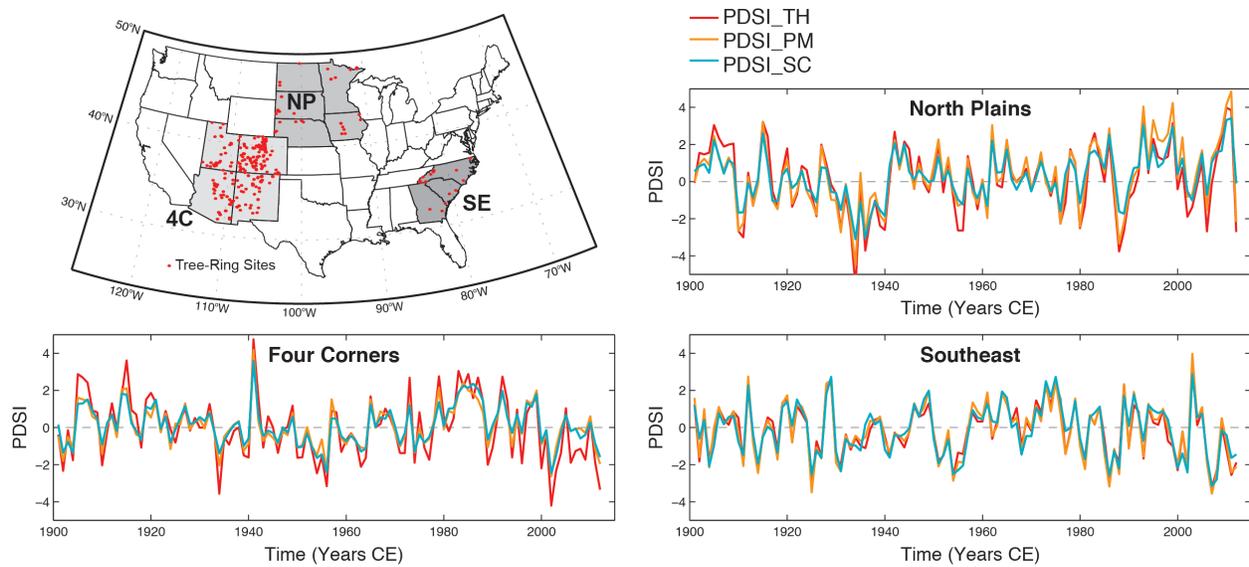
**Figure 8:** A comparison of reconstructed PDSI\_TH in the 4C region (see Figure 1) with collocated model estimates of PDSI\_TH, PDSI\_PM, normalized 30cmSM and normalized FCSM during the historical and projection intervals. Results are shown for the first ensemble member of the CanESM2 and CCSM4 model simulations to allow direct visual comparisons between the reconstructed and model variance. All time series have been centered over the 1901-1979 interval, the time period of common overlap. Reconstructions extend prior to 1800, but the 1800-2100 CE interval is chosen for ease of visual comparison.

**Figure 9:** Same as in Figure 8, but for the North Plains region (see Figure 1).

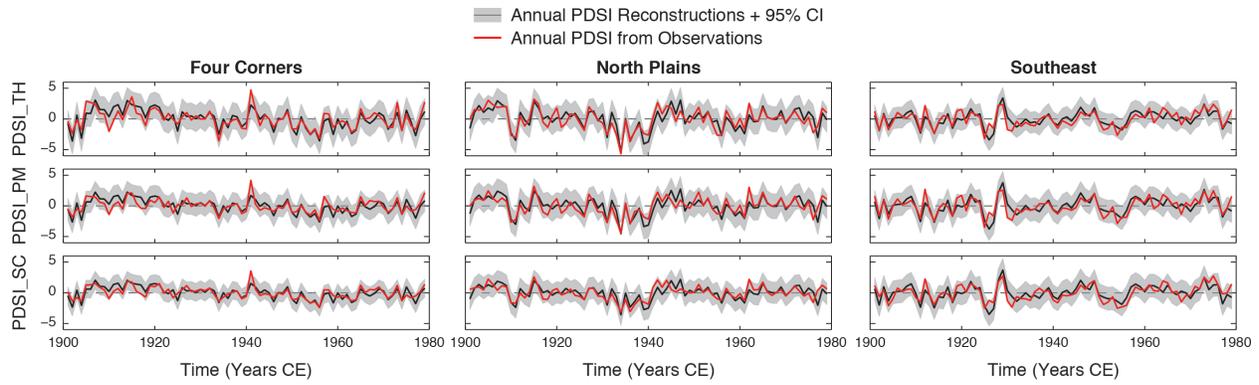
**Figure 10:** Same as in Figure 8, but for the Southeast region (see Figure 1).

