



Retrieval of the canopy chlorophyll content from Sentinel-2 spectral bands to estimate nitrogen uptake in intensive winter wheat cropping systems

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ARTICLE INFO

Keywords:

Nitrogen content
Canopy chlorophyll content
Artificial neural network
Red-edge bands
Sentinel-2
Scaling issue
Intensive cropping systems

ABSTRACT

One of the most common approaches to reducing the environmental impact of nitrogen (N) fertilisation in intensive agrosystems is to adjust the N input of the crop requirement. This adjustment is frequently related to the nitrogen nutrition index (NNI) based on the concepts of the critical and actual N absorbed (kg/ha) in the crop canopy (respectively, N_C and CNC). Accurate estimation of the N_C and CNC at the field scale over large areas based on freely available satellite imagery is thus a key issue to address. Relying on a large dataset of farmers' fields, this study highlights the high correlation ($R^2 = 0.90$) between the wheat CNC and canopy chlorophyll content (CCC) retrieved from Sentinel-2 (S2) with an Artificial Neural Network (ANN). The estimation is related to errors of 4 and 21 kg/ha (depending on the growing stage), which is a promising result for evaluating the NNI. There are four major outcomes from this result: (i) the importance of working at the canopy level; (ii) the independence of the relationship to the considered cultivars; (iii) the dependence of the relationship on the growing stage; and (iv) the potential to use only the 10 m S2 bands, opening the way for precision agriculture. In parallel, estimation accuracies were investigated for the three biophysical variables (BV) related to the CNC and N_C , i.e., the green area index (GAI), leaf chlorophyll content (Cab) and CCC. From this analysis, the added value of the red-edge bands for improving the estimation of the 3 BVs of interest was quantified as was the performance reduction related to the field heterogeneity.

1. Introduction

A fertilisation adjustment to the actual crop need by splitting is crucial, especially for crops with a high nitrogen (N) fertilisation level. Fractioning aims for the optimum economic outcome, the limitation of the lodging of cereals and disease development and minimisation of environmental losses and associated impacts. In many intensive wheat cropping systems in Europe as well as in south-eastern Australia and in Mexico, for example, N fertilisation is usually split in 2 to 3 fractions. The first fraction is applied at the tillering stage, corresponding to growing stages 25 to 29 on the BBCH scale (Lancashire et al., 1991), and the second fraction during stem elongation (from stage 30). The third fraction, conditioning the protein content and the potential yield, is applied between the stages of flag leaf pointing and flag leaf fully unfolded (stages 37–39). Estimation of the crop N content (in %) during stages 37 and 39 provides crucial information that allows the adjustment of fertilisation to the crop need, thus avoiding over-fertilisation. In Belgium, the rate of each N fraction is defined according to the qualitative balance-sheet method developed in the “Livre Blanc” (Meza

et al., 2016). In Mexico, the GreenSat program relies on the Normalised Difference Vegetation Index (NDVI) derived from SPOT observations at the critical period to advise the farmers (GreenSat, 2017). The recent Sentinel-2 (S2) constellation combines a high revisit frequency (5-day revisit cycle) and spatial resolution (10 m - 20 m) with systematic global acquisition and an open access policy, which is promising in the development of operational farming services in near real time. In addition to the visible and near-infrared (NIR) wavelengths, the S2 Multi Spectral Instrument (MSI) includes 3 bands in the red-edge region centred at 705, 740 and 775 nm, which were found to be of great interest for crop monitoring. In addition to the importance of the red-edge region in estimating the leaf chlorophyll *a* and *b* content (Cab) demonstrated in several papers (Boochs et al., 1990; Filella and Penuelas, 1994; Daughtry et al., 2000; Perry and Roberts, 2008), simulation studies highlighted the potential of S2 red-edge bands for retrieving the Leaf Area Index (LAI) and Cab (Delegido et al., 2011; Schlemmer et al., 2013; Clevers and Gitelson, 2013; Frampton et al., 2013; Peng et al., 2017). However, these studies were based on the use of vegetation indices solely and S2 simulated data, either from radiative transfer

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<https://doi.org/10.1016/j.rse.2018.06.037>

Received 16 September 2017; Received in revised form 14 June 2018; Accepted 24 June 2018

Available online 11 July 2018

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model simulations or from spectrometer measurements at a very high spatial resolution, which paves the way for the development of operational farming services at the national scale, including the rational use of fertilisers through precision agriculture at the parcel level. However, very few results have concerned actual farmers' fields, focusing instead on N content ranges observed only in experimental trials.

