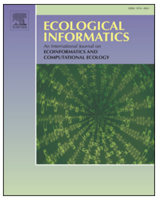
Ecological Informatics 35 (2016) 1–8

Contents lists available at ScienceDirect

Ecological Informatics

journal homepage: www.elsevier.com/locate/ecolinf



Hyperspectral indices based on first derivative spectra closely trace canopy transpiration in a desert plant

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ARTICLE INFO

Article history:
Received 26 November 2015
Received in revised form 10 June 2016
Accepted 22 June 2016
Available online 25 June 2016

Keywords:
Arid ecosystem
Canopy transpiration
Hyperspectral indices
Derivative spectra
Haloxylon ammodendron

ABSTRACT

A clear understanding of transpiration of arid ecosystems and its underlying mechanisms is critical for accurate prediction of long-term water and energy fluxes in such ecosystems, which have gradually been recognized to play major roles on a global scale. Unlike traditional measurements of transpiration that are generally time-consuming, expensive, and often unfeasible, remote sensing techniques such as hyperspectral indices are widely utilized as the only approach to obtain such information on a large scale. However, compared with other biochemical and biophysical parameters, few studies on hyperspectral indices have been applied to estimate canopy transpiration. In this study, we focused on a native dominant plant in the arid land of central Asia, *Haloxylon ammodendron*, to explore the featured spectra and to develop proper hyperspectral indices for estimating transpiration. This was based on a simultaneous dataset of original canopy-reflectance spectra as well as its first derivatives with transpiration estimated from sap flow. The results indicated that the derivative spectra-based indices are more effective for tracing canopy transpiration compared with its counterpart that was based on the original reflectance. The identified best index for estimating canopy transpiration was dSR(660,1040) based on the first-derivative spectra, which had a coefficient of determination (R^2) of 0.54. The index is also relatively stable concerning spectral resolutions. Results obtained in this study should help lay the basis for using remote sensing data to estimate transpiration.

1. Introduction

Globally, about 40% of the Earth's terrestrial surface is covered by arid and semi-arid ecosystems (Naithani et al., 2012). Understanding the physiological conditions of dry ecosystems and the underlying mechanisms is critical for accurate prediction of long-term variations of carbon, water, and energy fluxes in such ecosystems. Transpiration—defined as the process of water movement through a plant—is a basic process that is regulated over short time-periods by stomatal conductance (g_s) (McDowell et al., 2008). The efficient acquisition of field flux data for arid and semi-arid ecosystems needs to be addressed to improve current and future understanding of long-term ecosystem carbon, water, and energy fluxes (Naithani et al., 2012).

Sap flow measured using the Stem Heat Balance (SHB) or the Thermal Dissipation Probe (TDP) technique has been widely used to provide species-specific transpiration rates (Baldocchi, 2005; Čermák et al., 1995; Ewers et al., 2002) and for continuous estimation of leaf and canopy g_s since the 1980s (Granier, 1987; Grime and Sinclair, 1999; Xia et al., 2006; Huang et al., 2010). Although this method can be applied to various plants and can monitor over a continuous period of time, measurements of transpiration by the SHB and TDP methods can be invasive, time-consuming, expensive, and often unfeasible, which has led to increased attention being paid to remote sensing data to estimate transpiration.

The common approach of applying remote sensing data to estimate evapotranspiration generally involves energy balance, e.g., the surface temperature of the vegetation (Boegh et al., 1999), or more sophistical models like the Surface Energy Balance System (SEBS) (Su, 2002), Internalized Calibration (METRIC) model (Allen et al., 2007), and the Surface Energy Balance Algorithm for Land (SEBAL) model (Bastiaanssen et al., 1998). Although these algorithms can calculate the fluxes independently from land cover with remote sensing data inputs (Bastiaanssen et al., 1998), it is an indirect and complex approach that is based on remote sensing of the surface energy balance rather than establishing straightforward relationships between fluxes and reflectance (Devitt et al., 2011; Loukas et al., 2005).

With the development of hyperspectral remote sensing and imaging spectrometry, it is now possible to provide straightforward relationships

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http://dx.doi.org/10.1016/j.ecoinf.2016.06.004
1574-9541/

between various biological status parameters and reflected information. Although there are many empirical approaches for relationship analysis, vegetation indices remain a simple and popular method due to their ability to remove disturbances caused by external factors. Vegetation indices have also been proposed for use in monitoring biomass, phenology (periodic change), and the biochemical and physiological conditions of plants and canopies (Peñuelas and Filella, 1998), e.g., spectral indices were used for tracing photosynthetic efficiency (Gamon et al., 1992; Inoue et al., 2008) and photosynthetic pigments (chlorophyll and carotenoids) concentrations (Blackburn, 1998; Cheng et al., 2013; Wang and Li, 2012; Yi et al., 2014), as well as leaf area index estimations (Delegido et al., 2013; Gonsamo and Pellikka, 2012; Haboudane et al., 2004; Li and Wang, 2013; Liu et al., 2014).

