1 **Satellite Detection of Soil Moisture Related Water Stress Impacts on Ecosystem**
2 **Productivity using the MODIS-based Photochemical Reflectance Index**

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Abstract

Satellite remote sensing provides continuous observations of vegetation properties that can be used to estimate global terrestrial ecosystem gross primary production (GPP). The Photochemical Reflectance Index (PRI) has been shown to be sensitive to vegetation photosynthetic light use efficiency (LUE), GPP and canopy water-stress. Here, we use the NASA EOS MODIS (Moderate Resolution Imaging Spectroradiometer) based PRI with eddy covariance CO₂ flux measurements and meteorological observations from 20 tower sites representing major plant functional type (PFT) classes within the continental USA (CONUS) to assess GPP sensitivity to soil moisture related water stress. The sPRI (scaled PRI) metric derived using MODIS band 13 as a reference channel (sPRI₁₃) shows generally higher correspondence with tower GPP observations than other potential MODIS reference bands. The sPRI₁₃ observations were used as a proxy for soil moisture related water supply constraints to LUE within a satellite data driven terrestrial carbon flux model to estimate GPP (GPP_{PRI}). The GPP_{PRI} calculations show generally favorable correspondence with tower GPP observations ($0.457 \leq R^2 \leq 0.818$), except for lower GPP_{PRI} performance over evergreen needleleaf forest (ENF) sites. A regional model sensitivity analysis using the sPRI₁₃ as a water supply proxy indicated that water restrictions limit GPP over more than 21% of the CONUS domain, particularly in drier climate areas where atmospheric moisture (VPD) deficits alone are insufficient to represent both atmosphere demand and water supply controls affecting productivity. Our results indicate strong potential of the MODIS sPRI₁₃ to represent soil moisture related water supply controls influencing photosynthesis, with enhanced (1-km resolution) delineation of these processes closer to the scale of *in situ* tower observations. These observations may provide an effective tool for characterizing sub-grid spatial heterogeneity in soil moisture related controls that inform coarser scale observations and estimates determined from other satellite observations and global carbon, and climate models.

- 46 **Keywords:** Photochemical reflectance index (PRI), Soil moisture, Gross primary production (GPP),
- 47 MODIS, TCF LUE model

1. Introduction

Gross Primary Production (GPP), representing the sum of gross carbon (CO₂) uptake by plant photosynthesis, is a key component of the terrestrial carbon cycle (Potter et al. 1993; Yang et al. 2007). Accurate and reliable global estimation and monitoring of GPP is challenging due to a range of factors, including heterogeneity in vegetation conditions and environmental processes affecting photosynthesis. *In situ* observations from tower eddy covariance measurements have been used to track CO₂ exchange between terrestrial ecosystems and the atmosphere (Baldocchi et al. 2001); the associated tower measurements of net ecosystem CO₂ exchange (NEE) can be used to estimate GPP at the level of a local tower footprint (~1 km²) and with daily temporal fidelity useful for detailed analysis of stand level processes. At present, over 650 flux tower sites are represented within the global FLUXNET network, providing detailed time series measurements of NEE, water vapor and energy exchange between terrestrial ecosystems and the atmosphere (Baldocchi et al. 2001). However, a major constraint of these observations for global GPP assessment and monitoring is their limited spatial representation and sampling bias relative to the global range of vegetation and climate conditions (Schimel et al. 2014).

Alternatively, satellite remote sensing provides spatially contiguous observations of vegetation and ecosystem properties that can be used for estimating GPP over a global domain (Running et al. 2004). Canopy light use efficiency (LUE) defines the rate of assimilation of canopy absorbed photosynthetically active radiation (APAR) into vegetation biomass, and provides a basis for estimating GPP using remote sensing (Chapin et al. 2002). The LUE concept, based on the original logic of Monteith (1972), is a commonly used modeling approach for estimating GPP, expressed as the product of APAR and LUE (Running et al. 2004; Potter et al. 1993; Xiao et al. 2004a, b; Yuan et al. 2007). LUE is spatially and temporally dynamic according to various physical and environmental factors, including plant functional type (PFT), terrain, soil and environmental conditions (Madani et al. 2014). LUE is reduced from optimal

or maximum levels for unfavorable environmental conditions, including water supply restrictions, excessive atmospheric moisture deficits, and cold temperatures (Goerner et al. 2011; Ahl et al., 2004).

The LUE modeling approach proposes a direct proportional relationship between GPP and APAR, with biophysical parameters that are readily derived from satellite remote sensing (Running et al. 2004). A variety of LUE models have been developed for monitoring GPP (Hilker et al. 2008). The MOD17 LUE algorithm (Running et al. 2004) is the basis for the NASA EOS MODIS (Moderate Resolution Imaging Spectroradiometer) global operational GPP product, which is derived using satellite based estimates of the canopy absorbed fraction of photosynthetically active radiation (fPAR), and ancillary daily surface meteorology inputs from global reanalysis data, including incoming solar radiation, atmosphere vapor pressure deficit (VPD), and minimum daily air temperature (Ta). The Terrestrial Carbon Flux (TCF) model (Kimball et al. 2009; Yi et al. 2013) uses a similar LUE logic, but includes additional frozen temperature and soil moisture (SM) related environmental constraints on the GPP calculations; the TCF model is the basis of the NASA SMAP (Soil Moisture Active Passive) Mission Level 4 Carbon (L4_C) model being used for global operational estimation of GPP and net ecosystem CO₂ exchange (NEE) using SMAP informed observations as primary environmental inputs (Entekhabi et al. 2014).

Photosynthesis and plant-atmosphere exchange of CO₂ and water vapor are strongly influenced by the supply of water to leaves from the soil via uptake by roots and atmosphere moisture deficit (Xiao et al. 2004a; Leuning et al. 2005). In the MOD17 algorithm, VPD provides the sole moisture control to photosynthesis; while VPD can explain the effects of atmospheric water demand regulating leaf stomatal closure and canopy gas exchange, there is no provision for evaluating impacts from soil water supply variations, which can introduce large model uncertainty (Leuning et al. 2005). The TCF model includes a representation of SM related water supply constraints to LUE and GPP, but a detailed

understanding of regional and seasonal LUE and GPP responses to SM is lacking (Turner et al. 2003; Leuning et al. 2005; Xiao et al. 2004a).

