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# Hyperspectral response of agronomic variables to background optical variability: Results of a numerical experiment

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#### ABSTRACT

Understanding how biophysical and biochemical variables contribute to the spectral characteristics of vegetation canopies is critical for their monitoring. Quantifying these contributions, however, remains difficult due to extraneous factors such as the spectral variability of canopy background materials, including soil/crop-residue moisture, soil-type, and non-photosynthetic vegetation (NPV). This study focused on exploring the spectral response of two important agronomic variables (1) leaf chlorophyll content ( $C_{ab}$ ) and (2) leaf area index (LAI) under various canopy backgrounds through a global sensitivity analysis of wheat-like canopy spectra simulated using the physically-based PROSAIL radiative transfer model. Our results reveal the following general findings: (1) the contribution of each agronomic variable to the simulated canopy spectral signature varies considerably with respect to the background optical properties; (2) the influence of the soil-type and NPV on the spectral response of canopy to  $C_{ab}$  and LAI is more significant than that caused by soil/crop-residue moisture; (3) spectral bands at 560 and 704 nm remain sensitive to  $C_{ab}$  while being least affected by the impacts of variations in the NPV, soil-type and moisture; (4) the near-infrared (NIR) spectral bands exhibit higher sensitivity to LAI and lower background effects only in the cases of soil/crop-residue moisture but are relatively strongly affected by soil-type and NPV. Comparative analysis of the correlations of twelve widely used vegetation indices with agronomic variables indicates that LICI (LAI-insensitive chlorophyll index) and Macc01 (Maccioni index) are more effective in estimating  $C_{ab}$ , while OSAVI (optimized soil adjusted vegetation index) and MCARI2 (modified chlorophyll absorption ratio index 2) are better LAI predictors under the simulated background variability. Overall, our results highlight that background reflectance variability introduces considerable differences in the agronomic variables' spectral response, leading to inconsistencies in the VI- Cab /-LAI relationship. Further studies should integrate these results of spectral responsivity to develop trait-specific hyperspectral inversion models.

#### 1. Introduction

Plants are an essential component of the terrestrial ecosystem. Leaf area index (LAI), as an indicator of vegetation growth (Ma *et al.*, 2018), and the leaf chlorophyll content (henceforward referred to as  $C_{ab}$ ), as an indicator of the photosynthetic capacity of vegetation (Croft *et al.*, 2017), are two of the most important vegetation variables that control

water, energy and carbon exchange processes in the terrestrial biosphere. Knowledge of the spatial distribution of the LAI and  $C_{ab}$  is therefore crucial to assess the terrestrial carbon and water balance and to forecast agricultural yield, especially facing the challenges of global change (Chen *et al.*, 2019; Gitelson *et al.*, 2003; Houborg *et al.*, 2013; Huang *et al.*, 2015). Remote sensing can provide such information by enabling the non-destructive estimation of LAI and  $C_{ab}$  at regional to

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Fig. 1. Reflectance spectra of 55 backgrounds used as input into the PROSAIL model: (a) bare soil at seven different relative water contents (RWC), (b) crop residue with seven different levels of moisture content, (c) 17 contrastive soil types, and (d) 24 NPV.

global scales (Croft *et al.*, 2020; Fang *et al.*, 2019). The retrieval of LAI and  $C_{ab}$  from remote sensing data relies on the fact that the optical properties of leaves and the canopy correlate strongly with vegetation amount and leaf composition (Asner, 1998; Jacquemoud *et al.*, 2009). Consequently, an in-depth understanding of how the LAI and  $C_{ab}$  determine the vegetation spectral behavior – including vegetation indices (VIs) – under the effects of external factors is vital for a more accurate estimation of LAI and  $C_{ab}$  from remote sensing data. In this respect, the effects of changing soil background characteristics deserve more attention as, generally, even within a small agricultural field, the background optical properties vary spatially and temporally (Baret and Guyot, 1991; Li *et al.* 1993). Such spatiotemporal variations in background reflectance are the main source of uncertainty in satellite-derived LAI or  $C_{ab}$  products (Darvishzadeh *et al.*, 2008a, 2019; Eitel *et al.*, 2009; Verrelst *et al.*, 2010).

Numerous studies have used simulations based on radiative transfer models (RTMs) to analyze the sensitivity of surface reflectance of a soilvegetation system, usually through either local sensitivity analysis (LSA) or global sensitivity analysis (GSA) methods. LSA involves the qualitative analysis of the relationships between the spectral characteristics and a specific biophysical or biochemical parameter while keeping the remaining variables fixed. This has been successfully applied to evaluate the spectral sensitivity of agronomic variables to different soil types and water contents (Bach and Verhoef, 2003; Díaz and Blackburn, 2003; Huete *et al.* 1985; Morcillo-Pallarés *et al.*, 2019). However, LSA cannot identify and quantify the influential and noninfluential variables – and their mutual interdependences – that govern the spectral signatures at different wavelengths over the entire input variable space (Saltelli and Annoni, 2010). Such assessments have important implications for selecting optimal wavelengths for the estimation of LAI and  $C_{ab}$ . Moreover, previous applications of LSA rarely included the spectral response in the shortwave infrared (SWIR) bands that are configured in popular satellite sensors (e.g., Landsat-8 OLI, Sentinel-2 MSI) and commonly used for LAI retrievals (Amin *et al.*, 2021; Dong *et al.*, 2020). By contrast, GSA quantifies simultaneously the contribution of various model input parameters to the reflected electromagnetic radiation (Gu *et al.*, 2016; Mousivand *et al.*, 2014; Wang *et al.*, 2019; Xiao *et al.*, 2014), and is therefore typically preferable over LSA. In previous studies, however, GSA has often ignored the sometimes high spatiotemporal variability in the background optical properties.

To gain maximum understanding, sensitivity analyses should include major factors which contribute to the spectral variability of background materials. Typically, in many agricultural ecosystems, the background spectrum is highly heterogeneous due to different soil types, organic carbon contents, fertilizer treatments, amounts and type of nonphotosynthetic vegetation (NPV, e.g., crop residue, litter, senescent grass), and surface water and roughness status. Therefore, it is imperative to better elucidate the spectral response of vegetation variables under different background conditions.