Recently, more attention has been paid to quantifying physiological traits, including plant water status, through hyperspectral indices. However, compared with other parameters, there are few reported studies on transpiration or water potential. Only recently have a few remotely sensed vegetation indices been developed to assess water potential or transpiration (Dzikiti et al., 2010; Marino et al., 2014; Marshall et al., 2016). The study of Dzikiti et al. (2010) on Satsuma mandarin trees revealed that the water index (WI) and a narrow-band spectral ratio of the reflectance at 960 and 950 nm wavelengths gave the best predictions of midday stem (or xylem) water potential with $R^2 = 0.77$ and 0.79, respectively, but only for trees with severe drought stress. The stem (or xylem) water potential is the water status of non-transpiring leaves normally enclosed in darkened air-tight bags, which gives an indication of the water status of the tree's xylem as a function of the balance between transpired losses and water uptake from the soil (Dzikiti et al., 2010). However, there are fewer studies on transpiration. Marino et al. (2014) proposed that WI has a good correlation ($R^2 = 0.668$) with whole-plant transpiration of a drought-tolerant species, Olive (*Olea europaea* L.), but only the water index of R_{900}/R_{970} was tested in their research. A recent study by Marshall et al. (2016) on crops (cotton, maize, and rice) in the Central Valley of California suggested that the Hyperspectral Normalized Difference Vegetation Index (HNDVI) has a strong relationship ($R^2 = 0.68$) with transpiration. To the best of our knowledge, no other study has linked hyperspectral indices directly with transpiration, especially for drought-tolerant plants.

Furthermore, hyperspectral indices based on derivative spectra have been shown to reduce additive constants and to minimize soil background effects and to be a potentially feasible method for exploiting hyperspectral data in vegetated areas (Curran et al., 1990). Some types of so-called derivative indices (DIs) have already been used for estimating leaf nitrogen, chlorophyll variations, and fluorescence detection (Lamb et al., 2002; Zarco-Tejada et al., 2003). It has also been shown that chlorophyll-induced changes can be captured in the primary derivatives of the reflectance spectra (Kochubey and Kazantsev, 2007). This inspired us to examine whether derivative indices could also be used to trace plant transpiration.

The main objective of the present study was to fill the knowledge gap by examining the synchronous data of both transpiration and reflected spectra from which hyperspectral indices that closely trace the change of transpiration can be developed based either on the original or primary derivative spectra. In detail, the aims included: 1) to verify straightforward statistical relationships between transpiration and reflected/derivative spectra; 2) to develop corresponding hyperspectral indices either from original or primary derivative spectra to trace canopy transpiration; 3) to identify the best indices based on the different performances of hyperspectral indices. We selected a dominant native species from a desert environment, *Haloxylon ammodendron*, as the main material for the study. *Haloxylon ammodendron* is a shrub or a small tree that is well distributed in the arid land of northwestern China, which covers an area of 4.5×10^6 km^2 and accounts for nearly half of the territory of China (Zheng and Wang, 2014a), as well as in the arid land of central Asia.

2. Materials and methods

2.1. Study site

The sample plot (44°17′N,87°56′E; 475 m above sea level) was set inside the Integrated Remote Sensing Experimental Site (1 km × 1 km), which is located at the southern edge of the Gurbantonggut Desert in northwestern China and is 20 km north of Fukang Station of Desert Ecology, Xinjiang Institute of Ecology and Geography, Chinese Academy of Sciences (see Fig. 1 for location). This region has a continental arid temperate climate, with an annual mean temperature of 5.0–5.7 °C, but the extreme minimum and maximum temperature can reach −40 °C and 40 °C, respectively. The annual mean precipitation of this region is only 80–160 mm, and 40% occurs during the growing season (from May to October), while pan evaporation here can reach about 2000 mm (Li and Wang, 2012; Xu et al., 2007). The vegetation coverage of this plot is about 16%. *Haloxylon ammodendron* is the dominant species in this plot, and a few companion species, such as *Salsolapraecox*, *Erodium oxyrrhynchum*, and *Corispermum lehmannianum*, can be found during spring under the irrigation of snow-melt water (Zhao et al., 2009; Zheng and Wang, 2015). All field measurements were conducted in this plot.

2.2. Field measurements

2.2.1. Sap flow and canopy-scale transpiration

Six representative *Haloxylon ammodendron* trees were selected for sap flow measurement in the growing seasons from May to October of 2011 to 2014. Granier-type sensors (thermal dissipation probe method; Granier, 1985) were inserted at 20-mm depth into the tree trunk with diameters ranging from 5 to 16 cm at a height of 30 cm. To prevent direct solar heating and to minimize environmentally induced temperature variations, all Granier sensors were installed on the northern side of trees and sealed with silicone caulk to protect them from precipitation and moisture. Meanwhile, white foils were applied under the trees to protect the sensors from long-wave radiation from the ground (Zheng and Wang, 2015).

Sap flux density (m^3 m^{-2} s^{-1}) was calculated using the empirical calibration described in Lu et al. (2004) from recorded data by Granier sensors. All sensors were connected to a data logger (DT80, Thermo Fisher Scientific Pty Ltd., Australia), where data was recorded every 5 min during the growing season from May to October. All sensors and the data logger were powered by a 12-V battery that was charged by a solar panel. Canopy-scale transpiration (E) is expressed as sap flux on a sapwood area basis and was calculated from sap flux density and sapwood area (Schaeffer et al., 2000).

2.2.2. Canopy-reflectance spectra

Canopy hyperspectral spectra data (350–2500 nm in 1-nm steps) of the sap flow of six trees were recorded with a field spectroradiometer (ASD FR, USA). Measurements for each tree were always made in clear weather conditions once a month at key growth stages during the growing seasons from May to October of 2011 to 2014 except 2012 due to instrument failure. All spectra were measured with a 25° field-of-view at the nadir direction about 1-m above the tree. A white Spectralon reference panel was used before each canopy measurement to convert the spectral radiance measurements to reflectance. Five scans were made every time and were averaged to produce the final canopy spectra. Measurements each month were always taken around 12:00 local time to maintain similar sun heights.

