Normalized difference spectral indices for estimating photosynthetic efficiency and capacity at a canopy scale derived from hyperspectral and CO\textsubscript{2} flux measurements in rice

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Received 30 December 2006; received in revised form 30 March 2007; accepted 21 April 2007

Abstract

We explored simple and useful spectral indices for estimating photosynthetic variables (radiation use efficiency and photosynthetic capacity) at a canopy scale based on seasonal measurements of hyperspectral reflectance, ecosystem CO\textsubscript{2} flux, and plant and micro-meteorological variables. An experimental study was conducted over the simple and homogenous ecosystem of an irrigated rice field. Photosynthetically active radiation absorbed by the canopy (APAR), the canopy absorptivity of APAR (fAPAR), net ecosystem exchange of CO\textsubscript{2} (NEEC\textsubscript{CO2}), gross primary productivity (GPP), photosynthetic capacity at the saturating APAR (\(P_{\text{max}}\)), and three parameters of radiation use efficiency (\(ε_N\): NEE\textsubscript{CO2}/APAR; \(ε_G\): GPP/APAR; \(φ\): quantum efficiency) were derived from the data set. Based on the statistical analysis of relationships between these ecophysiological variables and reflectance indicators such as normalized difference spectral indices (NDSI\([i,j]\)) using all combinations of two wavelengths (\(i\) and \(j\) nm), we found several new indices that were more effective than conventional spectral indices such as photochemical reflectance index (PRI) and normalized difference vegetation index (NDVI = NDSI\[near-infrared, red\]). \(ε_G\) was correlated well with NDSI\[710, 410\], NDSI\[710, 520\], and NDSI\[530, 550\] derived from nadir measurements. \(φ\) was best correlated with NDSI\[450, 1330\]. NDSI\[550, 410\] and NDSI\[720, 420\] had a consistent linear relationships with fAPAR throughout the growing season, whereas conventional indices such as NDVI showed very different relationships before and after heading. Off-nadir measurements were more closely related to the efficiency parameters than nadir measurements. Our results provide useful insights for assessing plant productivity and ecosystem CO\textsubscript{2} exchange, using a wide range of available spectral data as well as useful information for designing future sensors for ecosystem observations.

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Keywords: CO\textsubscript{2} flux; Eddy covariance; fAPAR; GPP; Hyperspectra; Radiation use efficiency; Spectral index

1. Introduction

Assessment of photosynthetic functioning is one of the most important bases for the diagnosis and prediction of plant growth, as well as carbon exchange between ecosystems and the atmosphere. A great deal of research effort has been directed towards the assessment of crop yield and ecophysiological variables using remote sensing in optical, thermal, and microwave wavelength domains together with modeling approaches (e.g., reviews by Moran et al., 1997; Inoue, 2003; Olioso et al., 2005). Remotely sensed optical signatures have proved useful for estimating ecological variables such as leaf area index (LAI) and the absorptivity of photosynthetically active radiation (fAPAR; Asrar et al., 1984; Daughtry et al., 1983; Huete, 1988) that affect photosynthetic capacity. The relationship between fAPAR and spectral indices such as normalized difference vegetation index (NDVI) have been examined in detail with theoretical and experimental analyses (Asrar et al., 1989; Baret & Guyot, 1991; Myneni & Williams, 1994). Several important physiological variables, such as chlorophyll and nitrogen concentration, that affect
photosynthetic efficiency are also related to reflectance signatures (e.g., Inada, 1985; Inoue et al., 1998; Gitelson & Merzlyak, 1997; Yoder & Pettigrew-Crosby, 1995). It is obvious that efficiency and capacity are related to each other during long growth periods. However, in the context of ecosystem monitoring at high temporal resolution, we use the term “photosynthetic-efficiency variable” to indicate photosynthetic rates per unit of absorbed radiation and the term “photosynthetic-capacity variable” for potential photosynthesis at canopy scales, such as fAPAR and the canopy photosynthesis at the saturating APAR \( (P_{\text{max}}) \). In other words, the former is related to “rate”, whereas the latter is related mainly to “size”. Furthermore, stomatal or canopy conductance and canopy transpiration are also estimated using remotely sensed canopy temperatures with energy balance models (e.g., Inoue et al., 1990, 1994; Olioso et al., 1999; Taconet et al., 1995). These variables strongly control photosynthetic efficiency. Nevertheless, direct estimation of photosynthetic efficiency and capacity is an important research target for remote sensing.

In the past few decades, remote sensing has become more and more crucial in the study of biogeochemical cycles such as carbon, water, and energy exchange between ecosystems and the atmosphere in the context of global climate change (e.g., Grace, 2005; Roy & Saugier, 2001). One recent effort for systematic data acquisition and analysis is the Spectral Network (SpecNet) proposed by Gamon et al. (2006). Advanced concepts, methodologies, or achievements in agricultural remote sensing have been applied to various types of natural and managed ecosystems. For example, the use of fAPAR in a simple mechanistic model (e.g., Monteith, 1977) has been employed in a range of applications for rough assessment of net primary productivity (NPP) at various scales using remote sensing (e.g., Goetz et al., 1999; Maisongrande et al., 1995; Potter et al., 1993; Ruimy et al., 1994; Turner et al., 2002; Verostraete et al., 1996).