The objectives of this paper are: (1) to quantify the contributions of LAI and  $C_{ab}$  to the full-wavelength spectral response (400–2400 nm), as well as to commonly available VIs, when background optical properties are variable, and (2) to determine the spectral regions where LAI and/or  $C_{ab}$  most strongly affect the canopy spectral characteristics while being minimally influenced by variations in background reflectance. To address these goals, extensive numerical experiments based on radiative transfer simulations were conducted to generate representative spectral datasets. Research objectives were investigated for a setting simulating

#### Table 1

Main variables of PROSAIL in the global sensitivity analysis. In bold, the eight non-fixed variables of interest.

Variable	Symbol	Unit	Range	Refs.
Leaf structure parameter	Ν	-	1.0-2.5	Liu <i>et al</i> . (2012)
Leaf chlorophyll content	$C_{ab}$	$\mu g/cm^2$	5-100	Xu et al. (2019)
Leaf carotenoid content	$C_{xc}$	$\mu g/cm^2$	8	Liang <i>et al.</i> (2015)
Brown pigment content	$C_{\rm bp}$	-	0	Xu et al. (2019)
Equivalent water	$C_{\rm w}$	cm	0.0043-	Feret et al.
thickness			0.0713	(2011)
Dry matter content	Cm	$g/cm^2$	0.0008-	Feret et al.
			0.0331	(2011)
Leaf area index	LAI	$m^{2}/m^{2}$	0.1-10	Liang et al.
				(2015)
Average leaf inclination angle	ALA	0	30-80	Verger <i>et al.</i> (2014)
Hot-spot parameter	$S_{\rm L}$	-	0.2	Xiao et al.
				(2014)
Background brightness factor	α	-	0-1	Verrelst et al. (2015b)
Solar zenith angle	$\theta_s$	0	20-60	-
Viewing zenith angle	$\theta_{v}$	0	0	-
Relative azimuth angle	$\varphi_{sv}$	0	0	-
Fraction of diffuse incoming solar radiation	skyl	-	0.1	Zhang <i>et al</i> . (2016)

wheat canopies (*Triticum aestivum* L.) as well as other continuous crop canopies similar to wheat.

#### 2. Materials and methods

#### 2.1. Background spectra

Mimicking vegetation spectra with variable backgrounds requires realistic spectra from background materials and appropriate canopy reflectance models. Spectral reflectance of various soil types in China were collected from (i) a subset of the ICRAF-ISRIC spectral library (the International Centre for Research in Agroforestry-International Soil Reference and Information Centre) as described by Garrity and Bindraban (2004), and (ii) the CSSL spectral library (the Chinese Soil Spectral Library) described in Shi et al. (2014). The ICRAF-ISRIC spectral library includes 245 soil profiles collected from 47 locations in China. The CSSL spectral library contains 1581 soil samples derived from 16 soil groups of the Genetic Soil Classification of China (GSCC). Fifty-one reflectance spectra of NPV were acquired from the ECOSTRESS spectral library (the ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station, see Meerdink et al., 2019 for details). To avoid data redundancy caused by similar soil or NPV spectra in these three independent spectral libraries and to better sample the feature space, we used the spectral angle mapping classification method (Kruse et al., 1993) to identify several representative spectra based on the following equation:

$$\alpha_{XY} = \cos^{-1} \left\lfloor \frac{\sum_{i=1}^{n} (x_i y_i)}{\sqrt{\left(\sum_{i=1}^{n} x_i^2\right)} \times \sqrt{\left(\sum_{i=1}^{n} y_i^2\right)}} \right\rfloor$$

where,  $X = (x_1, x_2, ..., x_n)$  and  $Y = (y_1, y_2, ..., y_n)$  are two different soil spectral vectors with *n* wavebands;  $\alpha_{XY}$  is the spectral angle between *X* and *Y* and ranges from 0 to  $\pi/2$  ( $\alpha_{XY} = 0$  means that *X* and *Y* are completely similar, while  $\alpha_{XY} = \pi/2$  means that *X* and *Y* are entirely different).

Using the criterion that two different spectra with a spectral angle  $\alpha$  < 0.05 would be identified as similar reflectance (Jia *et al.*, 2016), the spectral reflectance curves of 1826 soil and 51 NPV were classified into 17 soil and 24 NPV groups, respectively. In addition, a set of average spectra generated from a dataset containing 70 crop-residue and soil at

seven moisture levels (Quemada and Daughtry, 2016) was used to mimic the canopy spectral variation due to differences in water contents of the ground underneath the canopy. In total, 55 different background reflectance spectra were assessed (Fig. 1): 17 soil types, 24 NPV, 7 soil moisture contents, and 7 crop-residue moisture contents. The chosen background spectra display highly distinct spectral contrast linked to soil type, composition, texture, and surface conditions, which permits to assess the impacts of a wide range of natural backgrounds. As a limitation it has to be noted however that the spectra come from different sources and are not mutually inclusive – in particular the (hypothetical) averages of the subsets (a) to (d) in Fig. 1 would not match each other.

#### 2.2. Global sensitivity analysis

We used the extended Fourier amplitude sensitivity test method (EFAST, Saltelli *et al.*, 2008), implemented in the software package SimLab (ver. 2.2, SIMLAB, 2009) to perform the global sensitivity analysis of the simulated datasets. The EFAST is a variance-based GSA method which has recently gained wider attention in agricultural modeling (Jin *et al.*, 2018; Xu *et al.*, 2019). The sensitivity measures of EFAST include the first-order sensitivity index  $S_i$ , which reflects the individual contribution of each input parameter to the model output, and the total-order sensitivity index  $ST_i$ , which represents the overall contribution of each parameter and the remaining parameters). Both sensitivity indices can be expressed as follow:

$$S_i = \frac{V_i}{V}$$

$$ST_i = S_i + \sum_{j \neq i} S_{ij} + \dots + S_{1,2,\dots,k}$$

where  $V_i$  ( $V_i = V[E(Y|x_i)]$ ) represents the first-order variance for each input factor; V is the attribution of total output variance and calculated according to  $V = \sum_{i=1}^{k} V_i + \sum_{i=1}^{k} \sum_{j>i}^{k} V_{ij} + \dots + V_{1,2,\dots,k}$ ; and  $V_{ij}$  ( $V_{ij} = V[E(Y|x_i, x_j)] - V_i - V_j$ ) to  $V_{1,2,\dots,k}$  represent the interactions among k factors (see Saltelli *et al.*, 2010, for further details on EFAST).