A number of studies have demonstrated the potential of the Photochemical Reflectance Index (PRI) for better understanding LUE and potentially improving GPP estimation. The PRI, calculated as $(R_{531} - R_{ref}) / (R_{531} + R_{ref})$, uses canopy reflectance at 531 nm (R_{531}), which can detect changing pigments in the xanthophyll cycle (Gamon et al. 1992) from a reference reflectance (R_{ref}), giving the PRI the ability to detect changes in photosynthetic activity. Several studies have successfully tested alternative PRI reference wavelengths using both airborne and satellite based remote sensing. A 550nm reference based PRI explained over 90% of diurnal variability in LUE for both nitrogen-stressed and irrigated sunflower crop canopies, but showed less LUE sensitivity under water stressed conditions (Gamon et al. 1992). A 570 nm reference based PRI was significantly correlated with midday photosynthetic rates for a range of vegetation types (Gamon et al. 1997). A 667 nm reference based PRI explained more than 75% of variability in tower-based LUE over boreal broadleaf deciduous forest using MODIS top-of-atmosphere reflectances, which produced better PRI performance than atmospherically corrected MODIS data (Drolet et al. 2005).

The PRI has been used to account for leaf to canopy level temporal variations in LUE over a range of different climate and vegetation conditions (Garbulsky et al. 2008, 2011; Gamon et al. 1992; Filella et al. 1996, 2009; Drolet et al. 2005, 2008; Goerner et al. 2011; Peñuelas et al. 2011). Previous studies using PRI as a LUE proxy to estimate productivity have yielded considerably more agreement with tower GPP observations than the MODIS productivity algorithm (MOD17), especially during seasonal dry periods (Goerner et al. 2009; Garbulsky et al. 2008). MODIS-based PRI studies have also shown strong correspondence with tower-based LUE observations under a range of conditions (Drolet et al. 2005; Drolet et al. 2008).

Alternatively, the PRI could be considered as a water stress indicator, distinguishing between well-watered and water stressed plants (Thenot et al. 2002). A weak relationship between the LUE of a water-limited canopy and the PRI was found by Gamon et al. (1992) when using a 550 nm reference reflectance band. Improved PRI relationships have also been found using longer wavelength references (Gamon et al. 1992). The PRI has also demonstrated sensitivity to diurnal changes in physiological indicators of water stress, such as stomatal conductance and stem water potential, though it is also sensitive to canopy structure and soil background variations (Suárez et al. 2008). Suárez et al. (2009) successfully used the remotely sensed PRI as a water stress indicator in annual and perennial irrigated crops. Time-series of airborne PRI observations normalized by incoming photosynthetically active radiation (PAR) also tracked changes in tree water status under different irrigation regimes (Suárez et al. 2010). Goerner et al. (2009) found that the MODIS-based PRI could track ecosystem LUE even during severe summer droughts in a Mediterranean forest, indicating PRI sensitivity to water stress. The PRI was also found to track observed inter-annual LUE variability associated with prolonged water stress in a water-limited Mediterranean pine forest (Moreno et al. 2012).

The PRI is sensitive to other factors in addition to canopy water stress, including species related differences in canopy structure and sensor observation view angles, which may limit PRI utility at regional or global scales (Barton and North. 2001; Hilker et al. 2010; Hernández-Clemente et al. 2011; Garbulsky et al. 2011). Continuous PRI observations from satellite optical and near infrared (NIR) remote sensing are strongly constrained over many areas by low solar illumination, cloud and atmosphere aerosol contamination, and sensor orbital swath gaps (Goerner et al. 2009; Hilker et al. 2009; Drolet et al. 2005, 2008). Fortunately, the PRI derived from MODIS is capable of relatively fine scale (~1-km resolution and daily time step) observations, while similar observations from MODIS sensors on both Terra and Aqua satellites may reduce PRI data gaps. However, there remains much uncertainty regarding relationships between the PRI and underlying environmental control factors at regional to

continental scales. PRI utility as an indicator of spatially and temporally dynamic plant water stress factors affecting GPP is also unclear. The potential of the PRI to improve understanding and model representation of water supply constraints affecting LUE and GPP requires further investigation across a diversity of vegetation and climate conditions.

In this study, we compared several MODIS PRI formulations using different reference bands against tower site based surface soil moisture and GPP observations spanning a continental US (CONUS) domain. The PRI formulation with the best performance was used as a surrogate for soil moisture (SM) related water supply controls on GPP in the TCF LUE model. PRI correlations with surface soil water content and eddy covariance CO₂ flux measurement based LUE observations were also compared for tower sites representing diverse regional vegetation and climate conditions. Informed by MODIS PRI and tower biophysical observations, the TCF model was used to evaluate the relative importance of SM related water stress influencing GPP spatial and seasonal variations. A regional map of estimated mean daily GPP during the study period (2003-2006) was also derived using active SM related water supply controls in the TCF model defined using the best performing MODIS PRI formulation. An alternative model GPP map was generated using no active water supply control, while the difference between the two maps was used for assessing the regional impact of PRI and SM related water supply constraints to vegetation productivity.

2. Materials and Methods

In this study, the potential of the PRI to represent LUE and GPP sensitivity to SM related water stress was investigated. The sensitivity of TCF model derived daily GPP simulations to estimated soil water constraints were evaluated over a large CONUS climate and vegetation gradient, and multi-year (2003-2006) study period. Alternate model simulations were conducted both with and without an active SM control on estimated GPP. Most of the tower study sites included *in situ* daily measurements of

volumetric soil water content (SWC) within the upper soil layer (Table 1), which were used with spatially continuous MODIS PRI data as alternative inputs for defining the TCF model GPP response to SM related water supply constraints; the resulting model simulations were used to estimate the low SM induced reduction in LUE and associated sensitivity of GPP to spatial and temporal SM and PRI variations. The model GPP results were compared with tower eddy covariance CO₂ flux measurement derived daily GPP observations representing major regional PFT classes to evaluate model performance and SM related water supply constraints on GPP. The TCF LUE model SM functional response was calibrated for different PFT classes by adjusting prescribed maximum and minimum SM levels using a Monte Carlo Markov Chain (MCMC) based iterative reduction of root mean squared error (RMSE) differences between daily model simulations and GPP observations at selected tower PFT calibration sites (Table 1). The calibrated model GPP results were then validated against daily GPP observations from a larger number of tower monitoring sites. The correlation coefficient (r) metric was used to characterize the sign and magnitude of correspondence between MODIS PRI and tower-based LUE, and SWC observations. Model performance was evaluated using coefficient of determination (R²), RMSE and mean relative error (MRE=[GPP_{sim}-GPP_{obs}]/GPP_{obs}*100%) differences between TCF model GPP simulations (GPP_{sim}) and co-located tower observations (GPP_{obs}). The calibrated model parameters from PFT representative tower calibration sites (Table 2) were then used with MODIS PRI and land cover classification data, and other ancillary inputs for spatial extrapolation and estimation of GPP over the CONUS domain.

