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Tracking Ecosystem Water Use Efficiency of Cropland by Exclusive Use of MODIS EVI Data

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Abstract: One of the most important linkages that couple terrestrial carbon and water cycles is ecosystem water use efficiency (WUE), which is relevant to the reasonable utilization of water resources and farming practices. Eddy covariance techniques provide an opportunity to monitor the variability in WUE and can be integrated with Moderate Resolution Imaging Spectroradiometer (MODIS) observations. Scaling up *in situ* observations from flux tower sites to large areas remains challenging and few studies have been reported on direct estimation of WUE from remotely-sensed data. This study examined the main environmental factors driving the variability in WUE of corn/soybean croplands, and revealed the prominent role of solar radiation and temperature. Time-series of MODIS-derived enhanced vegetation indices (EVI), which are proxies for the plant responses to environmental controls, were also strongly correlated with ecosystem WUE, thereby implying great potential for remote quantification. Further, both performance of the indirect MODIS-derived WUE from gross primary productivity (GPP) and

evapotranspiration (ET), and the direct estimates by exclusive use of MODIS EVI data were evaluated using tower-based measurements. The results showed that ecosystem WUE were overpredicted at the beginning and ending of crop-growth periods and severely underestimated during the peak periods by the indirect estimates from MODIS products, which was mainly attributed to the error source from MODIS GPP. However, a simple empirical model that is solely based on MODIS EVI data performed rather well to capture the seasonal variations in WUE, especially for the growing periods of croplands. Independent validation at different sites indicates the method has potential for broad application.

Keywords: water use efficiency; cropland; MODIS; vegetation index; GPP; ET

1. Introduction

Water use efficiency (WUE) is defined as the ratio of photosynthetic carbon uptake over transpiration, and has been widely recognized as an important link between global carbon and water cycles in terrestrial ecosystems [1,2]. Plants assimilate CO₂ through photosynthetic activity, which is always accompanied by the water loss that regulates the land surface exchanges between the biosphere and the atmosphere [3]. The exchanges of both CO₂ and water vapor are controlled by stomatal aperture for leaf-level WUE [4]. However, ecosystem-level WUE changes with vegetation types and the surrounding environmental conditions [5]. The variability in WUE is closely related to the reasonable utilization of water resources and survival strategies, as well as responses to the changing hydrological environment [6,7]. Especially for agriculture, WUE is important for agronomy and making optimal irrigation management decisions.

Increasing atmospheric CO₂ concentration has increased global mean temperature in the 20th and early 21st centuries [8]. In response to the higher temperature, plant transpiration and soil evaporation can enhance water consumption, which has the potential to increase the severity, frequency, and duration of soil moisture stress. Conversely, higher CO₂ concentration can trigger stomatal closure that may limit the extent of water loss by plant transpiration [9]. Further, in some systems, the higher temperatures will extend the plant's phenological period with an earlier spring and a later fall, which can cause more water to be consumed by terrestrial ecosystems [10]. In addition, land use/land cover changes, primarily the expansion of cropland from forest, grassland, and wetland, are deemed responsible for 20%–25% of the increase in atmospheric CO₂ over the past 150 years [11]. Given the rapid expansion of urbanization and industrialization, the demands on water are continuously increasing which further ramp up the pressure to decrease agricultural water consumption [12]. Technologies for improving crop WUE are critical for sustainable yield and food security. Therefore, quantifying large-scale ecosystem WUE is vital for diagnosing how current farming practices influence WUE and identifying opportunities for improvement without yield penalty.

At the ecosystem level, the eddy covariance (EC) technique has become one of the powerful tools used to characterize the dynamics of WUE as the ratio of gross primary production (GPP) over evapotranspiration (ET) [13–15]. By combining EC fluxes with remote sensing information, it is possible to extrapolate these site-level measurements of plant functional characteristics to a much

larger area with ecosystem models [16–19]. As an important proxy of terrestrial carbon and water coupling, both processes of CO₂ sequestration through photosynthesis and loss of water by evapotranspiration are closely related to the biophysical properties (e.g., biomass, leaf area, and growth stage) and environmental factors [20–23]. With the development of MODIS GPP and ET algorithms, currently large-scale ecosystem WUE can be calculated as the ratio of GPP to ET in accordance to its definition. Although Tang *et al.* [24] evaluated how global WUE of terrestrial ecosystems distributed and changed in the past decade using remotely-sensed products on an annual time scale, the correspondence between MODIS WUE estimates and tower-based WUE measurements at short time scales remains unclear. In fact, precise information on seasonal variations in WUE is more significant for agricultural water management [25–27]. There is an important need to examine the capacity of applying MODIS GPP and ET products to monitor the variability in crop WUE. Meanwhile, alternative approaches involving direct estimation of WUE from satellite data need to be explored.

Therefore, this study aims to answer:

- (1) How do environmental factors control the changes in WUE from flux measurements in corn/soybean rotation systems?
- (2) How well do the MODIS-derived WUE estimates from GPP and ET perform in capturing the seasonal dynamics in WUE of croplands? What are the possible sources of error?
- (3) Can we develop an alternative method that is based directly on the remotely-sensed data to improve the accuracy in WUE estimates of corn and soybean?

2. Materials and Methods

2.1. Site Descriptions

This study was conducted using EC flux data from an agricultural site in the midwestern part of the United States, near Champaign, Illinois (40.0062 °N, 88.2904 °W). The site (US-Bo1) is part of the research network in the global energy and water cycle experiment described by Lawford [28] as well as the international network for terrestrial carbon fluxes described by Baldocchi *et al.* [13]. This site has been operational since 1996, which aims to obtain long-term information about energy, water, and CO₂ fluxes and their environmental controls for improving soil-vegetative-atmosphere transfer models. The field was managed as continuous no-till with alternating years of corn and soybean crops (corn in the odd years and soybean in the even years). Soil type is silt loam consisting of three soil series (Dana, Flanagan, and Drummer). The micrometeorological tower placement in the field provides a fetch over a continuous crop with 300 m to the west, 700 m to the east, 500 m to the south, and 200 m to the north. For the corn and soybean crops, plant heights are typically 3.0 m and 0.9 m with the peak leaf area index (LAI) of 5.5 and 5, respectively. Climate of the region is temperate continental with the prevailing winds during the summertime from the south. A detailed description of the site can be found in Meyers and Hollinger [29] and Bernacchi *et al.* [30].

To independently evaluate the transferability of the developed model, the crop site (US-Ro1; 44.7143 °N, 93.0898 °W) located at the University of Minnesota's Rosemount Research and Outreach Center, approximately 25 km south of St. Paul, Minnesota, was also used. Waukegan silt loam is the main soil type with high organic carbon content (about 2.6%) on the surface layer and

varying thickness between 0.3 m and 2.0 m with coarse outwash sand and gravel. This field has the same temperate continental climate with a regional growing season that usually starts in late May and ends in October. In contrast to US-Bo1, this site was a conventional-till management corn/soybean annual rotation field (corn in the odd years and soybean in the even years). Apart from this, both sites are rain-fed farming systems. Further information can be obtained from Baker and Griffis [10] and Kalfas *et al.* [31].