**Figure 11:** (top row) Mean PDSI\_PM, normalized 30cmSM and normalized FCSM for the last two decades (2080-2099 CE) of the 21<sup>st</sup>-century projection interval (ensemble member 1) from the CanESM2 model. (bottom row) Agreement between the sign of the wetting (blue) or drying (brown) as projected by the three variables in the 2080-2099 CE interval. The total percentage of grid cells that agree on the wetting or drying trends are provided in the lower left hand part of the comparison maps. The boxes defined by dashed lines indicate the regions extracted from the 0.5°x0.5° NADA, observation and model grids as representative of the 4C, NP and SE regions.

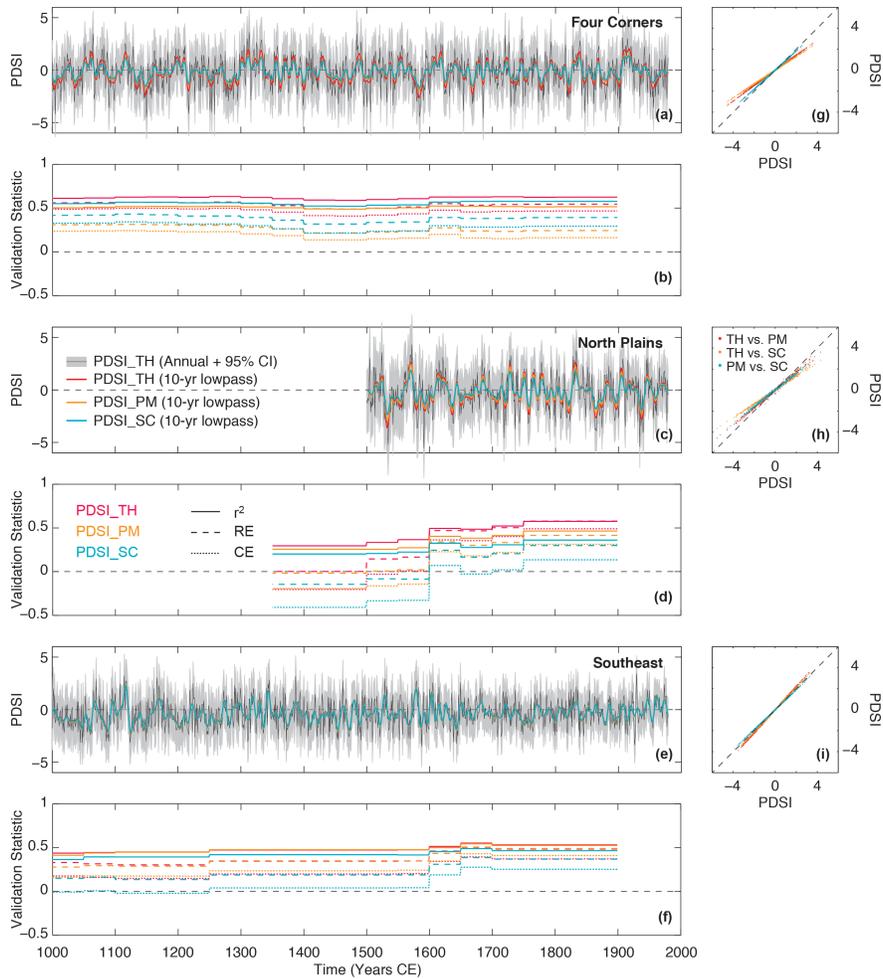
**Figure 12:** Same as in Figure 11, but for the CCSM4 model.