2.1 LUE model description

GPP was derived using the TCF LUE model framework (Kimball et al. 2012; Yi et al. 2013) as:

$$GPP = LUE_{max} * f(Ta) * f(VPD) * f(SM) * f(FT) * fPAR * PAR \quad (1)$$

where LUE_{max} is the maximum or potential light use efficiency of the vegetation canopy prescribed for individual biomes or PFT classes; $f(Ta)$, $f(VPD)$, $f(SM)$ and $f(FT)$ are dimensionless (0-1) response

functions ranging from 0 (fully constrained) to 1 (no constraint) that define LUE reductions for unfavorable environmental conditions, including low T_a , high VPD; low SM and frozen conditions (FT), respectively. The product of the PAR and canopy intercepted fraction of PAR (fPAR) terms represent the daily amount canopy APAR available for photosynthesis. The LUE_{max} term and parameters that define the above functional response characteristics are prescribed for each PFT within a general Biome Properties Look-Up Table (BPLUT, Table 2), based on the assumption that spatial variations in these response coefficients are conservative within individual biomes. The LUE FT reduction factor was set to 1 (no frozen constraint) in this investigation, given the study emphasis on predominantly non-frozen growing season conditions within the CONUS domain. The LUE and GPP functional response to low soil moisture conditions was defined as:

$$f(SM) = \begin{cases} 0 & SM \leq SM_{min} \\ \frac{SM - SM_{min}}{SM_{max} - SM_{min}} & SM_{min} < SM < SM_{max} \\ 1 & SM \geq SM_{max} \end{cases} \quad (2)$$

where SM_{min} and SM_{max} represent the respective minimum and maximum plant-available SM levels within the rooting zone, which vary by PFT classes. The SM data is normalized to a relative range of 0-1 for defining the SM scalar response in Eq. (2). In this study, SM_{min} and SM_{max} were optimized in the TCF LUE model using *in situ* SWC and MODIS sPRI₁₃ observations; the MCMC optimization involved minimizing RMSE differences between modeled GPP and tower observations (Table 2).

2.2 Tower study sites

In this study, daily eddy covariance CO₂ fluxes (Baldocchi et al. 2001) from the FLUXNET La Thuile synthesis dataset (Level 4 gap-filled) and supporting biophysical measurements from 20 CONUS tower sites representing 49 site-years were selected (Figure 1), while additional site information is summarized in Table 1. The data records selected for each tower site extend from 2003 to 2006. The tower sites

selected for this study span a broad regional climatic gradient encompassing arid, subtropical-Mediterranean, and temperate climate zones. The selected tower sites also represent a range of PFT classes, including cropland (CRO), grassland (GRA), shrubland (SHR), evergreen needleleaf forest (ENF) and deciduous broadleaf forest (DBF). The ratio of annual precipitation to potential evapotranspiration (PET) was calculated from *in situ* precipitation measurements and local PET estimates at each tower site, and used as a climate Aridity Index (AI; UNESCO, 1979) to distinguish regional differences in potential water stress impacts to productivity across sites. The AI categories include hyperarid ($AI < 0.03$), arid ($0.03 \leq AI < 0.2$), semi-arid ($0.2 \leq AI < 0.5$), dry sub-humid ($0.5 \leq AI \leq 0.65$), and humid ($AI > 0.65$) climate conditions. Approximately 67% of the tower sites were used for model development and PFT specific calibration (Cal), while all of the study sites were used for model validation (Table 1). Tower-based LUE was calculated as the product of tower GPP observations (GPP_t), MODIS fPAR and tower PAR measurements ($LUE = GPP_t / (fPAR * PAR)$), and used to evaluate tower level LUE and SWC correspondence.

For the TCF simulations, we combined cereal (C_3) and broadleaf (C_4) crop types into a single cropland class (CRO), since some of the tower CRO sites (e.g. US-Bo1, US-Ne2 and US-Ne3) had both C_3 and C_4 crop rotations (e.g. maize and soybean) during the study period that are not effectively represented by the static land cover classification.

2.3 Data used to support PRI development and LUE model simulations

2.3.1 MODIS data processing

We used the daily 1-km resolution Terra and Aqua MODIS Level 1B reflectance product (MOD/MYD021KM) to derive the PRI for each tower site. The daily 1-km MODIS geolocation product (MOD/MYD03) was used to define MOD/MYD021KM location and sensor zenith angle information for each grid cell. The daily 1-km MODIS cloud mask product (MOD/MYD35_L2) was used to identify and remove lower quality reflectance data under cloudy conditions (Drolet et al. 2005, 2008; Goerner et al.

