Upscaling key ecosystem functions across the conterminous United States by a water-centric ecosystem model

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[1] We developed a water-centric monthly scale simulation model (WaSSI-C) by integrating empirical water and carbon flux measurements from the FLUXNET network and an existing water supply and demand accounting model (WaSSI). The WaSSI-C model was evaluated with basin-scale evapotranspiration (ET), gross ecosystem productivity (GEP), and net ecosystem exchange (NEE) estimates by multiple independent methods across 2103 eight-digit Hydrologic Unit Code watersheds in the conterminous United States from 2001 to 2006. Our results indicate that WaSSI-C captured the spatial and temporal variability and the effects of large droughts on key ecosystem fluxes. Our modeled mean (±standard deviation in space) ET (556 ± 228 mm yr^{-1}) compared well to Moderate Resolution Imaging Spectroradiometer (MODIS) based (527 ± 251 mm yr^{-1}) and watershed water balance based ET (571 ± 242 mm yr^{-1}). Our mean annual GEP estimates (1362 ± 688 g C m^{-2} yr^{-1}) compared well (R^2 = 0.83) to estimates (1194 ± 649 g C m^{-2} yr^{-1}) by eddy flux-based EC-MOD model, but both methods led significantly higher (25–30%) values than the standard MODIS product (904 ± 467 g C m^{-2} yr^{-1}). Among the 18 water resource regions, the southeast ranked the highest in terms of its water yield and carbon sequestration capacity. When all ecosystems were considered, the mean NEE (−353 ± 298 g C m^{-2} yr^{-1}) predicted by this study was 60% higher than EC-MOD's estimate (−220 ± 225 g C m^{-2} yr^{-1}) in absolute magnitude, suggesting overall high uncertainty in quantifying NEE at a large scale. Our water-centric model offers a new tool for examining the trade-offs between regional water and carbon resources under a changing environment.

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1. Introduction

[2] Evapotranspiration (ET), water yield, gross ecosystem productivity (GEP), net primary productivity (NPP), ecosystem respiration (Re), and net ecosystem exchange (NEE) (i.e., NEE = -NEP, where NEP is net ecosystem productivity) are the key ecosystem functions [*Xiao et al.*, 2008, 2010; *Beer et al.*, 2010; *Jung et al.*, 2010; *Tian et al.*, 2010; *Xiao et al.*, 2010] that directly affect many ecosystem services, including providing stable and high quality water, moderating climate, sequestering atmospheric carbon dioxide, and protecting biodiversity. Understanding the tightly coupled water and carbon cycles is critical to evaluating regional and global biogeochemical cycles under a changing climate [*Law et al.*, 2002; *Nemani et al.*, 2003; *Beer et al.*, 2007, 2010]. Quantifying water and carbon balances at regional and continental scales is essential for land managers and policy makers to develop sound mitigation and adaptation strategies in response to global change.

[3] Although it is well known in ecology that water is a major control to plant growth and productivity [*Chapin et al.*, 2004; *Noormets et al.*, 2008; *Domec et al.*, 2009], water and carbon have long been treated as two separated entities. Many existing ecosystem models have some forms of coupling between carbon and water, mostly related to the effects of soil moisture on photosynthesis process. However, these models have rarely been validated with both carbon and water flux measurements [*Hanson et al.*, 2004; *Noormets et al.*, 2006; *Domec et al.*, 2010; *Tian et al.*, 2010]. Similarly, the hydrologic community has long ignored the feedbacks

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between plants and the water cycles, and hydrological modeling results are often assessed only with streamflow measurements at the watershed outlets, rarely with direct ET or soil moisture measurements [*Vörösmarty et al.*, 1998; *Hay and McCabe*, 2002]. Part of the reasons is that ET remains the least quantifiable water balance components at all scales [*Zhang et al.*, 2001; *Mu et al.*, 2007; *Allen*, 2008; *Zhou et al.*, 2008; *Sun et al.*, 2010]. The science of ecohydrology, that specifically addresses the interactions of hydrologic (i.e., ET) and ecological processes, is rapidly developing to offer the basis to address trade-offs between carbon sequestration and water use [*Jackson et al.*, 2005, 2009; *Vose et al.*, 2011] and between crop production and water resources [*Liu et al.*, 2009].

[4] Carbon and water exchange are inherently coupled by several mechanisms. The photosynthesis processes are mainly controlled by radiation and soil water availability, stomatal conductance, and leaf biomass and chemistry [*Chapin et al.*, 2004], all of them being the key factors regulating ecosystem ET [*Sun et al.*, 2010]. Seasonal patterns of ET rates together with precipitation regulate soil moisture storage, a key factor that determines ecosystem productivity [*Noormets et al.*, 2008, 2010]. This connection between ET and GEP has been used in continental and global GEP modeling [*Beer et al.*, 2007, 2010]. Similarly, Re is constrained by soil temperature and moisture [*Wen et al.*, 2006] as well as the quality and quantity of the carbohydrate substrates, which in turn depend on GEP [*Davidson et al.*, 2006]. Understanding the coupling of carbon, water and other biogeochemical elements across ecosystems at a large scale is critical to address modern environmental problems [*Finzi et al.*, 2011].

[5] Several methods have been proposed in recent years to quantify water and carbon fluxes and their interactions at a large scale. These include (1) empirical machine-learning techniques [*Xiao et al.*, 2008, 2010, 2011; *Jung et al.*, 2009; *Zhang et al.*, 2011] that involve developing regression models using large amounts of empirical measurements from the eddy flux networks and satellite remote sensing data; (2) process-based models driven by remote sensing data of landcover and biophysical parameters. Models such as CASA, PnET, Biome-BGC, TEM, DELM, simulate partial or the full biogeochemical cycles of carbon, water, and nutrients [*Field et al.*, 1995; *Aber et al.*, 1996; *Running et al.*, 2004; *Zhao et al.*, 2005, 2006; *Mu et al.*, 2007; *Xiao et al.*, 2009; *Tian et al.*, 2010]. *Schwalm et al.* [2010] conducted a comprehensive evaluation of the performance of 22 popular carbon cycle models using 220 site-years of CO_2 flux data; (3) atmospheric inverse modeling [*Deng et al.*, 2007] method that infers NEE from a network of CO_2 concentration measurements; and (4) inventory methods that estimate ecosystem productivity (i.e., NPP) from long-term forest inventory data [*Pacala et al.*, 2001] and do not account for annual climatic variability and are not designed to examine interactions between carbon and water.

[6] The objectives of this study included (1) developing and validating a new integrated model (WaSSI-C), to account for large-scale monthly water and carbon balances using limited input parameters and variables; and (2) applying the model to 2,103 large basins in the conterminous United States to examine spatial and temporal patterns of water and carbon exchange. We adopted an approach characteristic of data-model fusion methods with a focus on the interactions of water and carbon cycles at the monthly scale.

[7] We hypothesized that if ecosystem water and carbon fluxes are strongly coupled at the monthly scale [*Law et al.*, 2002; *Beer et al.*, 2007], a water-centric approach can be used to quantify carbon fluxes with a reasonable accuracy. The WaSSI-C model presented in this study is composed of an existing water balance model (WaSSI) and a set of biome-specific apparent water use efficiency relationships as estimated from 968 site-years of eddy covariance data. The ET, GEP, Re, and NEE prediction models were first developed using site level data of the eddy flux network and other hydrological experimental stations. Next, these algorithms were incorporated into the existing WaSSI model and applied to the conterminous United States for the period of 2001–2006 corresponding to the time period when Moderate Resolution Imaging Spectroradiometer (MODIS) products of ET, GPP, and NEE are available. The simulated spatial and temporal distributions of continental ET, GEP, and NEE were compared to estimates by several independent sources including national historical watershed runoff databases, improved MODIS-based ET and GPP products, and gridded GPP and NEE databases developed by integrating eddy flux measurements and remote sensing data.

2. Model Development, Validation, and Databases

[8] We explicitly examined spatial and temporal patterns of water and carbon interactions at the monthly and annual scales for 2001–2006, a period over which remote sensing data are available for model validation. Ecosystem ET is modeled as a function of with a monthly hydrologic model Water Supply Stress Index Model (WaSSI) [*Sun et al.*, 2008], and the carbon fluxes are estimated from the derived ET using eddy covariance-based biome mean water use efficiency (WUE = GEP/ET). The latter represents an update to the models reported by *Law et al.* [2002].

[9] The new WaSSI-C model operates at a monthly temporal scale and a variable spatial scale depending on the area of each land cover within a watershed. The model simulates the full monthly water and carbon balances, including ET, soil moisture content, water yield, GEP, Re, and NEE for each of the eight land cover categories within a watershed, and then aggregates the fluxes to the entire basin using a area-weighted average approach (Figure 1). The basins are the eight-digit Hydrologic Unit Code (HUC) watersheds designated by the Watershed Boundary Dataset [*Natural Resources Conservation Service*, 2009]. Hydrologic units are a widely used geographic framework for the conterminous United States in water resource management and natural resource conservation. Each unit defines a geographic area representing part or all of a surface drainage basin or a combination of drainage basins. We used a total of 2,103 basins across the conterminous United States with a size ranging from 11 to 22,965 km^2 with a median value of 3,207 km^2.