2.3. Reported indices for estimating transpiration/water potential

Some hyperspectral indices have been reported to estimate transpiration or plant water potential, and these have mostly been based on ratios or normalized ratios (Dzikiti et al., 2010; Eitel et al., 2006;

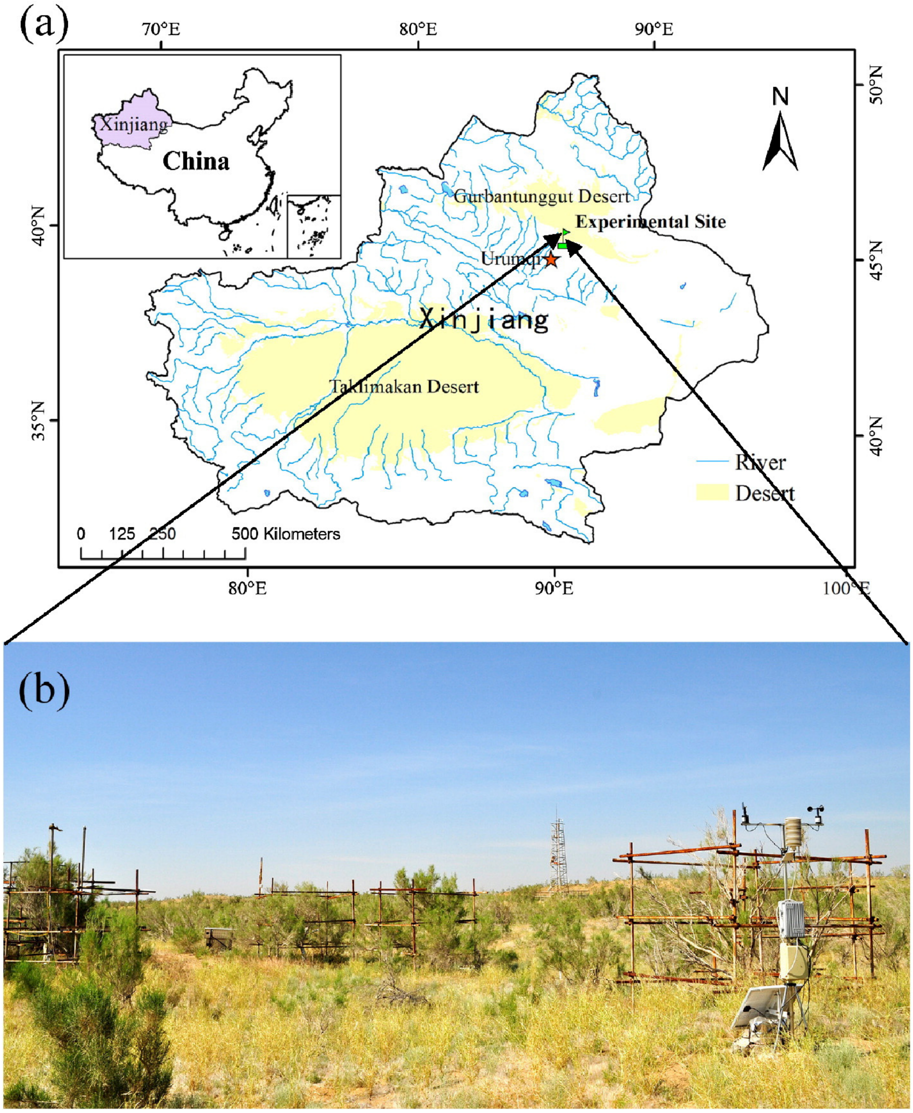

Fig. 1. Location of experimental site (a) and *Haloxylon ammodendron* plot (b).

Marino et al., 2014; Marshall et al., 2016; Stimson et al., 2005). In this study, seven reported indices from the published literature (Table 1) were selected and validated with our measured datasets. To the best of our knowledge, except for the study on crop transpiration by Marshall et al. (2016), only one attempt by Marino et al. (2014) was published to assess whole-tree transpiration using canopy spectral reflectance indices. Nevertheless, we have included indices for water potential as well due to its inherent links with transpiration. For each index, a polynomial regression was fit between the index values and the plant transpiration to be predicted.

Table 1
Published hyperspectral indices for estimating transpiration or water potential.

Spectral index	Formula	Reference
Hyperspectral Normalized Difference Vegetation Index	$HNDVI = \frac{R_{814}-R_{672}}{R_{814}+R_{672}}$	Marshall et al. (2016)
Water Index	$WI = \frac{R_{900}}{R_{970}}$	Marino et al. (2014)
Normalized Difference Water Index	$NDWI = \frac{R_{860}-R_{1240}}{R_{860}+R_{1240}}$	Stimson et al. (2005)
Reflectance Index	R_{970}	
Normalized Difference Vegetation Index	$NDVI = \frac{R_{860}-R_{690}}{R_{860}+R_{690}}$	
Maximum Difference Water Index	$MDWI = \frac{R_{,\max1500-1750}-R_{,\min1500-1750}}{R_{,\max1500-1750}+R_{,\min1500-1750}}$	Eitel et al. (2006)
Simple Ratio Index	$SR = \frac{R_{960}}{R_{900}}$	Dzikiti et al. (2010)