2.2. Satellite-Derived MODIS Products and Processing

Currently, satellite-based products of terrestrial GPP and ET from NASA MODIS have been developed and experienced ongoing improvement during the past decade [17,24]. Zhao *et al.* [16] identified important errors in the old GPP product (Collection 4) owing to the problems in the upstream inputs. Then, these GPP estimates were amended through improving the algorithms and perfecting the necessary parameters, which generated the enhanced Collection 5 MOD17 products. The 8-day composites of MODIS LAI/FPAR (fraction of photosynthetically active radiation) data with the resolution of 1-km were introduced into the processing methods of GPP as remote sensing-based vegetation properties. The information in the QA (quality-assessment) flags were used to gap-fill the missing data in the time-series MODIS LAI/FPAR product resulting from clouds. Near real-time meteorological data are obtained from the National Center for Environmental Prediction (NCEP) to drive the algorithm. The continuous 8-day MODIS GPP values are summed up to generate monthly and annual GPP estimates. Further, the global evapotranspiration data can be used to quantitatively evaluate the regional soil water status and energy balance, which is key for agricultural water management. The potential effects of changes in global climate, land use/land cover, as well as natural disturbances such as wildfires on regional surface energy change and water cycles can also be examined with long-term ET products. Mu *et al.* [32] developed the global satellite remote sensing-based ET product (MOD16A2) with an improved algorithm using MODIS and ground-based meteorological observations. These improvements included: (1) separating dry canopy surface from the wet that caused water consumption by evaporation from the intercepted water and the plant transpiration; (2) treating land surface evaporation as the sum of the saturated and moist soil surface; (3) inclusion of daytime and nighttime components; (4) estimation of the soil heat flux value as radiation partitioned from the land surface; and (5) improving the estimates of canopy and aerodynamic resistances, as well as the vegetation cover fraction. Both NTSG (Numerical Terradynamic Simulation Group of the University of Montana) MODIS GPP and ET products with an 8-day time scale can be obtained freely from the web site [33].

In addition, the 8-day composite land surface reflectance (MOD09A1, with resolution of 500 m) data from one MODIS pixel where the US-Bo1 and US-Ro1 lie were downloaded from the Oak Ridge National Laboratory's Distributed Active Archive Center web site [34]. The version of MODIS data is collection 5. The enhanced vegetation index (EVI) derived from blue, red, and near-infrared (NIR) bands has proved to be sensitive to vegetation production, plant transpiration and growth stages [35–37]. Huete *et al.* [38] defined EVI as:

$$EVI = 2.5 \frac{\rho_{nir} - \rho_{red}}{\rho_{nir} + (6\rho_{red} - 7.5\rho_{blue}) + 1} \quad (1)$$

where ρ_{mir} , ρ_{red} , and ρ_{blue} are the spectral reflectances in MODIS bands 2, 1, and 3, respectively. Time-series EVI data are used to analyze the correlation with variations in ecosystem WUE, and to develop an alternative method for quantifying crop WUE.

2.3. Site-Specific Climate and Flux Data

In this study, our analysis is based on continuous observations of land-surface exchanges during 2001–2006 at US-Bo1 site and during 2005–2006 at US-Ro1 site [39]. The product provides measurements of ecosystem-scale water flux (LE), CO₂ flux, meteorological variables including solar radiation (R_g), air temperature (T_a), soil temperature/moisture, vapor pressure deficit (VPD), precipitation (P), and the estimates of GPP derived from the measured NEE using the methodology proposed by Reichstein *et al.* [40] at half-hour, daily, weekly (8-day), and monthly time scales [17]. Both the marginal distribution sampling (MDS) approach and the artificial neural network (ANN) method are used to gap-fill the original CO₂ flux data. Generally, the ANN method is slightly superior to the MDS method [40,41]. Thus, the gap-filled results of NEE and GPP data based on the ANN method are used. The 8-day period, level-4 data are analyzed in this study. Therefore, flux tower and MODIS observation periods are consistent for comparison. In addition, the missing data resulting from system failures, stable atmospheric conditions or rejection of poor data were gap-filled using standardized approaches to provide complete data sets [40,42].

Crop WUE can be characterized in many different ways in terms of scientific disciplines as well as the temporal and spatial scope of interest [43]. The ecosystem-level definition is used in this study, which is also closely related to ecosystem models. It is defined as:

$$\text{WUE} = \text{GPP} / \text{ET} \quad (2)$$

The seasonal variations in WUE can be described using 8-day WUE ($\text{g}\cdot\text{C}\cdot\text{kg}^{-1}\cdot\text{H}_2\text{O}$). ET (mm/day) was inferred from the observed latent heat fluxes (LE, W/m^2) as:

$$\text{ET} = \text{LE} / \lambda \quad (3)$$

where λ is the amount of energy required to evaporate 1 kg liquid water to vapor (about 2,454,000 J).

2.4. Statistical Analysis

Pearson correlation analysis was conducted to assess the relationship between ecosystem WUE and the controlling environmental factors at the annual corn/soybean rotation field using SPSS 19.0 (Chicago, IL, USA). Performance of MODIS-derived WUE from GPP and ET was evaluated with tower-based measurements using the EC technique, and the main error sources were also explored through comparison of both processes. We also developed an alternative method to help capture the seasonal variations in WUE of croplands. Both fields (US-Bo1 and US-Ro1) were planted with corn in the odd years, and with soybean in the even years. Considering the differences in photosynthetic pathways between C₃ plant (soybean) and C₄ plant (corn), the site-level data at US-Bo1 were split into a training set (Corn year—2001 and 2003; soybean year—2002 and 2004) and a validation set (2005 for corn and 2006 for soybean), respectively. To evaluate the model's performance, coefficient of determination (R^2), root mean squared error (RMSE), scatterplots, and seasonal variations in predicted WUE *versus* tower-based WUE

were compared. A well-calibrated model should have a small *RMSE* compared to the total variances as well as the *R*² value close to 1. Finally, the transferability of the calibrated model was further tested at the independent US-Ro1 site. An overview of our research approach is shown in Figure 1.