This simple approach using fAPAR and radiation (or light) use efficiency \( (\varepsilon) \) has been widely used to estimate crop biomass, yield, or NPP (e.g., Choudhury, 2000). fAPAR is estimated from spectral indices such as NDVI \( (\frac{R_{\text{NIR}} - R_{\text{red}}}{R_{\text{NIR}} + R_{\text{red}}}) \) or a simple ratio \( (SR = \frac{R_{\text{NIR}}}{R_{\text{red}}}) \); e.g., Asrar et al., 1984; Baret & Guyot, 1991; Kumar & Monteith, 1982) and applied to a model (e.g., Nouvellon et al., 2000; Ruimy et al., 1994), where \( R_{\text{NIR}} \) and \( R_{\text{red}} \) are reflectance at near-infrared and red wavelength regions, respectively (hereafter, the term Rx indicates spectral reflectance at a wavelength \( x \) nm). The relationship is little affected by pixel heterogeneity, LAI, or variation in leaf orientation and optical properties (e.g., Pinter et al., 1985), but is affected by background, atmospheric, and bidirectional effects (Myneni & Williams, 1994) and by phenological stages and senescence. For instance, the NDVI-fAPAR relationship is largely different between before and after heading (anthesis) in most crops (e.g., Asrar et al., 1989; Choudhury, 2000; Daughtry et al., 1983; Inoue & Iwasaki, 1991; Inoue et al., 1998). In this approach, \( \varepsilon \) is first defined as the ratio of dry matter production (dDM) to APAR for season-long periods (e.g., Shibles & Weber, 1966). \( \varepsilon \) may be assumed to be constant under non-stressed conditions, but it is affected by stresses, phenological stages, and the physical environment (Choudhury, 2000; Kimiy et al., 1989; Sinclair, 1994). Hence, it may be inappropriate to assume that \( \varepsilon \) is constant and that the fAPAR-NDVI relationship is consistent for entire growth periods, especially when the model is applied to the assessment of canopy carbon exchange at a short (e.g., daily) time resolution over different phenological stages.

The photochemical reflectance index \( (\text{PRI} = [R_{531} - R_{570}]/[R_{531} + R_{570}]) \) is closely related to photosynthetic radiation use efficiency of plant leaves (Gamon et al., 1992; Peñuelas et al., 1995). R531 is presumed to detect the photochemical reaction in the xanthophyll cycle that dissipates excess light to protect the photosynthetic apparatus, while R570 is used as a reference assumed not to be affected by changes in short-term stress events (Peñuelas & Filella, 1998). Its simplicity, using only two wavelengths, is an attractive feature since it may meet the specifications for a range of available airborne and satellite sensors; thus a number of studies have examined the usefulness of PRI using various datasets and approaches (Barton & North, 2001; Drolet et al., 2005; Filella et al., 1996; Gamon et al., 1997; Inoue & Peñuelas, 2006; Rahman et al., 2001; Thenot et al., 2002; Trotter et al., 2002). Nevertheless, its applicability at canopy or ecosystem scales is not well known, and the use of remotely sensed signatures in the assessment of primary productivity (NPP or gross primary productivity, GPP) and net ecosystem CO2 flux (NEE_CO2) awaits further methodological innovations. Synergy of remote sensing signatures in ecosystem functioning models that include photosynthetic processes is promising (e.g., Inoue & Olioso, 2006), but simple and direct means are still a very attractive approach. Nevertheless, canopy-scale investigations of PRI and other spectral indices based on \textit{in situ} measurements of CO2 flux and hyperspectral measurements over homogenous ecosystems are still lacking (e.g., Peñuelas & Inoue, 2000), so that useful indices may yet be undiscovered.

Therefore, the objective of this study was to explore the significant and/or consistent relationships for remote sensing of photosynthetic-efficiency and-capacity variables such as \( \varepsilon \) and fAPAR. We made seasonal measurements of hyperspectral reflectance, ecosystem CO2 flux, and plant and micrometeorological variables over an irrigated rice field. The dataset from this simple and homogenous ecosystem facilitates efficient extraction of more significant relationships. In general, hyperspectral measurements allow various analyses such as multiple linear regression, principal component regression, partial least squares regression, and derivatives (e.g., Adams et al., 1999; Grossman et al., 1996; Takahashi et al., 2000), or assimilation techniques using a radiative transfer model such as PROSPECT+SAIL (e.g., Jacquemoud, 1993). Nevertheless, here we focus mainly on the comparative usefulness of the simple normalized difference spectral indices (NDISIs) using narrow band reflectance, instead of the whole spectrum for wider applications.
2. Materials and methods

2.1. Experimental site

The experimental site was a typical paddy field area in Tsukuba, central part of Japan (36°03’N, 140° 01’E, 15 m above sea level). Measurements were made in an irrigated rice paddy field (100×50 m) in 2003 and 2004. The field was surrounded by similar rice fields extending the area to 1.5×1.0 km. The soil was clay loam that was classified to grey lowland paddy soil (Cultivated Soil Classification Committee of Japan, 1995) and typic endoaquepts (Soil Survey Staff, 1992). Rice seedlings (Oryza sativa L., cv. Koshihikari) were transplanted in early May and harvested in mid-September. The paddy field was managed based on standard management practices for the region. The field was flooded all the time except for a mid-summer drainage period of about a week and the pre-harvest period, which is the most common practice for rice cultivation in Japan.