2.4. Identification and evaluation of new spectral indices

Five common types of indices based on the original reflected spectra, as well as the first-derivative spectra from the original reflectance data, were applied for this study: (1) a simple reflectance (R) or derivative spectra (dR) index; (2) a simple ratio (SR) index; (3) a simple difference (SD) index; (4) a normalized difference (ND) index; and (5) a double-difference (DDn) index, which was designed to solve the "peak jump" of the first derivative of the reflectance in deriving chlorophyll because it represents the changes in the first derivative in the red-edge region where chlorophyll varies (Le Maire et al., 2004; Wang and Li, 2012) as shown in Eqs. (1)–(5):

$$R(\lambda1) = R_{\lambda1} \tag{1}$$

$$SR(\lambda1, \lambda2) = \frac{R_{\lambda1}}{R_{\lambda2}} \tag{2}$$

$$SD(\lambda1, \lambda2) = R_{\lambda1} - R_{\lambda2} \tag{3}$$

$$ND(\lambda 1, \lambda 2) = \frac{R_{\lambda 1} - R_{\lambda 2}}{R_{\lambda 1} + R_{\lambda 2}} \tag{4}$$

$$DDn(\lambda 1, \Delta) = 2R_{\lambda} - R_{\lambda - \Delta} - R_{\lambda + \Delta} \tag{5}$$

where R_{λ} is the reflectance at a certain wavelength λ when testing the reflectance indices, and the DIs based on the first-derivative spectra are termed with a prefix "d" as dR, dSR, dSD, dND, and dDDn, respectively.

A Spearman rank correlation was performed for all possible combinations of wavelengths for a given index type with a wavelength step of 5 nm based on field-measured datasets (a total of 60 synchronous data-pairs of canopy transpiration and reflectance). For each type of index, index values were calculated using two (or one) random available wavebands (or increments of wavebands, △) in the 350–2500-nm region, and polynomial regressions (linear to the first order) were fit between the index values of the given combination of wavebands and the sap flux density recorded at the time of spectra measurement. The coefficient of determination (R^2) and the root mean square error (RMSE; Eq. (6)) were used to select the best band combination of each type of index and to compare different type of indices in this study. For a given type of index, the best band combination should have the highest R^2 and the lowest RMSE, and the best type of index should also have the highest R^2 and lowest RMSE.

$$\text{RMSE} = \sqrt{\frac{\sum_{j=1}^{n} \left(y'_j - y_j\right)^2}{n}} \tag{6}$$

with y_j' indicating the predicted value, y_j indicating the observation for the jth spectrum, and n indicating the number of spectra.

3. Results

3.1. Variations in canopy-scale transpiration and reflectance spectra and their correlations

Although measurements of both canopy-scale transpiration and reflectance were continuously carried out across several growing seasons from 2011 to 2014, synchronous data were only available in 2011 and 2014 due to an unexpected failure of the spectroradiometer in 2012 and poor-quality sap flow measurements in 2013 that failed to pass the quality check. Hence, all further analysis was based on the synchronous measurements in 2011 and 2014. The sap flux density values of the six representative *Haloxylon ammodendron* trees recorded in 2011 when the spectra measurements were conducted each month were extracted for the canopy transpiration calculation and are presented below as an example.

Seasonal variation in the sap flow, as well as the canopy spectra, was evident throughout the growing seasons (Fig. 2). The maximum transpiration rate, which occurred in September of tree No. 4, reached a value of 7.7×10^{-5} m^3 m^{-2} s^{-1} while the minimum value was 2×10^{-6} m^3 m^{-2} s^{-1}, which occurred at the end of the growing season in October of tree No. 2. In general, at the start and end of the growing season (June and October, respectively), the transpiration rates were quite low with values around 1×10^{-5} m^3 m^{-2} s^{-1}. The transpiration peaked in September with values around five times that of the values recorded in June and October.

Fig. 2(b) shows the canopy reflectance of six representative *Haloxylon ammodendron* trees measured from June to October. Generally, the canopy had the lowest reflectance at the start of the growing season (June). Although monotonically seasonal variations of the reflectance values associated with transpiration cannot be identified through the whole wavelength range (350–2500 nm), peak and trough characteristics can easily be identified within the domains of some bands. Troughs can be identified around wavelengths 1000 nm and 1200 nm, while peaks can be captured around wavelengths 800 nm and 1300 nm.

Fig. 3 illustrates the correlation analysis results for each wavelength of both the original reflectance and the derivative spectra. The results clearly show that the correlation coefficients between transpiration and the original reflectance from wavelength 350 nm to 2500 nm are within limits ranging from approximately −0.40 to 0.35 while the best correlation between the first-derivative spectra and transpiration reached −0.63 at 670 nm. In addition, positive or negative significant correlations at the wavelengths around 700 nm and 1200 nm were identified. On the other hand, insignificant correlations (correlation coefficients around 0) between the first-derivative spectra values and transpiration can be found within the wavelength domains of 850–900 nm and 950–1100 nm.