2011). Reflectance data with sensor view zenith angles lower than 40° were selected and averaged within 3x3 km grid cell windows centered over each tower location, as the PRI is sensitive to variations in sun/sensor geometry (Drolet et al. 2005, 2008). If both MOD021KM and MYD021M data were available for a certain day, averaged reflectance values from the two products were used. We applied no atmospheric corrections to the reflectance data based on evidence from previous studies indicating higher PRI and LUE correlations using top-of-atmosphere reflectance data instead of estimated surface reflectance (Drolet et al. 2005; Goerner et al. 2009, 2011; Moreno et al. 2012). We also found that PRI data derived using non-atmosphere corrected MODIS reflectance data were largely consistent with alternative PRI calculations derived using a Multi-Angle Implementation of the Atmosphere Correction MODIS reflectance record (MAIAC, Lyapustin et al. 2012), justifying the use of the more abundant top-of-atmosphere reflectance data (*see supplementary materials*). The PRI was therefore derived from MODIS top-of-atmosphere reflectance data for band 11 (526-536 nm) and five alternative reference bands, including band 1 (620-670 nm), 4 (545-565 nm), 10 (483-493 nm), 12 (546-556 nm) and 13 (662-672 nm) from the daily 1-km MOD/MYD021KM record. Here the PRI is defined as:

$$PRI = \frac{R_{11} - R_{ref}}{R_{11} + R_{ref}} \quad (3)$$

where R_{11} is the MODIS band 11 reflectance and R_{ref} is the corresponding reference reflectance obtained from MODIS bands 1, 4, 10, 12 or 13, respectively. The PRI is then scaled (sPRI) to obtain only positive values (Rahman et al. 2004; Drolet et al. 2005):

$$sPRI = (PRI + 1)/2 \quad (4)$$

The daily fPAR record from the 1-km MODIS MOD15A2 product was also extracted and averaged within 3x3 km grid cell windows centered over each tower site, similar to the PRI processing, and used as

dynamic inputs for the TCF model based GPP calculations. Temporal Linear interpolation was used to derive daily fPAR values from good quality (QC) 8-day MODIS fPAR records at each tower site.

2.3.2 Regional analysis data

Regional mean daily GPP was estimated over the CONUS domain through regional application of the TCF LUE model using gridded daily surface meteorological data from the global Modern-Era Retrospective analysis for Research and Application (MERRA) reanalysis (Reichle et al. 2011). Daily meteorological inputs were obtained for the study period (2003-2006), including VPD, Ta, and incoming shortwave radiation (SWrad). The MERRA meteorological data were spatially interpolated from their native (0.5° by 0.67°) spatial grid to a finer 0.01° by 0.01° resolution using nearest-neighbor resampling. Other geospatial data used to support the model analysis included MODIS daily reflectance (MOD/MYD021KM) data used to construct the PRI, and MODIS fPAR (MOD15A2) and land cover (MCD12Q1 type 5) data used as model inputs. For this study, all MODIS products and model input data were resampled to a consistent 0.01° by 0.01° (~1 km by 1 km) CONUS spatial grid and geographic projection.

Evergreen broadleaf forest (EBF) represents approximately 1.1% of the CONUS domain, but there were insufficient tower observations for this PFT class within the domain for effective TCF model calibration; we therefore used other EBF tower sites from the global FLUXNET archive located within the same latitude range as the CONUS domain for model SM calibration (results not shown). Less than 0.01% of the CONUS domain is represented by deciduous needleleaf forest (DNF), which was also not represented by the regional tower observations; DNF areas were therefore screened from the model simulations.

3 Results

3.1 PRI sensitivity to tower-based LUE, GPP and soil moisture

Several sPRI versions were derived from Eq. (3) using different MODIS reference wavelengths, including band 1 (sPRI₁), 4 (sPRI₄), 10 (sPRI₁₀), 12 (sPRI₁₂), and 13 (sPRI₁₃). The sPRI₁₃ results explain a greater proportion of daily GPP_f variability for most tower sites (Table 3). However, GPP_f shows higher correspondence with sPRI₁₀ at the ENF sites, with generally secondary sPRI₁₃ performance at these sites. The tower GPP_f observations also show generally stronger correspondence with sPRI₁₃ ($0.004 \leq R^2 \leq 0.692$) than SWC ($0.001 \leq R^2 \leq 0.491$) at most sites, except for US-Ne3 (CRO), US-Blo (ENF) and US-NR1 (ENF) (Table 3). Overall, the sPRI₁₃ results indicate the highest potential to track GPP_f seasonality over the broadest range of PFT classes and environmental conditions. Therefore, the sPRI₁₃ results were selected for further analyses.

Seasonal variations in MODIS sPRI₁₃ and tower GPP_f, and SWC observations are presented in Figure 2 for selected tower sites representing major CONUS PFT classes and climate (AI) regimes. The sPRI₁₃ is generally directly proportional to GPP_f, while both parameters show a similar seasonal progression despite the variable PFT and climate conditions represented. However, the apparent GPP_f and sPRI₁₃ responses to SWC variability are relatively complex and follow general climate moisture gradients. Both vegetation metrics (GPP_f and sPRI₁₃) show a general inverse relationship with SWC during the growing season at the CRO, DBF and ENF sites consistent with soil moisture drawdown by actively growing vegetation. However, SWC variability is more directly proportional to the vegetation metrics at the arid SHR and GRA sites, consistent with larger characteristic soil moisture related constraints to vegetation growth at these drier climate sites. The vegetation metrics at the semi-arid ENF site also show evidence of transient shifts to a direct response to SWC variability following the peak summer growth period; these results are consistent with an increase in soil moisture constraints to productivity during mid-summer and early fall periods when SWC levels are at seasonal lows.

The distribution of tower site correlations between MODIS sPRI₁₃ and tower-based LUE, and SWC observations in relation to characteristic woody and non-woody tower PFT classes, and climate aridity (AI) conditions is shown in Figure 3. The correlations are derived from mean monthly composites of the daily observations to reduce impacts from higher temporal frequency variations on the seasonal relationships. The sign and magnitude of the sPRI₁₃ and SWC correlation varies with AI, and is similar to the correlation pattern observed between the tower LUE and SWC observations. Positive correlations between sPRI₁₃ and SWC are generally found at arid sites (AI<0.2), while negative correlations predominantly occur at wetter sites (AI>0.5), similar to the tower LUE and SWC correlation pattern, and consistent with the SWC and productivity relationships indicated in Figure 2. The sPRI₁₃ is favorably correlated with SWC at most sites, with the highest correspondence at the arid US-Ton site ($r=0.763$). However, lower sPRI₁₃ and SWC correspondence was found for some sites, including US-Arm (irrigated CRO), US-Bo1 (humid CRO) and US-FR2 (SHR).