To investigate the spectral response of agronomic variables with different background scenarios, the EFAST global sensitivity analysis was performed using simulations with the well-known radiative transfer model PROSAIL (Berger *et al.*, 2018; Jacquemoud *et al.*, 2009) that could produce nadir-viewed canopy reflectance (from 400 to 2400 nm in 1 nm increments), assuming negligible atmospheric effects. The MATLAB code for PROSAIL can be downloaded at http://teledetection.ipgp. jussieu.fr/prosail/. To parameterize the PROSAIL model in a plausible manner, a combination of (i) *prior* knowledge (Liu *et al.*, 2012; Verger *et al.* 2014; Xu et al., 2019; Zhang *et al.* 2016) from site-specific information gathered in field campaigns of wheat, and (ii) related published literature (Feret *et al.*, 2011; Liang *et al.*, 2015; Xiao *et al.*, 2014) were used to assign the specific ranges of the main model input variables of wheat-like canopies (Table 1). All parameters were varied independently as information about possible covariation was not available.

For an informative sensitivity analysis, the sample size of input parameters should be as large as possible. On the other hand, the computational costs of the simulation increase with sample size. To assess how sample size affects the convergence of the sensitivity indices, we ran a set of the EFAST global sensitivity analysis with a gradually increasing sample size and then computed the total-order sensitivity index of the widely-used NDVI (normalized difference vegetation index) based on the narrowband reflectance at 670 and 800 nm from PROSAIL simulations, corresponding to eight variables. Substantial variations in the total-order sensitivity index of each input parameter of the PROSAIL model were observed when the sample size is  $\leq 10\ 000$  while it is more stable for a sample size of 30 000 (Fig. 2). As no more fluctuations occurred after 35 000 simulations, a final sample size of 40 000 samples



Fig. 2. Analysis of the impact of the total number of samples (*N*<sub>s</sub>) on the stability of global sensitivity analysis for NDVI with PROSAIL based on the extended Fourier amplitude sensitivity test.

Table	2
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A set of vegetation indices e	examined in	this	paper
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Spectral index	Formulation	Estimation or Elimination	Refs.
MSAVI, Modified soil adjusted vegetation index	$0.5[2R_{800} + 1 - \sqrt{(2R_{800} + 1)^2 - 8(R_{800} - R_{670})}]$	Background effect	Qi et al. (1994)
OSAVI, Optimized soil adjusted vegetation index	$(1+0.16)(R_{800}-R_{670})/(R_{800}+R_{670}+0.16)$	Background effect	Rondeaux et al. (1996)
NDVI, Normalized difference vegetation index	$(R_{800} - R_{670})/(R_{800} + R_{670})$	LAI	Rouse et al. (1974)
MSR, Modified simple ratio	$[(R_{800} \ / R_{670}) - 1] / \sqrt{(R_{800} \ / R_{670}) + 1}$	LAI	Chen (1996)
MCARI2, Modified chlorophyll absorption ratio index 2	$1.5[2.5(R_{800} - R_{670}) - 1.3(R_{800} - R_{550})]$	LAI	Haboudane et al. (2004)
	$\overline{\sqrt{\left(2R_{800}+1\right)^2-\left(6R_{800}-5\sqrt{R_{670}}\right)-0.5}}$		
sLAIDI, Standardized LAI Determining Index	$S(R_{1050} - R_{1250})/(R_{1050} + R_{1250})$ , where S = 5	LAI	Delalieux et al. (2008)
CI <sub>RE</sub> , Red-edge chlorophyll index	$(R_{750} / R_{710}) - 1$	Chlorophyll	Gitelson et al. (2006)
MTCI, MERIS terrestrial chlorophyll index	$(R_{754} - R_{709})/(R_{709} - R_{681})$	Chlorophyll	Dash and Curran (2004)
Macc01, Maccioni index	$(R_{780} - R_{710})/(R_{780} - R_{680})$	Chlorophyll	Maccioni et al. (2001)
LICI, LAI-insensitive chlorophyll index	$\left( R_{735} \left/ R_{720} \right) - \left[ \left( R_{573} - R_{680} \right) \left/ \left( R_{573} + R_{680} \right) \right] \right.$	Chlorophyll	Li et al. (2020)
MCARI <sub>(705, 750)</sub> /OSAVI <sub>(705, 750)</sub>	$[(R_{750} - R_{705}) - 0.2(R_{750} - R_{550})] \Big(rac{R_{750}}{R_{705}}\Big)$	Chlorophyll	Wu et al. (2008)
	$\frac{\left[\frac{(1+0.16)(R_{750}-R_{705})}{R_{750}+R_{705}+0.16}\right]}$		
PRI, Photochemical reflectance index	$(R_{531} - R_{570})/(R_{531} + R_{570})$	Photosynthetic efficiency	Gamon et al. (1992)

was selected to distinguish between influential and noninfluential parameters. Thus, a total of 40 000 combinations of the eight model parameters (*N*,  $C_{ab}$ ,  $C_w$ ,  $C_m$ , LAI, ALA,  $\alpha$ ,  $\theta_s$ ) were randomly generated (following uniform distribution) within the predefined ranges by using EFAST, resulting in the generation of 40 000 canopy spectra by running PROSAIL in the forward mode. Contrary to Widlowski *et al.* (2015), in the simulations, effects of leaf/canopy clumping were not considered, nor were the effects of background anisotropy. Then, the influence of the background on the contribution of  $C_{ab}$  and LAI to canopy reflectance as well as the twelve VIs selected (given in Table 2) was examined by repeatedly running EFAST for each of the 55 background spectra (i.e., 7 soil moisture contents + 7 crop-residue moisture contents + 17 soil types + 24 NPV types).

