

## Dependence of spectral characteristics on parameters describing CO<sub>2</sub> exchange between crop species and the atmosphere\*\*

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**A b s t r a c t.** The aim of this paper is to demonstrate that spectral vegetation indices are good indicators of parameters describing the intensity of CO<sub>2</sub> exchange between crops and the atmosphere. Measurements were conducted over 2011-2013 on plots of an experimental arable station on winter wheat, winter rye, spring barley, and potatoes. CO<sub>2</sub> fluxes were measured using the dynamic closed chamber system, while spectral vegetation indices were determined using SKYE multispectral sensors. Based on spectral data collected in 2011 and 2013, various models to estimate net ecosystem productivity and gross ecosystem productivity were developed. These models were then verified based on data collected in 2012. The R<sup>2</sup> for the best model based on spectral data ranged from 0.71 to 0.83 and from 0.78 to 0.92, for net ecosystem productivity and gross ecosystem productivity, respectively. Such high R<sup>2</sup> values indicate the utility of spectral vegetation indices in estimating CO<sub>2</sub> fluxes of crops. The effects of the soil background turned out to be an important factor decreasing the accuracy of the tested models.

**K e y w o r d s:** spectral vegetation indices, net ecosystem productivity, gross ecosystem productivity, crops, dynamic chambers, multispectral sensors

### INTRODUCTION

Net ecosystem productivity (NEP) is a parameter that describes the balance of all processes of carbon dioxide (CO<sub>2</sub>) exchange between the ecosystem and the atmosphere – the difference between the amount of CO<sub>2</sub> assimilated by plants within the photosynthesis and respiration of the ecosystem (Kirschbaum *et al.*, 2001; Law *et al.*, 2002). NEP values are given from the point of view of carbon dioxide gains or losses by the ecosystem: they are positive when

photosynthesis (expressed as gross ecosystem productivity, GEP) exceeds the respiration process at the ecosystem scale (ecosystem respiration, R<sub>eco</sub>). In turn, negative values of this parameter indicate excess respiration over photosynthesis, and thus carbon losses by the ecosystem.

In the vast majority of studies on measurements of CO<sub>2</sub> fluxes, eddy covariance (EC) systems were applied (Cheng *et al.*, 2009; Middleton *et al.*, 2009; Rossini *et al.*, 2010; Sakowska *et al.*, 2014; Urbaniak *et al.*, 2016). Measurements of gas fluxes conducted using this technique, despite many advantages (Goulden *et al.*, 1996; Moncrieff *et al.*, 1996; Verma, 1990), have also some limitations. For instance, the application of the EC technique is limited to relatively large (the flux ‘footprint’ varies from tens of meters to several kilometres), flat, and homogeneous surfaces (Urbaniak *et al.*, 2016). Apart from the EC technique, gas fluxes exchanged between the ecosystem and the atmosphere are also measured using *e.g.* the chamber technique, applied in this paper (Juszczak, 2013; Urbaniak *et al.*, 2016). It is a method based on point measurements and, therefore, is very well adapted to heterogeneous surfaces, in which EC systems may not be applied. A significant limitation of the chamber method is connected with the high labour and time intensity of the performed measurements.

Due to the considerable limitations of both the EC and the chamber methods, the focus in recent years has increasingly been placed on the need to estimate parameters describing CO<sub>2</sub> exchange between vegetation and the atmosphere based on remote sensing data. In the vast majority of studies, which are conducted at present at the ground level, spectral characteristics are measured using various types of automatic systems (Ide *et al.*, 2010; Meroni *et al.*, 2011;

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Nakaji *et al.*, 2007, 2008; Sakowska *et al.*, 2015, 2016). In order to facilitate the presentation of optical measurements within more than one spectral range, spectral vegetation indices (*VI*s) were introduced as algebraic dependencies of reflectance ( $\rho$ ) at various wavelengths ( $\lambda$ ). Thanks to these procedures, *VI*s may be presented in the form of one dimensionless value, sensitive to a specific characteristic of the analysed surface. These indices are extensively used to estimate various parameters of soil surfaces and the vegetation cover (Liang, 2004).

The normalised difference vegetation index (*NDVI*) is one of the most commonly applied *VI*s (Rouse *et al.*, 1973). It is calculated based on spectral reflectance measurements acquired in the visible (RED) and near-infrared (NIR) regions. *NDVI* is a spectral indicator of the greenness of the vegetation cover, *i.e.* a complex of such parameters as the canopy cover and structure, leaf area index, leaf chlorophyll content, as well as the physiological status of the vegetation (Liang, 2004; Zarco-Tejada *et al.*, 2005; Zhang *et al.*, 2005). Numerous studies have been conducted on the dependence of *NDVI* on different parameters of the vegetation cover, including CO<sub>2</sub> fluxes exchanged between the vegetation cover and the atmosphere. Emphasis has been particularly placed on its relationship with *GEP* (Rossini *et al.*, 2012; Sakowska *et al.*, 2014; Skinner *et al.*, 2011; Wang *et al.*, 2004) and *NEP* (Hassan *et al.*, 2006; Propastin and Kappas, 2009; Veroustraete *et al.*, 1996). The seasonal variation of CO<sub>2</sub> fluxes exchanged between different ecosystems and the atmosphere was successfully assessed based on different *VI*s including *NDVI* (Rossini *et al.*, 2012; Wang *et al.*, 2004; Zhang *et al.*, 2005). Relationships based on *NDVI* work best when the analysed vegetation cover is neither too dense nor too sparse. At high densities of the vegetation cover, the effect of saturation of *NDVI* values at a certain level and a lack of its further growth with an increase in the parameters estimated by this index can be observed (Carlson and Ripley, 1997; Uzdicka *et al.*, 2012). As a consequence of the saturation effect, the application of *NDVI* to estimate CO<sub>2</sub> fluxes may result in a considerable underestimation of these fluxes (Zarco-Tejada *et al.*, 2005). Different modifications of *NDVI* aiming at the minimisation of the saturation effect have been proposed *e.g.* simple ratio (*SR*), modified simple ratio (*MSR*), and wide dynamic range vegetation index (*WDRVI*). The *SR* index does not provide linear relationships with the vegetation biophysical parameters, since although it is highly sensitive to their changes at high plant densities, at the same time it has low sensitivity when the density of the vegetation cover is low (Jackson and Huete, 1991). The *SR* index was modified to *MSR* in order to obtain more linear relationship between spectral data and biomass (Chen, 1996). *WDRVI* was developed by Gitelson (2004) to obtain the same effect, although at a much better adaptation of the calculation methodology to the specific crop character.