2.2. Hyperspectral reflectance measurements

Canopy reflectance spectra were obtained under clear sky conditions near midday using a portable spectro-radiometer (FieldSpec- FR, ASD). Spectral range and the field of view of the sensor were 350–2500 nm and 25°, respectively. Spectral resolution (full-width-half-maximum; FWHM) was 3 nm for the region of 350–1000 nm and 10 nm for 1000–2500 nm, while the sampling interval was 1.4 nm and 2 nm for each region, respectively. These signatures were used to derive spectra at 1 nm interval using cubic spline interpolation functions. We used these spectral data at 1-nm intervals in this study because they could carry the maximum information at narrow wavelengths. The spectrometer was equipped with a 2-m optical fiber to allow measurements from higher positions. Reflectance measurements were taken at nadir-looking and off-nadir angles (40–45°) from 2 m above the canopy. The off-nadir measurements were added because we presumed that they would carry more physiological information on photosynthetic efficiency since little background is viewed within the field of view (Takebe et al., 1990) and because the increasing number of sensors would allow directional measurements (Chen et al., 2003). More than 30 measurements were made each time, moving over the canopy, and averaged for spectral analyses. Spectral reflectance was derived as the ratio of reflected radiance to incident radiance estimated by a calibrated white reference (Spectralon, Labsphere).

2.3. Flux measurements

Net ecosystem exchange of CO₂ (NEE_CO₂) was measured using an open-path eddy covariance system, which consisted of a sonic anemometer (DA-600, Kaijo) and an infrared gas analyzer (LI-7500, LI-COR). The sensors were mounted 3.0 m above the ground. Half-hour flux densities of CO₂, water vapor, sensible heat, and momentum were calculated from the covariance between the vertical wind velocity, w, and the respective quantities. The effect of air density fluctuations on the measurement of CO₂ and water vapor fluxes was corrected following Webb et al. (1980). Quality control of the fluxes was based on the standard methodology as described in a previous report (Saito et al., 2005). We assumed that the measured flux was representative for the field since all surrounding rice fields were managed by similar standard practices. It was also confirmed that the majority of the footprint was within the field based on a preliminary assessment using a footprint model (Fan et al., 1992; Kljun et al., 2004) with in situ measurements of micrometeorological data and remotely-sensed images (Inoue et al., 2005).

2.4. Micrometeorological and plant measurements

Basic micrometeorological data were recorded throughout the growing season: global solar radiation and net radiation (CNR1, Kipp & Zonen), incident and reflected photosynthetically active radiation (PAR; LI-190, LI-COR), transmitted PAR (LI-191, LI-COR), air temperature and relative humidity (HMP-45A, Vaisala), soil heat flux density (MF-81, Eko), and volumetric soil water content (TDR100, Campbell). The 1-m long PAR sensor (LI-191) was placed across three rows below the canopy to obtain spatially representative values. These data were sampled every 5 s, and 15-min averages of the sampled data were recorded using a data logger (CR23X, Campbell). The fraction of absorbed photosynthetically active radiation (fAPAR) was derived from PAR measurements as \( \frac{1-r_c}{(1-r_0)\tau_c} \), where \( r_c \) and \( \tau_c \) are the reflectance and transmittance of the canopy and \( r_0 \) is the reflectance of the ground.

Ten stocks of rice plants were sampled every 2 weeks during the growing season. The rice samples were divided into roots, stems, leaves (green or dead), and panicles, and the green leaf area was measured using an optical area meter (AAM-7, Hayashi Denkoh) to determine the LAI. All plant parts were dried at 70 °C for 2 weeks to determine dry biomass.

3. Results and discussion

3.1. NEE_CO₂ and canopy photosynthetic variables

Fig. 1 shows the seasonal changes in NEE_CO₂ in the rice field. The NEE_CO₂ was low for several weeks after transplantation, but CO₂ uptake during midday became obvious even at low LAI. The midday peak value of NEE_CO₂ increased with increasing LAI and decreased rapidly during the late ripening period, although it is was strongly affected by incoming PAR intensity. The photosynthetic rate was much lower during the ripening stage than during the early vegetative stage, with similar or larger values of green LAI. These differences are presumably due to senescence, increasing respiration, and decreasing PAR intensity at the active leaves. In general, CO₂ flux from the water surface
beneath the rice canopy is low compared to plant CO₂ flux, since soil microbial respiration is strongly suppressed by the water layer (Miyata et al., 2000). Nighttime NEEₐ, i.e., ecosystem respiration (Rₑ), increased across growth stages and was highly correlated with air temperature (r=0.81 in 2003 and 0.80 in 2004). Rₑ during the night was expressed as an exponential function of air temperature (tₐ):

\[ Rₑ = a \exp(b tₐ) \]  (1)

where a and b are parameters.

Since the Rₑ is the sum of plant and microbial respiration, by definition, and it is not proportional to photosynthesis, the photosynthetic activity of ecosystems may be represented better by GPP than by NEEₐ, NPP, or other variables. Hence, we derived GPP values from NEEₐ using the following equation, assuming that the relationship derived above (Eq. (1)) could be applied during the day:

\[ \text{GPP} = -\text{NEE}_\text{CO₂} + Rₑ \]  (2)

Here, NEEₐ is positive when CO₂ is emitted from the ecosystem into the atmosphere, while GPP and Rₑ are both positive.