Furthermore, assuming measured canopy radiance with a black background is theoretically controlled by the scattering properties of the vegetation layer only, "pure" vegetation spectra were generated by inserting "zero" for background reflectance in the simulation (Jean-Baptiste Feret, personal communication; Gao *et al.*, 2000). Note that this is equivalent to a canopy bounded by a fully absorbing background (Shabanov *et al.*, 2000). The global sensitivity of pure vegetation spectra and their VIs (termed "pure" VI hereafter), was also calculated. Then, a comparison between the spectral response of a canopy with a scattering background (e.g., impacted by soil-type, soil moisture, NPV, crop-residue moisture) and that with a non-reflecting – and hence non-interfering – background, was studied to gain insight into how variation in the spectral response of agronomic variables owned solely to vegetation elements (see Appendix A for interested reader, not shown here for brevity).

#### 3. Results

## 3.1. Variations of canopy spectral signatures to chlorophyll and LAI for different background optical properties

The background-induced changes in the canopy's spectral response to  $C_{ab}$  and LAI are shown in Fig. 3 based on the mean and the standard deviation (sd) of the  $S_i$  criterion. Differences in  $S_i$  at a certain wavelength (as displayed by sd) reveal how much the contribution of the two agronomic variables (Cab and LAI) varies, owing to background variability. Although canopy reflectance around 530-590 nm and around 690–710 nm is generally more sensitive to  $C_{ab}$  than in other spectral regions, the same spectral regions are also closely affected by background variations, not yet well described in the literature. We found that, due to the variability of background spectra, the leaf-level chlorophyll-sensitive wavebands in the visible and red-edge regions of the spectrum are altered. For example, spectral bands of high sensitivity to Cab appear near 560 and 704 nm for variations in soil-type, near 570 and 700 nm for NPV, and near 595 and 695 nm for variations in soil or cropresidue moisture content (Fig. 3a). On the other hand, the impact of variations in backgrounds relative to Cab at 560 and 704 nm is less strong compared to the impacts on other peak positions. Consequently, the use of canopy reflectance at 560 and 704 nm as predictors of Cab estimates is



**Fig. 3.** The first-order sensitivity indices with associated error (mean  $\pm$  standard deviation) of hyperspectral canopy reflectance to (a)  $C_{ab}$  and (b) LAI for 55 different background scenarios, including soil-type, soil moisture, NPV, and crop-residue moisture. Higher (lower) values of standard deviation indicate larger (less) disturbing effects of the respective background. Note that the  $S_i$  of canopy reflectance is restricted to 400 to 800 nm for  $C_{ab}$  as chlorophyll is transparent to infrared radiation (Knipling 1970).



**Fig. 4.** The first-order sensitivity indices ( $S_i$ ) as measures of the VIs response to  $C_{ab}$  and LAI using global sensitivity analysis and the coefficient of determination ( $R^2$ ) for the relationships between VIs and  $C_{ab}$  and LAI based on the synthetic datasets. The left panels represent the boxplots of  $S_i$ , and the right panels are error bars of  $R^2$  denoting the standard error in the mean across 55 different background scenarios.

desirable. This finding provides powerful support for spatially explicit monitoring of chlorophyll content using Sentinel-2 data, which have green and red-edge bands with center wavelengths of 560 and 704 nm, respectively. The canopy reflectance around 680 nm, which matches the chlorophyll absorption peaks, is closely related to  $C_{ab}$  only when considering variations in background moisture but is strongly affected by soil-type and NPV. Importantly, the sensitivity of canopy reflectance around 680 nm to  $C_{ab}$  decreases with increasing background moisture.

The impacts of background spectral properties on the response of canopy reflectance to changes in LAI vary with wavelength. As shown in Fig. 3b, spectral variations associated with soil-type and NPV impose a greater influence on the LAI-related spectral response of the spectral windows 450–530, 630–690 and 774–900 nm than does soil or cropresidue moisture. For instance, at the pigment-absorption features (around 487 and 675 nm) LAI explains  $28\% \pm 18\%$  and  $44\% \pm 12\%$  (when varying soil types) and  $26\% \pm 16\%$  and  $30\% \pm 16\%$  (when varying NPV) of variations in canopy reflectance, respectively, as opposed to  $5\% \pm 10\%$  and  $10\% \pm 10\%$  (when varying soil moisture) and  $3\% \pm 3\%$  and  $13\% \pm 5\%$  (when varying crop-residue moisture), respectively. Furthermore, canopy spectral response in the NIR range (774–900 nm) to LAI over background cases of soil-type and NPV is less strong than the response with a more or less wet background. In contrast, in the range 1900–2400 nm, differences in soil or crop-residue moisture affect the spectral response to LAI more than differences in soil

#### Table 3

The maximum sensitivity (mean  $\pm$  sd) of canopy reflectance at different spectral regions to variations of leaf-level chlorophyll content based on EFAST.

Canopy background	Visible region Wavelength (nm)	Contribution (%)	Red-edge region Wavelength (nm)	n Contribution (%)
Soil-type Soil moisture NPV	560 595 570	$64 \pm 6$ 71 $\pm 1$ 67 $\pm 7$	704 695 700	$\begin{array}{c} 56 \pm 7 \\ 70 \pm 2 \\ 62 \pm 8 \end{array}$
Crop-residue moisture	595	$71\pm1$	695	$69\pm1$
Fully absorbing background	585	62	695	62

types, particularly at water absorption features (around 1930 nm).