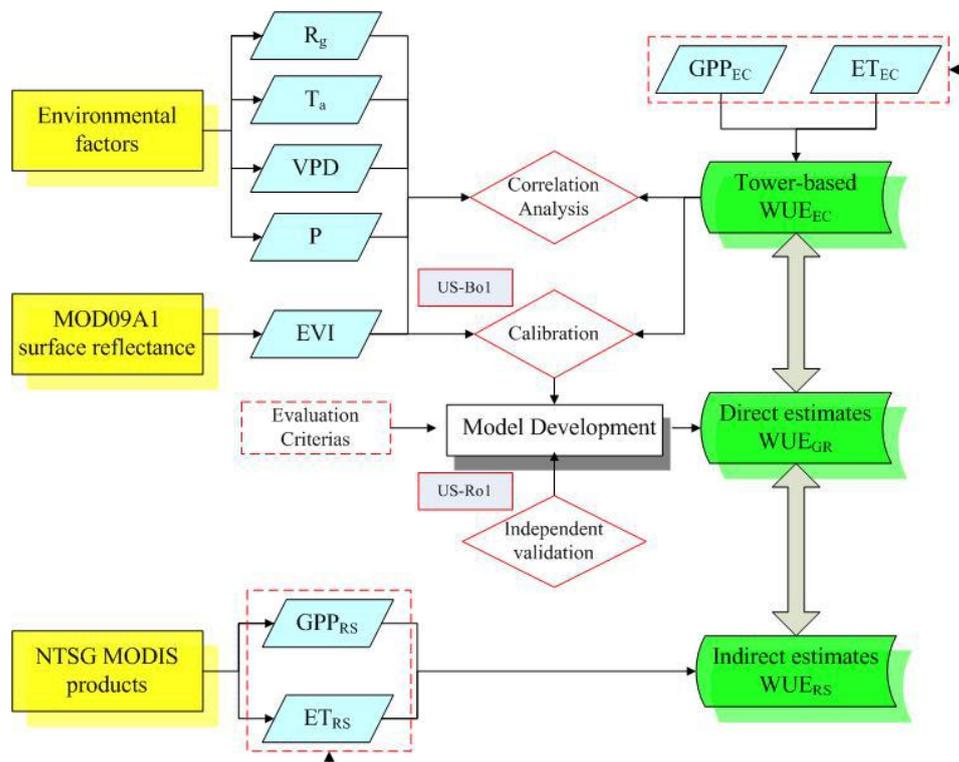


Figure 1. Overview of the research approach. R_g, T_a, VPD and P are observed at the flux tower sites. EVI are derived from the MODIS data. WUE_{EC}, WUE_{RS}, and WUE_{GR} refer to ecosystem water use efficiency from flux tower measurements, the indirect estimates from NTSG MODIS products and the direct estimates based on MODIS EVI data, respectively. In addition, the data from US-Bo1 are used for calibration and another US-Ro1 site is used for independent validation of the developed model.

3. Results and discussion

3.1. Seasonal Variations in Crop WUE with Environmental and Biological Controls

Climate of the region is northern continental, with short, moist growing periods in summer and cold, relatively dry winters, which has a profound effect on crop growth and the functional properties related to carbon and water budgets [23,44,45]. Crop growing season, including corn and soybean, in this region generally starts in late May to the end of October. The relationships between averaged 8-day tower-based WUE and the environmental conditions including R_g, T_a, VPD, P and MODIS-derived EVI data observed at US-Bo1 site during 2001 to 2006 are shown in Figures 2 and 3. Figure 2 shows the time-series of meteorological data and Figure 3 exhibits the variations in tower-based WUE. The statistical significance is examined using Pearson’s correlation analysis (Table 1). We find that time-series of WUE data have distinct seasonal cycles that strongly covary with R_g and T_a. During winter months, because low temperature and frozen soils inhibit the plant growth and photosynthetic activities,

WUE values are nearly zero. As temperature rises in the spring planting season, crops begin to grow and ecosystem photosynthetic capacity gradually increases accompanied by plant transpiration. Ecosystem WUE of both corn and soybean reached its peak value during about late July and early August, and then declined until the harvest in October. The C_4 plant-corn showed greater sensitivity to solar radiation than temperature in contrast to the C_3 plant-soybean (Table 1). In addition, despite the prominent role that R_g and T_a play as the main drivers of crop WUE, peak periods show a minor hysteresis effect. Except during the winter months, VPD remains at a suitable value over most of the growing period. The VPD around 10 hPa appear to be near optimal for stomatal aperture. Thus, VPD values are at best moderate, but not excessively high during these measurement periods. Moreover, VPD was more closely correlated to corn WUE than soybean WUE. Both of the two flux sites depend on precipitation during cultivation and no irrigation was applied. Approximately 63% of the annual precipitation occurred during the cultivation-period. Although it was not significantly correlated to WUE on 8-day periods, natural rainfall is vital to crop growth as the only water supply.