In the conditions of sparse vegetation cover, the main issue with estimating various parameters based on spectral data is connected to the contribution of the soil background to the measured signal (Baret and Guyot, 1991; Huete, 1988; Rondeaux *et al.*, 1996). In order to minimise this effect, Huete (1988) introduced a modification of *NDVI* and proposed the soil adjusted vegetation index (*SAVI*). *SAVI* works relatively well for plant cover with visible soil interspaces. A certain limitation in its application results from the fact that the parameter *L* used for calculation is a coefficient that in theory should be variable, depending on the density of the vegetation cover. For very dense vegetation cover, *L* should be 0, while for low vegetation cover density, it is ~1. Since the value of vegetation cover density is rarely ever known, optimisation of this parameter is highly approximate. However, the results of analyses made by Huete (1988) indicated that although optimal *L* values were different for different amounts of biomass in a given area, *L* of 0.5 was optimal for a very wide spectrum of conditions. Thus, the adoption of such a value of this parameter results in a reduction of soil disturbances in various types of vegetation cover (Panda *et al.*, 2010).

After Huete (1988), soil effects were considered in many other studies and a considerable number of *VI*s, which correct for the influence of soil brightness when vegetative cover is low, was developed. These include the transformed soil adjusted vegetation index (*TSAVI*: Baret and Guyot 1991), modified soil adjusted vegetation index (*MSAVI*: Qi *et al.*, 1994), and optimised soil adjusted vegetation index (*OSAVI*: Rondeaux *et al.*, 1996). All of these *VI*s are based on various modifications of parameter *L* in *SAVI*. According to the results of studies conducted to date (Rondeaux *et al.*, 1996) on homogeneous meadows and arable fields in temperate latitudes, the best results among indices of this group are provided by *OSAVI*. This index was used *e.g.* by Daughtry *et al.* (2000), Flowers *et al.* (2001), Haboudane *et al.* (2002) and Zarco-Tejada *et al.* (2005).

The photochemical reflectance index (*PRI*) is a spectral index that is sensitive to changes in carotenoid pigments in live foliage and is used as an indicator of the light use efficiency in the process of photosynthesis (Gamon *et al.*, 1992). Its relationship with biophysical parameters of the vegetation cover has also been confirmed by many studies (Coops *et al.*, 2010; Garbulsky *et al.*, 2011; Goerner *et al.*, 2011; Middleton *et al.*, 2009). Seasonal changes in *PRI* illustrate seasonal changes in the concentration of carotenoid pigments in plants (Stylinski *et al.*, 2002). Short-term changes in *PRI* reflect short-term changes in the photosynthesis light use efficiency (at constant carotenoid contents in plants: Goerner *et al.*, 2011) as a result of various stress factors (Gamon *et al.*, 1992, 1997).

The availability of simultaneous acquisition of near-surface spectral observations and CO<sub>2</sub> flux measurements obtained with the eddy covariance technique has increased

in recent years. One of the most widely applied approaches to modelling GPP based on spectral data is the light-use efficiency (LUE) model proposed by Monteith (1972, 1977), in which GPP is modelled as a function of the fraction of photosynthetically active radiation absorbed by vegetation (fAPAR), the incident photosynthetically active radiation (PAR), and the conversion efficiency of absorbed energy to fixed carbon (light-use efficiency) (Rossini *et al.*, 2012). Another approach to estimate GPP is based on a simplified version of Monteith model. In this approach, there is no need to estimate fAPAR and light use efficiency with the use of spectral vegetation indices. Based on the assumption that chlorophyll is related to the presence of photosynthetic biomass, recent studies (Gitelson *et al.*, 2008; Harris and Dash, 2010) suggest that GPP can be estimated through direct correlation with chlorophyll-related indexes (Rossini *et al.*, 2012) or sun induced fluorescence (Migliavacca *et al.*, 2017; Rossini *et al.*, 2010).

Studies on the relationships of the spectral characteristics of the vegetation cover with CO<sub>2</sub> fluxes measured using the chamber technique have been conducted relatively rarely till now (Boelman *et al.*, 2003; Dagg and Lafleur, 2010; Perez-Priego *et al.*, 2015). However, considering that both chamber and spectral measurements can be performed at a small scale of crop fields where the EC technique cannot be applied, our aim was to demonstrate how these two methods can be successfully combined to develop simple empirical models which allow estimation of the GEP and NEP of different crops with remote sensing.

#### MATERIALS AND METHODS

Measurements of the biophysical and spectral characteristics of the vegetation cover were taken in the Experimental Teaching Station in Brody (52°26'18" N, 16°17'40" E) on fields of a multi-year experiment conducted by the Department of Agronomy, Poznań University of Life Sciences. The cultivation experiment was established as early as 1957 and covers plots grown in monoculture and in crop rotation (with four blocks in each). In both cropping systems, seven crop species are grown, differing in the levels of mineral or organic fertilisation (11 fertiliser combinations).

The measurements presented here were recorded in 2011–2013, solely in plots of one selected fertiliser combination (N<sub>min</sub>, K<sub>2</sub>O, P<sub>2</sub>O<sub>5</sub> – 90, 120 and 90 kg ha<sup>-1</sup>, respectively as well as Ca) grown in the seven-year crop rotation system (potato plants – Vineta, spring barley – Nadek, winter triticale – Witon, 1 and 2-year alfalfa – Alba, winter wheat Turkis, winter rye – Dańkowskie Złote). Analyses were conducted on four crop species: winter wheat, winter rye, spring barley, and potato plants.

The 40 year period mean annual air temperature at a height of 2 m above the ground in the experimental area is 7.9°C, while the mean annual precipitation is 571 mm

(based on measurements recorded over 1959–1999 at the weather station of the Brody Experimental Station). The dominant soils in the analysed area are lessive soils, with the grain size composition of light and heavy loamy sands, of medium depth, lying over light loams. According to the FAO classification, they are classified as *Albic Luvisols* (Blecharczyk, 2002). The length of the vegetation period is between 216 to 228 days.