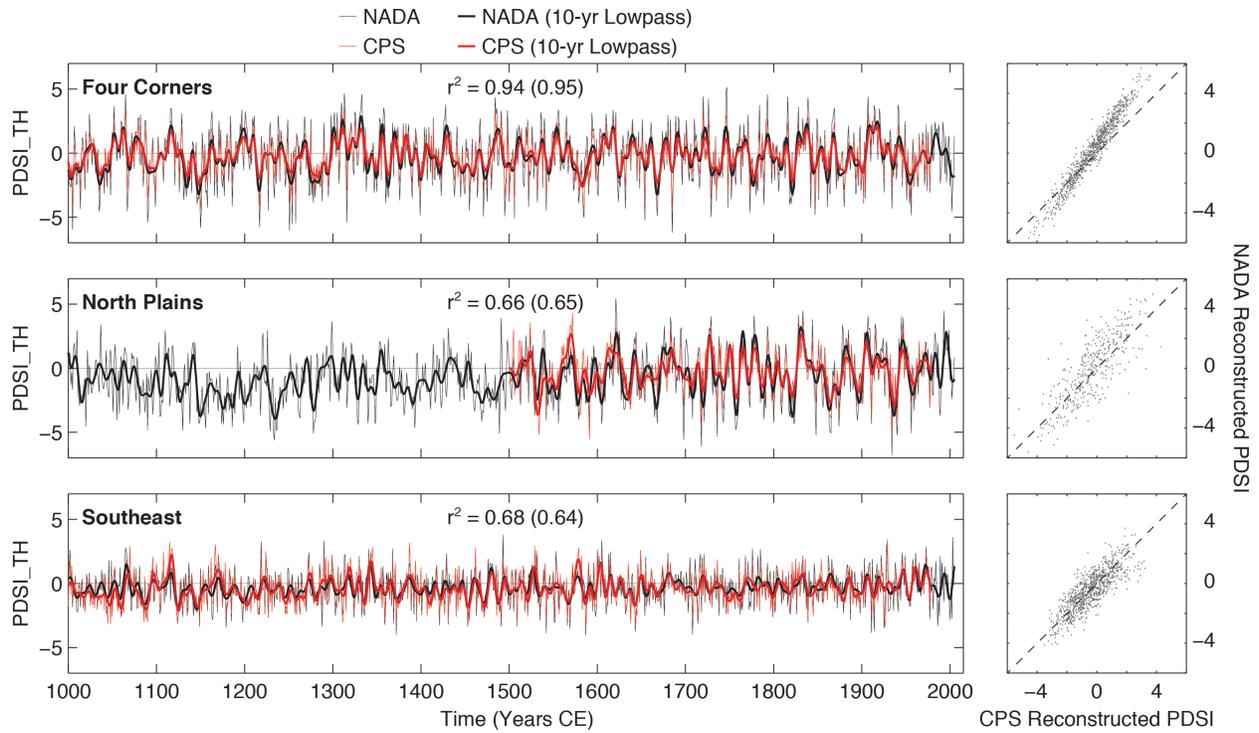
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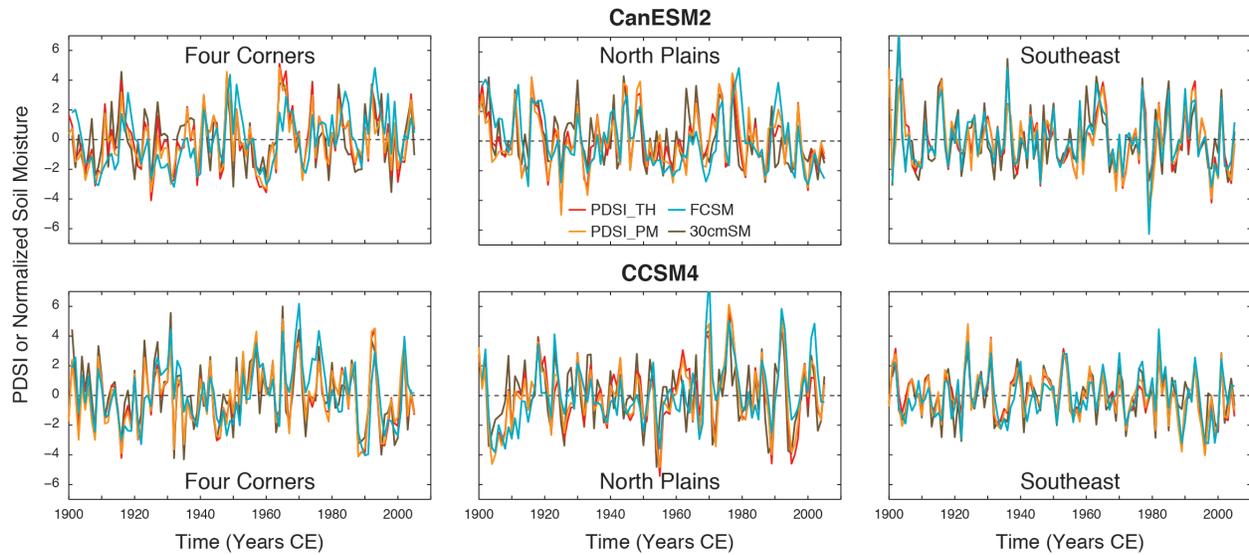
**Figure 2.** Targeted regional PDSI time series calculated from observational data for the PDSI\_TH, PDSI\_PM and PDSI\_SC formulations and the associated CPS reconstructions and 95% confidence intervals. Reconstructions and observationally-based estimates are shown during their common period of overlap from 1901-1979 CE, which also comprises the calibration/validation interval for the reconstructions.