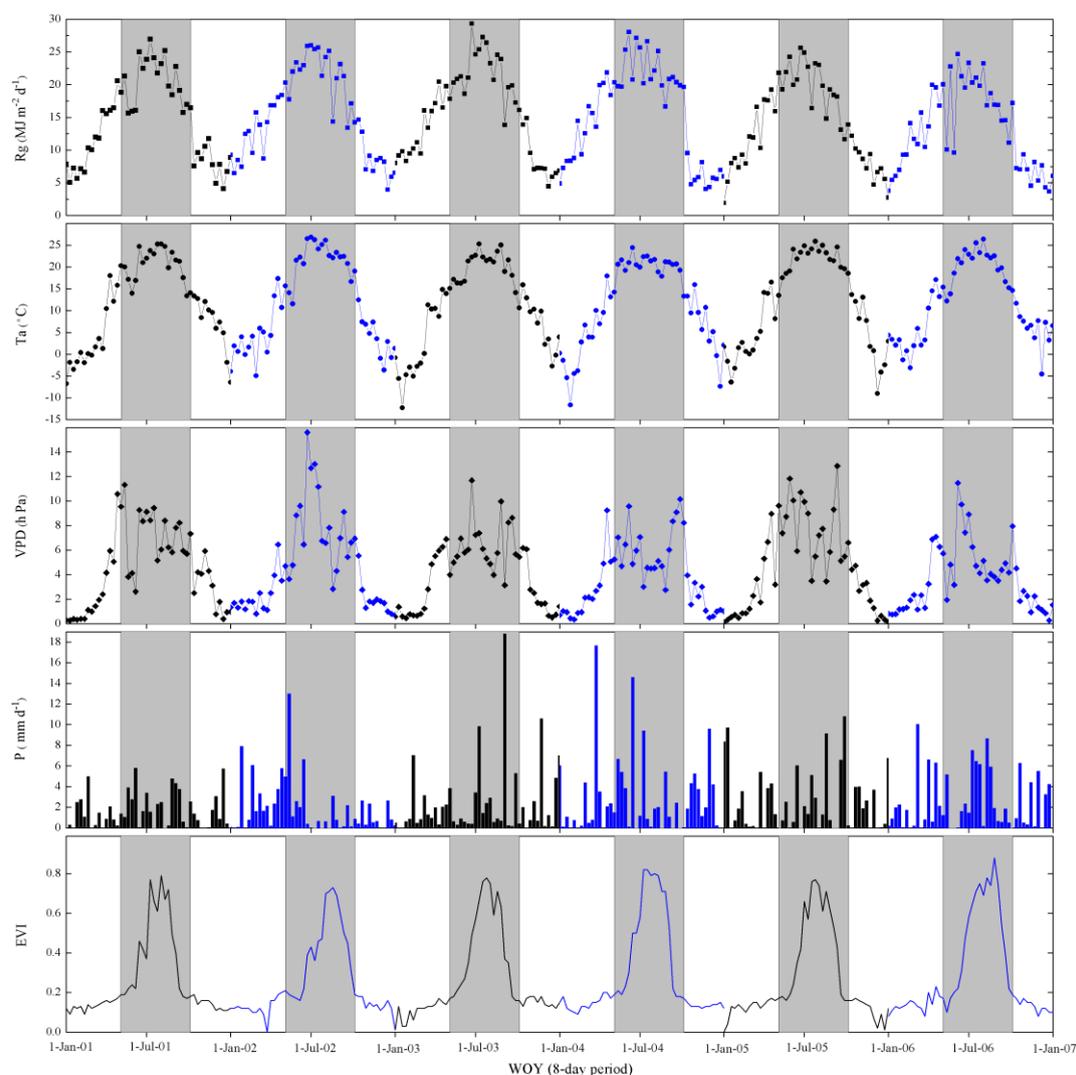


Figure 2. Seasonal and interannual variations of solar radiation (R_g), air temperature (T_a), vapor pressure deficit (VPD), precipitation (P) and enhanced vegetation index (EVI) observed at the annual corn/soybean rotation field (US-Bo1) during 2001–2006, with the growing season highlighted.

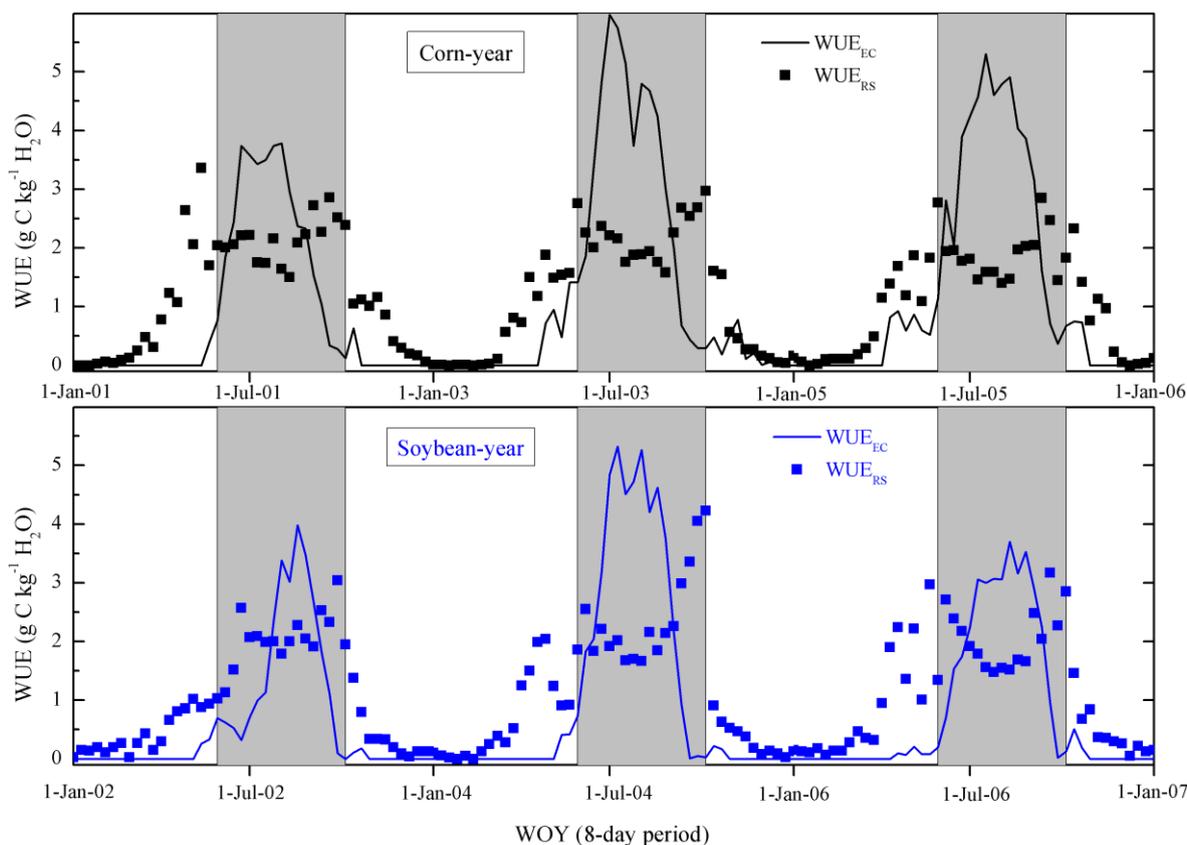


Figure 3. Seasonal variations of ecosystem water use efficiency from flux tower measurements (WUE_{EC}) and estimates from MODIS products (WUE_{RS}) at the flux tower site US-Bo1 during 2001–2006 (corn in the odd years and soybean in the even years).

Table 1. Correlations between 8-day tower-based WUE and satellite-driven EVI data with the controlling environmental factors at the annual corn/soybean rotation field.

Crop Type	-	GPP	ET	R_g	T_a	VPD	P	EVI
		($g\ C\ m^{-2}\ d^{-1}$)	($mm\ d^{-1}$)	($MJ\ m^{-2}\ d^{-1}$)	($^{\circ}C$)	(h Pa)	($mm\ d^{-1}$)	
Corn	WUE	0.982 **	0.818 **	0.740 **	0.673 **	0.503 **	0.147	0.906 **
	EVI	0.906 **	0.911 **	0.857 **	0.738 **	0.545 **	0.094	–
Soybean	WUE	0.978 **	0.732 **	0.533 **	0.577 **	0.248 **	–0.029	0.950 **
	EVI	0.931 **	0.784 **	0.604 **	0.686 **	0.385 **	–0.021	–

Note: ** Correlation is significant at the 0.01 level. * Correlation is significant at the 0.05 level. R_g , T_a , VPD and P are observed at the flux tower sites. Time series of EVI data are derived from the MODIS data.