#### 3.2. Sensitivities and correlations of VIs for various backgrounds

The response of VIs to background variations requires focal attention as VIs are extensively applied in the large-scale retrieval of vegetation variables. Fig. 4 visualises the sensitivities of different VIs to variations in leaf chlorophyll content or LAI and the correlations between agronomic variables and the VIs under all scenarios. In general, background influences from soil-type and NPV result in relatively high uncertainties in the  $C_{ab}$ -VIs relationships derived from simulations, while the effect of background moisture variability is minor (Fig. 4a) since the arithmetic combination of spectral bands employed in these chlorophyll-related indices reduce the effects of background moisture. The PRI remains highly sensitive to  $C_{ab}$  for all backgrounds except soil-type, in which the resulting PRI exhibits the worst performance with 13% interquartile range (IQR) of  $S_i$  and the coefficient of determination ( $R^2$ ) of  $0.59 \pm 0.07$ (mean  $\pm$  sd). The CI<sub>RE</sub> is slightly less sensitive to changes in  $C_{ab}$  ( $S_i$  =



**Fig. 5.** The modelled influences of soil type or moisture on canopy reflectance for twelve canopy densities (LAI = 0.1, 0.5, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 7, 8) based on PROSAIL. The distributions of all other PROSAIL parameters are kept constant (i.e., N = 1.5;  $C_{ab} = 25 \ \mu g/cm^2$ ;  $C_{xc} = 8 \ \mu g/cm^2$ ;  $C_{bp} = 0$ ;  $C_w = 0.01 \ cm$ ;  $C_m = 0.004 \ g/cm^2$ ; ALA = 57°;  $\theta_s = 37^\circ$ ), and only the set of background spectra is changed according to Fig. 1. The light-colored areas depict the variations in the canopy reflectance with background variability.

56% ± 3%), and is moderately closely related to  $C_{ab}$  ( $R^2 = 0.57$  on average), followed by MCARI/OSAVI<sub>(705, 750)</sub> with the lowest  $S_i$  of 34% ± 1% and  $R^2$  of 0.33 (on average). It is worth noting that the MCARI/OSAVI<sub>(705, 750)</sub> response to  $C_{ab}$  is only slightly affected by background variability, partly attributed to the OSAVI-based 705 nm feature. By contrast, Macc01 and LICI are better estimators of chlorophyll content across various background conditions, as evidenced by the relatively higher sensitivity ( $S_i > 79\%$  on average) and better relationships with  $C_{ab}$  ( $R^2 > 0.75$  on average), followed by MTCI with  $S_i$  of 66% ± 1% and  $R^2$  of 0.66 (on average). In theory, the LICI is recognized to be independent of LAI (Li *et al.*, 2020) with only a marginal  $S_i$  (< 1%, see Fig. B illustrating the GSA results for each of the selected VIs) that is lower compared to Macc01 with average  $S_i = 4\%$ , and hence is the most robust chlorophyll-related index of the VIs tested here.

Compared to the chlorophyll-related indices, background optical variability more strongly influences the LAI-related indices (Fig. 4b). Specifically, the strong impacts of background optical properties on LAI quantifications using VIs are to be expected in agricultural land with contrastive soil types and NPV. On the contrary, the effects of varying moisture contents are a much less concern.

The different responses of NDVI to LAI with varying soil moisture (with IQR of about 6%) indicate that NDVI is subject to variability associated with soil brightness (Huete, 1988; Huete and Tucker, 1991). Background influences from soil-type and NPV, aside from brightness, also cause more differences in the responsiveness of NDVI to LAI (with IQR of about 8% on average), and so does MSR (with IQR of about 6.8% on average). For this reason, the NDVI-LAI relationships vary significantly among different canopy backgrounds ( $R^2$  varied from 0.2 to 0.4). These outcomes partly explain the inconsistency of many experimental NDVI-LAI relationships, especially for seasonal crop growth monitoring at a global scale (Liu et al., 2012; Liu and Huete, 1995; Xu et al., 2020). Although the sLAIDI is little affected by the interference of chlorophyll effects (with minimal  $S_i < 0.01\%$ ) and yielded good results for certain specific background scenarios, it performs very poorly with respect to LAI (with  $R^2$  of 0.26  $\pm$  0.06 on average individually) in the cases of soil-type and NPV variation. MCARI2 is superior to NDVI, MSR, and sLAIDI because it shows a relatively stable response to LAI over soil backgrounds (with rather small IQR, < 1.5%) and reduced susceptibility to chlorophyll concentration (with  $S_i < 2\%$ ). The MCARI2-LAI relationship is also less sensitive to the variability of soil background reflectance (as evinced by the sd of  $R^2 < 0.01$ ). These results corroborate the well-established idea that MCARI2 is a significant improvement in monitoring crop LAI for precision agriculture (Haboudane et al. 2004).

In comparison with the above discussed LAI-related indices, soilcorrected VIs, including OSAVI and MSAVI respond to LAI with minimal interference of background moisture (this is especially the case for the OSAVI with relatively higher sensitivity, as evinced by the median of  $S_i$  with about 52% and IQR of about 1%). Out of the 12 VIs, only OSAVI displays a potential to estimate LAI despite soil-type background variations ( $R^2$  of 0.36  $\pm$  0.004). This result confirms the earlier findings by Thenkabail *et al.* (2000) that the soil-corrected VIs are valuable when remote monitoring of agricultural crops are studied on widely varying soils. However, OSAVI and MSAVI suffer from poor performance, respectively, due to variations introduced by NPV, as confirmed by larger deviations in  $R^2$  (with sd = 0.2 and 0.3, respectively).

#### 4. Discussion

This work is an attempt to unveil variations in the spectral response of two important agronomic variables, namely,  $C_{ab}$  and LAI, under various background scenarios. It shows that background optical variability can cause significant deviations in the spectral response to  $C_{ab}$  and LAI between different backgrounds and can lead to substantial alterations in the VI-  $C_{ab}/$ -LAI correlations.

#### 4.1. Wavelength selection to background optical variability

The use of wavelength selection for chlorophyll or LAI inversion has been well studied. For example, Verrelst et al. (2016a) pointed out that  $C_{ab}$  is reasonably well correlated with reflectance at 500, 564, 710, and 714 nm. Zhang et al. (2021) suggested the sensitivity wavelengths at 455, 545, 571, 615, 641, 662, 706, 728, and 756 nm for the retrieval of  $C_{ab}$ . Concerning LAI, the sensitive spectrum were extracted from the 680 nm and 910 nm (Thenkabail et al., 2002), 740 nm (Horler et al., 1983), 970 nm and 1725 nm (Le Maire et al., 2008) wavelength. Even so, in contrast to earlier findings only analyzing a scenario with a single soil type, our analyses conclude that background optical variability may result in inconsistencies in the specific feature-sensitive wavelengths chosen over different sites (environments and conditions), further supporting the idea of Mitchell et al. (2012), who using in-situ data figured out the selected wavelengths particularly affected by NPV. As Table 3 shown, the chlorophyll-sensitive peak of canopy spectra in the visible spectral region is observed to have a "blue shift" (towards shorter wavelengths) due to background variability associated with soil-type (the peak located at 560 nm) and NPV (the peak located at 570 nm). In contrast, the peak (at 595 nm) is detected as a "redshift" (towards longer wavelengths) because of background variations linked to moisture contents, whereas the highest sensitivity occurred at 585 nm with a fully absorptive background. The maximum sensitivity of canopy spectra in the red-edge range of 690 to 730 nm shifts toward a longer wavelength only in the cases of soil-type (at 704 nm) and NPV (at 700 nm), as compared to its peak at 695 nm with a fully absorbing background. Consequently, there remains a lack of universality and consistency in the selection of the feature-sensitive wavebands as remote sensing of agriculture frequently involves the measurement of soil and non-vegetation components, which alter plants' spectral characteristics, especially over the semi-arid agricultural landscape where mixed soil-plant litter/residues.