CO<sub>2</sub> fluxes were measured with a dynamic chamber system, composed of a non-transparent chamber facilitating measurements of ecosystem respiration (R<sub>eco</sub>) as well as a transparent chamber to measure NEP fluxes. Measurements of R<sub>eco</sub> and NEP were used to calculate GEP. The dark chamber was made from white PVC, while the transparent chamber was made from PLEXIGLAS (Evonik Industries, Darmstadt, Germany). Each chamber had walls of 3 mm thickness and was 78 x 78 x 50 cm in size. Both chambers were equipped with two fans of 1.4 W each (to ensure effective air mixing inside the chambers), a pressure equilibration system, and a temperature sensor (T-107, Campbell Scientific, USA) installed inside the chamber (in a radiation protection shield at a height of 30 cm from the lower edge). In order to measure CO<sub>2</sub> concentrations changing in the course of measurements, a home-made measurement system with a Li-820 analyser (LICOR, USA) was used. Air circulated between the chamber and the analyser within a closed loop. The measurement system comprised a CR1000 data logger (Campbell Scientific, USA) recording data on CO<sub>2</sub> concentration every 5 s (Chojnicki *et al.*, 2010; Juszczak, 2013; Juszczak *et al.*, 2012, 2013). Additionally, a SKP215 sensor (Skye Instruments Ltd. UK) installed in the chamber was also used to measure the intensity of incoming photosynthetically active radiation (PARi) during the NEP measurements, while a set of T-107 thermistors (Campbell Scientific, Utah, USA) was used to measure soil temperature at 2 and 5 cm depths.

The chambers were placed on PVC soil frames (75 x 75 cm) inserted to a depth of ~15 cm. In each experimental plot, two frames were installed (at a distance of 1 m). Due to the plant height changing during the growing season, extensions were used in order to increase the height of the whole chamber set (to a maximum of 1.5 m). Chamber measurements were performed every 3–4 weeks, on cloudless days, during daytime hours from sunrise to late afternoon. Measurements of NEP and R<sub>eco</sub> were taken one directly after another to facilitate GEP calculations (as a sum of NEP and R<sub>eco</sub>). Due to the high air temperatures in the summer and the potential overheating of the transparent chamber, the temperature in that chamber was stabilised using cooling pads installed on the frame inside the chamber headspace (Drösler, 2005). The duration of chamber closure ranged from 120 to 180 s in the transparent and non-transparent chamber, respectively.

**Table 1.** Spectral vegetation indices calculated for this study ( $\rho$  – spectral reflectance at a given wavelength  $\lambda$ ,  $L$  – parameter characterizing the density of the vegetation cover; in this study, in calculations of *SAVI* its optimal value (Huete 1988) was set to 0.5)

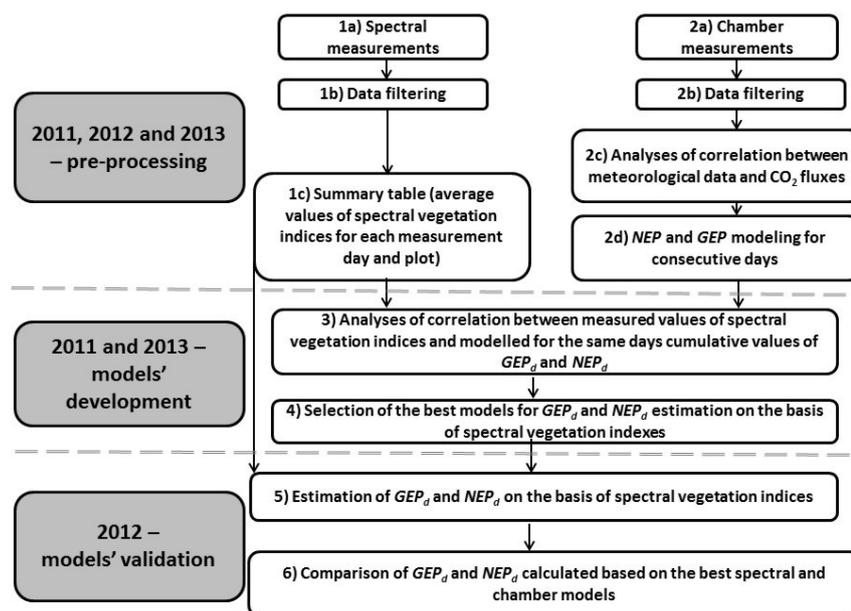
Spectral vegetation index	Formulation	Reference
Normalized difference vegetation index ( <i>NDVI</i> )	$NDVI = \frac{\rho_{850} - \rho_{670}}{\rho_{850} + \rho_{670}} \quad (1)$	Rouse <i>et al.</i> (1973)
Simple ratio ( <i>SR</i> )	$SR = \frac{\rho_{850}}{\rho_{670}} \quad (2)$	Jordan (1969)
Modified simple ratio ( <i>MSR</i> )	$MSR = \frac{SR - 1}{SR^{0.5} + 1} \quad (3)$	Chen (1996)
Soil adjusted vegetation index ( <i>SAVI</i> )	$SAVI = \frac{\rho_{850} - \rho_{670}}{\rho_{850} + \rho_{670} + L} (1 + L) \quad (4)$	Huete (1988)
Optimised soil adjusted vegetation index ( <i>OSAVI</i> )	$OSAVI = \frac{\rho_{850} - \rho_{670}}{\rho_{850} + \rho_{670} + 0.16} \quad (5)$	Rondeaux <i>et al.</i> (1996)
Wide dynamic range vegetation index ( <i>WDRVI</i> )	$WDRVI = \frac{0.2\rho_{850} - \rho_{670}}{0.2\rho_{850} + \rho_{670}} \quad (6)$	Gitelson (2004)
Photochemical reflectance index ( <i>PRI</i> )	$PRI = \frac{\rho_{570} - \rho_{531}}{\rho_{570} + \rho_{531}} \quad (7)$	Gamon <i>et al.</i> (1992)

A total of 37 measurement campaigns were conducted over 2011–2013 (12 in 2011, 17 in 2012, and 8 in 2013).  $\text{CO}_2$  fluxes ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ) were calculated based on the gas concentration change over the closure time using the linear approach (Juszczak *et al.*, 2012, 2013). For each measurement campaign, relationships between measured  $R_{\text{eco}}$  and air and soil temperatures were found (Lloyd and Taylor, 1994) as well as between GEP and  $\text{PAR}_i$  (Michaelis-Menten, 1913). The protocols of data analysis and flux modelling applied were identical to those in Eickenscheidt *et al.* (2015). The obtained relationships were used together with model  $\text{CO}_2$  fluxes in the periods between the measurement campaigns. Modelling was conducted with a 30-minute step, using air or soil temperature (to calculate  $R_{\text{eco}}$ ) and  $\text{PAR}_i$  (to estimate GEP) measured at an automatic weather station located 50 m from the plots. Based on the values of modelled fluxes, cumulative seasonal  $R_{\text{eco}}$ , GEP, and NEP ( $\text{NEP} = \text{GEP} - R_{\text{eco}}$ ) were calculated.