As a proxy of the biological properties that reflected the response of vegetation to environmental controls, time series MODIS-derived EVI data also showed a strong consistency with seasonal and interannual variations in ecosystem WUE. 8-day EVI data presented fairly similar patterns as WUE during the growth period of crops. Moreover, the vegetation index captured well the beginning and ending of the crop growing season in 2001–2006. EVI started to increase in late May, reached peak values during peak growth (July–August), and declined after crop senescence or harvest (October). Correlation coefficients between EVI and WUE reached 0.906 for corn and 0.950 for soybean, respectively. As illustrated in Table 1, it again demonstrated its significant relationship with processes of

both GPP and ET that were consistent with previous findings in forests [44,46], crops [6,37], and grasslands [2,47].

3.2. Comparisons of Tower-Based WUE and the MODIS Estimates from GPP and ET

Figure 3 shows the performance of MODIS-derived WUE estimates (WUE_{RS}) from GPP and ET in explaining the variability in EC measurements (WUE_{EC}) at the crop flux site. Changes in WUE_{EC} were tracked by WUE_{RS} with reasonable consistency for both corn and soybean. However, there existed two pronounced discrepancies. MODIS WUE estimates greatly overpredicted tower-based WUE at the beginning and ending of crop-growth periods whereas ecosystem WUE during the peak periods were severely underestimated, especially for the C_4 plant-corn. This comparison reveals large uncertainties in the coupling processes between carbon and water cycles as represented in the MODIS GPP and ET products. These uncertainties may stem from the algorithm, various upstream inputs, as well as the specific parameters stored in a Biome Properties Look-Up Table (BPLUT). A single value for agricultural lands without considering the differences between C_3 and C_4 must be problematic. Thus, further analysis is needed to diagnose the errors.

Seasonal patterns of GPP and ET from flux observations and the corresponding MODIS estimates are compared to explore the potential reasons for differences between WUE_{EC} and WUE_{RS} . As shown in Figure 4, the MODIS ET product performed reasonably well with measured ET during both corn years and soybean years except several 8-day periods. Overall, the percentage deviation of multiyear mean annual ET_{EC} and ET_{RS} was less than 5%. However, large discrepancies existed in the seasonal dynamics between GPP_{EC} and GPP_{RS} . Similar to the variability in ecosystem WUE, crop GPP was overestimated at the emergence stage and after harvest, and was severely underestimated during the peak growth periods. The percentage difference during the corn planting years was up to 30% in contrast to less than 10% for the soybean years. In addition, we also found that 8-day patterns of MODIS GPP product during 2001 to 2006 were nearly identical without considering the differences between C_3 and C_4 photosynthetic pathways for corn and soybean crops. It suggests that improvement of the MODIS GPP product needs to consider this point for the purpose of monitoring crop WUE accurately.

Ecosystem WUE of corn is generally higher than that of soybean. Statistical analyses for the flux tower site US-Bo1 during 2001–2006 found that tower-based WUE of corn during the crop-growth period ranged from $2.22 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ to $3.10 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ with the mean value of $2.81 \text{ g C kg}^{-1} \text{ H}_2\text{O}$, while soybean WUE_{EC} spanned between $1.58 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ and $2.83 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ with the average value of $2.16 \text{ g C kg}^{-1} \text{ H}_2\text{O}$. These differences are related to the plant physiological pathways, as well as the leaf structure and architecture that differ between corn (C_4 plant) and soybean (C_3 plant) [48,49]. C_4 crops are generally found to have high phosphoenolpyruvate carboxylase activity [50,51]. Theoretically, water use efficiency of plants is affected by the leaf-to-air CO_2 concentration difference and VPD [52]. Recent studies [53,54] have shown the existence of further internal resistances into the leaf (called mesophyll conductance) that may constrain as much as stomata the CO_2 diffusion pathway and are also key actors in controlling and determining plant WUE. Under the same background and environmental conditions, WUE of a C_3 crop is apparently lower than C_4 crop because CO_2 concentration is still higher in C_4 leaves than in C_3 leaves [51,55]. Therefore, the characteristics of species determine a larger WUE for C_4 plant than for C_3 plant. In addition, many studies have found

that C₄ vegetation exhibited increasing WUE in response to rising atmospheric CO₂ concentration by reducing the stomatal aperture as well as the transpiration rate compared with C₃ species [6,56,57]. We hypothesize that the lack of this C₃/C₄ distinction in the biome-specific parameters in BPLUT causes substantial uncertainty in the MODIS GPP product and the estimation of WUE.