2.1. Water Supply Stress Index Model

[10] The original WaSSI model was developed to examine impacts of multiple stresses, including climate change, land cover/land use change and water demand, on watershed hydrology and water stresses [*Sun et al.*, 2008]. The model simulates the full monthly water fluxes for each of the eight land cover categories within a watershed, and then aggregates each fluxes to the entire basin using area-weighted

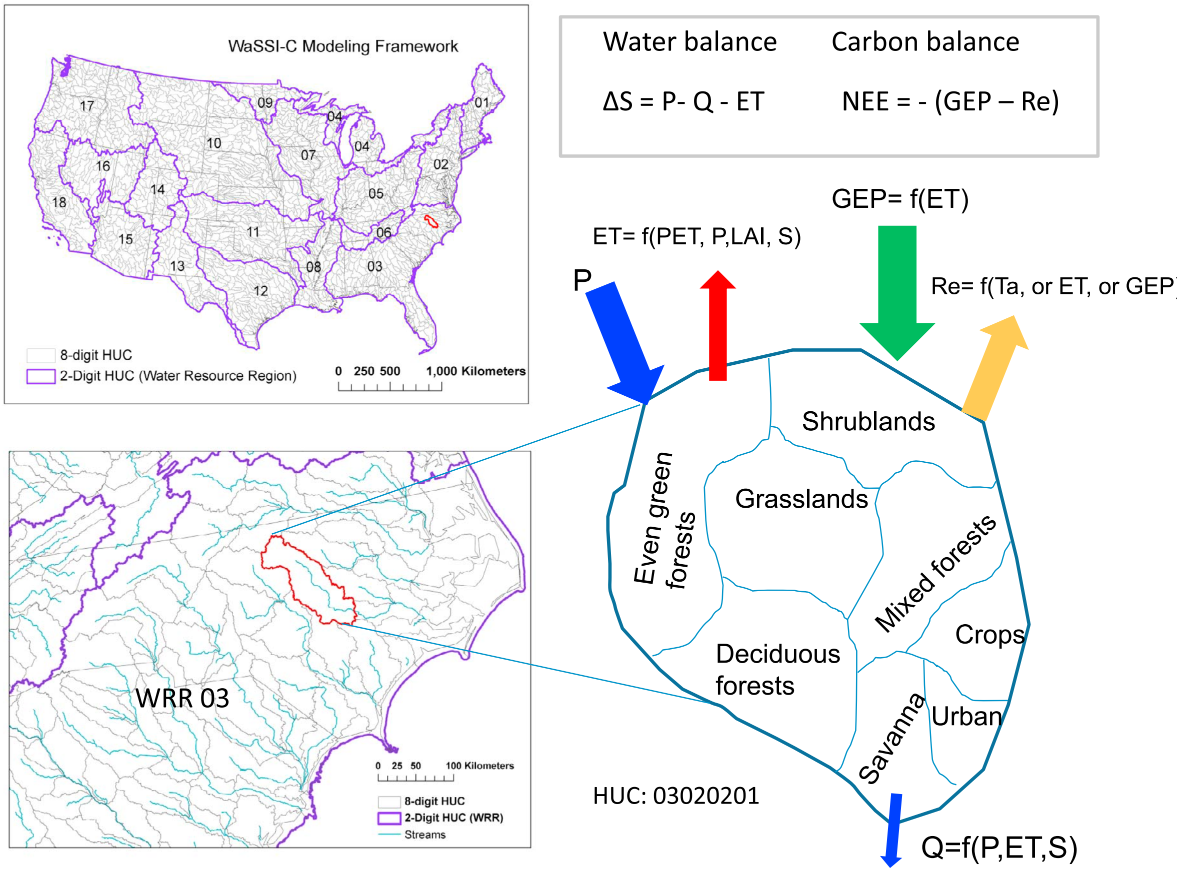

Figure 1. Sketch of conceptual framework of WaSSI-C model for an eight-digit Hydrologic Unit Code watershed with mixed land covers.

averaging (Figure 1). The hydrologic fluxes include ET, infiltration, soil storage, snow accumulation and melt, surface runoff, and base flow, and discharge was routed through the stream network from upstream to downstream watersheds (Figure 1). Estimation of infiltration, soil storage, and runoff processes was accomplished through the integration of algorithms from the Sacramento Soil Moisture Accounting Model and STATSGO-based soil parameters. The model was driven by watershed-averaged monthly precipitation and mean air temperature that were scaled from gridded historical PRISM climate data (Table 1).

[11] The core of the WaSSI model is an empirical ET model derived from a data set of ecosystem-level ET measurements based on eddy covariance or sapflow techniques at thirteen sites [*Sun et al.*, 2011]. These sites represented a range of biomes that span a large climatic gradient, ranging from subtropical rain forests in the humid Appalachians in the southeastern United States to the hot dry woodlands in eastern Australia, and from forested wetlands on the Atlantic coastal plain in the southeastern United States to the grasslands and shrub lands and cultivated croplands in the semiarid Inner Mongolian region of northern China. Management practices also varied widely across sites. The geographic range of the sites varied in latitude from 43.5°N to 33.7°S and in longitude from 83.8°W to 150.8°E. The annual mean air temperature ranged from 0.6 to 17.6°C and mean annual precipitation from 300 to > 1800 mm yr^{-1}. Monthly total ET rates from each site were scaled from half-hour measurements using either the standard eddy covariance methods or sapflow + canopy interception methods. Ancillary data, such as monthly averaged leave area index (LAI), *P*, and climatic variables were assembled from field measurements to develop a regression model for predicting ET. In developing and applying the ET regression model across the United States, it became clear that a single equation could not capture the spatial variability in ET as predicted by MODIS estimates and water balance approaches. In particular, we observed that ET in forested regions (i.e., forest cover percentage >20%) in northern latitudes (e.g., >40°N) required a unique form of the ET regression model to accurately replicate measured data. For forested regions at high latitudes (>40°N) dominated by winter precipitation in the northeastern United States, the following ET equation was applied:

$$\mathrm{ET} = 0.4^*\mathrm{PET} + 7.87^*\mathrm{LAI} + 0.00169^*\mathrm{PET}^*\mathrm{P}$$

$$R^2 = 0.85\ \mathrm{RMSE} = 14.5\left(\mathrm{mm\ month}^{-1}\right), n = 147, \mathrm{p} < 0.0001$$

For other regions,

$$\mathrm{ET} = 0.174^*\mathrm{P} + 0.502^*\mathrm{PET} + 5.31^*\mathrm{LAI} + 0.0222^*\mathrm{PET}^*\mathrm{LAI}$$

$$R^2 = 0.86\ \mathrm{RMSE} = 14.0\left(\mathrm{mm\,month}^{-1}\right), n = 147, p < 0.0001$$

where LAI was monthly averaged leaf area index measured on site or derived from continental MODIS products [*Myneni*

Table 1. Databases for WaSSI-C Model Development, Parameterization, and Validation

Data Set	References Source	Usage	Original Resolution	Time Period
Eddy flux data	FLUXNET (http://www.fluxnet.ornl.gov/)	model development	>240 sites	Vary
Climate (monthly P and air T)	PRISM Climate Group (http://prism.oregonstate.edu/)	parameterization	4*4 km^2	1960–2007
Streamflow	U.S. Geological Survey (USGS) (http://waterwatch.usgs.gov/index.php/?m = romap3&w = download)	for regional ET validation	eight-digit HUC	1901–2006
Land cover	Moderate Resolution Imaging Spectroradiometer (MODIS) (http://modis.gsfc.nasa.gov/)	parameterization	1*1 km^2	2001
Leaf area index	Moderate Resolution Imaging Spectroradiometer (MODIS) http://modis.gsfc.nasa.gov/	parameterization	1*1 km^2	2001–2006
Soil properties	STATSGO-based Sacramento Soil Moisture Accounting Model Soil Parameters and NOAA-NWS Hydrology Laboratory, Office of Hydrologic Development	parameterization	1*1 km^2	N/A
GEP	wall-to-wall maps published by *Xiao et al.* [2010]	validation	1*1 km^2	2000–2006
NEE	wall-to-wall maps published by *Xiao et al.* [2008]	validation	1*1 km^2	2000–2006

et al., 2002]. Potential ET (PET) was calculated with Hamon's method that used air temperature and potential daytime length and was widely used due to its simplicity and reliability comparing to more complex methods [*Vörösmarty et al.*, 1998; *Lu et al.*, 2005].

[12] The above two equations do not account for soil water availability's effect on ET and thus may cause overestimation errors under extreme dry conditions. To correctly close the water balance, the ET predicted by the regression models was further constrained. Using the two-soil-layer SAC-SMA model algorithm, the WaSSI model compares ET demand to soil water storage, and limits ET if soil water is insufficient to meet the demand. Soil moisture for ET is withdrawn sequentially from the upper soil layer tension water storage (i.e., soil water tension between field capacity and the wilting point), upper layer free water storage (i.e., soil water tension between saturation and field capacity), and from the lower layer tension water storage until the demand is met or until available soil water has been depleted.

2.2. The Carbon Models

[13] It has been shown that ecosystem ET and GEP are closely coupled at a monthly scale [*Law et al.*, 2002]. The original relationships for forest ecosystems have been successfully used in a number of modeling studies, but the availability of data has increased by orders of magnitude, and we reevaluated these relationships, as well as developed them for nonforest ecosystems that were not covered by *Law et al.* [2002]. The relationships between GEP and ET were evaluated using level 4 data of FLUXNET LaThuile data set (http://www.fluxdata.org) which were integrated to a daily scale. These values were further integrated to a monthly scale for the analyses presented here. Of the 968 site-years of data 935 and 905 site-years were available for analyzing GEP-ET and Re-Ta relationships, respectively. The data covered 244 and 233 separate sites, respectively and spanned 11 IGBP land cover classes. The relationships of monthly GEP with ET, and Re versus GEP were estimated using linear regression procedures (SAS v9.1.3, Cary, NC). For GEP-ET relationship, the intercept was forced through the origin (Table 2), and the coefficients of determination increased over those with nonzero intercept. Thus, the slope of GEP-ET regression model represented an integrated GEP-based water use efficiency.