3.2 Impact of soil moisture related controls on GPP for different PFT classes

Three sets of TCF LUE model simulations were conducted at each of the tower study sites. The tower SWC measurements and MODIS sPRI₁₃ observations were used as alternative inputs to define SM related water supply controls in the calibrated LUE model for estimating daily productivity at each site (GPP_{swc} and GPP_{PRI} , respectively). GPP was also estimated from the LUE model without using an active SM constraint (GPP_{nsm}). The resulting GPP_{PRI} calculations show generally stronger correspondence with the tower GPP observations (GPP_f) than GPP_{nsm} or GPP_{swc} for all CRO, SHR, and DBF sites (Table 4); these sites are generally located in arid and semi-arid areas (AI<0.50, Table 1) where low SM levels are expected to be a stronger limitation on photosynthesis. The GPP_{PRI} results for these sites show 5.3 to 14.6 percent greater R^2 correspondence, and 4 to 11 percent lower RMSE differences (-0.063 to -0.497 g C m⁻² d⁻¹) with GPP_f relative to the GPP_{swc} results (Table 4). For the GRA sites, GPP_{PRI} shows slightly lower

performance against the tower observations than GPP_{swc} , indicated by 4.1% lower R^2 correspondence, 9% larger RMSE ($+0.221 \text{ g C m}^{-2} \text{ d}^{-1}$) and 3.8% higher MRE; however, the GPP_{pri} results show 15.9% better R^2 performance than GPP_{nsm} at these sites, since SM is still expected to be a major limiting factor for these drier ($0.32 \leq AI \leq 0.66$) climate sites. However, the GPP_{pri} results show degraded performance relative to GPP_{swc} for the ENF sites, indicated by lower R^2 correspondence and higher RMSE differences.

The GPP_{pri} and GPP_f correspondence is generally better when just the tower calibration sites are considered ($0.547 \leq R^2 \leq 0.826$) relative to all tower sites ($0.457 \leq R^2 \leq 0.818$), except for ENF. For example, GPP_{pri} shows 9.1% improved R^2 correspondence and 4.7% lower RMSE ($-0.123 \text{ g C m}^{-2} \text{ d}^{-1}$) with GPP_f for the GRA calibration sites, relative to the results from all GRA tower sites. For the CRO calibration sites, GPP_{pri} shows 5.9% greater R^2 correspondence, 12.2% lower RMSE ($-0.494 \text{ g C m}^{-2} \text{ d}^{-1}$) and 1.5% lower MRE differences with GPP_f relative to all CRO tower sites examined. Overall, the use of MODIS $sPRI_{13}$ as a water supply constraint factor in the TCF LUE model produces generally consistent or improved model performance over alternative estimates derived using SM inputs from *in situ* tower site measurements (GPP_{swc}) or no active water supply constraint (GPP_{nsm}) for most PFT classes examined except ENF.

3.3 Regional GPP extrapolations using MODIS PRI inputs

The spatial pattern of estimated mean daily (2003-2006) GPP_{pri} over the CONUS domain is presented in Figure 4a. The model results show relatively higher productivity in CRO and DBF areas in the northeast, upper mid-west and central areas of the domain, consistent with characteristically higher LUE and productivity levels for these PFT classes (Madani et al. 2014; Guanter et al. 2014). Lower productivity areas include semiarid GRA and SHR areas of the southwest and western USA (Figure 4a). The resulting GPP_{pri} pattern is also similar to satellite based GPP observations derived from the GOME-2 Solar-Induced canopy Fluorescence (SIF) record (Guanter et al. 2014). These results indicate that GPP_{pri} provides an effective delineation of productivity patterns and temporal dynamics, consistent with both

regional tower observations and characteristic productivity patterns spanning a large regional climate and vegetation gradient. However, GPP_{PRI} was unresolved for approximately 2.0% of the domain due to extensive spatial and temporal gaps in the MODIS (Terra and Aqua) band 13 reflectance data used to define PRI reference conditions, particularly for sparsely vegetated drier climate areas in the western and southwest portions of the domain.

The spatial pattern of differences between GPP_{PRI} and GPP_{nsm} as a percentage of GPP_{nsm} ($\Delta GPP = (GPP_{PRI} - GPP_{nsm})/GPP_{nsm} * 100$) indicate the regional impacts of SM related water supply constraints to productivity (Figure 4b). Large SM constraints (ΔGPP up to -60%) occur in the interior GRA dominated northwest; the regional climate in these areas is mostly arid and semi-arid, where SM is the primary factor limiting plant photosynthesis (Kurc and Small, 2007). Productivity is also strongly limited by SM in southwest CONUS areas (indicated by large ΔGPP), where vegetation is predominantly SHR with semi-arid, arid or subtropical-Mediterranean climate (Figure 4b). However, SM is less of a limiting factor to productivity (indicated by smaller ΔGPP differences) in eastern areas of the domain dominated by CRO and DBF vegetation, and a temperate-continental climate (Figure 4b). Overall, these results indicate that vegetation productivity is strongly limited by SM related water supply constraints (ΔGPP exceeding -25%) over approximately 21% of the CONUS domain (Figure 4b).

4 Discussion

This study investigated the potential of the MODIS-based PRI to track soil moisture related water supply constraints on vegetation productivity for a diverse set of regional climate and vegetation conditions within the CONUS domain. Model productivity calculations derived using the MODIS-based $sPRI_{13}$ as a surrogate for SM related water supply constraints (GPP_{PRI}) showed significantly improved performance over GPP_{nsm} at the CRO, SHR, DBF and GRA tower sites (Table 4). The GPP_{PRI} also outperformed GPP_{swc} at the CRO, SHR, and DBF sites (Table 4). These results indicate that the MODIS $sPRI_{13}$ metric is an effective

surrogate for SM related plant water supply constraints to model simulated GPP relative to tower GPP_f observations encompassing diverse CONUS climate and vegetation conditions. The correlation pattern between tower-based LUE and *in situ* SWC measurements across a regional tower site climate moisture gradient shows generally positive correlations at drier sites ($AI < 0.2$) and negative correlations at wetter sites ($AI > 0.5$), consistent with greater soil moisture restrictions to vegetation photosynthesis in drier climate areas and minimal SWC restrictions in wetter climate zones (Figure 3); the correlations between $sPRI_{13}$ and SWC observations show a similar regional pattern, confirming $sPRI_{13}$ sensitivity to soil moisture variability and associated controls on photosynthesis.