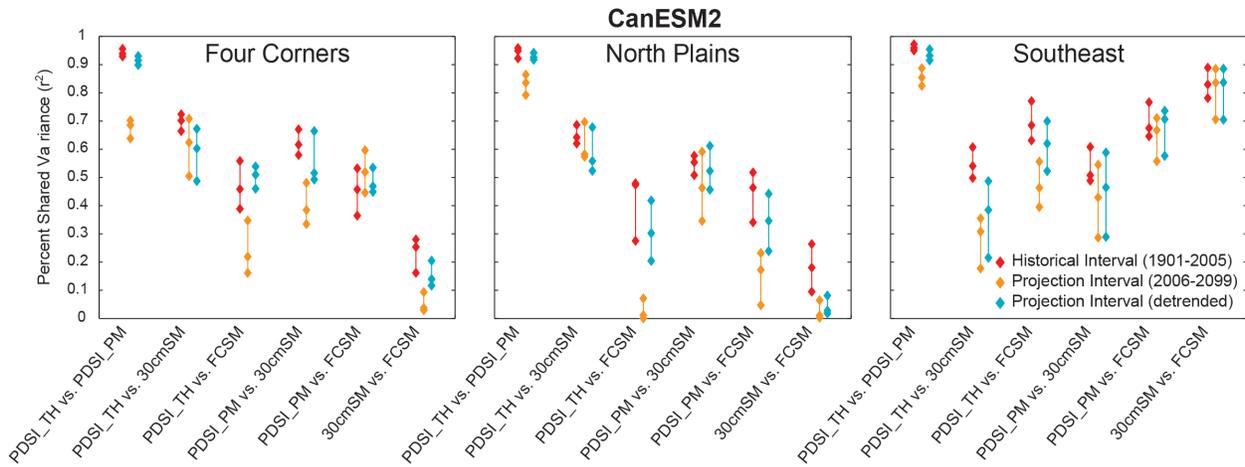
**Figure 3.** PDSI reconstructions using the CPS method and three regional PDSI target series using the PDSI\_TH, PDSI\_PM and PDSI\_SC formulations (a, c, and e). The 10-yr lowpass time series for each PDSI reconstruction (filtered using a 10-point butterworth filter) are also shown in panels a, c and e, while each panel also plots the annual PDSI\_TH and associated 95% confidence intervals for reference. Panels b, d and f plot resolved variance, RE and CE cross-validation statistics for each of the regional PDSI reconstructions as a function of each 50-yr nest. Figure legends for panels a-f are given in panels c and d. Comparisons between the annually-reconstructed PDSI values are shown in the scatter plots in panels g-i, in which each value of reconstructed PDSI is plotted against the other. Scatter plots do not include the calibration/validation interval from 1901-1979 and plot a dashed 1:1 line for reference.



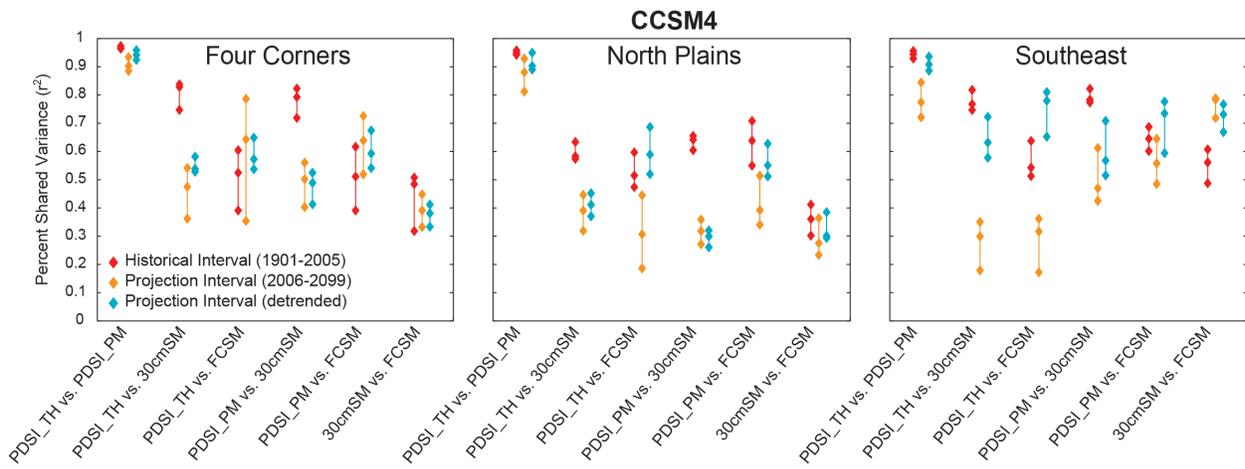
**Figure 4.** Comparisons of reconstructed PDSI\_TH from this study using CPS and the regional averages of the gridded NADA product over the targeted CPS reconstruction domains. Time series plot both annual values and the 10-yr lowpass filtered time series using a 10-point butterworth filter. The shared variance ( $r^2$ ) between the annual (filtered) CPS and NADA time series over their periods of overlap are shown within each plot in the left column. Scatter plots for the annual CPS and NADA values are shown in the right column of the figure with one-to-one lines shown for reference.