![Fig. 1. Seasonal change of net ecosystem CO₂ exchange (NEEₐ) in a rice field measured by eddy covariance method in 2004. Negative NEEₐ values indicate the flux from the atmosphere into the ecosystem. Solid lines indicate the incident PAR. Solid lines indicate the incident PAR. Dates for transplanting, heading, and harvesting were DOY123 (May 2), DOY208 (July 28), and DOY253 (September 9), respectively.](image)

![Fig. 2. Seasonal change of APAR-GPP relationship. Data points represent half-hourly measurements available for each week in 2003.](image)

We derived two indicators of canopy radiation use efficiency at the time of remote sensing measurements from half-hourly data.

\[ \varepsilon_N = \frac{\text{NEE}_\text{CO₂}}{\text{APAR}} \]  (3)

\[ \varepsilon_G = \frac{\text{GPP}}{\text{APAR}} \]  (4)

To infer the photosynthetic functioning of the canopy, we also derived quantum efficiency and maximum GPP by...
applying a light-photosynthesis curve to the APAR-GPP relationship. It was obvious that the APAR-GPP relationship was not linear in either daily or weekly scatter plots (Fig. 2). Although both linear (e.g., Campbell et al., 2001) and hyperbolic formulae (e.g., Wall & Kanemasu, 1990) have been used to represent the APAR-GPP relationship, the linear and hyperbolic formulae do not express the lower part of the relationship very well. Hence, we applied the asymptotic exponential equation as follows:

\[
GPP = \frac{P_{\text{max}}}{\left(1 + \frac{1}{\varphi} \exp \left(-\frac{\varphi \text{APAR}}{P_{\text{max}}} \right)\right)}
\]

where \(\varphi\) is the initial slope of the curve (quantum efficiency) and \(P_{\text{max}}\) is the photosynthetic capacity at the saturating APAR. The coefficient of determination for all curve fitting was as high as 0.98, so both daily and weekly parameters were derived accordingly. The overall patterns of seasonal change were similar for \(P_{\text{max}}\) and LAI, while both \(\varphi\) and \(\varepsilon_G\) were high at the early vegetative stage but decreased drastically with plant growth (Fig. 3). The seasonally integrated value of radiation use efficiency is consistent for each crop species, especially when there are no environmental stresses (Monteith, 1977; Sinclair, 1994), and it is often assumed to be constant in growth models. Nevertheless, it is obvious that the photosynthetic-efficiency variables do change and are affected by growth stage and environmental conditions.

We examined the effect of time scale on the estimates of radiation use efficiency at different integration periods to assess whether the instantaneous (often near midday) remote sensing measurements could provide robust information on the photosynthetic status of vegetation over longer terms. Fig. 4 compares \(\varepsilon_G\) values derived for midday 30 min \((\varepsilon_{G,30 \text{ m midday}})\), 1 day \((\varepsilon_{G,\text{day}})\), and 1 week \((\varepsilon_{G,\text{week}})\). We found significant linear relationships among all three values. However, it should be noted that \(\varepsilon_{G,\text{day}}\) was 4% lower than \(\varepsilon_{G,30 \text{ m midday}}\) and \(\varepsilon_{G,\text{week}}\) was 22% lower than \(\varepsilon_{G,\text{day}}\). These differences are mainly due to diurnal or daily changes in PAR intensity. The values of \(\varepsilon_{G,30 \text{ m midday}}\) represent the efficiency at midday under clear sky conditions, whereas both \(\varepsilon_{G,\text{day}}\) and \(\varepsilon_{G,\text{week}}\) values incorporate all data under various weather conditions including cloudy and rainy conditions. Under cloudy conditions, for example, the radiation use efficiency could be higher because a higher percentage of irradiance is diffuse and more effectively penetrates the canopy and because leaf photosynthesis is more efficient at weaker light intensity (Campbell et al., 2001). Hence, in general, the relationship of GPP (or \(\varepsilon_G\)) at different time scales largely depends upon variability in environmental conditions (such as PAR and water availability) as well as the response of efficiency to such conditions (e.g., Sims et al., 2005). Nevertheless, our results strongly suggest that one midday measurement would be a good indicator for inferring the potential values of radiation use efficiency or those for longer periods using ancillary data such as daily PAR.

3.2. Relationship of photosynthetic-efficiency variables with reflectance spectra

Fig. 5 shows the seasonal change in reflectance spectra obtained over the rice canopy with different levels of LAI, biomass, \(P_{\text{max}}\), and \(\varphi\). Wavelength windows around 1430 nm and 1910 nm were eliminated due to strong disturbance by atmospheric vapor. The spectra just after transplanting (05/12)

![Image](image1.png)

Fig. 3. Seasonal change of photosynthetic capacity \((P_{\text{max}})\), quantum efficiency \((\varphi)\), and radiation use efficiency \((\varepsilon_G)\) for the rice canopy. These parameters were determined for weekly sets of GPP and APAR data in 2003.

![Image](image2.png)

Fig. 4. Relationship between the values of radiation use efficiency \(\varepsilon_G\) at the time scale of 30 min \((\varepsilon_{G,30 \text{ m midday}})\), one day \((\varepsilon_{G,\text{day}})\), and one week \((\varepsilon_{G,\text{week}})\).
were similar to those of shallow rivers or ponds but already showed a slight trough at the chlorophyll absorption wavelength (670 nm). The reflectance in the red wavelengths decreased with plant growth until the time of heading (near maximum LAI), but decreased again during the ripening period until harvesting. A similar seasonal trend was found in the blue wavelengths (420–540 nm). In contrast, green (540–580 nm) and near-infrared (700–1350 nm) wavelengths increased throughout the growth period until harvesting. The range of change was much higher in the near-infrared region than in the visible region during the vegetative stage (i.e., before heading), whereas it was inverse during the ripening stage (i.e., from heading to harvesting). The post-harvest surface (09/27) showed typical spectra for crop residues. In accordance with the above trends, the spectrum of the post-harvest surface (09/27) was largely different from the spectra during the ripening stage in red and blue regions, while it was slightly different in the green and near-infrared regions. Reflectance in shortwave-infrared regions showed a trend similar to the near-infrared, but was less sensitive to vegetation change during the vegetative stage (e.g., see lines for 06/14, 07/05, and 08/03). This trend was more obvious at longer wavelengths (2000–2300 nm). These spectra are determined largely by the spectral features of photosynthetic pigment, water, and lignin/cellulose, as well as the background surface (Curran, 1989; Jacquemoud, 1993). Nevertheless, we assume these spectra also carry a number of minor spectral responses to the ecophysiological or biochemical functioning of vegetation.