[14] Ideally, ecosystem carbon fluxes should be independently derived from one another. However, scaling Re solely from temperature (Ta) led to very high estimates over hot and dry desert ecosystems that are grouped together with shrub lands in the IGBP classification scheme. To obtain more realistic estimates at the continental scale, Re must be constrained by moisture availability and vegetation activity that are both controlling factors of Re [*Davidson et al.*, 2006]. GEP provided such an integrative constraint, and while future development calls for independent Re estimates, current data availability limits global application of unbounded Re-Ta relationships. While the correlation between Re and GEP was strong in the current data set (Table 3), recent analyses suggest it may have been exaggerated by the assumptions implicit in the gap-filling protocols [*Vickers et al.*, 2009, 2010; *Lasslop et al.*, 2010]. Although there are strong reasons for the correlation to exist between productivity and respiration [*Lasslop et al.*, 2010], the strength of the relationship in monthly data is strongest in comparison to the strength in shorter and longer time domains, and unrelated to the possible artificial correlations introduced in the gap-filling process. Finally, monthly NEE was modeled as the difference between GEP and Re (NEE = Re − GEP). A model comparison study by *Schwalm et al.* [2010] suggests models that estimate NEE as the difference between GEP and Re perform better than others. Nevertheless, future

Table 2. Regression Model Parameters for Estimating Monthly GEP as a Function of ET, GEP = a*ET

Land Cover	Number of Flux Tower Sites	a ± SD	R^2
Croplands	29	3.13 ± 1.69	0.78
Closed Shrublands	6	1.37 ± 0.62	0.77
Deciduous Broadleaf Forest	32	3.20 ± 1.26	0.93
Evergreen Broadleaf	16	2.59 ± 0.54	0.92
Evergreen Needleleaf	69	2.46 ± 0.96	0.89
Grasslands	44	2.12 ± 1.66	0.84
Mixed Forests	12	2.74 ± 1.05	0.89
Open Shrublands	11	1.33 ± 0.47	0.85
Savannas	4	1.26 ± 0.77	0.80
Wetlands	15	1.66 ± 1.33	0.78
Wet Savannas	6	1.49 ± 0.36	0.90

Table 3. Regression Model Parameters for Estimating Monthly Ecosystem Respiration as a Function of GEP, Re = m + n GEP

Ecosystems	Number of Eddy Flux Sites	m ± SD	n ± SD	R^2
Cropland (CRO)	29	40.6 ± 3.84	0.43 ± 0.02	0.77
Closed Shrublands	3	11.4 ± 15.62	0.69 ± 0.15	0.74
Deciduous Broadleaf Forest (DBF)	32	30.8 ± 2.93	0.45 ± 0.03	0.83
Evergreen Broadleaf Forest (EBF)	11	19.6 ± 8.74	0.61 ± 0.06	0.63
Evergreen Needleleaf Forest (ENF)	70	9.9 ± 2.24	0.68 ± 0.03	0.8
Grasslands (GRA)	44	18.9 ± 2.31	0.64 ± 0.02	0.82
Mixed Forests (MF)	12	24.4 ± 4.24	0.62 ± 0.05	0.88
Open Shrublands (OS)	8	9.7 ± 3.03	0.56 ± 0.08	0.81
Savannas (SAV)	3	25.2 ± 3.23	0.53 ± 0.07	0.65
Wetlands (WET)	15	7.8 ± 3.04	0.56 ± 0.03	0.8
Wet Savanna (WSA)	6	14.7 ± 2.75	0.63 ± 0.04	0.74

efforts in WaSSI-C development will focus on independent estimation of GEP and Re as outlined above.

2.3. WaSSI-C Model Validation

2.3.1. Model Validation Methods

[15] The WaSSI-C model was developed from site-level data and applied to eight-digit HCU watersheds. We validated the model against remote-sensing based GEP and NEE estimates with a spatial resolution of the watershed. For ET validation, two data sets were used: (1) derived from the watershed water balance method published by the U.S. Geological Survey (USGS), and (2) acquired from the MODIS ET products [*Mu et al.*, 2010]. For carbon flux, modeled GEP and NEE fluxes were compared to the standard MODIS-GPP product [*Zhao et al.*, 2005] and gridded GPP and NEE data derived from eddy covariance (EC) and MODIS data (EC-MOD) [*Xiao et al.*, 2008, 2010, 2011]. To be consistent with terminology, we referred to the GPP data sets of both sources as GEP hereafter in this paper. The performance of the model in predicting ET, GEP, and NEE was evaluated qualitatively using scatterplots and difference maps, quantitatively using Root Mean Square Error (RMSE) and Coefficients of Determination (R^2) and the slopes of the linear regression models. We validated the model against various reference products of annual ET, GEP, NEE, and monthly ET.

2.3.2. Databases for Model Validation

2.3.2.1. MODIS-ET

[16] Remote sensing–based ET models have been developed in recent years to estimate regional-scale ET and water balances [*Cleugh et al.*, 2007; *Mu et al.*, 2007; *Fisher et al.*, 2008; *Zhang et al.*, 2010]. *Mu et al.* [2010] further improved the MODIS ET algorithms by (1) simplifying the calculation of vegetation cover fraction; (2) calculating ET as the sum of daytime and nighttime components; (3) adding soil heat flux calculation; (4) improving estimates of stomatal conductance, aerodynamic resistance and boundary layer resistance; (5) separating dry canopy surface from the wet; and (6) dividing ground moisture conditions into saturated and moist surfaces. The MODIS ET algorithm employs reanalysis surface meteorological data (0.05° resolution) from NASA's *Global Modeling and Assimilation Office* [2004] with MODIS land cover, albedo, LAI and the Fraction of Absorbed Photosynthetically Active Radiation (FPAR) inputs for regional and global ET mapping and monitoring. The global ET product has been evaluated using AmeriFlux flux data sets with variable success [*Mu et al.*, 2007]. We aggregated the new 1 km^2 ET data set [*Mu et al.*, 2010] to the eight-digit HUC level by averaging monthly ET (sum of 8 day values) of all cells for each watershed.

2.3.2.2. ET Data Derived From Waters Balance of Gauged Watersheds

[17] In addition to the MODIS-ET for WaSSI-C model validation, we also acquired historic runoff (Q) data (Table 1) from the U.S. Geological Survey (USGS) to estimate annual ET as the difference between precipitation (P), runoff, and change in surface and groundwater storage, ET = P − Q ± ΔS. This method (hereafter USGS-ET) represented an independent approach for estimating regional ET flux at an annual scale. The change in water storage is negligible for a normal year or over a long-term period, and the water balanced equation can be simplified as ET = P − Q. However, ET may be greatly overestimated or underestimated at the annual scale during extreme wet or dry years due to a positive or negative change in soil water storage, respectively [*Donohue et al.*, 2007]. In addition, natural streamflow characteristics of many watersheds have been altered by water management practices such as interbasin transfer, groundwater pumping, and large-scale irrigation, resulting in measurement errors in Q, and thus estimated ET. These potential sources of error were not accounted for in the current version of WaSSI-C.

[18] Not all the watersheds within the large basins modeled in this study were gauged for streamflow measurements. Continental-scale eight-digit HUC watershed-level runoff databases were consequently estimated by combining historical daily flow data collected at approximately 6000 USGS stream gauges. The drainage basin areas of these gauged streams ranged from 10 to 180,000 km^2. We identified 2103 valid eight-digit HUC watersheds for this study to use.

2.3.2.3. MODIS-GEP (MOD17A3)

[19] We scaled the 8 day, 1 km^2 resolution MODIS GEP (MOD17A3) data (Table 1) to the eight-digit HUC watershed level to compare to our model results. The original GEP data were developed using Monteith's logic that calculated GEP as a function of light use efficiency (ε), minimum air temperature, vapor pressure deficit, absorbed photosynthetically active radiation (APAR), and shortwave radiation [*Running et al.*, 2004]. MODIS GEP has been used in many applications including the evaluation of water stress by integrating with the BIOME-BGC model [*Mu et al.*, 2007] and long-term ecosystem productivity trend analysis at the global scale [*Nemani et al.*, 2003]. MODIS GPP products have been evaluated by eddy flux measurements across many biomes [*Turner et al.*, 2006; *Zhang et al.*, 2008] and used to predict plant diversity in semiarid Inner Mongolia [*John et al.*, 2008], estimate wheat yield, and scale up site level GEP into estuarine wetlands of the Yangtze delta [*Yan et al.*, 2008].

2.3.2.4. Gridded GPP and NEE Data Sets

[20] To provide an independent estimate of carbon flux, we also acquired continental 1 km^2 GEP and NEE data developed by *Xiao et al.* [2008, 2010, 2011]. The data sets were constructed by a data-driven approach that combined