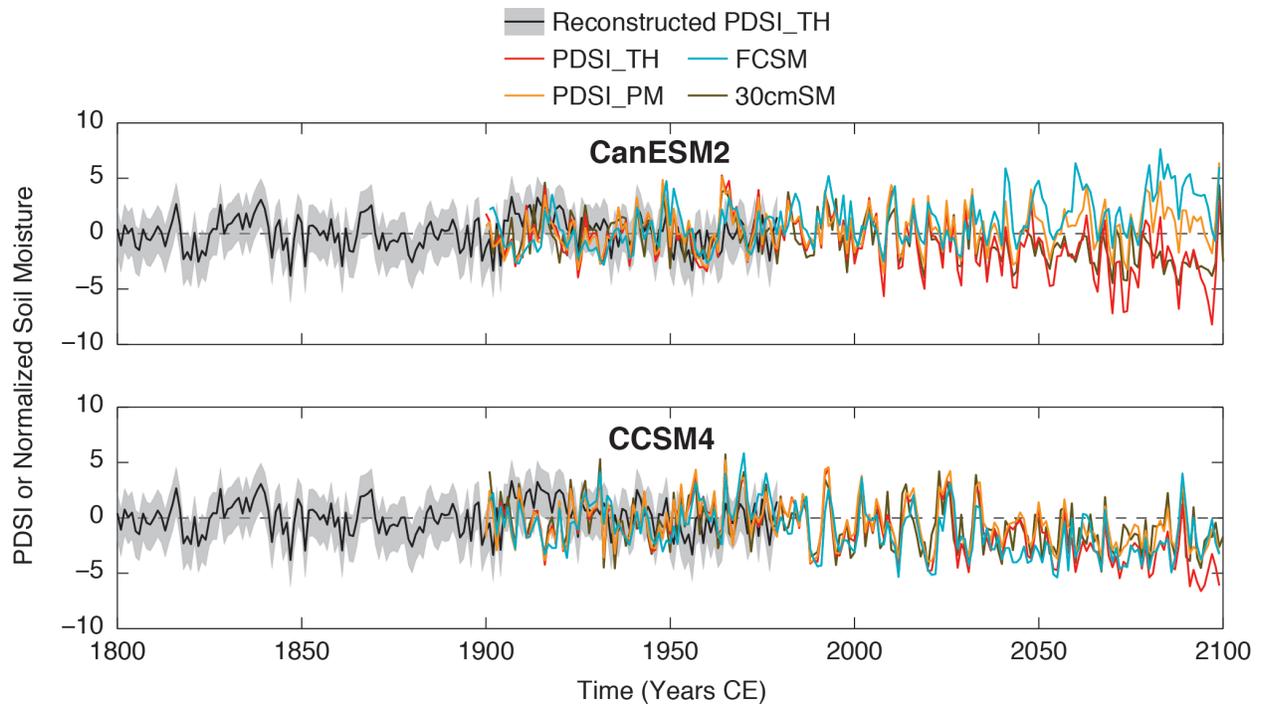
**Figure 5:** Regional model estimates of PDSI\_TH, PDSI\_PM, normalized 30cmSM and normalized FCSM during the historical interval (1901-2005 CE) in the CanESM2 and CCSM4 models. The first ensemble member of each model is plotted (interannual  $r^2$  estimates across all five ensemble members are shown in Figures 6 and 7). In all cases, PDSI or soil moisture normalizations used the 1901-2005 CE intervals as a baseline, but time series are recentered from 1901-1979 CE to match the calibration/validation interval of the PDSI reconstructions.