Radiometric measurements were taken using two four-channel SKR1850 sensors (SKYE Instruments Ltd., Llandrindod Wells, UK) installed at the zenith-nadir position on a portable SKL908 device (Spectrosense2+, SKYE Instruments Ltd., Llandrindod Wells, UK). Multispectral measurements were conducted for radiation incident and reflected from the vegetation cover, at four wavelengths  $\lambda$  (530, 570, 670, and 850 with 10 nm bandwidth). On this basis, it was possible to calculate six spectral *VIs* – *NDVI*, *SR*, *MSR*, *SAVI*, *OSAVI*, *WDRVI*, and *PRI* (Table 1).

In the years 2011–2013, a total of 36 spectral measurement campaigns were conducted. Measurements were taken in the same plots and for crop species, in which chamber measurements of gas exchange were recorded. The measurements were organised in most cases on the same days as the chamber measurements; however, under unfavourable conditions (*e.g.* due to clouds), these measurements were taken on the first sunny and cloudless days following the chamber measurements. Spectral measurements were recorded solely from 10:00 to 14:00 local time.

During the multispectral measurements performed with the Spectrosense2+ device, the sensor directed downwards measured the spectral radiance of the investigated area with a 25° field of view. The measurement results were recorded in nanoamperes (nA). The size of the area from which the collected signal originates, depends on the height of the installed sensor. For measurements conducted within this study (at a sensor mounted at a constant height of 1.80 m above the ground), it was a circular area with a radius of 0.4 m and surface area of 0.5 m<sup>2</sup>. A sensor directed upwards is equipped with a cosine diffuser, which expands its field of view to 180°. This diffuser facilitates the application of Lambert cosine law to calculate spectral hemispheric irradiance and to express radiation fluxes in  $\mu\text{mol m}^{-2} \text{ s}^{-1}$ . Both sensors take measurements at exactly the same moment, thus preventing any errors resulting from variability in the weather conditions.



**Fig. 1.** Algorithm for the analysis of data collected in the course of spectral and chamber measurements and their interdependencies.

Measurements were taken on each plot in three replications located at a distance of 30 cm from one another. The value of the spectral vegetation index characterising a given plot was the arithmetic mean of three measurements. Spectral data filtering included rejecting the data acquired when the diffusion index (calculated as the ratio between diffuse and total PARi) exceeded 50%.

Since not all measurement campaigns for CO<sub>2</sub> exchange and spectral measurements were performed on the same days and because the number of chamber measurements for each day and crop was different, we decided to use modelled values of CO<sub>2</sub> fluxes to determine the relationship between NEP and GEP fluxes and vegetation indices. Daily sums of modelled NEP (NEP<sub>d</sub>) and GEP (GEP<sub>d</sub>) were used to develop relationships with spectral indices for days when optical measurements were taken. The results obtained for the training dataset (2011 and 2013) were used to develop the best models to estimate NEP<sub>d</sub> and GEP<sub>d</sub> based on spectral vegetation indices. For each index, four regression types were analysed: linear, logarithmic, exponential, and power. For all analysed plant species, the best models were selected for the estimation of CO<sub>2</sub> fluxes based on individual indices. When evaluating the models, the following statistical parameters were considered: coefficient of determination (R<sup>2</sup>) and normalised root mean square error (NRMSE). The models characterised by the highest R<sup>2</sup> and lowest NRMSE were selected as the best.

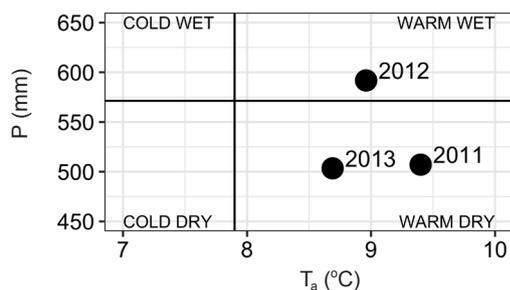
Data collected during 2012 were used as an independent dataset to validate the developed models. Each model was fitted against training dataset consisting of data collected in 2011 and 2013 and the resulting parameterization was used to estimate CO<sub>2</sub> fluxes of 2012.

In the final step, the best models were used to estimate CO<sub>2</sub> fluxes based on spectral vegetation indices interpolated linearly between the conducted measurement campaigns for 2012. The developed seasonal courses of CO<sub>2</sub> fluxes were then compared to seasonal courses of NEP<sub>d</sub> and GEP<sub>d</sub> derived from chamber CO<sub>2</sub> modelling. These analyses were conducted for the same period between the middle of April (when the first spectral measurements were taken in all years) to the middle of August (the last spectral measurements taken). The scheme for our data analysis is given in Fig. 1.

## RESULTS

Manual chamber and spectral measurements at Brody were performed from April 2011 to August 2013; they covered three growing periods: 2011, 2012, and 2013. The mean annual air temperatures and annual precipitation sums for these three years are presented in Fig. 2. Considering the mean values of temperature and sums of precipitation, 2012 was a warm and wet year (mean air temperature: 8.9°C and sum of precipitation: 592 mm), while 2011 and 2013 were warm and dry years with average air temperature of 9.4 and 8.7°C and sum of precipitation of 507 and 503 mm, respectively.