Two main approaches were developed to estimate the N content from reflective optical measurements: (i) direct methods that relate surface reflectance to the N status, generally through the use of vegetation indices (Haboudane et al., 2002; Wang et al., 2012; Clevers and Gitelson, 2013; Li et al., 2014a; Kusnierek and Korsaeth, 2015; Chen, 2015; Feng et al., 2016) and (ii) indirect methods first relating the surface reflectance to the *Cab* and then the *Cab* to the N content (Cartelat et al., 2005; Baret et al., 2007a; Houles et al., 2007; Schlemmer et al., 2013; Feng et al., 2015; Zhou et al., 2016; Zhao et al., 2016). Indeed, based on plants grown under controlled conditions, Evans (1989) demonstrated that leaf *Cab* is significantly correlated to the total leaf N content for winter wheat ($R^2 = 0.94$) and more generally for C3 plants. Nevertheless, radiation in the visible and NIR wavelengths is sensitive to both the *Cab* and the *LAI* (Baret et al., 2007a). In this context, relating N to *Cab* at the canopy level increases the accuracy of N estimation and its robustness across time (Houles et al., 2007). Schlemmer et al. (2013) found that switching to the canopy level acted as a normalisation factor, increasing the coefficient of determination of the relationship between N and *Cab* from 0.73 to 0.94. Given the results from these studies and the importance of estimating N at the field level to adjust the fertilisation advice, in addition to the *Cab*, two biophysical variables (BV) at the canopy level were considered in this study, i.e., the green area index (*GAI*) and the canopy chlorophyll content (*CCC*). The *CCC* is defined as the product of the *GAI* and the *Cab* expressed in grams per unit leaf area (g/m^2) (Houles et al., 2007; Clevers et al., 2017). Conversely to the *LAI*, which refers only to the green leaves of the crop, the *GAI* includes all the green photosynthetically active elements of the canopy, including stems, inflorescences and others (Duveiller et al., 2011). The *GAI* is thus more closely related to what is actually recorded by the satellite instrument.

For each approach, empirical methods relate vegetation indices to the variable of interest by means of statistical relationships, while physically based methods often involve the combination of a Radiative Transfer Model (RTM) and machine-learning algorithms to estimate several BVs, including the *GAI* and *Cab*. Empirical methods of estimating either *Cab* or the N content are simple, computationally efficient and provide accurate results according to numerous studies (Marshall and Thenkabail, 2015). Recently, Clevers et al. (2017) showed a high potential in estimating *Cab*, *LAI* and *CCC* with vegetation indices based on S2 images in one trial potato field. However, since the spectral signature of a crop is driven by many factors that vary in time, space, climatic conditions and vegetation types, empirical methods based on vegetation indexes are not generic and frequently require local calibration. On the other hand, physically based methods are able to cope with the non-linearity of the relationship between the BV and the measured reflectance (Verrelst et al., 2012). These models simulate the radiation within the canopy to describe the mechanistic interactions between the BV and the canopy reflectance, thereby increasing the likelihood of transferability (Houborg and Boegh, 2008; Marshall and Thenkabail, 2015).

In the context of the development of operational farming services, this study focuses on physically based methods, which present the advantages of being calibrated once and being applicable at large scale. The N content is then estimated via an indirect approach with an artificial neural network (ANN) trained on canopy radiative transfer simulations. The main criteria in selecting this approach are: (i) RTMs are based on knowledge of the physical processes involved in photon transport within vegetation canopies (Verger et al., 2011); (ii) the approach is based on an ANN, which is potentially more accurate than other estimation techniques since it optimises directly over the

variables of interest (Baret and Buis, 2008); (iii) in situ data are not mandatory for the calibration of the regression model, making them applicable at a large scale with a short processing time; and (iv) it is possible, using an ANN, to test the influence of the new red-edge spectral bands on performance retrieval. Nonetheless, the training process and database, including a priori statistical distributions and co-distributions of the BVs, have a major impact on retrieval performances and are often not sufficiently documented (Verger et al., 2011; Sehgal et al., 2016). Another pertinent physically based method would be the Gaussian processes that provide uncertainty bars and demonstrate similar or higher accuracy than the ANNs (Verrelst et al., 2012). Nonetheless, Camacho et al. (2017) moderated these results. The root mean square error (RMSE) between the ground and estimated *GAI* obtained with the Gaussian processes was 0.05 less than with the ANN, which is low compared to the measurements errors. In addition, considering wheat and barley, the ANN were over-performing (RMSE = 1.16 versus 1.39). We decided thus to rely on the ANN implemented in the BV-NET tool (Weiss and Baret, 1999), which is freely available upon request and has already shown good performances in the literature. The BV-NET tool was used to develop operational and validated products at both the kilometric and decametric scales and allowed the development of the CYCLOPES product, which was derived from the VEGETATION sensor (Baret et al., 2007b) in the past and was also used to generate the *LAI* retrieval algorithm provided in the SNAP toolbox, the Sentinel-2 for Agriculture system (Bontemps et al., 2015) and S2 products on demand with global coverage made available by Vuolo et al. (2016).