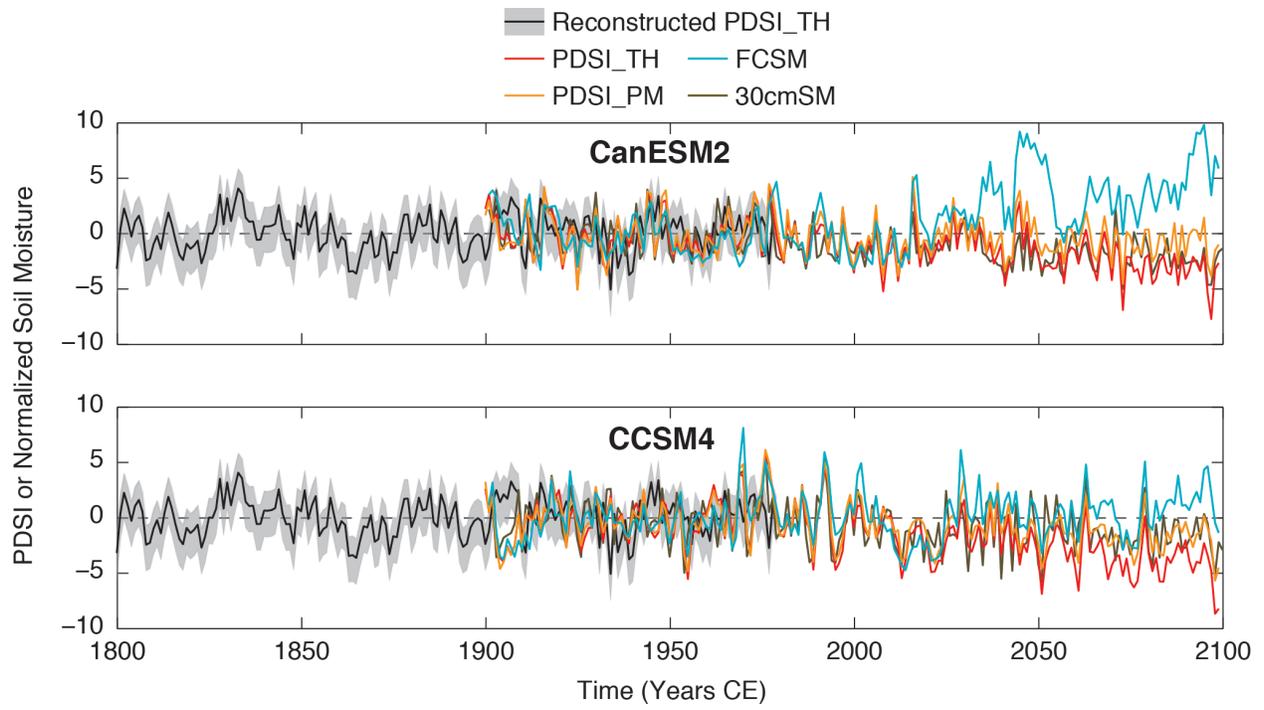
**Figure 6:** Regional shared variances ( $r^2$ ) among the collection of soil moisture metrics in the CanESM2 model simulations during the historical (1901-2005 CE) and projection (2006-2099 CE) intervals. Vertical diamond triplets correspond to the maximum, minimum, and median shared variance across the five members of the ensemble. Detrended results have been computed for the projection interval after removing a linear trend over the same period.