Arrows in Fig. 5 indicate the wavelengths used to calculate the majority of previously reported spectral indices such as NDVI, SAVI, PRI, WI, SIPI, NPQI, GRI, SWWI, RV1, WDVI, MSAVI, EV1, GEMI, NDMI1, NDMI2, and BI (Peñuelas & Filella, 1998; definitions of these indices are given in Tables 1 and 2). The spectral widths for broad-band indices were determined based on the specifications of Landsat-TM. We examined the relationship of three efficiency parameters, $\epsilon_N$, $\epsilon_G$, and $\phi$, with these conventional indices, with the reflectance ($R_i$) at
a single wavelength \((i\ \text{nm})\), and with NDSIs using all combinations of two separate wavelengths \((i\ \text{and} \ j\ \text{nm})\),

\[
NDSI[i,j] = (R_i - R_j)/(R_i + R_j)
\]

(6)

In theory, \(NDSI[i,j] = -NDSI[j,i]\) and the range of NDSIs is from \(-1\) to \(1\). This normalization is effective at canceling atmospheric disturbance or other error sources as well as to enhancing and standardizing the spectral response to observed targets (e.g., Qi et al., 1994). For example, NDVI (i.e., a specific index \(NDSI[830, 660]\) in our generalized expression) has been widely used in scientific and operational applications (e.g., see reviews by Inoue & Olioso, 2006; Moran et al., 1997). Other well known indices such as PRI are in a similar formulation (Tables 1 and 2). In principle, NDSIs using consecutive wavelengths have a role similar to the first derivative.

The correlation coefficients between reflectance at a single wavelength and the three radiation use efficiency parameters are shown in Fig. 6a. Both \(\varepsilon_N\) and \(\varphi\) were highly correlated with near-infrared wavelengths \((r = -0.75 \sim -0.8)\), while \(\varepsilon_G\) was best correlated with \(R710\) \((r = 0.7)\) and less correlated with longer wavelengths. There was an obvious peak at around 550 nm, but the visible region was not highly correlated in general. The line for \(\text{NEE}_CO_2\) looks nearly inverse to the others simply because the signs of \(\text{NEE}_CO_2\) and the other parameters are inverse (negative \(\text{NEE}_CO_2\) means ecosystem \(CO_2\) uptake); nevertheless, it is interesting that a peak at around 710 nm (the so-called red-edge) was found only in \(\varepsilon_G\) and not in \(\varepsilon_N\) or \(\varphi\). The response in near-infrared regions was very flat with two minor peaks (970 and 1130 nm).

Fig. 7 shows a contour map of the coefficient of determination \((r^2)\) between \(\varepsilon_G\) and NDSIs with the two wavelengths on the \(x\) and \(y\) axes. The map provides an overview of the statistical significance of NDSIs for all combinations of two wavelengths. It allows efficient extraction of significant peak-wavelengths as well as the extent of the effective regions for assessment of each target variable. There are several narrow peaks (reddish) and deep troughs (bluish). Some steep walls are also found (e.g., around the 530 vs. 560 nm region). Therefore, selection of effective wavelengths should be made carefully so as not to span such steep-wall regions, since even a small bias could largely reduce the potential significance.

Table 1 summarizes the statistical significance of the conventional indices and selected NDSIs in the estimation of canopy photosynthetic variables. The NDSIs were selected on the basis of the contour map, a part of which is shown in Fig. 7. \(\varepsilon_N\) was best correlated with NDSI[542, 550] \((r^2 = 0.660)\), followed by NPQI using R415 and R435 \((r^2 = 0.512)\), while all other indices were poorly correlated.
Since \( \varepsilon_N \) is the ratio of \( \text{NEE}_{\text{CO}_2} / \text{APAR} \), the relationship between photosynthesis and spectral reflectance may be weakened due to the effects of plant respiration and microbial respiration. On the other hand, \( \varepsilon_G \) was correlated with \( \text{NDSI}_{[710, 410]} \) \( (\varphi^2 = 0.715) \), \( \text{NDSI}_{[710, 530]} \) \( (\varphi^2 = 0.711) \), and \( \text{NDSI}_{[530, 550]} \) \( (\varphi^2 = 0.711) \; \text{Fig. 8} \). \( \text{R550}, \text{R710}, \text{and R1122} \) were selected for multiple combinations because they may have some specific role in ecophysiological processes that directly or indirectly affect photosynthetic efficiency. \( \text{R550} \) normalized by near-infrared wavelengths (e.g., 830 nm) is best related to leaf nitrogen content (Inada, 1985) and rice canopy (Inoue et al., 1998; Takebe et al., 1990). Since nitrogen content is closely related to chlorophyll content and thus photosynthesis, \( \text{R550} \) may play an essential role in the estimation of photosynthetic efficiency. \( \text{R710} \) is positioned around the so-called red-edge wavelengths, which represent the large jump from the bottom of chlorophyll absorption \( (660–670 \text{ nm}) \) to the near-infrared plateau in typical vegetation spectra (Fig. 5). Therefore, it may have a role in normalizing the amount of vegetation when it is used with other visible wavelengths such as 410 or 530 nm. Considering the effective width and spectral resolution of the data, \( \text{R530} \) may have a role similar to that of 531 nm, which is used for PRI. Since the PRI using \( \text{R531} \) and \( \text{R570} \) was poorly correlated, but \( \text{NDSI}_{[530, 550]} \) was highly correlated, the use of 550 nm instead of 570 nm as a reference wavelength may significantly improve the estimation of photosynthetic efficiency.
The performance of PRI was surprisingly poor, although a number of papers have suggested that PRI would be useful for assessing photosynthetic radiation use efficiency (see review in the Introduction). Several attempts to apply PRI to ecosystem scales (e.g., Rahman et al., 2001), but its performance is not approved yet (Gamon et al., 2006; Sims et al., 2006). These reports suggest that PRI would work, to some extent, under “normal” rainfall conditions, but would work poorly for wider conditions including drought. These results coincide with similar results in other drought-prone systems where canopies undergo large structural changes (Filella et al., 2004; Gamon et al., 1992). Inoue and Peñuelas (2006) also confirmed a close relationship between PRI and photosynthetic radiation use efficiency (the ratio of net photosynthesis to incident PAR) at the leaf scale, but also found that the relationship was expressed as a function of soil water content. Hence, application of PRI to canopy or ecosystem scales may currently have critical limitations. More comprehensive investigations based on precise measurements at canopy scales would yield better spectral indices for assessment of photosynthetic activity or other ecophysiological variables. It is also obvious, on the other hand, that we need more systematic approaches to use remotely-sensed data in combination with ecophysiological process models for dynamic and accurate assessment of carbon, water, and biomass of plant ecosystems (e.g., Inoue & Olioso, 2006).