Although the "lambda-by-lambda" band-optimization algorithm could, in principle, determine the sensitive bands for a given experimental dataset (e.g., Thenkabail et al., 2004; Yu et al., 2014), it is suitable merely for field-scale measurements and not for large-scale monitoring. The spectral-band selection using Gaussian process regression (Verrelst et al., 2016a), random forest regression (Liu et al., 2019), and even multi-method ensembles consisting of partial least squares, random forest, and support vector machine regression (Feilhauer et al., 2015) seem more appropriate for band optimizations because of their capacity for band-ranking over very large datasets. Unfortunately, previous band-selection experiments have only put slight emphasis on the effects of variations in the spectral response of canopies with different backgrounds. Appropriate knowledge of background spectra is valuable for accurate discrimination of sensitivity or insensitivity bands from continuous spectra with narrow bandwidth. In future research, the spectral behavior of canopies with various backgrounds such as those given here may serve as prior knowledge to select an optimal set of spectral bands and thus improve the estimation of LAI and  $C_{ab}$ , particularly using spectral mixture analysis (e.g., Tits et al., 2013) or RTM inversion (e.g., Atzberger et al., 2013).

#### 4.2. Applicability of vegetation indices under various backgrounds

The studied background factors lead to changes in VIs for canopies with the same leaf optical properties and LAI (Barillé *et al.*, 2011). Our analyses further reveal that the impacts of different backgrounds on the VIs' sensitivities, as well as on the relationships between VI and agronomic variables, are highly dependent on the type of background (Fig. 4 and Fig. B).

Compared with other chlorophyll-related indices, the performance of PRI was more strongly influenced by background spectra linked to soiltype variability, followed by NPV. Soil background effects mainly involve two ways (Huete *et al.* 1985): (1) the brightness influences attributed to the variations in soil wetness, and (2) the "color" differences caused by variations of soil background material (e.g., soil type). Our results give an indication that PRI is more susceptible to variations in soil background with contrasting soil types, in agreement with the earlier discussion of Barton and North (2001), which may explain why remote sensing of photosynthesis using PRI over large areas on regional or national scale still remains highly uncertain (Garbulsky *et al.*, 2011). A recent research by Yang (2022) suggested that the combination of NDVI and the soil reflectance at 531 and 570 nm may possibly compensate for the soil background effects on PRI. In addition, Barton and North (2001) also noted that background contributes to PRI for canopies with LAI < 3.0. Our results could not confirm this phenomenon, as it would require an analysis of critical thresholds of vegetation cover corresponding to background effects using LSA, which is beyond the scope of the current study.

Several authors (Main *et al.*,2011) pointed out that a canopy index modified to include the red-edge wavebands was superior to their predecessors with red or NIR band reflectance. However, two red-edge-based spectral indices selected here (i.e.,  $CI_{RE}$  and MCAR-I/OSAVI<sub>(705, 750)</sub>) performed not as well as expected. One of the reasons for this is that the background reflectance variability could confound the detection of the relatively subtle differences in canopy reflectance due to changes in leaf chlorophyll content (Daughtry *et al.*, 2000). Another explanation is that  $CI_{RE}$  and MCARI/OSAVI<sub>(705, 750)</sub> were initially formulated for canopy chlorophyll content variations (Gitelson *et al.*, 2005; Wu *et al.*, 2008), although both indices have also been found to provide accurate leaf-level estimations of foliar chlorophyll content (e. g., Gitelson and Solovchenko, 2017; Stuckens *et al.*, 2011).

In contrast to other chlorophyll-related indices, our analyses show that the MTCI, Macc01 and LICI were highly sensitive to changes in leaf chlorophyll while greatly suppressing the influence of background variability. This confirms previous studies (e.g., Li et al., 2020; Main et al., 2011). However, LAI also interferes with the retrieval of leaf chlorophyll content in the visible and red-edge regions. It has been shown in several studies (e.g., Croft et al., 2020; Qian et al., 2022) that there is a stratification in chlorophyll content (as measured by the MTCI) over regions with sparse- and dense-level vegetation cover due to the strong influence of LAI on MTCI. The LICI might be a plausible candidate for spatially-explicit monitoring of leaf chlorophyll content compared to MTCI over agro-pastoral transitional zones because the former is quite insensitive to both LAI and background variations. Nevertheless, the use of LICI for other vegetation types is yet to be confirmed (Chen et al., 2022) since it was originally developed for wheat and rice (Li et al., 2020). This paper demonstrates the potential of LICI for monitoring applications in wheat-like canopies and over heterogeneous agricultural regions.

In terms of LAI-related VIs, background spectra - especially associated with soil-type and NPV - have been shown to impose more significant effects on NDVI and MSR than on MCARI2 (Fig. 4b) although based on the same narrow bands (i.e., 670 and 800 nm). One possible reason is that the mathematical equations defining MCARI2 could better address the differences in the spectral response of each band under different backgrounds. Given the issue that the most relevant spectral information for LAI estimation varied with soil-type (Darvishzadeh et al., 2008a), it must be carefully considered when the NDVI-/MSR- LAI relationships are applied to imagery where green vegetation, soil-type, NPV components are aggregated. Nonetheless, MCARI2 exhibits a notable discrepancy in the correlations with LAI (as evinced by  $R^2$  with 0.34  $\pm$  0.02) due to the presence of NPV. It thus might be sub-optimum in cases where NPV is a significant and variable component of surface cover. These are interesting findings as earlier studies have mostly disregarded the occurrence of non-photosynthetic materials - particularly the appreciable amounts of standing litter present in no-tillage fields. More real data analysis on the effects of NPV on MCARI2 representing vegetation activity (e.g., LAI) is needed in agricultural applications.