The coefficients of determination (R<sup>2</sup>) for the relationship between NEP<sub>d</sub> and GEP<sub>d</sub> and spectral vegetation indices ranged from 0.12 to 0.83 and from 0.09 to 0.92 for NEP<sub>d</sub> and GEP<sub>d</sub>, respectively (Table 2), depending on the investigated crop. On this basis, a spectral vegetation index was selected for each species, which worked best in the estimation of NEP<sub>d</sub> as well as GEP<sub>d</sub> (Figs 3 and 4). For the



**Fig. 2.** Mean annual air temperatures ( $T_a$ ) and annual sums of precipitation ( $P$ ) at Brody Station for 2011, 2012, and 2013. Solid lines represent the 40-year average (1959-1999).

$NEP_d$ ,  $R^2$  for the best models based on spectral data ranged from 0.71 to 0.83 (Fig. 3A), while for  $GEP_d$  it was from 0.77 to 0.92 (Fig. 4B). The best results in the estimation of  $CO_2$  fluxes were recorded when applying *WDRVI* and *OSAVI* for winter wheat and *SAVI* and *OSAVI* for the other crops (Table 2, Figs 3 and 4). The weakest relationships were obtained using *PRI*.

The best models estimating  $NEP_d$  and  $GEP_d$  given in Figs 3 and 4 were applied to calculate the  $CO_2$  fluxes for the successive days in the growing season of 2012 (Fig. 5). Due to *VI*s saturation observed for winter rye (Figs 3-5), the spectral indices increased linearly with  $NEP_d$  and  $GEP_d$ , only up to a certain value of these fluxes. In the case of  $NEP$ , the spectral indices were saturated at  $NEP_d$  values exceeding  $9 \text{ g } CO_2\text{-C m}^{-2} \text{ d}^{-1}$ , while in the case of  $GEP_d$  – at  $18 \text{ g } CO_2\text{-C m}^{-2} \text{ d}^{-1}$ . Above these threshold values, the spectral vegetation indices remained at a constant maximum level despite a further increase in  $NEP_d$  and  $GEP_d$  (Fig. 5). Consequently, the values of  $NEP_d$  and  $GEP_d$  estimated based on spectral measurements for winter rye at the peak of the growing period are markedly underestimated compared to the values of  $NEP_d$  and  $GEP_d$  that were derived from the chamber model (Fig. 5). On the other hand, after the peak of the season,  $NEP_d$  fluxes calculated based on *VI*s are significantly overestimated for winter rye and spring barley. This effect may compensate for the underestimation of the fluxes in the peak of the growing season and even overestimate the overall cumulative fluxes calculated for the whole period (Table 3). Besides winter rye, *VI*s were not saturating with the increasing  $NEP_d$  and  $GEP_d$  and hence the fluxes modelled based on *VI*s can well reflect the seasonal dynamics of the  $CO_2$  exchange between the crops and the atmosphere.

In order to estimate the carbon budget for individual species and individual years, both in the case of the spectral and chamber models, the total  $CO_2$  fluxes were calculated for these periods. Overall, the models based on spectral data most frequently provided elevated cumulative  $NEP$  fluxes relative to those based on chamber data, except for winter wheat (Table 3). In the case of  $GEP$ , cumulative seasonal fluxes calculated from the spectral model were not differ-

ent for winter rye, spring barley, and potato, while winter wheat fluxes were nearly 40% smaller than those estimated based on the chamber related model.

## DISCUSSION

The high values of  $R^2$  obtained for models estimating  $NEP_d$  and  $GEP_d$  based on spectral data (supported by very good validation results) indicate that spectral vegetation indices are good proxies, which may be successfully used to estimate the  $CO_2$  fluxes exchanged between the vegetation cover and the atmosphere. The high accuracy for the relationship between  $CO_2$  fluxes and spectral vegetation indices has also been confirmed elsewhere (Gitelson *et al.*, 2008, 2012; Rossini *et al.*, 2012; Skinner *et al.*, 2011; Wang *et al.*, 2004). Significant problems observed in the case of such analyses, which were also found here, include:

- disturbance effects caused by a soil background;
- the weakest relationship obtained using *PRI*;
- the saturation effect of spectral indices found at high densities of the vegetation cover; and
- usually the insufficient amount of spectral measurements over the growing season and the need to linearly interpolate *VI*s between campaigns in order to estimate biophysical characteristics of the canopy.

Due to the disturbing effect exerted on *NDVI* by the soil background, the greatest accuracy was found for models based on indices reducing the impact of this effect, *e.g.* *SAVI* and *OSAVI*. Due to the specific canopy structure of cereals and potatoes, in the case of these species these effects are of great importance in terms of the accuracy of the estimates of  $CO_2$  fluxes based on spectral characteristics. This effect has also been recorded in studies of Baret and Guyot, 1991; Huete, 1988; Rondeaux *et al.*, 1996; and Qi *et al.*, 1994. The greatest values of the determination coefficients obtained using *SAVI* and *OSAVI* have also been confirmed by Borge and Leblanc, 2001; Glenn *et al.*, 2008; Mandal *et al.*, 2007; Yuetting *et al.*, 2008.