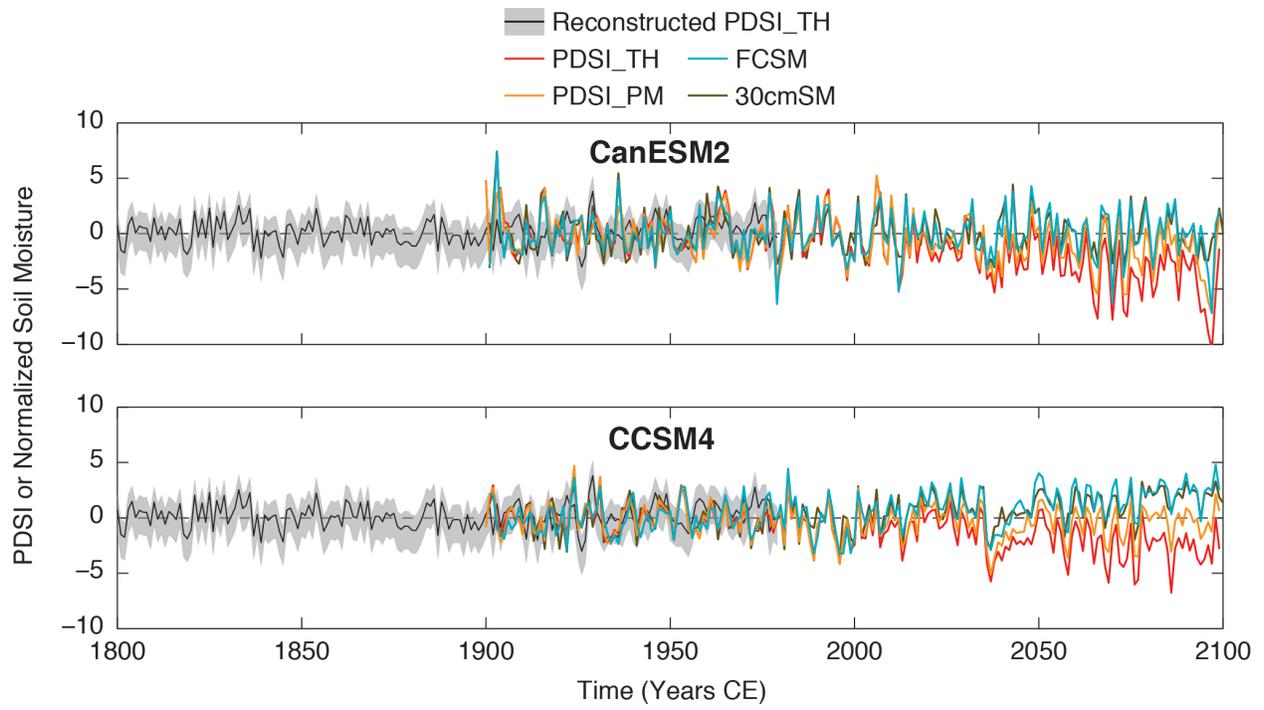
**Figure 7:** Same as in Figure 6, but for the CCSM4 model simulations. Maximum, minimum and median results were similarly computed from an ensemble of five simulations.



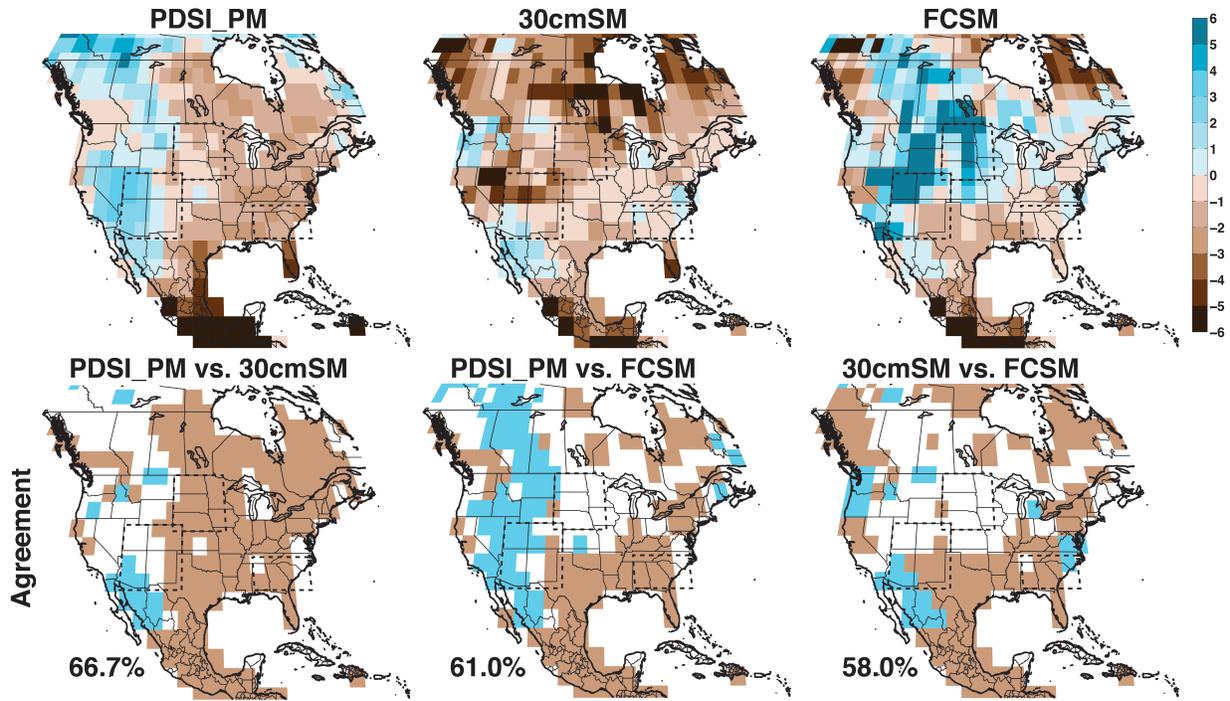
**Figure 8:** A comparison of reconstructed PDSI\_TH in the 4C region (see Figure 1) with collocated model estimates of PDSI\_TH, PDSI\_PM, normalized 30cmSM and normalized FCSM during the historical and projection intervals. Results are shown for the first ensemble member of the CanESM2 and CCSM4 model simulations to allow direct visual comparisons between the reconstructed and model variance. All time series have been centered over the 1901-1979 interval, the time period of common overlap. Reconstructions extend prior to 1800, but the 1800-2100 CE interval is chosen for ease of visual comparison.