3.2. Published indices

As indicated in Table 2, no published indices have shown a very good relationship with canopy transpiration of *Haloxylon ammodendron.* The coefficients of determination varied from the lowest of 0.06 (SR) to the highest of 0.21 (HNDVI), while RMSE was estimated to be within the range from 2.2×10^{-5} m^3 m^{-2} s^{-1} (HNDVI) to 2.3×10^{-5} m^3 m^{-2} s^{-1} (SR). Although HNDVI had a statistically significant relationship ($p < 0.01$) with whole-tree transpiration of *Haloxylon ammodendron*, its performance was yet to be satisfied ($R^2 = 0.21$).

3.3. Best indices identified from original reflectance

Five types of indices based on original canopy reflectance were examined for their potential to trace canopy transpiration. The results revealed that all of the best indices that were identified from the original reflectance measurements poorly estimated tree transpiration (Table 3). In detail, the highest coefficient of determination (R^2) of the

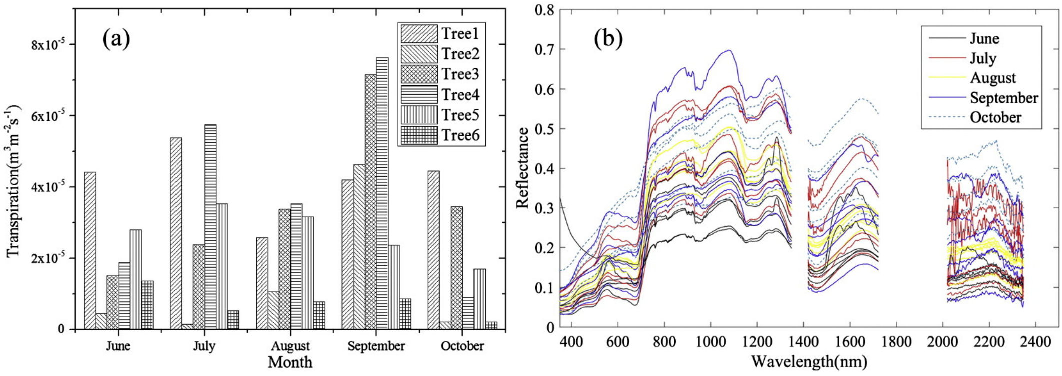

Fig. 2. Seasonal variation of transpiration (a) and canopy reflectance (b).

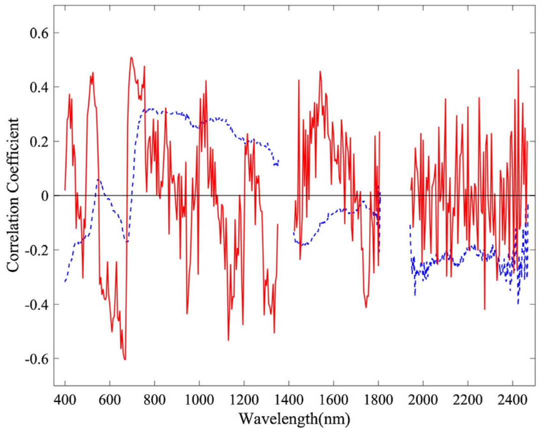

Fig. 3. Correlation between reflectance/the first-derivative spectra and transpiration.

R-type indices could only reach 0.11 at 2425 nm with the lowest RMSE of 2.2×10^{-5} m^3 m^{-2} s^{-1}. Similarly, the simple ratio (SR) and the normalized difference (ND) types of indices had low coefficients of determination (R^2) with transpiration. The identified SR and ND types of indices with the same band combination of 1525 nm and 2150 nm had the best correlation with transpiration ($R^2 = 0.22$ and $R^2 = 0.23$, respectively). The double-difference (DDn) type of indices had slightly higher coefficients of determination (R^2) with transpiration. The DDn index of the wavelength 2320 nm with a 50-nm △ had an R^2 of 0.35 with transpiration.

Among the five types of best indices based on reflectance, the simple difference (SD) type of indices, with the band combination of 2315 nm and 2370 nm, was more effective at estimating transpiration than any other type of indices and any other band combinations. The R^2 of SD (2315,2370) for estimating transpiration was 0.42. The regression performance on transpiration (R^2 and RMSE) based on the SD type of indices with different band combinations is illustrated in Fig. 4.

3.4. Derivative spectra-based indices

Similarly, five types of indices with all combinations of wavelengths based on derivative spectra were examined for their performance in tracing canopy transpiration. Much better correlations were obtained for the derivative spectra-based indices with canopy transpiration, as illustrated in Table 4.

The simple derivative spectra (dR) index, which uses only the first-derivative values of reflectance of one wavelength, had a much higher correlation with transpiration compared its counterpart of using the original spectra ($R^2 = 0.31$ vs. 0.11). Furthermore, the dND and dDDn types of indices based on derivative spectra also had certain improvements compared with their counterparts that were based on the original reflectance spectra. The normalized difference (dND) index with the wavelength combination of 755 nm and 1195 nm had a coefficient of determination (R^2) of 0.36, while the double-difference (dDDn) index of the wavelength 1195 nm with a 500-nm △ wavelength had an R^2 of 0.44 with canopy transpiration.

Table 2
Performance of reported indices in estimating transpiration for *Haloxylon ammodendron.*

Spectral index	Coefficient of determination	RMSE ($\times 10^{-5}$)	*p*
Hyperspectral Normalized Difference Vegetation Index	0.21	2.2	<0.01
Water Index	0.12	2.2	<0.05
Normalized Difference Water Index	0.12	2.2	<0.05
Reflectance Index	0.07	2.3	<0.05
Normalized Difference Vegetation Index	0.18	2.2	<0.05
Maximum Difference Water Index	0.12	2.3	<0.05
Simple Ratio Index	0.06	2.3	<0.1

Table 3
Results of five types of spectral reflectance-based indices for transpiration.