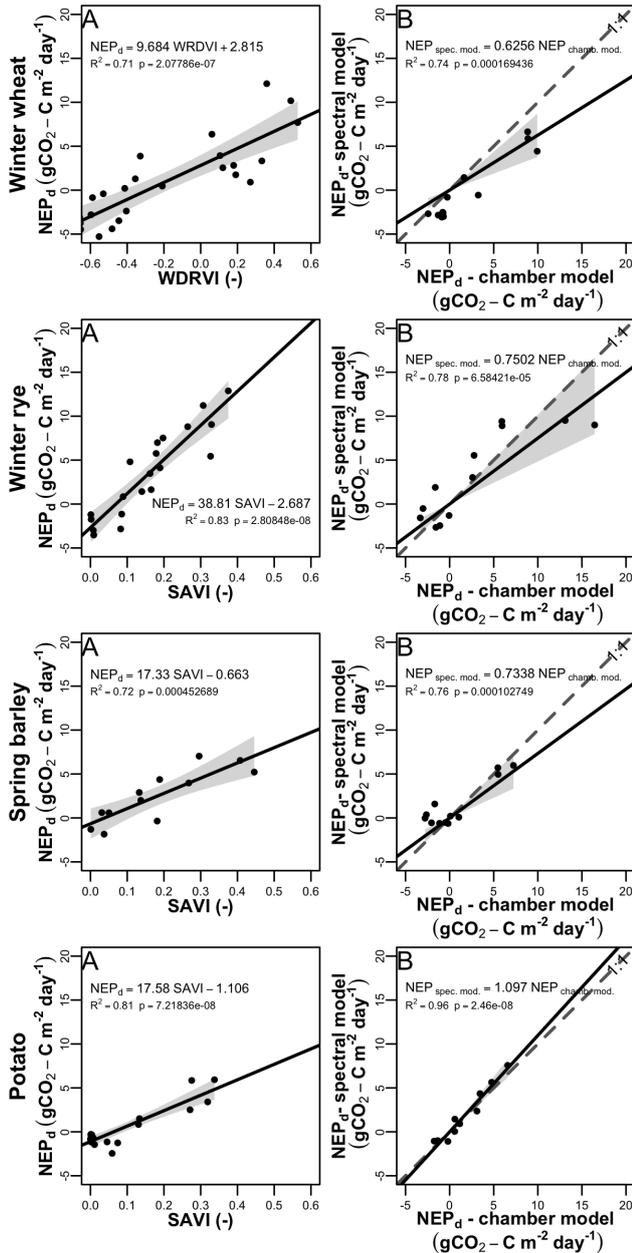
The worst results in the estimation of  $CO_2$  fluxes were found using *PRI*. This is probably connected with the fact that, apart from the contents of carotenoid pigments and light use efficiency, it is also influenced by several other factors, such as reflection from the soil background (as stated above – a highly significant factor in the case of the crops analysed in this study); proportions between direct and diffuse incoming radiation; structure of the canopy; the angle of solar rays; and sun-vegetation cover-sensor geometry (relative to the Sun as well as elements of the vegetation cover) (Grace *et al.*, 2007; Hall *et al.*, 2008; Louis *et al.*, 2005; Suarez *et al.*, 2008). Due to the measurement errors caused by these factors, although *PRI* works very well as an indicator of LUE at the leaf level (Filela *et al.*, 1996; Gamon and Surfus, 1999; Penuelas *et al.*, 1995, 1997), the accuracy of models based on this index is more limited if they are applied at the canopy level.

**Table 2.** Summary of statistics for regression models defining the relationship between NEP<sub>d</sub> and GEP<sub>d</sub> and spectral vegetation indices. The model was created on a set of data from 2011 and 2013 and it was validated using 2012 data

Crop	Index	Model (2011, 2013)				Model validation (2012)			
		Equation	n	R <sup>2</sup>	NRMSE (%)	n	R <sup>2</sup>	NRMSE (%)	
Winter wheat	NEP <sub>d</sub>	NDVI	$y = 12.65x - 4.81$	24	0.68	15	12	0.87	15
		SR	$y = -3.01 \ln(x) - 2.50$	23	0.66	15	12	0.79	16
		MSR	$y = -11.39x - 3.09$	22	0.62	16	12	0.58	23
		SAVI	$y = 28.77x - 2.51$	21	0.62	17	12	0.89	10
		OSAVI	$y = 22.79x - 3.19$	24	0.65	16	12	0.90	12
		WDRVI	$y = 9.68x + 2.81$	24	0.71	14	12	0.90	15
		PRI	$y = 142.1x + 29.05$	23	0.40	20	11	0.70	10
	GEP <sub>d</sub>	NDVI	$y = 11.80 x^{1.51}$	24	0.69	19	12	0.84	07
		SR	$y = -4.53 \ln(x) + 0.15$	23	0.75	14	12	0.74	17
		MSR	$y = -17.14x - 0.48$	22	0.64	17	12	0.57	23
		SAVI	$y = 43.56x + 0.10$	21	0.75	15	12	0.91	7
		OSAVI	$y = 38.70x^{1.30}$	24	0.78	14	12	0.90	8
		WDRVI	$y = 13.41x + 8.11$	24	0.73	15	12	0.83	10
		PRI	$y = 176.73x + 40.39$	23	0.31	24	11	0.61	12
Winter rye	NEP <sub>d</sub>	NDVI	$y = 11.47x - 3.46$	23	0.56	19	12	0.52	14
		SR	$y = -3.36 \ln(x) - 2.32$	23	0.60	18	11	0.49	25
		MSR	$y = -11.65x - 1.97$	21	0.60	18	12	0.35	24
		SAVI	$y = 38.81x - 2.69$	20	0.83	12	12	0.73	14
		OSAVI	$y = 29.95x - 3.65$	23	0.81	13	12	0.70	14
		WDRVI	$y = 8.32x + 3.25$	23	0.53	20	12	0.52	15
		PRI	$y = 123.72x + 27.21$	23	0.35	23	11	0.56	13
	GEP <sub>d</sub>	NDVI	$y = 15.43x - 0.58^7$	23	0.50	21	12	0.38	15
		SR	$y = -4.96 \ln(x) + 0.24$	23	0.64	17	11	0.32	26
		MSR	$y = -16.79x + 0.81$	21	0.60	18	12	0.34	24
		SAVI	$y = 55.82x - 0.35$	20	0.83	13	12	0.76	12
		OSAVI	$y = 58.07x^{1.49}$	23	0.79	13	12	0.73	12
		WDRVI	$y = 3.00 e^{4.36x}$	23	0.58	33	12	0.16	41
		PRI	$y = 167.93x + 40.97$	23	0.32	23	11	0.49	16