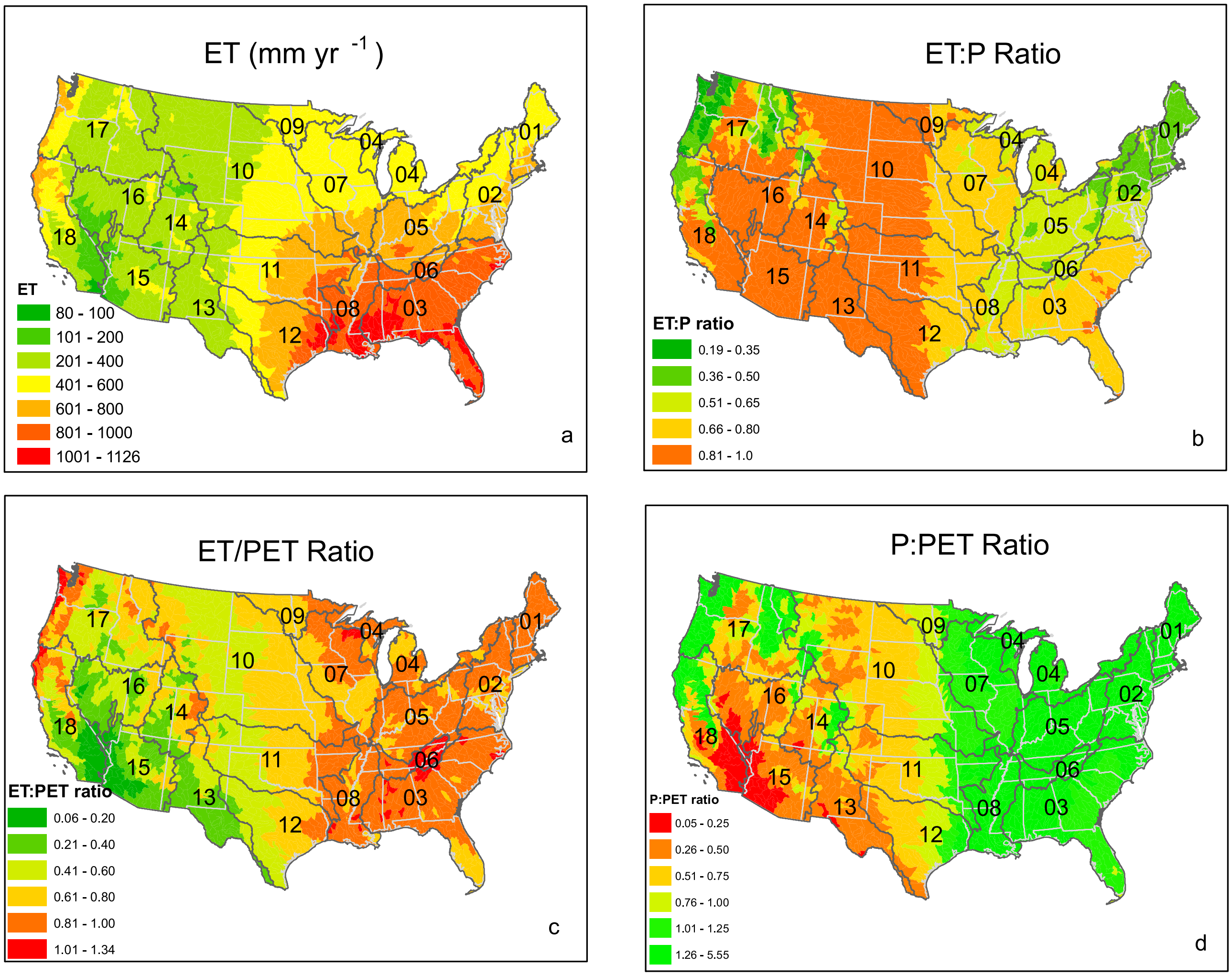

Figure 2. Spatial distributions of (a) mean annual evapotranspiration (ET) (mm yr^{-1}), (b) ET:P ratios, (c) ET:PET ratios, and (d) P/PET ratios across the conterminous United States over the period of 2001–2006 as simulated by the WaSSI-C model.

eddy covariance data and MODIS data to develop predictive GEP and NEE models. The explanatory variables in the models included vegetation type, surface reflectance, daytime and nighttime land surface temperature, enhanced vegetation index, and normalized difference water index. These variables could partly account for a variety of physical, physiological, atmospheric, hydrologic, and edaphic variables that affect ecosystem carbon exchange. The models, referred to as EC-MOD, were used to create gridded flux fields for temperate North America over the period of 2001–2006 [*Xiao et al.*, 2011]. We scaled the data set to the watershed scale for comparison purposes.

3. Results and Discussion

3.1. Spatial and Temporal Dynamics of ET

[21] Spatially, WaSSI-C predicted ET ranged from approximately 200 to 1200 mm yr^{-1}, and closely followed precipitation and temperature distribution patterns across the United States (Figure 2a). The 6 year spatial average (±spatial SD) was 556 ± 228 mm yr^{-1}. Due to both a warm (i.e., high PET) and wet climate (i.e., high precipitation), the water resource regions in the southeastern Untied States (e.g., WRR 03) had high annual ET, ET:PET and P:PET ratios, and a moderate ET:P ratios overall (Figure 2). WRR 01, 02, 5, and western parts of WRR 17 and 18 had the lowest ET:P ratios (<0.6), while the highest ET:P ratios (>0.8) were found in the arid western WRR (14, 15, 16) where ET was low (Figure 2b). Additionally, a few watersheds on the lower coastal plain in the southeastern United States also had high ET:P ratios. These watersheds were dominated by forests that consumed more water than other ecosystems [*Sun et al.*, 2010]. For the northeastern and the Pacific Northwest regions, ET was limited by energy in the winter months when precipitation (i.e., snow and rainfall) exceeded atmospheric demand. In contrast, in the arid western United States, precipitation generally limited ET in most of the seasons, thus ET was similar to P, and rarely equaled PET (Figure 2d).

[22] We compared modeled annual and monthly mean ET for 2001–2006 with MODIS-ET across the 2103 watersheds. We eliminated outliers in the MODIS-ET and the USGS-ET databases if the annual ET values were found to be unrealistically higher than precipitation, or if ET values substantially exceeded calculated PET. The data for those

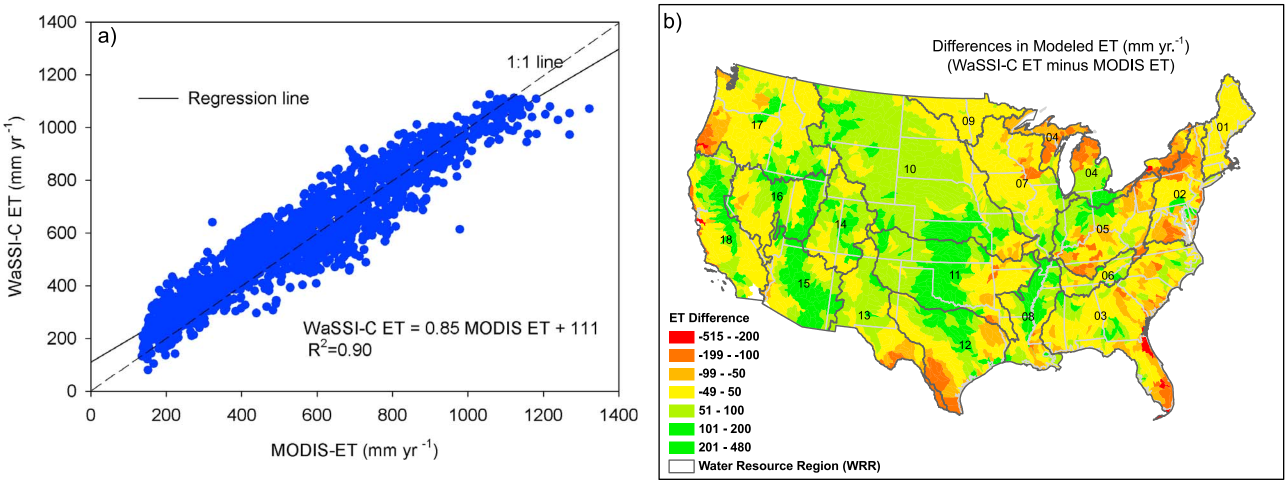

Figure 3. A comparison between mean (2001–2006) annual ET (mm yr^{-1}) by WaSSI-C and MODIS for (a) scatterplot and (b) spatial display of differences, across 2103 HUCs for the period of 2001–2006.

watersheds were not appropriate for model validation purposes and were considered to contain errors in the data. The USGS-ET water balance method only provided annual ET estimates. However, these annual estimates were still affected by annual changes in soil water storage, so we only evaluated model performance against average annual ET. As mentioned earlier, water resources management activities such as inter basin transfer and groundwater over withdrawal likely impacted the accuracy of ET estimates based on the water balance equation. The errors were more pronounced in the western United States where groundwater had been widely used for irrigation of agricultural crops.

[23] The comparison of our modeled annual ET against MODIS-ET and USGS-ET showed that the WaSSI-C model performed reasonably well (Figures 3 and 4). Modeled ET was highly correlated with MODIS-ET (R^2 = 0.90, RMSE = 70 mm yr^{-1}, $p < 0.001$) and USGS-ET (R^2 = 0.85, RMSE = 78 mm yr^{-1}, $p < 0.001$) methods. The scatterplots of modeled ET by WaSSI-C versus USGS-ET (Figure 3a) and MODIS-ET versus USGS-ET (not shown) indicated higher variability of P-Q values than WaSSI-C versus MODIS-ET for a few watersheds. The errors were likely related to watershed hydrologic alteration by human activities such as interbasin water transfers, groundwater recharge (e.g., missing surface water at gauging stations, and groundwater withdrawals added to surface water) that all affected the accuracy of ET estimates by the USGS-ET method. In spite of the discrepancies at individual watersheds, the cross-model validation suggested that both WaSSI-C and MODIS-ET models captured ET variability over space and time.

[24] As expected, the highest monthly ET occurred in July (85 ± 32 mm $month^{-1}$), and lowest ET in January (20 ± 13 mm $month^{-1}$). The seasonal patterns of mean monthly ET predicted by WaSSI-C matched very well with those of MODIS-ET (Figure 5). The two sets of ET predictions were significantly correlated to each other (R^2 = 0.80, RMSE = 14.3 mm $month^{-1}$, $p < 0.0001$, WaSSI-C ET = 142 + 0.73*MODIS-ET). MODIS-ET had a much higher

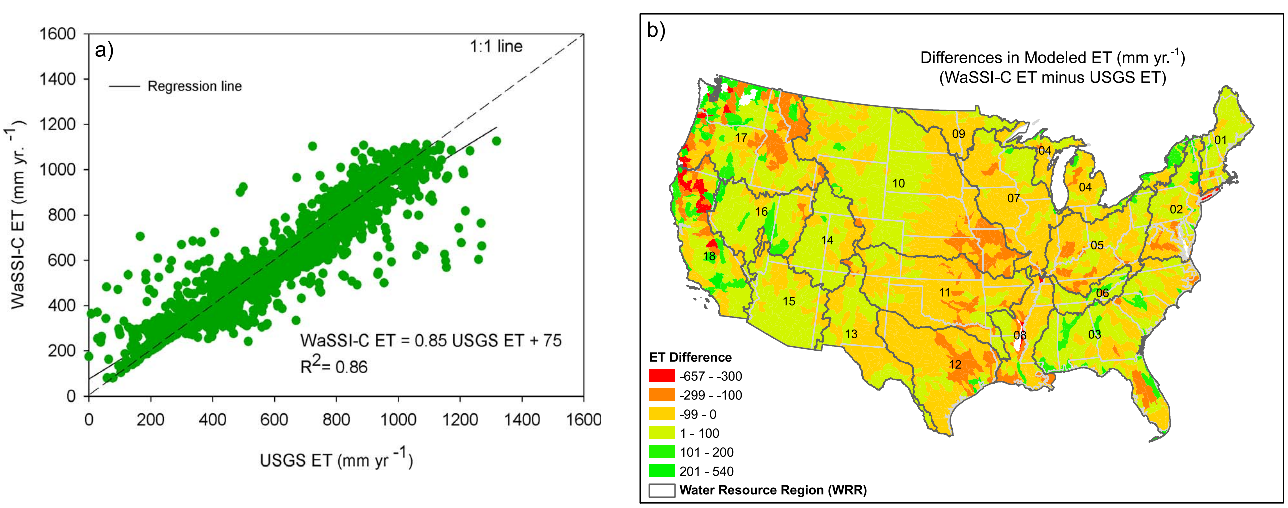

Figure 4. A comparison between mean annual ET (mm yr^{-1}) by WaSSI-C and the USGS-ET. (a) Scatterplot and (b) spatial display of differences, across 2103 HUCs for the period of 2001–2006.