As for R1122, we have long recognized that nearby wavelengths are often selected when estimating the amount of canopy nitrogen using seasonal reflectance measurements (e.g., Inoue et al., 1998). We presume that R1122 is related to the amount of canopy nitrogen because 1120 nm is the wavelength of lignin absorption (Curran, 1989), and lignin/cellulose content is inversely related to nitrogen content during the growing season.

The quantum efficiency $\varphi$ was best correlated with NDSI [450, 1330] ($r^2=0.773$). It is interesting that NDSI[403, 830] ($r^2=0.760$) and NDSI[420, 970] ($r^2=0.759$) using very far wavelengths were also highly correlated with $\varphi$, whereas some other NDSIs use nearby wavelengths such as NDSI[933, 940] ($r^2=0.762$), NDSI[933, 948] ($r^2=0.759$) and NDSI[1053, 1058] ($r^2=0.755$). The bandwidth is relatively broad for the former NDSIs (5–80 nm) and narrow for the latter NDSIs (3 nm) that have similar information as derivatives. The WI using R970, a weak absorption peak of water, has proved useful for detecting leaf water status (Peñuelas & Inoue, 1999). This may explain the high correlations of WI with $\varphi$ and $\varepsilon_G$, since leaf water status strongly affects photosynthetic efficiency. However, there is no literature that suggests the role of 933, and 940, or 948 nm, although our results suggest the 930–950 region may have potential when estimating $\varphi$.

In general, the newly explored hyperspectral indices were highly correlated with these efficiency variables, while most conventional indices were less well correlated. Only NPQI and WI had relatively high correlations with efficiency variables ($r^2=0.51–73$). This may be because most conventional indices were examined using measurements in a few broad bands such as those for Landsat-TM, while hyperspectral measurements allow optimum selection of the most significant wavelengths. The spectral width for selected NDSIs was fairly narrow (3–10 nm), which requires a high signal/noise ratio, but future image sensors should enable detection of low energy signatures at high spectral resolution.
A similar analysis was conducted for off-nadir measurements since we presumed that they would carry more physiological information on photosynthetic efficiency, as little background is within the field of view. Fig. 9 zooms in on a part of the contour map of \( r^2 \) between \( \varepsilon_G \) and NDSIs derived from off-nadir measurements. The region consisting of 400–440 nm vs. 400–500 nm has rather high \( r^2 \) values (reddish), while there is a deep trough around 410–530 nm vs. 500–580 nm region (bluish). It is interesting that the 400–420 nm regions showed a high correlation ridge along R422. Fig. 10 shows a close-up view of two significant parts in the contour map of \( r^2 \) between \( \varphi \) and NDSIs derived from off-nadir measurements. A ridge of high \( r^2 \) was found around 413 nm, while the other regions showed poor correlations (Fig. 10a). In contrast, relatively large regions had high \( r^2 \) values around the 1000–1120 nm vs. 1100–1130 nm and the 1130–1150 nm vs. 1160–1200 nm regions. There are deep troughs in other parts around the 1000–1130 nm vs. 1150–1170 nm and the 1020–1040 nm vs. 1020–1050 nm regions.