The *in situ* SWC measurements used in this study to estimate productivity (GPP_{swc}) and evaluate tower site vegetation growth represent upper layer soil moisture conditions that may not be an effective indicator of SM related water supply controls on vegetation activity, since the SWC measurements from a single point may not adequately represent heterogeneous SM conditions within the tower footprint ($\sim 1 \text{ km}^2$). The upper layer SWC measurements may also not adequately represent deeper root zone soil moisture conditions affecting photosynthesis (Neal, 2012; Kurc and Small, 2007; Reichstein et al. 2002), which may explain the generally low SWC correlations and low GPP_{swc} performance in relation to MODIS PRI and the tower-based LUE and GPP_f observations. The internal water storage capacity of woody plant tissues may also offset soil moisture demand (Borgogno et al. 2010; Reichstein et al. 2002), which may contribute to relatively lower daily SWC correspondence with PRI and vegetation productivity in forest and SHR areas (e.g. Table 4).

In situ soil moisture records from regional station networks are inconsistent and sparse, while spatial extrapolations of these data may not resolve large characteristic SM spatial heterogeneity (Wanders et al. 2012; Western et al. 2002). Alternatively, spatially contiguous soil moisture records are available from satellite observations or global model data reanalysis (Reichle et al. 2004; Albergel et al. 2012),

387 though currently available data records may be too coarse to resolve SM heterogeneity and associated
388 ecological constraints to photosynthesis approaching finer ($\sim 1 \text{ km}^2$) scale tower observations. The
389 MODIS sPRI₁₃ used in this study appears to provide an effective means for representing soil moisture
390 related plant water supply controls in the LUE model GPP_{PRI} simulations, and at relatively finer (1-km
391 resolution) spatial scales consistent with local tower measurement based GPP observations. The
392 regional model sensitivity analysis from this study indicates that SM related water stress impacts on
393 productivity are generally larger in semi-arid to arid climate zones within interior western, central and
394 southwest GRA and SHR areas of the domain (Figure 4b). The actual extent and severity of water
395 constrained areas is likely larger than indicated (Figure 4b) due to intensive land management and
396 irrigation of croplands, which may offset SM related water supply deficits influencing MODIS sPRI₁₃
397 sensitivity and associated GPP_{PRI} reductions. However, the MODIS sPRI₁₃ data shows substantial gaps
398 and information loss over high reflectance areas, including deserts and other sparse vegetation areas of
399 the southwest CONUS domain where soil moisture constraints on productivity are severe; MODIS band
400 13 has a relatively low reflectance threshold designed for ocean signal detection (Hu et al. 2011), which
401 results in signal saturation and sPRI₁₃ information loss over these higher reflectance land areas.
402 Alternative MODIS bands 1, 4, 10 and 12 have relatively higher reflectance thresholds, which may
403 provide alternative reference bands and sPRI formulations with better spatial and temporal coverage;
404 however, the alternative sPRI formulations evaluated in this study showed less sensitivity to GPP
405 seasonal dynamics than the sPRI₁₃ over most sites (Table 3), though other reference bands may provide
406 better sPRI sensitivity for some areas and PFT classes (e.g. ENF).

407 The MODIS-based sPRI₁₃ is sensitive to other factors influencing vegetation canopy reflectance and
408 environmental stress levels, including temperature extremes, atmosphere moisture deficits (VPD) and
409 canopy structure (e.g. fPAR). In this study, the sPRI₁₃ was only significantly correlated with VPD for the
410 DBF sites ($R^2=0.26$), while no significant sPRI₁₃ and VPD correlations were found for other PFT sites.

411 These results indicate that the PRI is uniquely sensitive to soil moisture related impacts on canopy
412 reflectance apart from atmosphere VPD effects. The $sPRI_{13}$ was found to be sensitive to vegetation
413 canopy structural changes indicated by favorable fPAR correspondence at most PFT sites, including CRO
414 ($R^2=0.460$), SHR ($R^2=0.371$), DBF ($R^2=0.618$) and GRA ($R^2=0.409$). The $sPRI_{13}$ was correlated with T_a at the
415 CRO, DBF and GRA tower sites, indicating that variations in daily T_a are a contributing factor affecting
416 $sPRI_{13}$ variability and associated cold temperature induced changes in GPP for these land cover types.
417 However, the $sPRI_{13}$ was not significantly correlated with T_a for the SHR and ENF sites. The SHR sites are
418 mainly distributed in the southwest portion of the CONUS domain, where cold temperatures may be
419 less of a constraint to productivity than low soil moisture levels. Low correspondence between $sPRI_{13}$
420 and fPAR, and T_a , and the poor performance of GPP_{PRI} for the ENF sites may reflect one or more factors,
421 including low characteristic seasonality in canopy fPAR for evergreen vegetation. Relatively cold-adapted
422 and highly clumped ENF canopies show generally higher reflectance across most spectral wavelengths
423 (Wong et al. 2015), which may result in low PRI sensitivity to photosynthetic changes. The PRI
424 seasonality is also dominated by both xanthophyll cycle activity and changes in leaf pigment pools
425 (relative to chlorophyll). The xanthophyll cycle is more active during warmer seasons, and mostly
426 inactive in the winter; thus, changes in leaf pigment pools rather than direct xanthophyll activity may
427 cause PRI changes during the spring transition period in ENF ecosystems that may vary from GPP
428 seasonal changes (Wong et al. 2015). Nevertheless, in this study, PRI calculated using MODIS reference
429 band 10 ($sPRI_{10}$) showed the best correspondence with tower GPP_f observations for the ENF sites (Table
430 3). Alternative TCF model GPP calculations derived using $sPRI_{10}$ as a SM surrogate produced better
431 correspondence with tower GPP_f observations for all ENF sites ($R^2 = 0.433$), than the $sPRI_{13}$ based GPP_{PRI}
432 results ($R^2=0.299$). Other studies also indicate potential utility for alternative PRI formulations as water
433 stress indicators for ENF (Hernández-Clemente et al. 2011). Thus a more flexible use of alternative

reference bands for different PFT classes may enhance PRI capabilities for regional water stress monitoring.