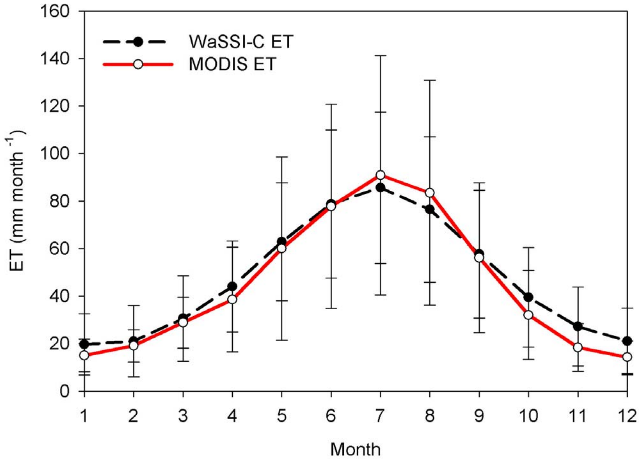

Figure 5. A comparison of mean monthly modeled ET by WaSSI-C versus MODIS estimates across 2103 HUCs for the period of 2001–2006.

spatial variability (SD = 30–50 mm month^{-1}) than did WaSSI-C modeled ET (SD = 25–30 mm month^{-1}) in the growing season.

3.2. Spatial and Temporal Distributions of GEP and NEE

3.2.1. Modeled GEP Comparisons

[25] We applied the uncalibrated WaSSI-C model to the continental United States and calculated GEP for each watershed and each month over the period of 2001–2006. Mean annual GEP (Figure 6) modeled by this study were compared to two other GPP products (Figures 7 and 8). Across the 2103 watersheds, mean modeled annual GEP was 1360 g C m^{-2} yr^{-1} and ranged from 200 to 3000 g C m^{-2} yr^{-1} (Figure 6). The total conterminous United States carbon uptake was 10.11 Pg C yr^{-1} during 2001–2006, which was higher than the mean GEP (7.06 Pg C yr^{-1}) estimated by *Xiao et al.* [2010] (Table 4). Since modeled GEP is directly proportional to ET in this study (Table 2), spatial patterns of GEP closely followed the ET distribution (Figure 2). The top three WRRs with high spatial mean annual GEP values were WRR08 and WRR06 (mean = 2400 g C m^{-2}yr^{-1}), and WRR03 (mean = 2336 g C m^{-2} yr^{-1}) located in the southern United States. WRR03 received the highest precipitation under a warm climate (i.e., high PET). In terms of total amount of ecosystem carbon uptake, the top three regions were WRR03 (1.7 Pg C yr^{-1} or 2337 g C m^{-2} yr^{-1}), WRR10 (1.37 Pg C yr^{-1} or 1057 g C m^{-2} yr^{-1}), and WRR11 (0.89 Pg C yr^{-1} or 1431 g C m^{-2} yr^{-1}).

[26] Our mean annual GEP correlated well with estimated EC-MOD GEP [*Xiao et al.*, 2010] (R^2 = 0.83, RMSE = 279 g C m^{-2} yr^{-1}, $p < 0.001$, GEP = 208 + 0.97 EC-MOD GEP) (Figure 7). Compared to EC-MOD, WaSSI-C estimates were 208 g C m^{-2} yr^{-1}, or about 10% greater on average (Figure 7a). The spatial distribution of difference was complex. WaSSI-C predicted higher GEP that EC-MOD in regions with high GEP values, such as the southern United States, but lower in the cool regions with low GEP, like in the northeastern United States and the Pacific Northwest (Figure 7b).

[27] We found a large discrepancy in annual GEP between WaSSI-C model predictions and MODIS-GEP (Figure 8). Our estimates were about 30% higher that estimate by MODIS GEP. This result was consistent with *Xiao et al.*'s [2010] observation that eddy flux-based model predictions are generally higher than MODIS-GEP for highly productive regions. The differences between WaSSI-C and MODIS GEP estimates were greatest at GEP > 1500 g C m^{-2} yr^{-1}. WaSSI-C GEP exhibited a weaker relationship with MODIS GEP (R^2 = 0.72, RMSE = 359 g C m^{-2} yr^{-1}, $p < 0.0001$, GEP = 231 + 1.25 MODIS GEP) than with EC-MOD.

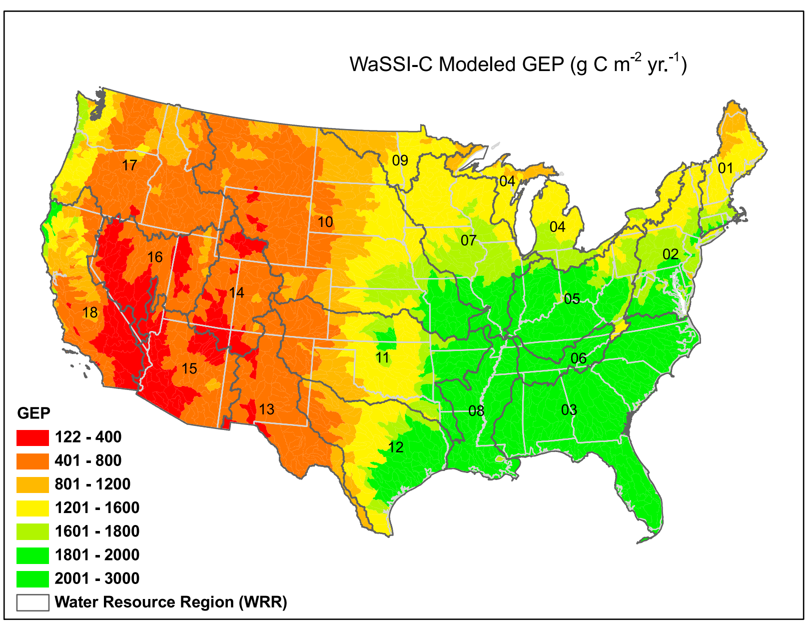

Figure 6. WaSSI-C simulated spatial distribution of mean annual GEP (g C m^{-2} yr^{-1}) for the conterminous United States over the period of 2001–2006.

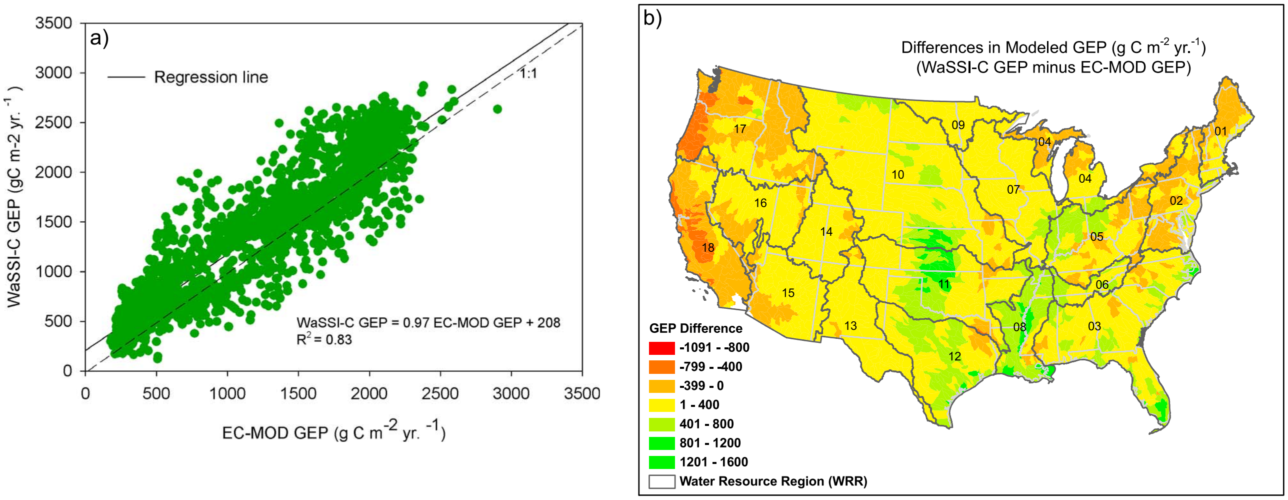

Figure 7. A comparison between mean annual GEP (g C m^{-2} yr^{-1}) estimates by WaSSI-C and EC-MOD. (a) Scatterplot. The dashed line is 1:1 line, and the solid line is regression line. (b) Spatial display of differences, across 2103 HUCs for the period of 2001–2006.

[28] The large differences found from this study could be attributed to several reasons: (1) Deficiency in MODIS-GEP algorithms related to the critical light use efficiency parameter [*Zhang et al.*, 2008] and inherent errors due to limitation of meteorological data. Comparing to tower-based measurements, a 20–30% error was not uncommon in MODIS-GEP [*Heinsch et al.*, 2006]. (2) Uncertainty of input parameters (i.e., LAI derived from MODIS products) and driving variables data (i.e., coarse meteorological data) for continental scale applications [*Zhao et al.*, 2006; *Xiao et al.*, 2010]. All models, including WaSSI-C, involved this type uncertainty. (3) Insufficient representation of some ecosystems within the FLUXNET as well as accurate land cover classification for our study. Past flux measurements are conducted mostly in mature or unmanaged forests, and the contribution of young or managed forests may be underrepresented in the current flux data sets. Additionally, model parameters are lumped to one biome without discrimination to age, ecosystem structures, tree species, or disturbances [*Amiro et al.*, 2010]. For examples, few flux towers exist for wetlands and savannas that represent the two ends of the water regime. A lack of representations of these biomes would result in large errors of GEP estimation. (4) The ET model used in this study does not account for other vegetation characteristics than LAI variability. One solution is to develop specific ET model for each biome when sufficient eddy flux tower data become available. Finally, measurement errors exist in flux data used since eddy covariance towers represent a single point in space that is integrated over the entire stand [*Oren et al.*, 2006].