Table 2 summarizes the statistical significance of the conventional indices and some selected NDSIs in assessment of photosynthetic-efficiency variables. As expected, among the conventional indices, PRI and NPQI were better correlated with \( \varepsilon_N \) \((r^2=0.636 \text{ and } 0.708, \text{ respectively})\), \( \varepsilon_G \) \((r^2=0.391 \text{ and } 0.601)\) and \( \varphi \) \((r^2=0.262 \text{ and } 0.500)\) than NDSIs from nadir measurements. Nevertheless, a closer relationship was found at NDSI[442, 435] for \( \varepsilon_N \) \((r^2=0.747; \text{ Fig. 11})\), NDSI[442, 416] for \( \varepsilon_G \) \((r^2=0.716; \text{ Fig. 12})\), and NDSI[1107, 1110] for \( \varphi \) \((r^2=0.766; \text{ Fig. 13})\). The spectral width at these peaks was as narrow as 1–3 nm in most indices. These results suggest that physiological information on photosynthetic efficiency may be better estimated by directional measurement than nadir measurement, as suggested by previous reports (e.g., Takebe et al., 1990). Since multi-angular measurements provide more accurate or extra information on vegetation canopies (Asner et al., 1998; Bicheron & Leroy, 1999), photosynthetic-efficiency variables may be included in the targets of such directional sensors. In case of off-nadir measurements, both \( \varepsilon_N \) and \( \varepsilon_G \) were related to NDSIs using visible wavelengths only, whereas NDSIs using water-related wavelengths (such as 970 and 1122 nm) were selected in nadir-measurements. This may be because the background was only slightly included, if at all, in the field of view in the off-nadir measurements. \( \varphi \) might be related to NDSIs using such water-related wavelengths since quantum efficiency represents the initial slope at weak light intensity and may be sensitive to leaf water status. The reflectance spectrum of the background surface was consistent during flooded conditions; nevertheless, water conditions in both background surfaces and plant leaves might have affected the results. Analyses using process models such as PROSPECT+SAIL with additional measurements would allow more detailed investigation of the effects of water in the background and in plants.
Fig. 10. A contour map of coefficient of determination ($r^2$) between $\phi$ and the normalized difference spectral indices (NDSIs) using the two separate wavelengths on $x$ and $y$ axes. A significant portion has been expanded out of a map for the entire wavelength regions to depict the details. Data are for off-nadir measurements.
3.3. Relationship of photosynthetic-capacity variables with reflectance spectra

Next, we investigated the relationship between hyperspectral reflectance and photosynthetic-capacity variables such as fAPAR and \( P_{\text{max}} \). The correlation coefficients between reflectance at a single wavelength and canopy photosynthesis parameters are shown in Fig. 6b. The response curves were quite similar for fAPAR, NEE\(_{\text{CO}_2}\), GPP, and \( P_{\text{max}} \); as explained for the efficiency variables in Fig. 6a, the line for NEE\(_{\text{CO}_2}\) is nearly inverse to the others due to the inverse sign of NEE\(_{\text{CO}_2}\). In general, near-infrared wavelengths were highly correlated

<table>
<thead>
<tr>
<th>Spectral indices (Off-nadir)</th>
<th>( \varepsilon_N )</th>
<th>( \varepsilon_G )</th>
<th>( \varphi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>NDSI[442, 435] ( \Delta [2, 2] )</td>
<td>0.747</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[442, 438] ( \Delta [2, 2] )</td>
<td>0.745</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[543, 548] ( \Delta [3, 2] )</td>
<td>0.720</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[422, 406] ( \Delta [2, 1] )</td>
<td>–</td>
<td>0.704</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[422, 416] ( \Delta [2, 2] )</td>
<td>–</td>
<td>0.716</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[422, 419] ( \Delta [2, 2] )</td>
<td>–</td>
<td>0.711</td>
<td>–</td>
</tr>
<tr>
<td>NDSI[413, 416] ( \Delta [1, 2] )</td>
<td>–</td>
<td>–</td>
<td>0.722</td>
</tr>
<tr>
<td>NDSI[962, 964] ( \Delta [1, 1] )</td>
<td>–</td>
<td>–</td>
<td>0.708</td>
</tr>
<tr>
<td>NDSI[971, 973] ( \Delta [1, 1] )</td>
<td>–</td>
<td>–</td>
<td>0.710</td>
</tr>
<tr>
<td>NDSI[1060, 1118] ( \Delta [20, 3] )</td>
<td>–</td>
<td>–</td>
<td>0.708</td>
</tr>
<tr>
<td>NDSI[1107, 1110] ( \Delta [2, 2] )</td>
<td>–</td>
<td>–</td>
<td>0.766</td>
</tr>
</tbody>
</table>

Notes: The NDSIs in this Table were selected on the basis of the contour map a part of which was shown in Figs. 9 and 10. Other notes are same as in Table 1.

Fig. 11. Relationship between \( \varepsilon_N \) and NDSI[442, 435] by off-nadir measurements.

Fig. 12. Relationship between \( \varepsilon_G \) and NDSI[422, 416] by off-nadir measurements.
with all variables ($|r|=0.7–0.9$). The highest correlation was found at around 720 nm for fAPAR, although the curve was rather flat over the near-infrared wavelengths. Peaks were found at around 550 and 670 nm, but the blue region (400–500 nm) was also relatively highly correlated with all capacity variables. These wavelengths may have significant roles in the assessment of capacity variables, although they must be normalized in some way.

Fig. 14 shows a contour map of $r^2$ between fAPAR and NDSIs for all combinations of two wavelengths from nadir measurements. In general, regions with high $r^2$ values are relatively broad compared to those for the photosynthetic-efficiency variables examined in the previous section. One obvious feature is the overall usefulness of the blue wavelengths (400–500 nm), although the red-edge region (around 700 nm) had a very deep trough (bluish) when combined with 400–670 nm wavelengths. Three peaks were also found over the near-infrared regions along 750 nm in combination with 970, 1120, and 1250 nm wavelength regions. These peak-regions extended from 740 nm toward longer wavelengths up to 900 nm, depicting the typical spectral response in green vegetation. On the other hand, 970 and 1120 nm might be selected due to their response to water content, as discussed before, while no potential feature was identified for 1250 nm in the literature.