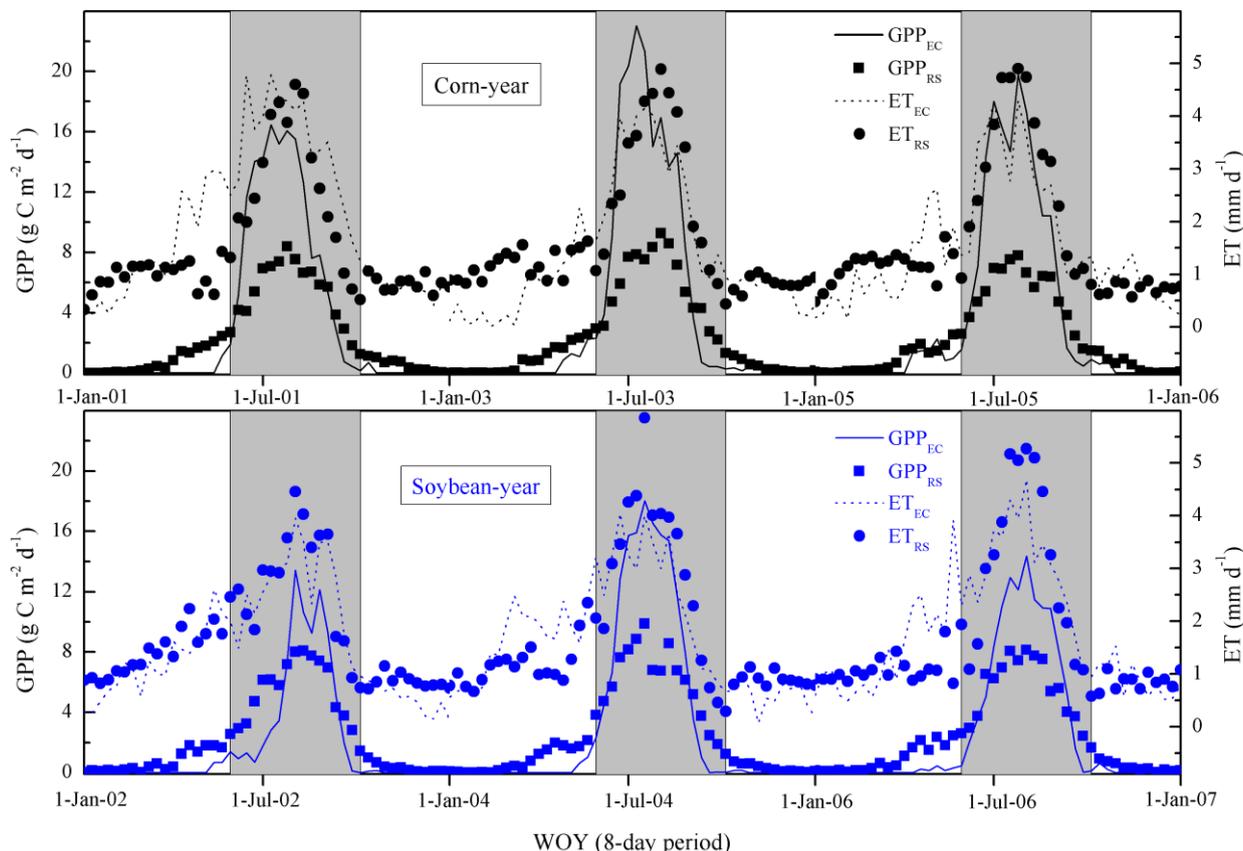


Figure 4. Comparison of seasonal dynamics in gross primary production and evapotranspiration between flux tower measurements (GPP_{EC} , ET_{EC}) and MODIS estimates (GPP_{RS} , ET_{RS}) at the flux tower site US-Bo1 during 2001–2006.

3.3. An Alternative Method to Estimate WUE Using MODIS EVI Data

Considering that large uncertainties exist in the MODIS WUE estimates from GPP and ET, an alternative method needs to be developed in order to extrapolate tower-based WUE measurements to different time and space scales. The strong relationship between time series of MODIS EVI data and ecosystem WUE also indicated this potential. Here, we established a regression model that was solely based on the 8-day EVI data. For the corn-planting year and soybean-planting year, crop WUE can be calculated using the following Equations (4) and (5), respectively:

$$WUE_{GR} = 7.245 \times EVI - 0.871 \quad (R^2 = 0.82; \text{RMSE} = 1.07) \tag{4}$$

$$WUE_{GR} = 6.601 \times EVI - 0.938 \quad (R^2 = 0.90; \text{RMSE} = 0.69) \tag{5}$$

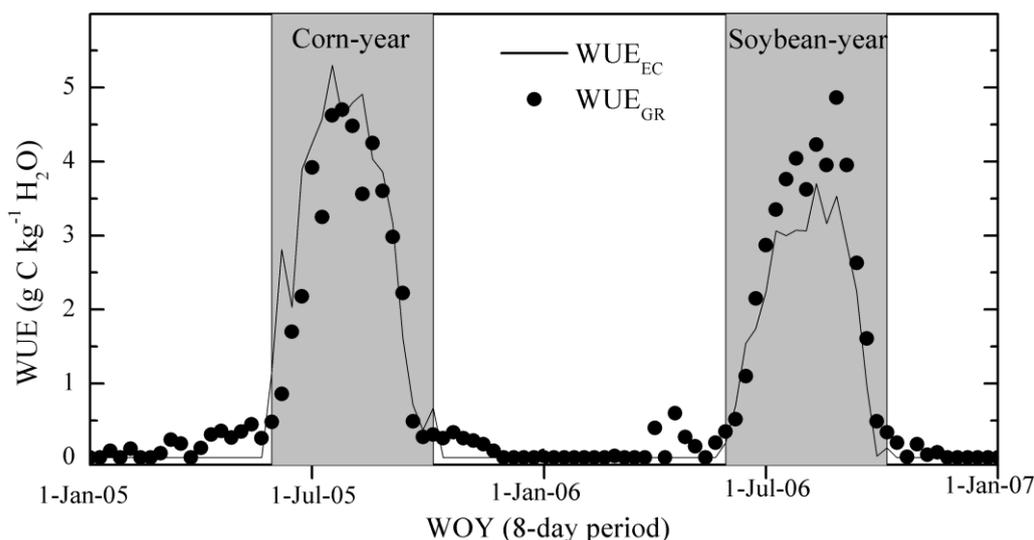


Figure 5. Seasonal dynamics in ecosystem water use efficiency from flux tower measurements (WUE_{EC}) and estimates based on MODIS EVI data (WUE_{GR}) at the flux tower site US-Bo1 during 2005 (corn) and 2006 (soybean), with the growing seasons displayed in gray.

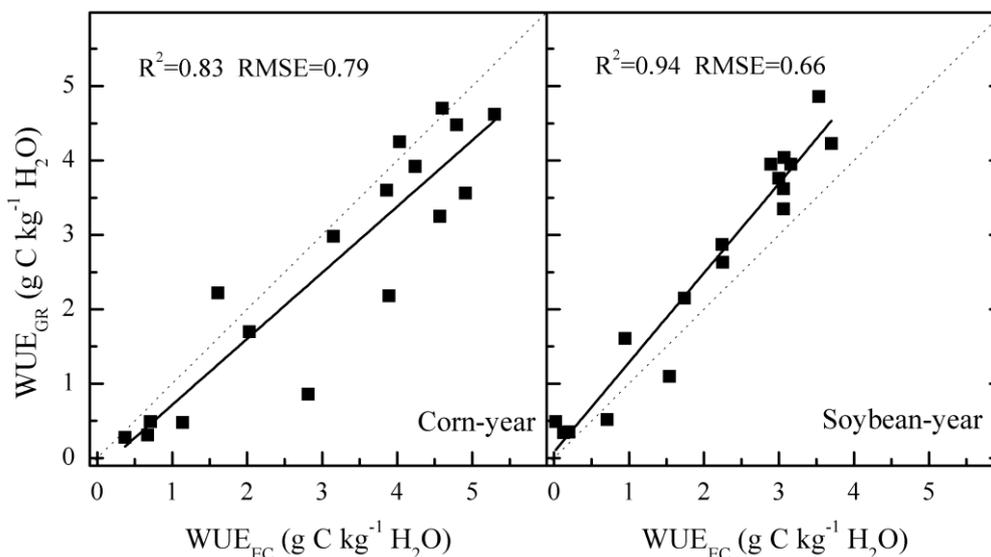


Figure 6. A scatterplot comparison between ecosystem WUE from flux tower measurements (WUE_{EC}) and estimates based on MODIS EVI data (WUE_{GR}) at the flux tower site US-Bo1 during the growing season of 2005 (corn) and 2006 (soybean).