3.2.2. Modeled NEE

[29] The WaSSI-C modeled spatial patterns of mean (2001–2006) annual NEE (Figure 9) were compared to estimates by EC-MOD (Figure 10). Across the 2103 watersheds, annual WaSSI-C modeled NEE varied from a carbon source of 200 g C m^{-2} yr^{-1} to a strong carbon sink of −1150 g C $m^{-2}yr^{-1}$ (Figure 9). The conterminous U.S. mean NEE was −353 ± 298 g C m^{-2} yr^{-1}, representing a total net

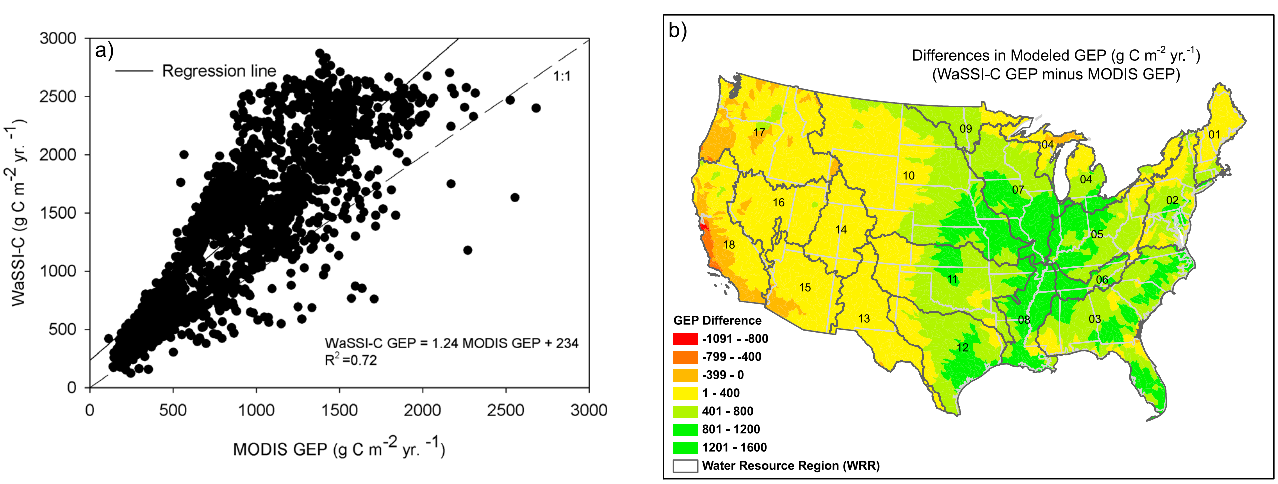

Figure 8. A comparison between mean annual GEP (g C m^{-2} yr^{-1}) estimates by WaSSI-C and MODIS. (a) Scatterplot and (b) spatial display of discrpencies across 2103 HUCs for the period of 2001–2006.

Table 4. Summary of Annual Conterminous United States, Regional, and Global Estimates of Carbon Fluxes

GEP	NEE or Carbon Sequestration (Absolute Values)	Methodology	Comments	Reference
	0.37–0.71 Pg C yr^{-1} (including C exports)	multiple methods	conterminous United States (1980–1989)	*Pacala et al.* [2001]
7.06 Pg yr^{-1}	1.21 Pg C yr^{-1} (all lands) 0.63 Pg C yr^{-1} (excluding croplands)	EC-MOD model; regression tree scaling up eddy flux data in the United States	conterminous United States (2001–2006)	*Xiao et al.* [2010, 2011]
NPP = 0.92–1.45 Pg yr^{-1}	0.54 Pg C yr^{-1} (all lands)	process-based ecosystem model	southern region (13 states)	*Zhang* [2008]
	0.36 Pg C yr^{-1}	coupling eddy flux data and remote sensing	U.S. Great Plains grasslands	*Zhang et al.* [2010]
NPP = 3.4 Pg C yr^{-1}	NEP = −0.12 Pg C yr^{-1} (carbon loss)	NASA-CASA model	continental United States (1982–1997)	*Potter et al.* [2006]
	0.12–0.23 Pg C yr^{-1}	NASA-CASA model	North America (1996–98)	*Potter et al.* [2003]
	0.666 Pg C yr^{-1} (net C absorption)	SOCCR Project; multiple methods and sources	North America	*Pacala et al.* [2007]
10.11 Pg C yr^{-1}	1.24 Pg C yr^{-1} (croplands, C export not included)	ET based, water-centric model parameterized with global eddy flux data	conterminous United States (2001–2006)	this study
	2.6 ± 1.7 Pg C yr^{-1}	model synthesis	global, deforestation excluded	*Denman et al.* [2007]
109.12 Pg C yr^{-1} (NPP = 56.02 Pg C yr^{-1})		MODIS	global	*Zhao et al.* [2005]
121.7 Pg C yr^{-1}		processes-based models	global	*Beer et al.* [2010]

carbon sequestration of 2.54 Pg C yr^{-1} during 2001–2006. When crop lands NEE were excluded from the calculations, the total NEE was reduced to 1.24 Pg C yr^{-1}. Because NEE was modeled linearly from GEP in this study (Tables 2 and 3), spatial patterns of NEE was closely related to GEP distribution (Figure 8). Similar to GEP distributions, when NEE was expressed on a unite area basis with croplands excluded, the top three WRRs were WRR6 (−554 g C m^{-2} yr^{-1}), WRR3 (−405 g C m^{-2} yr^{-1}), and WRR8 (−390 g C m^{-2} yr^{-1}) in the southeastern United States. These WRRs received abundant precipitation and radiation energy (represented by high PET in this study). In terms of contribution to total regional NEE, the top three regions were WRR03 (−0.30 Pg C yr^{-1}), WRR11 (−0.14 Pg C yr^{-1}), and WRR05 (−0.23 Pg C yr^{-1}).

[30] We found large differences in NEE estimates from those of *Xiao et al.* [2011] (Figure 10) and other limited continental-scale carbon sink values in the literature (Table 4). *Xiao et al.* [2008, 2011] estimated spatial mean NEE as −220 ± 225 g C m^{-2} yr^{-1} and total carbon sequestration of −1.21 Pg C yr^{-1} for all ecosystem included, or −0.63 Pg C yr^{-1} when croplands were excluded (Table 4). Correlations between the two data sets were significant (R^2 = 0.63, RMSE = 179 g C m^{-2} yr^{-1}, $p < 0.0001$, NEE = −120 + 1.06* EC-MOD NEE). Compared to EC-MOD, WaSSI-C predicted on average 33% higher NEE (Figure 8), even greater in

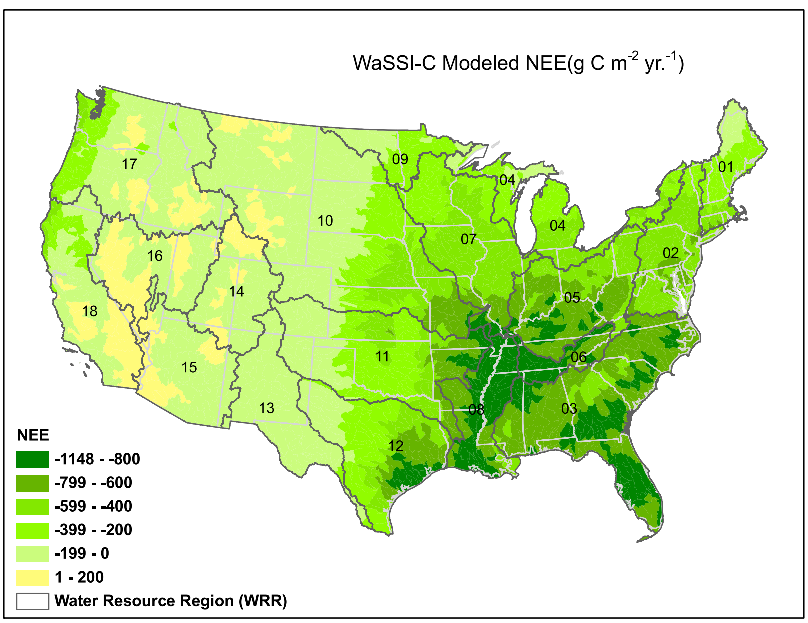

Figure 9. Spatial distribution of WaSSI-C simulated mean annual NEE (g C m^{-2} yr^{-1}) over the period of 2001–2006.

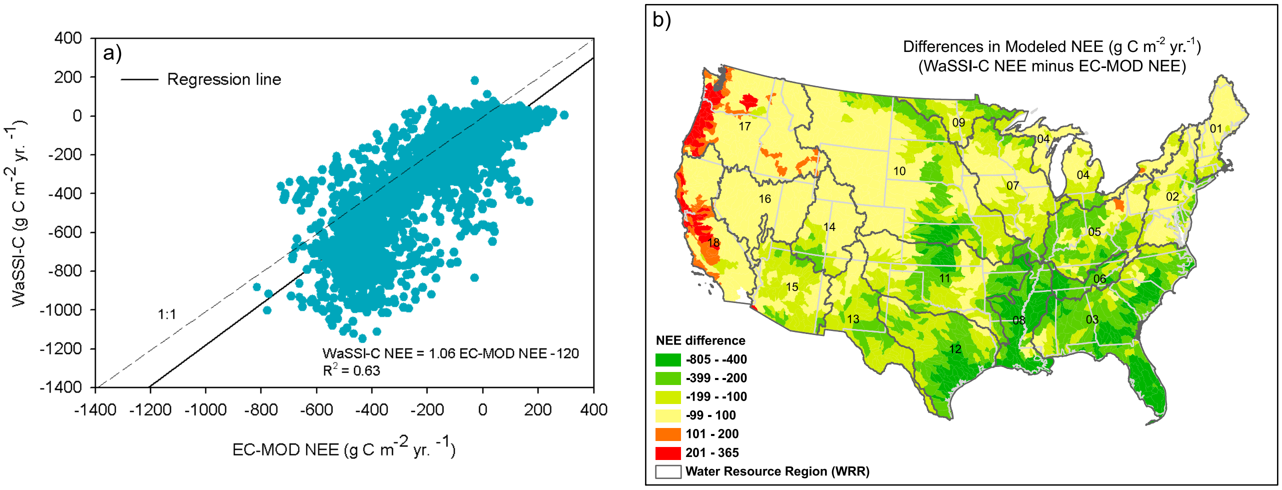

Figure 10. A comparison between mean annual NEE (g C m^{-2} yr^{-1}) estimates by WaSSI-C and EC-MOD. (a) Scatterplot and (b) spatial display of differences, across 2103 HUCs for the period of 2001–2006.

regions with high ET and GEP. The differences were highest in the southern United States in general, and in the Lower Mississippi Valley in particular, with a large contribution of croplands.