ANNs have been successfully used in several studies to estimate *Cab*. Suo et al. (2010) estimated leaf *Cab* from cotton using RGB camera images based on a three-layer ANN with a relative error of 8.4%. Based on hyperspectral images, Liu et al. (2010) reported an error of $2.6 \mu\text{g/cm}^2$ ($10 < \text{Cab} < 45 \mu\text{g/cm}^2$) for rice, and Kira et al. (2015) reported a coefficient of variation of 11.8% for trees' leaves. Similarly, based on an IRS-P6 satellite image, Sehgal et al. (2016) obtained a RMSE of $23.3 \mu\text{g/cm}^2$ ($25 < \text{Cab} < 65 \mu\text{g/cm}^2$) for wheat, and Verrelst et al. (2012) reported a relative RMSE (RRMSE) of approximately 20% for 9 crops, including wheat, based on the S2-simulated reflectance. We used the same algorithm as the one developed by Weiss and Baret (1999), further adapted and evaluated over different sensors (Baret et al., 2007b; Claverie et al., 2013; Li et al., 2015).

This study aims to assess the performance of an ANN on S2 images to estimate wheat *CCC* and its associated BVs, i.e., *GAI* and *Cab*, in an intensive agricultural landscape and to test the strength of the link between the BVs *Cab* and *CCC* and the N content at the leaf (%) and canopy (kg/ha) levels, respectively. The first objective of this study is to determine the impact of the S2 spatial resolution on the estimation of the BVs linked to the *CCC* and N content. We compared the retrieval accuracy of these variables of interest with the bands at 10 and 20 m resolution, including the new S2 red-edge bands centred at 705, 740 and 775 nm and the SPOT5 configuration. The possibility to estimate these BVs and the N content at 10 m resolution would offer important opportunities for operational precision farming applications. The second objective is to quantify the accuracy of the proposed method in estimating winter wheat N content at the canopy level at 10 and 20 m. The third objective is to investigate the impact of spatial heterogeneity due to different biomass levels in a field on the accuracy of the retrieved BVs. Unlike many studies based on N trials with a large range of variation in *Cab*, this analysis considers intensively managed farmers' fields and therefore addresses the small range of N variation effectively observed in productive fields.

2. Materials and methods

2.1. Satellite data

Both S2 surface reflectance time series for the 2016 and 2017 winter wheat growing seasons were processed using the MACCS (Multi-sensor

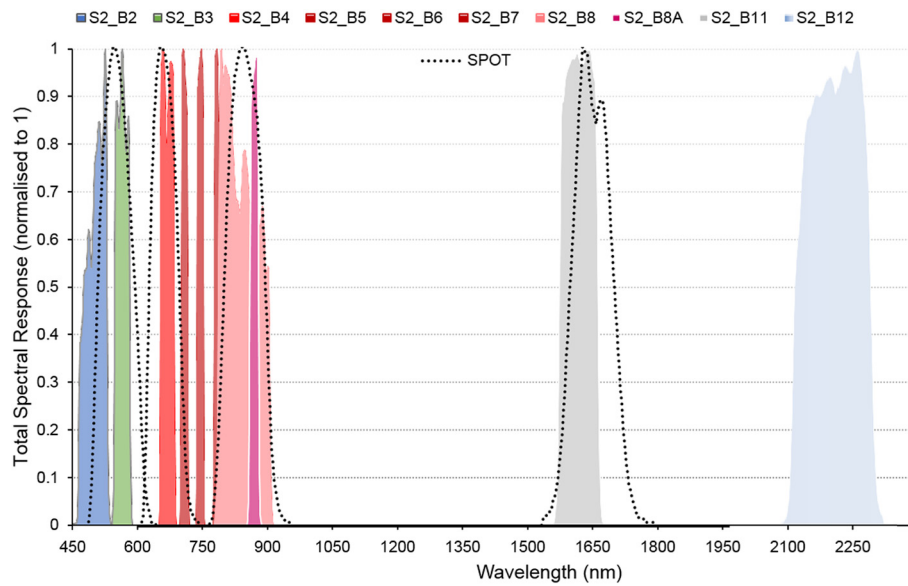


Fig. 1. Comparison of S2 and SPOT5 Take5 spectral response. S2 bands are displayed in solid curves and SPOT5 bands (respectively, 1 to 4) are in dashed black curves. Only the bands used in this study are presented.