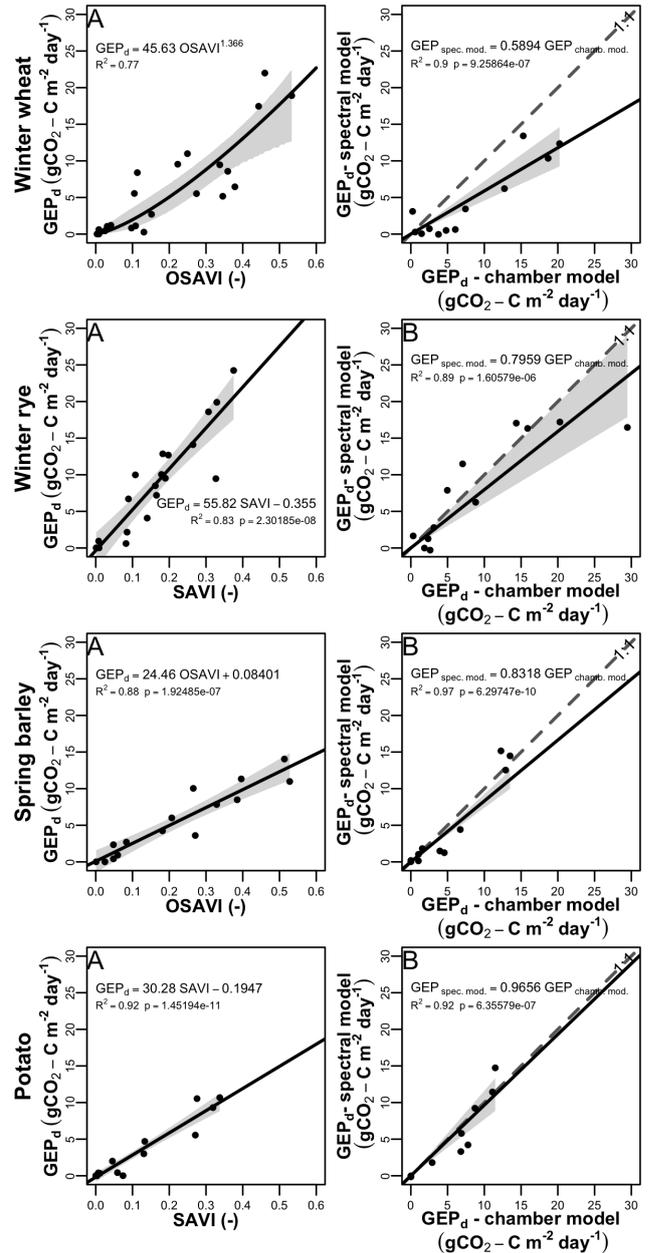
**Table 2.** Continuation

Crop	Index	Model (2011, 2013)				Model validation (2012)			
		Equation	n	R <sup>2</sup>	NRMSE (%)	n	R <sup>2</sup>	NRMSE (%)	
Spring barley	NEP <sub>d</sub>	NDVI	$y = 7.54x - 1.91$	15	0.54	23	12	0.71	12
		SR	$y = -1.52 \ln(x) - 0.60$	15	0.33	28	12	0.65	19
		MSR	$y = -5.81x - 0.89$	15	0.30	28	12	0.43	21
		SAVI	$y = 17.33x - 0.66$	12	0.72	16	12	0.81	14
		OSAVI	$y = 14.55x - 1.69$	15	0.63	21	12	0.79	12
		WDRVI	$y = 5.67x + 2.56$	15	0.54	23	12	0.80	10
		PRI	$y = 85.99x + 18.64$	15	0.31	28	11	0.10	12
	GEP <sub>d</sub>	NDVI	$y = 13.15x - 0.51$	15	0.83	13	12	0.95	6
		SR	$y = -3.18 \ln(x) + 1.04$	15	0.73	17	12	0.77	23
		MSR	$y = -12.10x + 0.45$	15	0.66	19	12	0.58	29
		SAVI	$y = 28.70x + 1.02^4$	12	0.84	19	12	0.93	12
		OSAVI	$y = 24.46x + 0.08$	15	0.88	11	12	0.95	7
		WDRVI	$y = 9.93x + 7.31$	15	0.82	14	12	0.93	8
		PRI	$y = 71.69x + 19.78$	15	0.11	30	11	0.01	24
Potato	NEP <sub>d</sub>	NDVI	$y = 7.25x - 1.30$	23	0.73	14	12	0.83	12
		SR	$y = -2.09 \ln(x) - 0.53$	18	0.68	15	11	0.90	25
		MSR	$y = -4.88x - 0.51$	21	0.49	19	12	0.77	18
		SAVI	$y = 17.58x - 1.11$	20	0.81	12	12	0.91	10
		OSAVI	$y = 11.97x - 1.21$	23	0.61	17	12	0.91	8
		WDRVI	$y = 6.92x + 3.52$	23	0.76	13	12	0.87	13
		PRI	$y = 59.21x + 12.13$	22	0.12	25	11	0.01	8
GEP <sub>d</sub>	NDVI	$y = 12.50x - 0.37$	23	0.86	13	12	0.99	5	
	SR	$y = -3.48 \ln(x) + 0.69$	18	0.80	14	11	0.95	22	
	MSR	$y = -8.93x + 0.74$	21	0.69	18	12	0.71	23	
	SAVI	$y = 30.28x - 0.19$	20	0.92	09	12	0.88	16	
	OSAVI	$y = 21.42x - 0.32$	23	0.77	17	12	0.93	10	
	WDRVI	$y = 11.50x + 7.73$	23	0.83	14	12	0.93	12	
	PRI	$y = 80.7x + 18.43$	22	0.09	31	11	0.04	15	



**Fig. 3.** Best models to estimate NEP<sub>d</sub> based on spectral vegetation indices (A) and their verification (B) - relationship between NEP<sub>d</sub> estimated from model (A) with NEP<sub>d</sub> calculated based on chamber measurements.