Index type	λ1	λ2 (or△)	Slope ($\times 10^{-4}$)	Intercept ($\times 10^{-4}$)	R^2	RMSE ($\times 10^{-5}$)	*p*
R	2425	–	−0.80	0.43	0.11	2.3	<0.05
SD	2315	2370	11.76	0.21	0.42	**1.8**	<**0.01**
SR	1525	2150	1.13	−1.07	0.22	2.1	<0.01
ND	1525	2150	3.01	0.02	0.23	2.1	<0.01
DDn	2320	50(△)	9.16	0.38	0.35	2.0	<0.01

However, the best type of indices among the above five was found to be the dSR type. This type of index, based on the first-derivative spectra with the wavelength combination of 660 nm and 1040 nm, was identified as the most effective hyperspectral index to estimate canopy transpiration with an R^2 of 0.54. The performance of linear regression analysis on transpiration based on dSR types of derivative spectra-based indices is illustrated in Fig. 5. The best derivative spectra-based index dSR(660,1040) is more effective than SD(2315,2370), which was identified from original reflectance, as shown in Fig. 6.

4. Discussion

4.1. Reported indices vs. newly developed indices

Empirical relationships between hyperspectral indices and physiological traits associated with plant water status, including whole-tree transpiration and plant water potential, have been constructed in order to conduct physiological traits estimation (Dzikiti et al., 2010; Eitel et al., 2006; Marino et al., 2014; Stimson et al., 2005). Although may lack of definitude mechanisms, such a data-oriented approach is important and also is an inevitable step towards clarifying underlying mechanisms.

Previous studies have indicated that the relationship between indices and plant water status decreased with decreasing water stress, suggesting that some spectral indices might show limited sensitivity to low and moderate levels of water stress (Asner et al., 2004; Ceccato et al., 2002; Gao, 1996; Imanishi et al., 2004; Peñuelas et al., 1993; Pu et al., 2003; Serrano et al., 2000; Stimson et al., 2005). It has been proposed that the WI and a narrow-band spectral ratio of reflectance at 960 nm and 950 nm wavelengths can give the best predictions of the midday stem (or xylem) water potential (Dzikiti et al., 2010). However, we could not find any hyperspectral index that can be applied for plants under severe drought stress, as in the case we are dealing with here.

The sensitivity of spectral indices to changes in plant water status is species-dependent (Eitel et al., 2006). In this study, hyperspectral indices that were proposed in previous studies (e.g., Marino et al., 2014; Marshall et al., 2016) were tested for tracing transpiration of the drought-tolerant plant *Haloxylon ammodendron*, a stem-succulent shrub and a typical desert plant that is dominant in most areas of central Asia deserts, which are under severe drought stress (Li and Wang, 2012). Apparently, none of them including HNDVI were able to trace the canopy transpiration of *Haloxylon ammodendron,* although HNDVI was suggested to have a strong relationship with crop transpiration (Marshall et al., 2016). The specific canopy structure of *Haloxylon ammodendron*, as well as serious soil background effects, may be important reasons for the low performance of HNDVI in tracing tree transpiration in arid land.

Several studies have highlighted that the use of wavelengths in the NIR are less sensitive to changes in leaf water status than wavelengths in the short-wave infrared (SWIR, 1300–2500 nm) range of the electromagnetic spectrum (Carter, 1991; Ceccato et al., 2002; Danson et al., 1992; Tucker, 1980). The canopy reflectance around wavelengths 1400 nm and 2500 nm are quite noisy, so they are not applicable on a canopy scale. We did not prove that any WIs, which are established

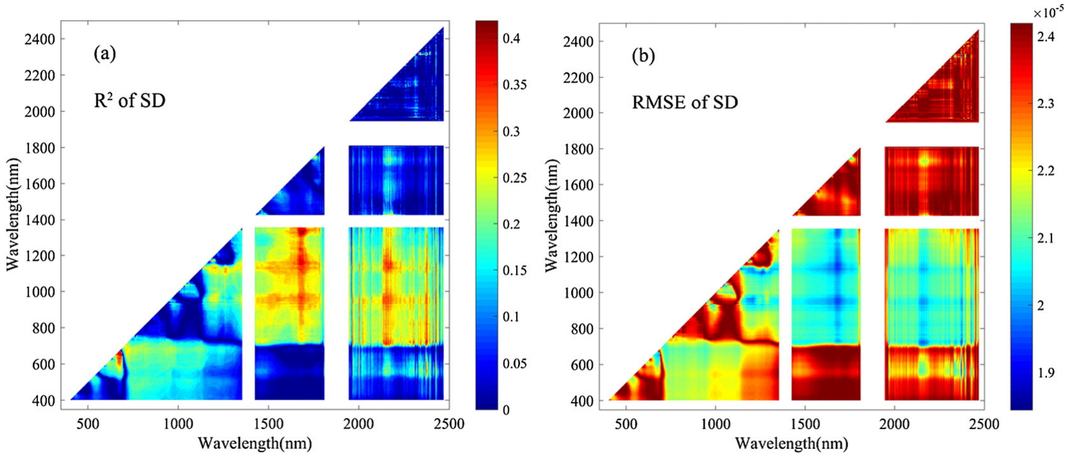

Fig. 4. Matrices representing the R^2 (a) and RMSE (b) of transpiration prediction with SD type of indices based on reflectance.