The performances of these empirical models (GR) was evaluated using scatter plots between the predicted (WUE_{GR}) vs. measured WUE (WUE_{EC}) and the seasonal variations between them in 2005 (corn-year) and 2006 (soybean-year). As shown in Figure 5 and 6, the seasonal patterns of WUE simulated by the GR model agreed reasonably well with the tower-based observations for both corn and soybean in 2005–2006, which also exhibited a nearly linear relationship. Compared with the indirect MODIS WUE estimates (WUE_{RS}) from GPP and ET in Figure 3, large discrepancies in ecosystem WUE at the beginning and ending of crop growing season and peak periods were generally reduced. This result may be explained by the underlying phenological information in the time-series of MODIS EVI data. A large

number of researchers have used time series of EVI data to extract phenology characteristics [36,58,59]. Chen *et al.* [60] also indicated that in order to precisely evaluate the land-surface mass (water and carbon fluxes) and energy budgets, we need to account for crop phenology in ecosystem models. *RMSE* of WUE_{RS} and WUE_{GR} with WUE_{EC} over the growing season were $2.24 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs $0.79 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ in 2005 for corn, and $1.58 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs $0.66 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ in 2006 for soybean. Therefore, this simple empirical model provides a very reasonable estimate of ecosystem-level WUE.

3.4. Independent Validation of the Proposed Models

Although the calibrated model developed at the US-Bo1 site provided fairly good estimates of crop WUE directly from MODIS EVI data, its applicability to other crop sites needs to be evaluated before spatial up-scaling of site-level observations to regional scale. Therefore, flux measurements at additional US-Ro1 crop site were used for independent validation.

Comparisons between both WUE_{RS} and WUE_{GR} with 8-day tower-based WUE_{EC} are shown in Figures 7–9. Validation of the empirical model at the independent US-Ro1 site also exhibited a significant improvement in ecosystem WUE simulation, especially for the soybean-planting year. The WUE estimates by exclusive use of MODIS EVI data captured the seasonal variations in ecosystem WUE in spite of a slight underestimation during the peak-growth period of the corn year, which may be ascribed to the effects of different farming practices on the vegetation index. Although both US-Bo1 and US-Ro1 sites are annual corn/soybean rotation fields, US-Bo1 is under continuous no-till treatment whereas US-Ro1 adopts conventional tillage management [10,29]. The scatter plots showed that R^2 and *RMSE* between WUE_{RS} with WUE_{EC} were 0.02 and $2.21 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs the values of 0.86 and $1.15 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ between WUE_{GR} and WUE_{EC} , respectively in 2005. During the soybean-planting year—2006, R^2 and *RMSE* between WUE_{RS} with WUE_{EC} were 0.23 and $1.61 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs 0.82 and $0.72 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ between WUE_{GR} and WUE_{EC} , respectively. Therefore, all crop WUE estimates have been improved substantially with the use of EVI.

However, owing to the diversity in climate conditions, crop types, and management practices [37,45,61,62], it is still challenging to develop a general a robust model for WUE estimation. For agriculture, monitoring ecosystem WUE of croplands in view of C_3 and C_4 photosynthetic pathways needs to be considered. Nevertheless, although our calibrated model for estimating 8-day WUE of corn and soybean captured the general tendencies, there still existed large discrepancies for individual periods such as the peak growing season of the corn-year at US-Ro1 (Figure 7). Normally, tower-based WUE of corn is generally higher than that of soybean. But the proposed models resulted in almost the same WUE values for both corn and soybean, which was not observed in the flux tower measurements. On one hand, the flux sites and dataset used for calibration remained rather limited, whereas diverse farming practices are implemented across the globe. This challenges the general application of such models. On the other hand, our analyses and simple model for typical cropping systems in the United States indicate there is good potential for upscaling WUE especially when water is not severely limited. Medrano *et al.* [63] showed that under water stress, plant WUE usually increased and GPP decreased. Therefore, it is necessary to examine the EVI-based models' sensitivities to drought during drought and non-drought years. Dong *et al.* [64] also compared four EVI-based models including the Vegetation Photosynthesis Model (VPM), Temperature and Greenness (TG) model, Greenness and Radiation (GR) model and

Vegetation Index (VI) model to estimate GPP of corn and soybean croplands and grasslands under drought conditions. They found that these four models had reasonably good agreement with the GPP estimated from EC-based observations in non-drought years, while the VPM model performed best, followed by the VI, GR and TG model in drought years that may be ascribed to the VPM model incorporating a satellite-based water index.

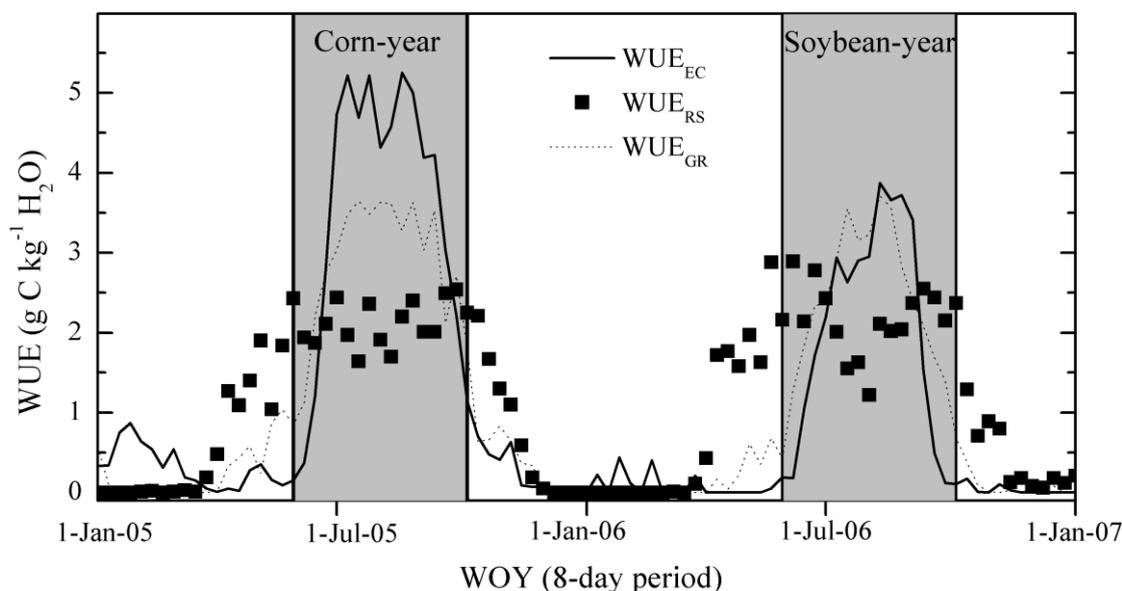


Figure 7. Seasonal dynamics in ecosystem WUE from flux tower measurements (WUE_{EC}), predicted from MODIS products (WUE_{RS}), and estimates based on MODIS EVI data (WUE_{GR}) at the flux tower site US-Ro1 during 2005 (corn) and 2006 (soybean).