[31] The large differences in predicted NEE could be attributed to several reasons. First, NEE was underestimated for ecosystems with high carbon sequestration potential across season and sites for EC-MOD estimates [*Xiao et al.*, 2008]. Second, radiation was not an input variable to estimate PET or ET by the WaSSI-C model due to model simplification, which can cause potential overestimate of NEE. PET was estimated using a temperature-based approach. However, it is well known that plant transpiration is very responsive to radiation. Large PET does not automatically translate to high transpiration or carbon assimilation at the ecosystem level even under a wet condition. For example, a recently cleared forest land may receive similar energy as a mature stand, but the low LAI of the young stand may result in relatively much less transpiration but higher soil evaporation than older stands [*Sun et al.*, 2010]. Therefore, we may have overestimated NEE for some areas (i.e., sparsely vegetated wetlands) in the southern United States where total ET was estimated rather high. In this case, a large portion of ET may be water evaporation (e.g., plant canopy interception + soil evaporation). The small number of flux tower sites (Table 2) may also misrepresent the true global patterns of ecosystem WUE, and further refinement of these estimates is bound to improve model performance. Third, unlike WaSSI-C, *Xiao et al.* [2008, 2011] did not use local precipitation and soil physical property data as model inputs

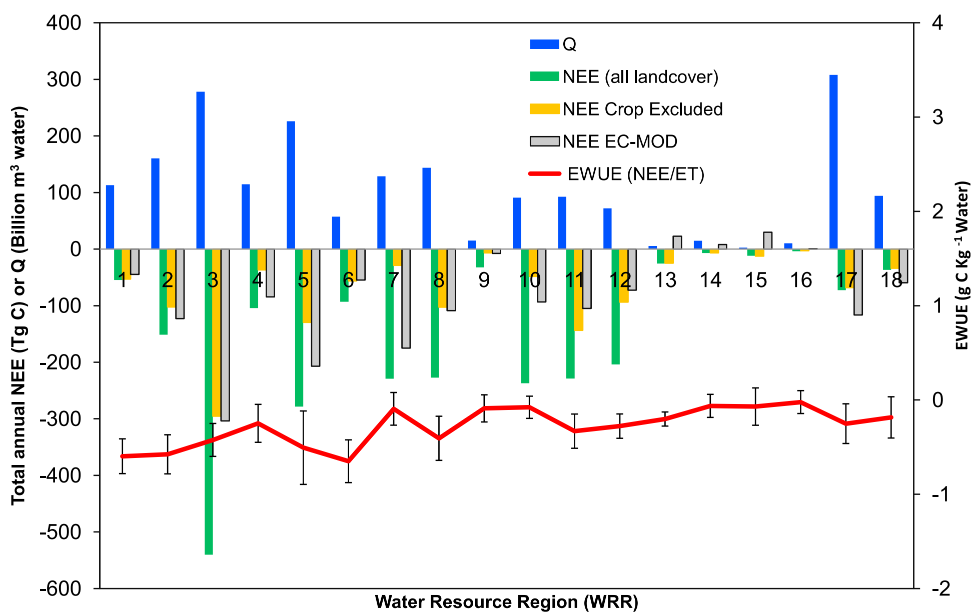

Figure 11. Summary of modeled mean annual water yield, carbon gain or loss expressed as Q (billion m^3 yr^{-1}) and NEE (Tg yr^{-1}), and ecosystem water use efficiency (EWUE) (NEE/ET, g C kg^{-1} H_2O) by water resource region (WRR).

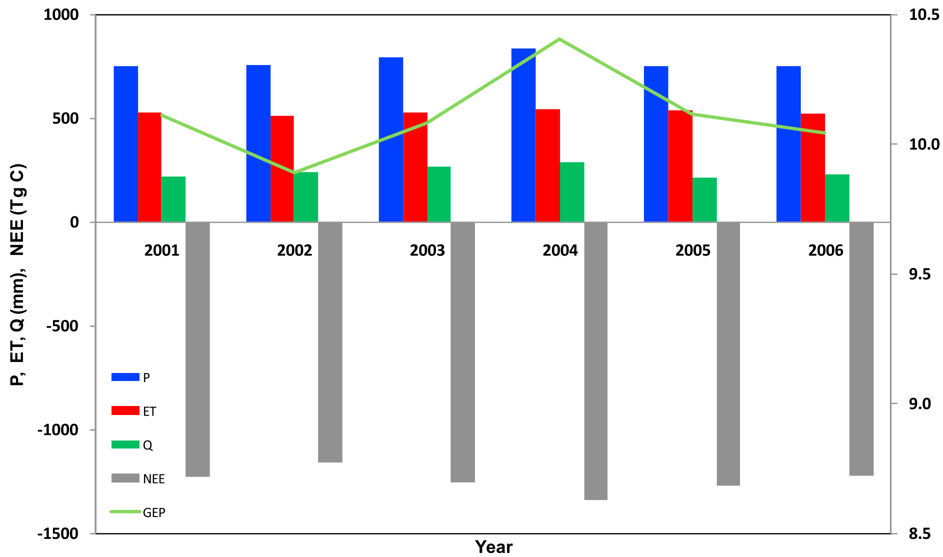

Figure 12. WaSSI-C modeled annual variability of key ecosystem fluxes in the conterminous United States during 2001–2006.

although the use of normalized difference water index derived from MODIS could partly account for soil moisture conditions. Bias could be introduced for regions that have high precipitation variability or where ET and plant carbon uptake is sensitive to soil water storage. In addition, neither model considered the effect of soil organic matters on NEE through Re, nor the effect of deep root functioning on NEE [*Domec et al.*, 2010], thus amplifying the effects of climatic variables on the differences. A recent comprehensive model evaluation study by *Schwalm et al.* [2010] found that all the 22 ecosystem models assessed performed poorly in matching observed CO_2 fluxes at a series of eddy flux sites, suggesting a large knowledge gap in modeling carbon cycle even at the site level.

[32] It could be confusing when comparing NEE values among studies that used different accounting methods and with a poor definition of carbon sequestration. This is especially troublesome when reporting the total sum values at the continental scale due to error propagation. A few studies have attempted to document the carbon sequestration strength for either the entire or certain geographic regions of the United States (Table 4). Although some consistency of carbon sequestration estimations was reported by previous studies [*Pacala et al.*, 2007; *Xiao et al.*, 2010, 2011], given the poor performance of existing models [*Schwalm et al.*, 2010], we argue a large uncertainty remains in reported U.S. ecosystem carbon sink and this study offers improved understanding and estimation of carbon fluxes and interactions between carbon and water.

3.2.3. Ranking of Water Resource Region According to Carbon and Water Fluxes

[33] Water yield volume and total carbon sequestration are summarized by water resource region (WRR) to rank their capacity of providing ecosystem services (Figure 11). Over the period of 2001–2006, we estimated a total water yield of 1.92 trillion m^3 yr^{-1}, an annual NEE of 1.24 Pg C yr^{-1} (croplands excluded) and mean water use efficiency of -0.57 ± 0.38 g C kg^{-1} H_2O^{-1} for the conterminous United States. The top three water production regions were WRR17, WRR03, and WRR05, each of which received highest precipitation and covered a large geographic region. The top three carbon uptake regions (i.e., WRR03, WRR05, and WRR10) overlapped two of the three regions identified by water yield. WRR10 had a similar total NEE as WRR 7, 8, 11, and 12. WRR17, located in the high latitude with low PET, exhibited relatively low NEE in spite of receiving large amount of precipitation in the dormant season. Although the magnitudes of estimated NEE by WRR were different between the WaSSI-C and EC-MOD models, the NEE ranking patterns for the two models were similar, suggesting model consistency in estimating NEE (Figure 11).

[34] Trade-offs between carbon and water at the regional scale can be evaluated by ecosystem water use efficiency (E_{WUE} = NEE:ET), representing the amount of carbon sequestered per unit of water consumed (g C · Kg^{-1} H_2O). This study showed that the E_{WUE} values of the most productive regions in both water and carbon (WRR03 and WRR05) were relatively high compared to those of the arid regions (WRR 13–16) or cool regions (WRR 10, 17, 18) that had low productivity (Figure 11). However, overall E_{WUE} was rather uniform across regions, suggesting mutual constraints between carbon and water fluxes.

3.2.4. Temporal Variability of ET, GEP, and NEE and the Roles of P

[35] The mean annual precipitation (P) for the conterminous United States during 2001–2006 was 775 ± 34 mm, about 8% lower than the long-term (1960–2007) mean of 847 mm. Year 2004 was a relatively wet year among the 6 years studied, resulting in higher GEP and NEE, and water yield (Q) than other 5 years (Figure 12). The severe drought in 2002 caused a noticeable decrease in GEP and NEE as a whole across the Untied States. In contrast, ET fluxes fluctuated little over the entire study period (Figure 12), suggesting carbon fluxes were more sensitive to precipitation change that ET as a large scale.