Table 4
Results of five types of derivative spectra-based indices for transpiration.

Index type	λ1	λ2 (or△)	Slope ($\times 10^{-4}$)	Intercept ($\times 10^{-4}$)	R^2	RMSE ($\times 10^{-5}$)	*p*
dR	670	–	−924.25	0.25	0.31	2.0	<0.001
dSD	755	1195	387.83	0.15	0.38	1.9	<0.001
dSR	660	1040	−0.11	0.20	0.54	**1.6**	**<0.001**
dND	755	1195	0.08	0.24	0.36	1.9	<0.001
dDDn	1195	500 (△)	−91.51	0.05	0.44	1.8	<0.001

indicators of plant water content, were very successful for estimation of transpiration at the canopy level as judged from the coefficients of determination.

Overall, the superiority of the newly developed indices may primarily be because they were identified based on transpiration rather than water potential, but the severe drought stress that none of the former studies dealt with might also be an important reason. In addition, the specific canopy structure of the drought-tolerant plant, as well as serious soil background effects, may also play important roles.

4.2. Original reflectance vs. first-derivative spectra

Much better indices based on the derivative spectra were identified in this study for estimating canopy transpiration. A good index generally includes information from both sensitive and inertial bands. Sensitive bands can closely capture the variations of transpiration while inertia bands for transpiration may reduce measurement errors. The identified best index based on derivative spectra dSR(660,1040) closely followed this rule. The wavelength of 1040 nm is within the range of stable bands while 660 nm is within the sensitive bands. The superiority of derivative spectra-based indices may partially rely on the fact that they general have more sensitive bands, as shown in Fig. 3, which clearly indicated that the best correlation of the first-derivative spectra (−0.63) was much better if compared with most correlation coefficients of original reflectance, which ranged from approximately −0.40 to 0.35.

Furthermore, soil background reflectance has been claimed to be the main reason for the superiority of the derivative spectra-based indices over the original reflectance-based indices, since soil background reflectance has been estimated to make a large contribution of reflected energy to the canopy-scale reflectance (Rondeaux et al., 1996). Derivative spectrum analysis has the advantage of reducing additive constants and minimizing such soil background effects and is a potential method for exploiting hyperspectral data in vegetated areas (Curran et al., 1990), especially for analyzing hyperspectral remote sensing data with soil background effects (Imanishi et al., 2004).

However, several original reflectance-based are available to reduce soil background effects, e.g., the soil-adjusted index (SAVI) by Huete (1988), the enhanced vegetation index (EVI) by Huete et al. (2002), and its modified version (EVI2) by Jiang et al. (2008). In order to further illustrate the effects of soil background reflectance on canopy transpiration estimation, we conducted linear regression analyses on measured transpiration with these types of indices. Both broad- and

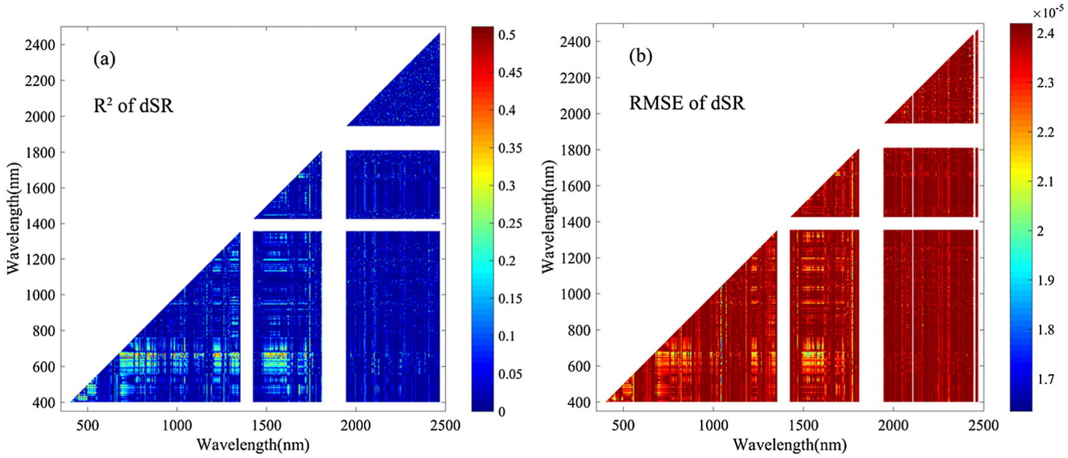

Fig. 5. Matrices representing the R^2 (a) and RMSE (b) of transpiration prediction with the dSR type of indices-based derivative spectra.