In addition to this, ecosystem WUE ultimately reflected the photosynthetic productivity per amount of water consumption; therefore, how to explain and quantify the variability of crop WUE from the environmental mechanisms remains essential. This study found that the WUE estimates from MODIS GPP and ET products performed poorly in capturing the seasonal dynamics of tower-based observations, which were mainly attributed to the uncertainties in the GPP estimates. A number of studies have indicated this deficiency [65,66]. Various efforts are ongoing to improve the GPP performance including the algorithm and data inputs. Xiao *et al.* [67,68] developed the satellite-based VPM model using MODIS EVI, land surface water index (LSWI) and climate data, and the predicted GPP values agreed reasonably well with observed GPP for both deciduous broadleaf forest and evergreen needleleaf forest. Wu *et al.* [69] calibrated the GR model for estimating monthly GPP at a wide range of ecosystems and provided better GPP estimates than the TG model and the standard MODIS GPP product. Peng *et al.* [70] also developed a simple model using a chlorophyll-related vegetation index to estimate crop GPP and accurately detected GPP variations in both irrigated and rainfed croplands in three Nebraska AmeriFlux sites. Based on these studies and our own work, there remains a need to improve the current MODIS GPP product and then re-evaluate our ability to estimate WUE.

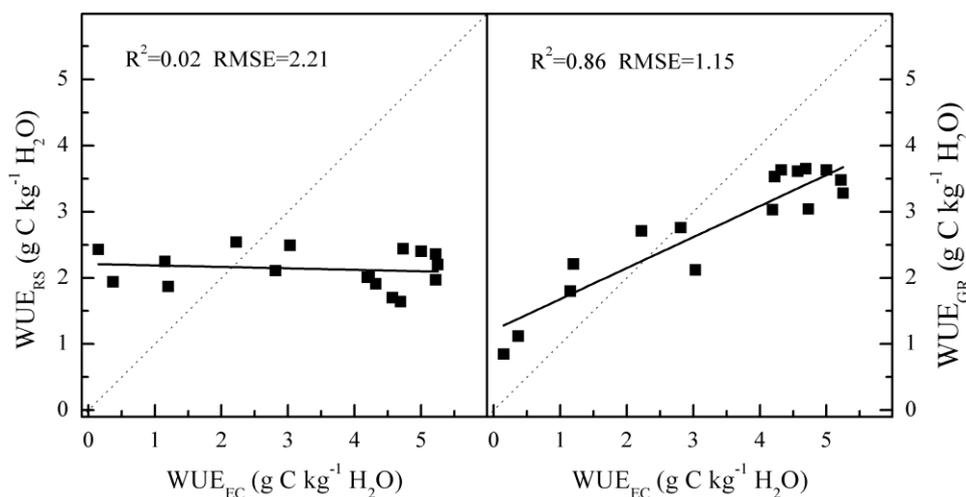


Figure 8. A linear comparison between ecosystem WUE from flux tower measurements (WUE_{EC}) with predictions from MODIS products (WUE_{RS}) and estimates based on MODIS EVI data (WUE_{GR}), respectively at the flux tower site US-Ro1 during the growing season of 2005 (corn).

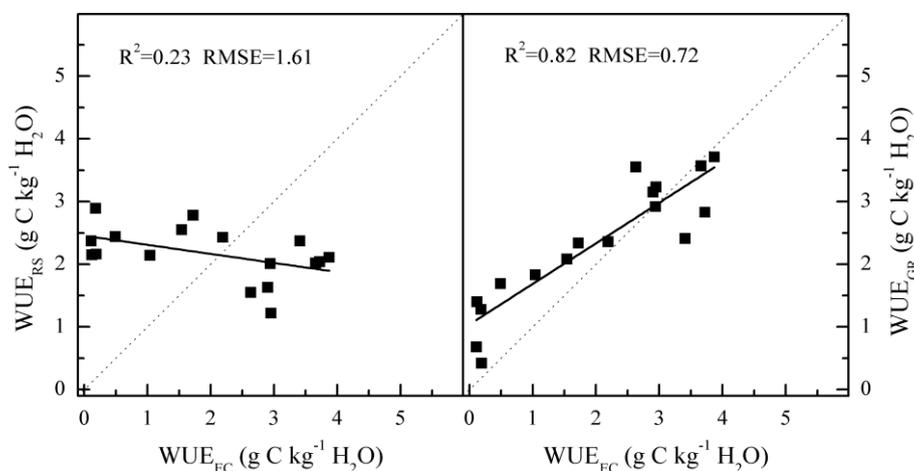


Figure 9. A linear comparison between ecosystem WUE from tower measurements (WUE_{EC}) with predictions from MODIS products (WUE_{RS}) and estimates based on MODIS EVI data (WUE_{GR}), respectively at the flux tower site US-Ro1 during the growing season of 2006 (soybean).

4. Conclusions

Quantitatively evaluating the spatiotemporal patterns of ecosystem WUE and the underlying mechanisms are of great significance for understanding the effect of hydrological change on the ecosystem carbon budget. In this study, we assessed the driving environmental controls on crop WUE at corn/soybean rotation fields. As a proxy of vegetation responses to environmental conditions, time-series MODIS EVI data showed a strong correlation with the variability in crop WUE. Regional and global WUE have been estimated by integrating MOD17 GPP and MOD16 ET products. However, we observed large discrepancies between WUE_{RS} and WUE_{EC} for a few 8-day periods. The overall $RMSE$ for corn and soybean were $2.24 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ and $1.58 \text{ g C kg}^{-1} \text{ H}_2\text{O}$, which was mainly attributed to the great

uncertainties in the MODIS GPP product. Fortunately, an alternative approach that is solely based time-series EVI data performed reasonably well in capturing the seasonal variations in crop WUE from EC flux sites. *RMSE* during the growing season of corn and soybean improved to $0.79 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ and $0.66 \text{ g C kg}^{-1} \text{ H}_2\text{O}$. Independent validation also showed the model's potential for broad application. During the corn-planting year and soybean-planting year, the *RMSE* between WUE_{EC} with WUE_{RS} and WUE_{GR} were $2.21 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs $1.15 \text{ g C kg}^{-1} \text{ H}_2\text{O}$, and $1.61 \text{ g C kg}^{-1} \text{ H}_2\text{O}$ vs $0.72 \text{ g C kg}^{-1} \text{ H}_2\text{O}$, respectively. This study also revealed that MODIS WUE estimates from the perspective of C_3 and C_4 may be a reasonable method to predict the seasonal patterns in WUE of farmland systems. Such analyses will be helpful for agricultural policy makers and managers to plan and implement strategic goals of water resource management and food supply.

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Author Contributions

Xuguang Tang and Hengpeng Li. contributed equally to design this study and write this manuscript including the figures and tables. Tim J. Griffis, Xibao Xu, Zhi Ding and Guihua Liu contributed significantly to the discussion of results and manuscript refinement.

Conflicts of Interest

The authors declare no conflict of interest.

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