The results of this investigation may be influenced by one or more factors affecting PRI data quality and sensitivity, empirical relationships and model assumptions. In this study we used top-of-atmosphere MODIS reflectance data screened for view zenith angles lower than 40° (Drolet et al. 2005, 2008) to reduce potential PRI sensitivity to sun and view angle effects, though this selection may be insufficient to fully account for sun/sensor geometry effects, introducing PRI uncertainties. However, a recent study indicated that MODIS PRI was not significantly affected by solar view angle and azimuth effects during the growing season at three forest sites in the eastern US (Sims et al. 2011). Though previous studies (Drolet et al. 2005; Goerner et al. 2009, 2011; Moreno et al. 2012) have demonstrated higher correlations between PRI and GPP/LUE using reflectance data without atmospheric corrections, the use of top-of-atmosphere reflectance may contribute additional uncertainty in our analysis since the atmosphere may influence each spectral band differently. The PRI and LUE may also be sensitive to other factors not directly represented in the TCF model, including effects of nutrient availability, land management, stand age and vegetation disturbance (e.g. Perez-Priego et al. 2015); these factors may introduce bias into the resulting model GPP calculations.

The tower GPP observations are based on model partitioning of eddy covariance measurements of net ecosystem CO₂ exchange (NEE). The method of model partitioning and gap-filling can introduce substantial bias in the tower derived GPP observations (Reichstein et al. 2005), which can affect model calibration and performance. Typical flux tower footprints have longitudinal length scales of 100-2000m, and changes in wind direction and speed can cause variations in the flux footprint (Schmid 1994; Baldocchi et al. 2001) and spatial mismatches between tower and satellite observations. Spatially averaged MODIS reflectance values from 3X3 grid cell windows over each tower location were used to

reduce these effects, but may also introduce additional uncertainties through regional smoothing of MODIS retrievals and model simulations relative to local tower observations, especially over spatially complex vegetation and terrain.

Further studies are needed over a global range of climate and vegetation conditions to clarify the range of effective PRI sensitivity, and SM related impacts on productivity. Other satellite observations may provide additional constraints for distinguishing water supply control factors influencing regional productivity, including solar-induced canopy fluorescence (Guanter et al. 2014; Guan et al. 2015), terrestrial water storage changes from satellite gravimetric measurements (Rodell and Famiglietti 2002), and soil moisture dynamics derived from lower frequency satellite microwave sensors (Entekhabi et al. 2010). The MODIS PRI appears to provide an effective tool for quantifying soil moisture related water supply impacts to GPP that are closer to the scale of local tower observations and land management activities, allowing potentially improved spatial delineation of heterogeneous vegetation water stress characteristics and seasonal climate impacts.

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716 List of Figure Captions

717 Figure 1. The spatial distribution of tower eddy covariance measurement sites used in the study;
718 background image shows the MODIS (MCD12Q1 type 5) land cover product, representing evergreen
719 needleleaf forest (ENF), evergreen broadleaf forest (EBF), deciduous needleleaf forest (DNF), deciduous
720 broadleaf forest (DBF), shrubland (SHR), grassland (GRA), cropland (CRO) including cereal and broadleaf
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724 arid shrubland (US-Ton) and grassland (US-Var); semi-arid cropland (US-IB1), deciduous broadleaf forest
725 (US-Dk2) and evergreen needleleaf forest (US-Dk3); arid shrubland (US-FR2) and grassland (US-Var) sites.
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730 tower site correlations are distributed along a regional moisture gradient indicated by the climate aridity
731 index (AI, X-axis), and denoted by the dominant PFT woody and non-woody growth form at each site.
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735 similar LUE and $sPRI_{13}$ correspondence with SWC (The dash line is 1:1 line).

736 Figure 4. Spatial pattern of (a) estimated average daily GPP (2003-2006) using $sPRI_{13}$ as a surrogate for
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738 difference between GPP_{PRI} and GPP_{nsm} expressed as a percentage of GPP_{nsm} ($\Delta GPP = (GPP_{PRI} - GPP_{nsm}) /$
739 $GPP_{nsm} * 100\%$), where GPP_{nsm} is calculated without an active SM constraint in the TCF model. State
740 boundaries are denoted by grey lines, while white areas denote barren or sparsely vegetated areas,
741 water bodies and other areas screened from the analysis.

742 Table 1. Summary of the 20 Ameriflux tower sites used in this study, including latitude, longitude, study
743 period, plant functional type (PFT), climate type, depth of *in situ* measured soil water content (SWC),
744 aridity index (AI), and whether the site is used for model calibration (Cal); key references are also
745 provided that give more detailed information for each site .

Site Name	Latitude	Longitude	Study period	PFT	Climate	Depth of SWC	* AI	Cal	Reference
**US-Arm	36.61	-97.49	2003-2005	CRO	SubTropical-Mediterranean	5 cm	0.42	Cal	Billesbach et al. (2004)
US-Bo1	40.01	-88.29	2003-2006	CRO	Temperate-Continental	5 cm	0.64	Cal	Meyers and Hollinger (2004)
US-IB1	41.86	-88.22	2006	CRO	Temperate-Continental	2.5 cm	0.44	Cal	Matamala et al (2008)
**US-Ne1	41.17	-96.48	2003-2004	CRO	Temperate-Continental	10 cm	0.44	Cal	Suyker et al. (2005)
**US-Ne2	41.16	-96.47	2003-2004	CRO	Temperate-Continental	10 cm	0.48		Suyker et al. (2004)
US-Ne3	41.18	-96.44	2003-2004	CRO	Temperate-Continental	10 cm	0.36		Suyker et al. (2004)
US-Dk2	35.97	-79.10	2003-2005	DBF	SubTropical-Mediterranean	10 cm	0.30	Cal	Oren et al. (2006)
US-MMS	39.32	-86.41	2003	DBF	SubTropical-Mediterranean	surface	0.31		Sims et al. (2005)
US-Blo	38.90	-120.63	2003-2006	ENF	SubTropical-Mediterranean	10 cm	0.37	Cal	Goldstein et al. (2000)
US-Dk3	35.98	-79.09	2003-2005	ENF	SubTropical-Mediterranean	30 cm	0.31	Cal	Katul et al. (2001)
US-Me2	44.45	-121.56	2004-2005	ENF	SubTropical-Mediterranean	30 cm	0.12	Cal	Law et al. (2004)
US-NR1	40.03	-105.55	2003	ENF	Boreal	5cm	0.13		Monson et al. (2005)
US-Goo	34.25	-89.87	2003-2006	GRA	SubTropical-Mediterranean	10 cm	0.66	Cal	Wilson and Meyers (2007)
US-IB2	41.84	-88.24	2006	GRA	Temperate-Continental	2.5 cm	0.55	Cal	Matamala et al (2008)
US-Var	38.41	-120.95	2003-2006	GRA	SubTropical-Mediterranean	surface	0.32	Cal	Baldocchi et al. (2004)
US-Bkg	44.35	-96.84	2005-2006	GRA	Temperate-Continental	10 cm	0.42		Xiao et al. (2010)
US-Dk1	35.97	-79.09	2003-2005	GRA	SubTropical-Mediterranean	10 cm	0.66		Oren et al. (2006)
US-Ton	38.43	-120.97	2003-2006	SHR	Dry (arid and semi arid)	surface	0.18	Cal	Baldocchi et al. (2004)
US-FR2	29.95	-98.00	2005	SHR	SubTropical-Mediterranean	5 cm	0.15	Cal	Xiao et al. (2010)
US-NC1	35.81	-76.71	2005-2006	SHR	SubTropical-Mediterranean	30 cm	0.52		Noormets et al. (2010)