Another peak was in the region around 1075 nm vs. 1100 nm. The most commonly used combination of red region (650–670 nm) and near-infrared region (800–1300 nm), i.e., NDVI, also showed a ridge of high $r^2$, although the significance seems secondary compared to some other peaks. According to the summary of useful NDSIs and conventional indices in the assessment of fAPAR (Table 1), fAPAR was well correlated with some conventional indices such as GEMI ($r^2=0.834$), SAVI ($r^2=0.801$), and WDV1 ($r^2=0.801$), while NDVI was less well correlated ($r^2=0.629$). Considering that these four indices use the same two bands (red and near-infrared wavelengths only), the adjustment employed in the former three indices seems effective in the assessment of fAPAR. Nevertheless, a much higher correlation was found at NDSI[550, 410] ($r^2=0.931$; Fig. 15b) and NDSI[720, 420] ($r^2=0.926$; Fig. 15c).

The NDVI-fAPAR relationship is very different in the vegetative and ripening stages (Asrar et al., 1989; Choudhury, 2000; Daugthry et al., 1983; Inoue & Iwasaki, 1991; Inoue et al., 1998). The lower correlation with NDVI in this analysis could be explained by the dependence of the relationship on phenology (Fig. 15a). In contrast, new indices using blue (410 and 420 nm), green (550 nm), and near-infrared (720 nm) wavelengths showed highly linear relationships with fAPAR for the entire growing period, with no phenology dependence. This feature should be attractive for extending the applicability of the fAPAR approach, since previous studies have focused on the vegetative stage only (Choudhury, 2000; Kiniry et al., 1989) or the phenology dependence has been otherwise neglected. Adjusting for background effects (like SAVI or MSAVI) to 410, 420, 550, and 720 nm wavelengths may bring further improvement in the assessment of fAPAR.

$P_{\text{max}}$ was moderately correlated with RVI ($r^2=0.667$), GRI ($r^2=0.662$), MSAVI ($r^2=0.594$), and four new indices, NDSI[518, 676], NDSI[620, 623], NDSI[620, 637], and NDSI[750, 761] ($r^2=0.65–0.66$). In principle, $P_{\text{max}}$ may not be highly correlated with actual measurements since $P_{\text{max}}$ is the potential photosynthesis at the highest incident radiation without any stresses. Nevertheless, it is noteworthy that these wavelengths are all in the chlorophyll a and b absorption region. These results suggest that conventional indices using red and near-infrared wavelength regions (e.g., RVI, GRI, and MSAVI) could be useful for a rough assessment of $P_{\text{max}}$. Carter (1998) showed that R701 was best correlated ($r^2=0.41$) with the “photosynthetic capacity” (observed maximum) in pine canopies, assuming that it could be estimated from photosynthetic measurements at the leaf level using a leaf chamber. It is reasonable that the significant wavelengths should be around the red-edge region, but should not necessarily agree with our results since the “capacity” variable of Carter (1998) is neither the efficiency nor capacity variable used in our study but a combination of both. Accordingly, it is also reasonable that
Carter (1998) found no significant relationship between PRI and the "capacity" variable.

4. Conclusions

Based on season-long measurements of CO₂ flux and hyperspectral reflectance in a homogenous ecosystem of flooded rice, we derived new spectral indices that will be useful for estimating canopy photosynthetic variables. NDSIs using narrow spectral bands were highly correlated with radiation use efficiency (εₙ, ε₄₅, φ) and capacity-related variables (fAPAR, Pₘₐₓ). Our selected indices were much more effective than conventional indices. ε₄₅ was best estimated by NDSI[410, 710], and fAPAR was best estimated by NDSI[550,410]. NDSI[550, 410] and NDSI[720, 420] had linear relationships with fAPAR throughout the growing period with no phenology dependence, whereas the phenology dependence of NDVI and similar indices has been a critical issue for the fAPAR approach. Some NDSIs, such as NDSI[933, 940], use wavelengths that are near each other, while several NDSIs (e.g., NDSI[450, 1330]) use widely spaced wavelengths. Also, some NDSIs, such as NDSI[1050, 1222], were a combination of only near-infrared wavelengths, while the photosynthetic pigments are directly related to visible wavelengths (400–700 nm). The contribution of some wavelengths in the near-infrared or shortwave-infrared regions (e.g., 970, 1050, 1120, 1222, and 1330 nm) may be attributed to the effects of water and lignin/cellulose to photosynthetic efficiency and capacity. It is also interesting that some NDSIs, such as NDSI [422, 406], had very sharp, significant peaks (1 to 3 nm), although several NDSIs, (e.g., NDSI[450, 1330]), were stable over relatively broad wavelength ranges (40 to 80 nm).

This experimental study was conducted in a rice paddy ecosystem that was rather simple and homogenous, with few confounding factors. Therefore, our results include potential ecophysiological relationships that might be common for various types of vegetation. These results provide useful insights for the assessment of radiation use efficiency and photosynthetic capacity in other ecosystems using a wide range of available spectral data. This information will also be useful for selection of sensors and for designing future sensors for ecosystem observations. Nevertheless, the underlying mechanisms for the NDSIs are not well identified at the moment, except for the well-known absorption features of major pigments and materials such as chlorophyll, xanthophyll, carotenoids, and water (Chappelle et al., 1992; Gamon et al., 1992; Inoue et al., 1993; Peñuelas & Filella, 1998). Further studies are needed to examine their applicability to other ecosystems and to investigate the ecophysiological and photochemical mechanisms to systematically account for the effects of biotic and abiotic stresses.

Acknowledgment

The authors would like to thank Drs. A. Olioso and F. Baret, INRA-CSE (Avignon, France) for their encouraging suggestions and information. We are also grateful to the useful comments from the anonymous reviewers. This study was supported in part
by the Global Environment Research Fund, Ministry of Environment of Japan.

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Fig. 15. Relationship of fAPAR with NDVI, NDSI[550, 410] and NDSI[720, 420] by nadir measurements.
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