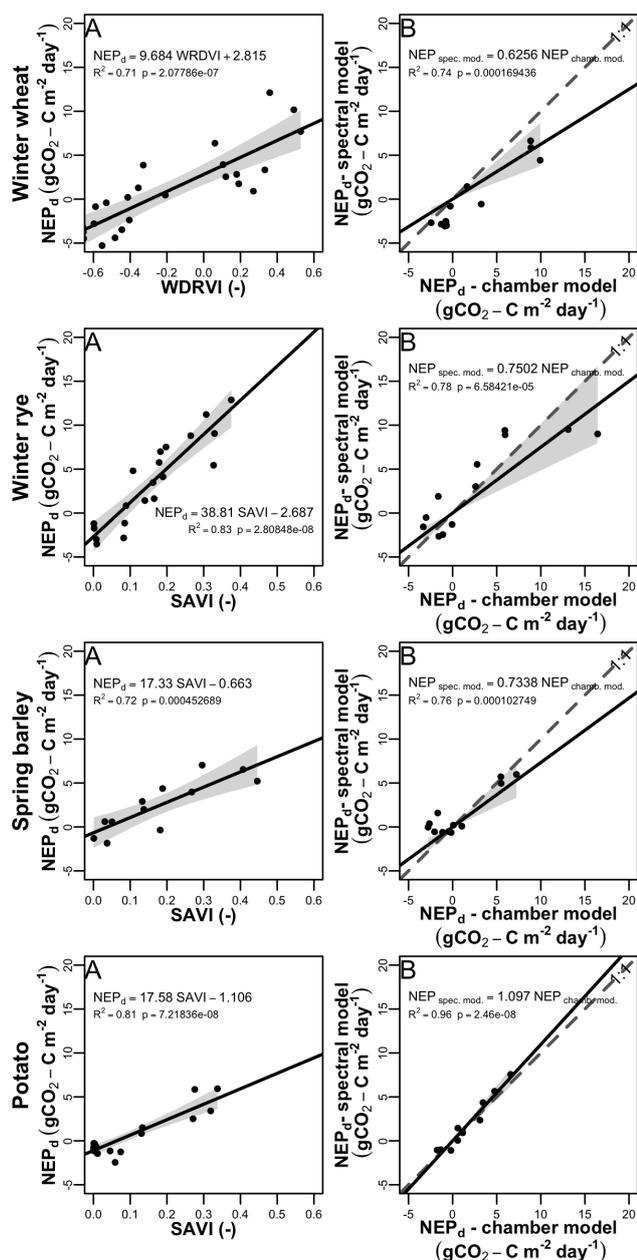
Saturation of spectral data at high values of biophysical parameters estimated by them is a phenomenon that has frequently been observed in studies concerning the interdependencies of various parameters of the vegetation cover (Brantley *et al.*, 2011; Tang *et al.*, 2005; Wang *et al.*, 2004; Zarco-Tejada 2005). In this study, this effect was only found in the case of winter rye. For this crop, the threshold values of biophysical parameters for this effect were exceeded already in April, *i.e.* relatively early in the growing season. That is why the spectral model of CO<sub>2</sub> fluxes does not reflect the seasonal variability of the fluxes



**Fig. 4.** Best models to estimate GEP<sub>d</sub> based on spectral vegetation indices (A) and their verification (B) - relationship between GEP<sub>d</sub> estimated from model (A) with GEP<sub>d</sub> calculated based on chamber measurements.

exchanged between the ecosystem and the atmosphere, as well as why the cumulative values of estimated seasonal GEP are underestimated. For other crop species considered in this paper, the saturation of the indices does not constitute a very significant factor disturbing the accuracy of estimates of carbon dioxide fluxes based on the spectral characteristics of the vegetation cover.

Besides saturation, another factor influencing the accuracy of the estimated fluxes is usually the insufficient frequency of the periodically performed manual measurements of crop canopy spectral characteristics. These



**Fig. 5.**  $NEP_d$  (A) and  $GEP_d$  (B) estimated for different crops based on the chamber model (grey line) and the spectral model (black line).

**Table 3.** A comparison of cumulative NEP and GEP values (kg CO<sub>2</sub>-C m<sup>-2</sup>) for the analysed crop species for the period from 18th April to 14th August of 2012: chamber model (A) and spectral model (B)

Crop	NEP		GEP	
	A	B	A	B
Winter wheat	0.25	0.13	1.20	0.74
Winter rye	0.28	0.50	1.34	1.17
Spring barley	0.02	0.25	0.73	0.71
Potato	0.20	0.30	0.72	0.78

measurements are conducted during sunny days and very often during periods with unfavourable weather conditions. The number of optical measurements is often limited to a few per season, which may have a pronounced effect on the values of biophysical characteristics of the canopy estimated with  $VIs$ . This may have the biggest effect in periods when vegetation is growing fast as the maximum value of the  $VIs$  may be not recorded during a peak of the growing season. Consequently, this may lead to underestimation of the estimated CO<sub>2</sub> fluxes or other biophysical characteristics of the canopy. Considering that number of spectral measurements taken on field is often limited, the  $VIs$  and biophysical parameters estimated with  $VIs$  need to be linearly interpolated between campaigns. What is more, relationships between  $VIs$  and biophysical characteristics of the canopy (*e.g.* CO<sub>2</sub> fluxes) are developed for sunny and cloudless days when spectral measurements were conducted. In consequence, this may lead to overestimation of the estimated parameters for cloudy days. Besides, due to linear interpolation, it is not possible to reflect daily dynamics of the estimated variables. Nevertheless, despite all of the weaknesses of such analyses, considering the results presented in this study,  $VIs$  are good proxies of the CO<sub>2</sub> fluxes exchanged between the canopies and the atmosphere and allow estimation of NEP and GEP with acceptable uncertainty.

However, we have to emphasise that the analyses performed in the paper are based on the point-based measurements and hence they cannot reflect the full spectrum of  $VIs$  variability on a field scale. Besides, we need to consider the site-specific conditions (*e.g.* soil), fertilization level, management practices, and local climate, which may significantly modify both fluxes and spectral characteristics of crops. Considering the above, the relationships estimated in the paper, although they can be good proxies for NEP and GEP, should not be extrapolated for other sites with other types of soils and climate.

## CONCLUSIONS

1. Models based on spectral vegetation indices calculated based on radiation in the ranges of reflectance measurements acquired and near-infrared proved to be

highly suitable for the estimation of seasonal fluctuations of daily sums of net and gross ecosystems productivity for crop species. Photochemical reflectance index turned out to be a much less suitable index for the estimation of these characteristics.

2. The effect of the soil background turned out to be an important factor disturbing the accuracy of models based on spectral vegetation indices. These effects are partly eliminated thanks to the application of soil adjusted vegetation index and optimised soil adjusted vegetation index, which were the best at the estimation of carbon dioxide fluxes exchanged between crops and the atmosphere for the crops analysed in this study.

3. The accuracy of models based on spectral indices was also affected by the effect of the vegetation indices saturation at high densities of vegetation canopy. For the crops analysed in this study, the reduced accuracy of the models caused by the saturation effect is still lower than its reduction as a result of the disturbing effects of the soil background. The boundary values of daily sums of net and gross ecosystems productivity, which when exceeded resulted in the spectral data saturation effect, were reached solely in the case of winter rye.

4. Overall, models based on values of spectral vegetation indices provide elevated values of daily sum of net ecosystem productivity while differences in daily sum of gross ecosystem productivity estimated based on vegetation indices and chamber model were not significant (besides winter wheat). Hence, we proved that for the crops considered in this study spectral vegetation indices are good proxies of daily sum of gross ecosystem productivity, and daily sum of net ecosystem productivity, although in the latter case fluxes are estimated with higher uncertainty.

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