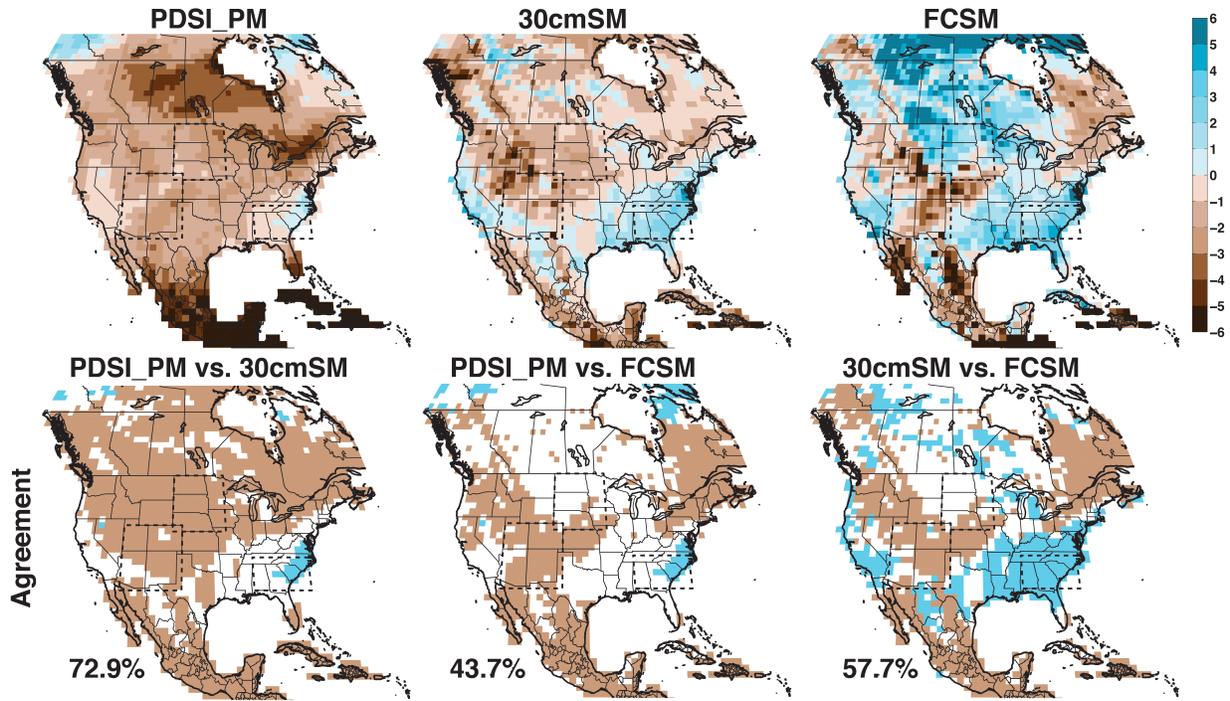
**Figure 9:** Same as in Figure 8, but for the North Plains region (see Figure 1).



**Figure 10:** Same as in Figure 8, but for the Southeast region (see Figure 1).



**Figure 11:** (top row) Mean PDSI\_PM, normalized 30cmSM and normalized FCSM for the last two decades (2080-2099 CE) of the 21<sup>st</sup>-century projection interval (ensemble member 1) from the CanESM2 model. (bottom row) Agreement between the sign of the wetting (blue) or drying (brown) as projected by the three variables in the 2080-2099 CE interval. The total percentage of grid cells that agree on the wetting or drying trends are provided in the lower left hand part of the comparison maps. The boxes defined by dashed lines indicate the regions extracted from the 0.5°x0.5° NADA, observation and model grids as representative of the 4C, NP and SE regions.



**Figure 12:** Same as in Figure 11, but for the CCSM4 model.