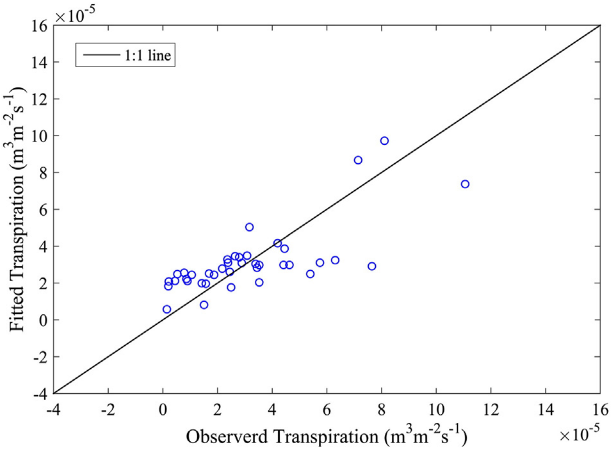

Fig. 6. Scatter diagrams of observed and estimated transpiration from the best index, dSR(660,1040), identified from derivative spectra.

narrow-band values were calculated for SAVI and EVI, where broadband indices used the average values of wavelengths while narrow-band indices used each wavelength within the domains of SAVI and EVI that firstly reported (Huete et al., 1994; Rocha and Shaver, 2009). The parameter L for SAVI was varied from 0 to 1 by an increment of 0.1. All possible combinations (different wavelengths or L) of SAVI or EVI were investigated for their relationships with transpiration. The results showed that the coefficients of determination (R^2) of EVI, EVI2, and SAVI with canopy transpiration were only 0.19, 0.20, and 0.21 ($L = 1$), respectively, in broadband mode. Furthermore, the R^2 of the identified best combination in narrow-band mode was 0.22 (SAVI, with $L = 1$). Astonishingly, the identified best narrow-band combinations (with the largest R^2 and lowest RMSE) for both EVI2 and SAVI were consistently found to be 841 nm and 670 nm.

The poor performance of both EVI and SAVI types may, on one hand, suggest that other factors besides soil background are also playing important roles if these types of indices functioned well as they were developed for. A leaf-scale study of transpiration and reflectance in which there was no effect contributed from soil background, again showed that derivative spectra-based indices performed much better than any other type of indices (Jin and Wang, unpublished). On the other hand, it is also possible that these types of indices have not minimized the soil background effects as claimed and are not suitable analyzing canopy transpiration. However, no matter what the reason is, the derivative spectrum analysis as applied in this study has largely eliminated all these effects, including soil background, and thus proves to be a feasible way for tracing canopy transpiration.

4.3. Stability of identified indices based on derivative spectra

In order to examine the stability of identified indices to spectral resolutions, we created three reflectance and corresponding derivative spectra at the resolutions of 1 nm, 5 nm, and 10 nm, respectively. This is an important step towards applying satellite-borne hyperspectral data to monitoring canopy-scale transpiration. Currently, the approximated bands at 10-nm intervals are close to the specification of some hyperspectral sensors, such as Hyperion and AVIRIS (Imanishi et al., 2004).

When we checked the performance of the best type of index (dSR) based on the derivative spectra at a wavelength step of 1 nm, we obtained a more effective derivative spectra-based index, dSR(647,1040), with a coefficient of determination (R^2) of 0.57. At 5-nm resolution, the best index was found to be dSR(660, 1040) with an R^2 of 0.54.

Indices with a wavelength step of 10 nm for the estimation of transpiration were also examined. The best index of the SR type to trace canopy transpiration was with the same band combination as that of dSR(660,1040), obtained with a wavelength step of 5 nm, while the best band combination of the dND type of index was found to be dND(620,1530) with an R^2 of 0.40.

4.4. Further study

To the best of our knowledge, there are very few studies that have ever applied hyperspectral indices to estimate transpiration. The importance of this study lies in that it has filled this knowledge gap, although the underlying physical and physiological mechanisms of the identified indices with transpiration remain a challenge.

Furthermore, we realized that all possible error sources related to both transpiration and reflectance measurements should be taken into account in future studies. It has been argued that sap flow methods (e.g., thermal dissipation probe, heat-pulse velocity) have different sensitivities to errors in actual sap flow estimates (González-Altozano et al., 2008; Madurapperuma et al., 2009; Steppe et al., 2010). In this study, Granier sensors (TDP method) were used for sap flux density measurements. Previous research on American beech (*Fagus grandifolia Ehrh.*) indicated that the TDP method underestimates the actual flow rate (Steppe et al., 2010). Besides, the sap flux density calculation involved a power function to estimate the sapwood area from the stem diameter (Zheng and Wang, 2014b), which could also lead to transpiration estimation errors. How to identify noise-resistant indices remains a challenge for future studies.

In addition, the sensitivity of spectral indices to changes in plant water status is often considered to be species-dependent (Eitel et al., 2006; Peñuelas et al., 1997; Sinclair et al., 1971). As such, other desert plants, for instance, *Tamarix ramosissima*, should also be addressed in following studies. In addition, only the first-derivative spectra have been extensively examined. It is still necessary to check whether there are effective or better indices based on the second-derivative spectra to detect transpiration.

Even so, we foresee that the identified dSR indices from the derivative spectra will have wide applications for rapid estimation of transpiration, especially in arid environments where soil background information plays a dominant role in reflected information.

5. Conclusions

Both published and newly developed hyperspectral indices have been examined for their applicability for estimating canopy transpiration of a drought-tolerant plant in a desert environment. The results suggest that the best indices identified from original reflectance are less effective at tracing seasonal variations in transpiration, while the derivative spectra-based indices can closely trace canopy transpiration. The identified best index was dSR(660,1040), which is based on the first-derivative spectra and had a coefficient of determination (R^2) of 0.54. This index is also relatively stable concerning spectral resolutions, which had similar bands at different resolutions. The results of this study should provide the basis for using remote sensing data for the estimation of transpiration.

Acknowledgments

Funds from the “973” Program (Grant No. 2012CB956204) and the NSFC project (Grant No. 41371364) are gratefully acknowledged.

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