[36] The low interannual variability of fluxes presented in Figure 12 might have masked the true coupling between

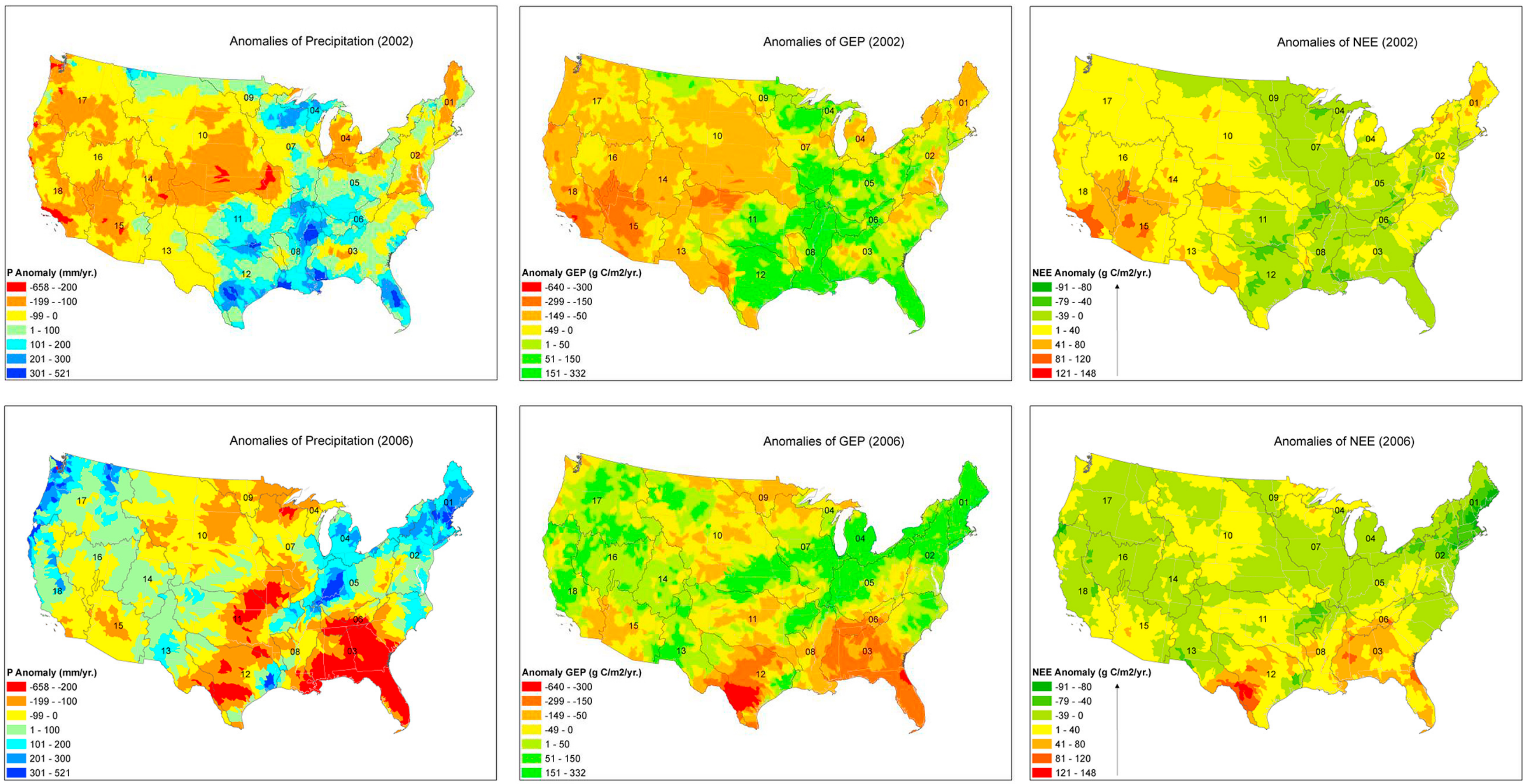

Figure 13. Anomalies of annual precipitation relative to the 48 year period 1960–2007 taken from the PRISM climate database and anomalies of GEP and NEE relative the 6 year mean in 2002 and 2006, showing impacts of server droughts on ecosystem fluxes. The arrows indicate an increase of carbon sequestration potential (more native in NEE).

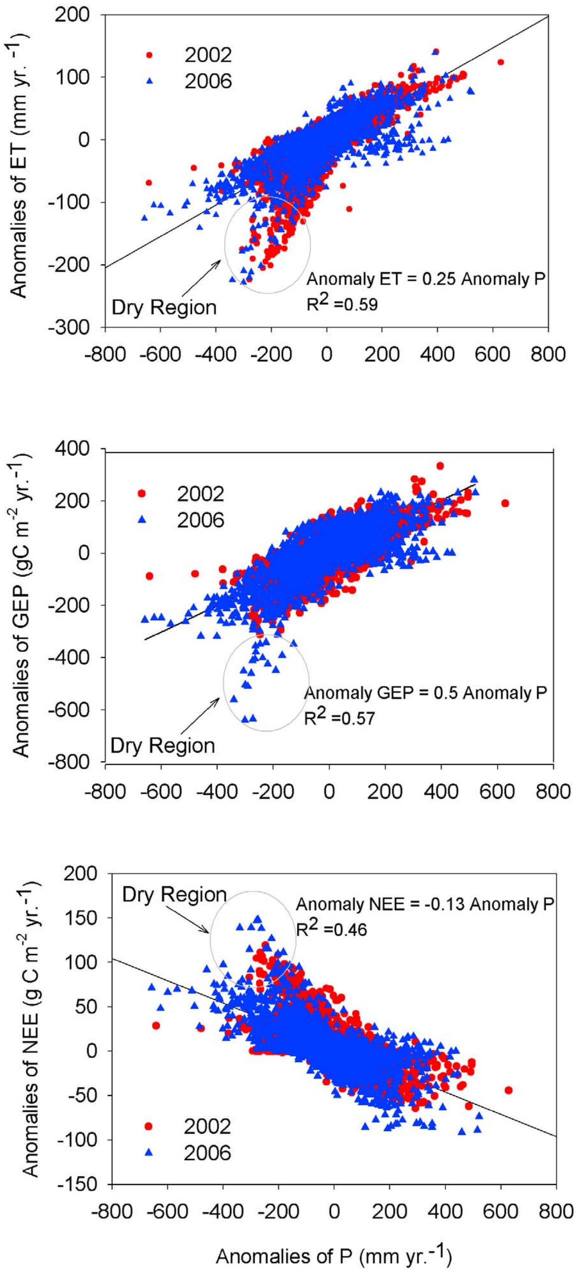

Figure 14. Relationships between anomalies of annual P and (top) annual ET, (middle) GEP, and (bottom) NEE, suggesting regional differential responses of ecosystem fluxes to changes in P in 2002 and 2006. Anomalies of P were relative to 48 year mean (1960–2007), while anomalies of ET, GEP, and NEE were relative to the mean of 2001–2006.

water and carbon processes. For example, year 2002 had the same annual precipitation as 2004 (757 mm), but the 2 years had rather distinct spatial patterns of carbon and water fluxes owing to spatial precipitation variability (Figure 13). The western and eastern regions experienced separate severe droughts in 2002 and 2006, respectively, resulting in large decreases in GEP and NEE. The regional decreases in GEP and NEE closely followed with the decreases in P (Figure 13). The reason was that modeled GEP and NEE was a linear function of ET which was controlled by P in most regions in the United States. Indeed, annual ET anomalies were strongly influenced by P, as were anomalies of GEP and NEE (Figure 14). We found that the ET fluxes were more sensitive to P in water-limited dry regions (e.g., WRR15) than in other regions. This was demonstrated by a severe shift to a steeper slope for the relationship between anomalies of ET and P compared to the overall relationship across the conterminous United States that has slope of 0.25 mm mm^{-1} (Figure 14). GEP and NEE had similar pronounced response to droughts for the arid regions. Annual ET generally increased with an increase in P at the annual scale, but we found the opposite for some watersheds (e.g., HUC 17100101–17100312) in WRR17 in the wet and cool Pacific Northwest. In this case, ET, GEP, and NEE decreased somewhat (in absolute values), up to 60 mm yr^{-1}, 100 g C m^{-2} yr $^{-1}$, 20 g C m^{-2} yr^{-1}, respectively, with the increase in annual P up to 380 mm yr^{-1} in 2006 (Figure 14). A close examination of seasonal precipitation patterns in 2006 found that the increase in annual P was due to an increase in winter precipitation whereas the growing season precipitation decreased compared to the long-term mean, consequently resulting in a decrease in ET, GEP, and NEE (absolute values) in the annual totals.

4. Conclusions

[37] We developed a water-centric carbon and water resource accounting model, WaSS-C, by linking a data-driven water balance model and simple relationships between GEP, Re, and ET as derived from global eddy flux databases. This approach was similar to *Beer et al.*'s [2007, 2010] water use efficiency approach to derive carbon fluxes from water fluxes. The main advantages of our model are twofold: (1) the algorithms were developed from eddy flux data and captured the essence of carbon and water interactions at the monthly scale, and (2) input data are widely available to run the model for prediction purposes. The model requires only two basic climatic variables (i.e., precipitation and air temperature) and two major remote sensing products (i.e., LAI, and land cover maps). As a result, it is highly transferable to other regions that have limited resources as a first estimation of water supply and ecosystem productivity.

[38] The model was applied to the 2103 basins in the conterminous United States. Model results suggest that most of the ecosystems in the United States are carbon sink at the annual timescale. When croplands were excluded, the carbon sink capacity of ecosystems of the conterminous United States was estimated to be 1.24 Pg C yr^{-1}. Terrestrial ecosystems produced about 1.92 trillion m^3 of fresh water annually. There was a large spatial and temporal variability in both water and carbon fluxes across the United States, largely due to climate and vegetation dynamics over space and time. The southeastern United States represented a region with a large carbon sink and high water yield. We found that carbon fluxes were strongly influenced by water availability during the growing seasons. This was especially true for arid regions where ET, thus GEP and NEE, was more sensitive to changes in precipitation.

[39] This study presents improved understanding and estimation of U.S. ecosystem water and carbon fluxes. The

spatial and temporal changes of ET modeled by WaSSI-C compared reasonably well with both MODIS-ET products and estimates based on streamflow data of gauged watersheds. Although modeled ET and GEP values by this study were compared well to several reference data sets, our NEE estimates were higher than those published by the published products, suggesting a large uncertainty in large scale NEE estimates in all methods used in this comparison study.

[40] Future studies should aim at closing the NEE estimation gaps among different regional modeling methods. Alternative physiologically based soil respiration models need to be incorporated into our water-centric model to fully account for ecosystem respiration fluxes. Eddy flux measurements and modeling efforts should focus on ecosystems that are currently not represented in the flux networks, such as wetlands and managed ecosystems that are under various natural and human disturbance regimes. In spite of the uncertainty and deficiencies identified, our model will be useful in helping natural resource managers construct water and carbon budgets and examine trade-offs between carbon sequestration and water supply at the regional scale.

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