We found that both OSAVI and MSAVI are quite insensitive to soil

brightness, relatively insensitive to soil "color" attributed to soil-type, but considerably affected by NPV. Prior studies (e.g., Li *et al.*, 2019) mostly focused on evaluating soil brightness and saturation effects for estimating LAI using soil-corrected VIs. However, aside from soil, the background of a given site consists of litter, crop residues, senescent grass, and sometimes moss. The optical properties of these materials differ greatly from that of the soil. More analysis is thus needed regarding the impact of NPV on soil-corrected VIs in areas with abundant non-photosynthetic materials. Our results imply that, regardless of the robustness of these indices based on the soil line concept (Baret *et al.*, 1993), the background effects of soil-type and NPV cannot be removed entirely.

In conclusion, this research provides a physically-based interpretation of why  $C_{ab}$  or LAI retrievals have low accuracy in some study sites (e.g., Pisek *et al.*, 2010). This can be at least partially attributed to the background spectra. To mitigate the effects of background spectral variations in the retrieval of terrestrial vegetation bio-geophysical properties, multi-angle spectral data (Gemmell, 2000) and new VI-correction methods have been recommended. The latter can be based on the fraction of canopy cover (e.g., Li *et al.*, 2016; Van Beek *et al.*, 2015; Yao *et al.*, 2014) or on the fractions of NPV and soil background (Verrelst *et al.*, 2008).

#### 4.3. Potential and Limitations

Numerical experiments based on radiation transfer simulations are essential to understand the spectral response of biophysical and biochemical parameters with different canopy backgrounds (e.g., Malenovský et al., 2008; Vincini et al., 2008). A unique advantage of this modelling is the ability to cover a wide range of scenarios while circumventing uncertainties related to measurement errors (Verrelst et al., 2010). Although the analysis presented here is based on the simulated data, our investigations showed that simulated and ground truth measurements of wheat canopy spectra are generally in good agreement (see Appendix B). These results suggest that our simulations are reliable representations of the contribution of  $C_{ab}$  and LAI on wheat-like canopy reflectance. In real-world experiments, explicitly quantifying these dynamic sensitivities is difficult since such wide-ranging and contrasting conditions cannot be easily generated through field campaigns. Our detailed analyses provide a good reference for other research groups studying the impacts of subsets of the backgrounds.

Considering the broad range of simulated vegetation properties (in Table 1), we expect these findings to be useful for remotely sensed monitoring of wheat and other crops with similar canopy structures to wheat (e.g., rice, barley, soybean, etc.). Similarly, as a wide range of background spectra were considered (Fig. 1), many different background effects could be included. Note that, even though the LAI values defined here had a large range (0.1 to 10), due to PROSAIL model without taking into account LAI phenology patterns at specific growth status, it might not present the dynamics of vegetation spectral response to seasonal canopy-background reflectance. A GSA involving coupled crop growth and radiative transfer models (e.g., Thorp *et al.*, 2012) would be a plausible way to evaluate the spectral-temporal behavior of crops to background properties.

Although the contribution of soil to canopy reflectance is often reported to be negligible for LAI > 3 or 4 (Goel, 1988), the results of our study showed that they still affect the crop canopy spectra (Fig. 5, Appendix C). Therefore, it is necessary to consider the spectral response of agronomic variables even in areas with dense vegetation coverage. Fig. 5 also demonstrates the need for a more comprehensive soil spectral library in which for a given soil type, many different water contents have been measured. Due to the lack of such data we had to run simulations for (i) soil type effects, and (ii) soil wetness effects separately from each other, leading to the two distinct sets shown in Fig. 5 with mutually no overlap.

#### 5. Conclusion

Unravelling the spectral response of agronomic variables despite different backgrounds is of fundamental importance for an effective Earth observation (EO)-based monitoring of crop physiological and phenological status. With the availability of spaceborne imaging spectrometers, this need further increases, as researchers and practitioners can now use/optimize subsets of spectral bands for their specific applications. In this respect, we highlighted that the contribution of each parameter to the spectral behavior of wheat-like canopies varies with the optical properties of canopy background, particularly associated with soil-type and NPV whose impacts are more significant than that caused by background moisture.

In terms of remotely-sensed chlorophyll content estimates, our analysis suggests that the canopy reflectance measurements at the 560 and 704 nm are desirable due to their relatively high sensitivity to  $C_{ab}$ , with minimum soil impact. On the other hand, the canopy spectra in the interval 774-900 nm is recommended for LAI estimation only for more or less wet background surfaces, while its sensitivity to LAI shows remarkable differences among cases of background soil-type and NPV. Comparing analyses of the sensitivities and correlations of VIs to  $C_{ab}$  and LAI for different canopy backgrounds demonstrates that background reflectance variability is a critical factor leading to substantial uncertainties in the estimation of C<sub>ab</sub> and LAI using EO data. Our analysis points out that LICI, Macc01 and OSAVI, MCARI2 potentially provide better estimates of Cab and LAI, respectively, because of their higher responsiveness to those agronomic variables at a reduced background influence. Notwithstanding, a single spectral index providing a generic algorithm for the two agronomic variables under all "disturbance factors" (comprising soil-type, NPV, irrigated components, etc.), is not realistic. An area-wide canopy background classification based on a priori landscape stratification thus seems indispensable for large-scale mapping of leaf chlorophyll content and LAI.

Additionally, our findings help to improve understanding of the subtle changes in the relationships between spectral features and  $C_{ab}$  and LAI over various background scenarios, which is one of the fundamental requirements for their successful retrieval via the current generation of hyperspectral satellite sensors (e.g., GF-5/AHSI, PRISMA, EnMAP), and those anticipated in the near future (e.g., CHIME, HISUI), and is thus pivotal for accurately diagnosing crop growth status. Although our findings need to be verified further with real-world experiments and/or actual imageries, this aspect is beyond the scope of the current study and will be addressed in our future studies.