746 *AI climate aridity: hyperarid ($AI < 0.03$), arid ($0.03 \leq AI < 0.20$), semi-arid ($0.20 \leq AI < 0.5$), dry sub-humid ($0.50 \leq AI \leq 0.65$), and
747 humid ($AI > 0.65$)

748 **Irrigated cropland site

749 Table 2 Biome properties look-up table used in this study to define different PFT environmental
750 response characteristics for the TCF LUE model GPP calculations; parameters include maximum LUE
751 (LUE_{max}), and maximum and minimum thresholds for air temperature (Ta_{max} , Ta_{min}), vapor pressure
752 deficit (VPD_{max} , VPD_{min}), *in situ* upper layer soil water content (SWC_{max} , SWC_{min}) and scaled PRI ($sPRI_{max}$,
753 $sPRI_{min}$).

	Ta_{max} (°C)	Ta_{min} (°C)	VPD_{max} (Pa)	VPD_{min} (Pa)	SWC_{max}	SWC_{min}	$sPRI_{max}$	$sPRI_{min}$	LUE_{max} (g C/MJ)
CRO	12.02	-8.00	5071	500	0.27	0.19	0.51	0.10	2.13
DBF	9.94	-6.00	4160	500	0.16	0.10	0.43	0.00	1.56
ENF	8.31	-8.00	4000	500	0.14	0.00	0.12	0.01	1.05
GRA	12.02	-8.00	5500	752	0.17	0.07	0.48	0.18	1.10
SHR	10.00	-8.00	4800	434	0.10	0.00	0.25	0.01	1.20

754

755 Table 3. Coefficients of determination (R^2) between different scaled PRI metrics calculated using
756 respective MODIS reference bands 1, 4, 10, 12 and 13 ($sPRI_1$, $sPRI_4$, $sPRI_{10}$, $sPRI_{12}$ and $sPRI_{13}$) and tower
757 observed GPP (GPP_f) across all tower study sites; R^2 correspondence between local tower daily SWC
758 measurements and GPP_f is also shown along with the dominant PFT class for each site. The maximum
759 scaled PRI correspondence for each tower site is shown in bold.

Site Name	PFT	$sPRI_1$	$sPRI_4$	$sPRI_{10}$	$sPRI_{12}$	$sPRI_{13}$	SWC
US-Arm	CRO	0.314	0.008	0.368	0.175	0.376	0.001
US-Bo1	CRO	0.231	0.006	0.173	0.008	0.524	0.005
US-IB1	CRO	0.343	0.029	0.272	0.006	0.497	0.450
US-Ne1	CRO	0.784	0.101	0.275	0.003	0.692	0.080
US-Ne2	CRO	0.445	0.104	0.203	0.049	0.491	0.004
US-Ne3	CRO	0.347	0.001	0.172	0.032	0.227	0.491
US-NC1	SHR	0.013	0.065	0.313	0.026	0.477	0.185
US-Dk2	DBF	0.038	0.087	0.202	0.003	0.579	0.225
US-MMS	DBF	0.058	0.063	0.159	0.006	0.585	0.252
US-Blo	ENF	0.008	0.002	0.208	0.034	0.100	0.112
US-Dk3	ENF	0.035	0.033	0.294	0.006	0.200	0.056
US-Me2	ENF	0.003	0.013	0.292	0.115	0.145	0.060
US-NR1	ENF	0.034	0.004	0.194	0.035	0.007	0.387
US-FR2	SHR	0.013	0.001	0.173	0.004	0.082	0.079
US-Ton	SHR	0.101	0.006	0.167	0.056	0.221	0.074
US-Bkg	GRA	0.059	0.015	0.089	0.030	0.287	0.217
US-Dk1	GRA	0.041	0.065	0.220	0.005	0.286	0.055
US-Goo	GRA	0.055	0.069	0.175	0.000	0.438	0.064
US-IB2	GRA	0.243	0.048	0.454	0.028	0.323	0.200
US-Var	GRA	0.393	0.011	0.127	0.031	0.415	0.187

761 Table 4. Comparisons of TCF modeled GPP using an active SM constraint driven by either *in situ* upper
762 layer soil water content (GPP_{swc}) or MODIS sPRI₁₃ (GPP_{pri}) inputs, and model simulated GPP without an
763 active SM constraint (GPP_{nsm}); model results are shown relative to corresponding tower observations
764 (GPP_f) for all study sites representing the major CONUS PFT classes.

PFT	GPP _{nsm}			GPP _{swc}			GPP _{pri}		
	R ²	RMSE	MRE	R ²	RMSE	MRE	R ²	RMSE	MRE
CRO	0.568	4.203	9.1%	0.518	4.546	-1.8%	0.664	4.049	-5.5%
SHR	0.629	1.482	0.3%	0.632	1.503	-1.1%	0.685	1.440	-3.4%
DBF	0.728	2.302	5.0%	0.717	2.356	0.6%	0.818	2.090	-4.2%
ENF	0.302	2.203	-3.1%	0.393	2.148	-9.7%	0.299	2.186	-9.7%
GRA	0.298	2.681	10.3%	0.498	2.367	-2.7%	0.457	2.588	-6.5%

765

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