#### **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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To further study background effects, the differences of the spectral response of a canopy over scattering backgrounds (shown in Fig. 3) was compared to that over a fully absorbing background (shown in Fig. A). Canopy reflectance in the 550–710 nm spectral region exhibits divergent responses to changes in  $C_{ab}$  between scattering backgrounds through comparison with those sensitivities of the totally absorbing background: the  $S_i$  is slightly higher (approximately 0–9%) over wet backgrounds and considerably lower (around 0–29%) across contrastive soil-type and NPV. This  $S_i$  difference is most pronounced in the red range (660–680 nm), notably with soil-type cases (over 20% lower than those  $S_i$  with a completely absorbing



Fig. A. Main effect and interactions of the EFAST sensitivity analysis on vegetation biophysical and biochemical parameters with a totally absorbing background.

background). This result corresponds to early findings that experimental measurements of red reflectance are susceptible to the effects of variable irradiance and background (Curran & Milton, 1983). Besides, equivalent water thickness ( $C_w$ ) explains about 31%–61% of the canopy reflectance variation in the SWIR wavelength longer than 1880 nm (termed "SWIR2" hereafter) under the zero-background case, much larger than LAI does with a contribution less than 12%. This result is an apparent difference with GSA results only concerning one specific soil background that LAI governed over 50% of the variation in SWIR2, greater than  $C_w$  does (e.g., Xiao *et al.* 2014; Verrelst *et al.*, 2015a, 2016b). This inconsistency is tentatively attributed to the fact that the background has a much higher single-scattering albedo in the SWIR2 spectral part than does green vegetation (Asner, 1998), so the SWIR2 reflectance of plant canopy mixed with the background is more sensitive to changes in LAI than that under the zero-background case in the absence of specular reflection. Furthermore, the sensitivity of canopy spectra in the NIR plateau (800–1300 nm) to LAI decreases dramatically while the sensitivity of red reflectance in the wavelength interval [665, 680 nm] and SWIR2 reflectance increases compared to those responsiveness in a totally absorbing background, respectively.

The comparison of the response of VIs over the scattering backgrounds with their "pure" counterparts responsiveness under fully absorbing background (as presented in Fig. B and C) illustrates the performance of the VIs (especially LAI-related indices) could be misleading due to background optical properties. The sensitivity of NDVI to LAI in the zero-background case ( $S_i = 7\%$ ) is far less than that with canopy backgrounds. Theoretically, the NDVI relies on the spectral contrast between red and NIR signatures (Rahman *et al.*, 2004). The NDVI-LAI insensitivity can be accounted for by the fact that the red-NIR contrast is fairly uniform under a 100% absorbing background due to multiple interactions within the canopy only, which is similar to the saturation of NDVI at high values of LAI. This result is in agreement with the findings of Gao *et al.* (2000). While the multiple scattering process in the vegetation background theoretically enhances the response of NDVI to LAI changes and thus the NDVI-LAI relationship has a larger correlation coefficient than that under totally absorbing background ( $R^2 = 0.04$ ). Likewise, the sensitivities and correlations of MSR-LAI and sLAIDI-LAI relationships are found to be larger than that with totally absorbing background ( $S_i = 12\%$  and 14%,  $R^2 = 0.09$  and 0.11, respectively). Note that this positive contribution of canopy background to spectral response of VIs only is observed for LAI-related VIs including NDVI, MSR, and



Fig. B. Results of the global sensitivity analysis (the mean values of the first-order sensitivity indices) for each of the selected vegetation indices across (a) scattering and (b) fully absorbing backgrounds.



Fig. C. Sensitivity and correlation of VI to (a) C<sub>ab</sub> and (b) LAI under conditions of a completely absorbing background.

sLAIDI responsiveness to LAI but are rarely found in VIs related to chlorophyll content. Overall, the results of the comparative analysis reveal that the contributions of agronomic variables to plant-canopy spectra depend on wavelength and differ considerably with the background scenarios. Such information is needed to the understanding of the narrowband EO data discerning subtle, but import, features related to plant phenotypes.

#### Appendix B

The performances of the PROSAIL are evaluated by comparison between measured and simulated reflectance. Similar works also have been carried out by Schlerf and Atzberger (2006) and Darvishzadeh *et al.* (2008b). The results (Fig. D) illustrate a good agreement between the measured and modelled wheat canopy spectra.



Fig. D. Measured (continuous line) and modelled (dashed black line) wheat canopy reflectance for different values of canopy LAI.

#### Appendix C

In the literature it is often stated that the contribution of soil to canopy reflectance might be negligible for LAI > 3 or 4. We tested this assumption further in our study through modelling. The relative changes in canopy reflectance (Diff) under different LAI values was calculated based on the equation (Sun *et al.*, 2020):

$$\text{Diff} = \left| \frac{Ref_2 - Ref_1}{Ref_1} \times 100\% \right|$$

where *Ref*<sub>1</sub> is the simulated canopy reflectance under one background reflectance, while *Ref*<sub>2</sub> is corresponding reflectance under another background reflectance.

Figs. E and F show that background optical variability continues to influence the canopy reflectance even when  $LAI \ge 6$ , even though such subtle differences in canopy reflectance might not be measurable from an optical sensor due to noise etc.



**Fig. E.** The modelled influences of NPV or crop-residue moisture on canopy reflectance with varying LAI values (LAI = 0.1, 0.5, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 7, 8) based on PROSAIL. The distributions of all other PROSAIL parameters are kept constant (i.e., N = 1.5;  $C_{ab} = 25 \ \mu g/cm^2$ ;  $C_{xc} = 8 \ \mu g/cm^2$ ;  $C_{bp} = 0$ ;  $C_w = 0.01 \text{ cm}$ ;  $C_m = 0.004 \text{ g} /cm^2$ ; ALA = 57°;  $\theta_s = 37^\circ$ ), and only the set of background spectra is changed.



Fig. F. Relative changes in canopy reflectance (Diff) under different LAI values. The horizontal dash line at 0 indicates no differences in reflectance due to background changes.

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