Atmospheric Correction and Cloud Screening) algorithm implemented in the Sentinel-2 for Agriculture system (Hagolle et al., 2010; Hagolle et al., 2015a; Hagolle et al., 2015b). The same algorithm was used to process the SPOT5 Take5 images for the sake of consistency of both datasets regarding radiometric calibration and atmospheric correction. Started in April 2015 by the CNES, the SPOT5 Take5 experiment lowered the orbit of SPOT5 by 3 km to obtain a 5-day revisit cycle with a constant observation angle for a limited number of sites. This experiment aimed at providing images with similar revisit frequency and resolution to the Sentinel-2 constellation, but with only 4 spectral bands (Fig. 1). SPOT5 Take5 level 2A surface reflectance images acquired between April and June 2015 and delivered by THEIA are used to compare the performance of the 2016 S2 time series to retrieve the GAI.

2.2. Field campaigns

Two types of in situ data were collected: a first set to assess the GAI retrieval performance from S2 versus from SPOT5 (first part of Table 1)

Table 1

Data acquired during the 4 field campaigns organised between April 2015 and 2017. The GAI was estimated through the growing seasons in 2015 and 2016. The variables linked to the CCC were measured during the key period of N application in the spring of 2016 and 2017. NC stands for Nitrogen Content, DM for Dry Matter Content and DHP for Digital Hemispherical Photograph. The agricultural practices in the fields studied for the CNC are given in Table 2.

Campaign	GAI growing season		CCC estimation	
Date	April–July 2015	March–July 2016	3rd N supply Early May 2016	2nd N supply Early April 2017
# fields	21	18	5 + 1 organic	4
Area (satellite)	SPOT5Take5 scene	Spread in Belgium (S2)	Spread in Belgium (S2)	Reduced area (S2)
BV retrieved Measurements	GAI DHP		GAI, Cab, NC, DM DHP, Dualex, destructive sampling: NC(%), DM	
ESU size	2 × 2 20 m pixels	2 × 2 20 m pixels	1 10 m pixel	1 10 m pixel
# samples (N)	125	83	15 + 23	10

and a second set to study the ability of S2 images to accurately estimate the CCC and consequently the N absorbed by the canopy, abbreviated to Canopy Nitrogen Content (CNC) (second part of Table 1). The first set of field campaigns took place in 2015 and 2016 during the winter wheat growing season to measure the GAI in a large sample of fields. Due to the cost of destructive sampling, the second set of field campaigns was completed to systematically acquire data on Cab, N and aboveground biomass in a limited number of fields during the key period of N application. In 2016, these fields corresponded to a sub-sample of the fields monitored for the GAI.

2.2.1. Study area

The first field campaigns took place from April to July 2015 over 21 fields located in the SPOT5 Take5 Belgian scene corresponding to an area characterised by intensive agriculture over a silty soil (called the “Silty region”). In 2016, 18 other fields geographically spread throughout Belgium were sampled from end of March to July (Fig. 2). To estimate the CCC during the key period of N application, a second set of campaigns took place in 6 fields in early May 2016 and in 4 fields in early April 2017, the key periods for the third and the second N supply in Belgium. All the data were collected in farmers' fields either in conventional or in organic farming, representing the agricultural practices of these intensive cropping systems. The selected fields were spread over 4 agricultural regions to capture the soil and climatic diversity of Belgium. Most fields were located in the Silty region, which is the largest region in terms of area. This agricultural land is the best and the most fertile, with cereal crops, including wheat, beet and potato, being the most common crops. Each studied field was sown with one unique cultivar of winter wheat (*Triticum aestivum* sp.). The mixture of cultivars was excluded to test the effect of cultivars on the CNC-CCC relationships. The agricultural practices (i.e., cultivar, sowing date and density, BBCH stage, N supply and yield) and the destructive measurements, including the dry matter content (DM) and N content (%), are reported in Table 2 for the 10 fields monitored for the CCC. In addition, an organic field was selected for its well-known heterogeneity due to very different sub-parcel management trajectories to study the heterogeneity effect on the retrieved BV accuracy. Indeed, this field was converted to organic practices in 2015 from the land consolidation of 7 conventional fields currently showing a large diversity in terms of soil structure and nutrients.

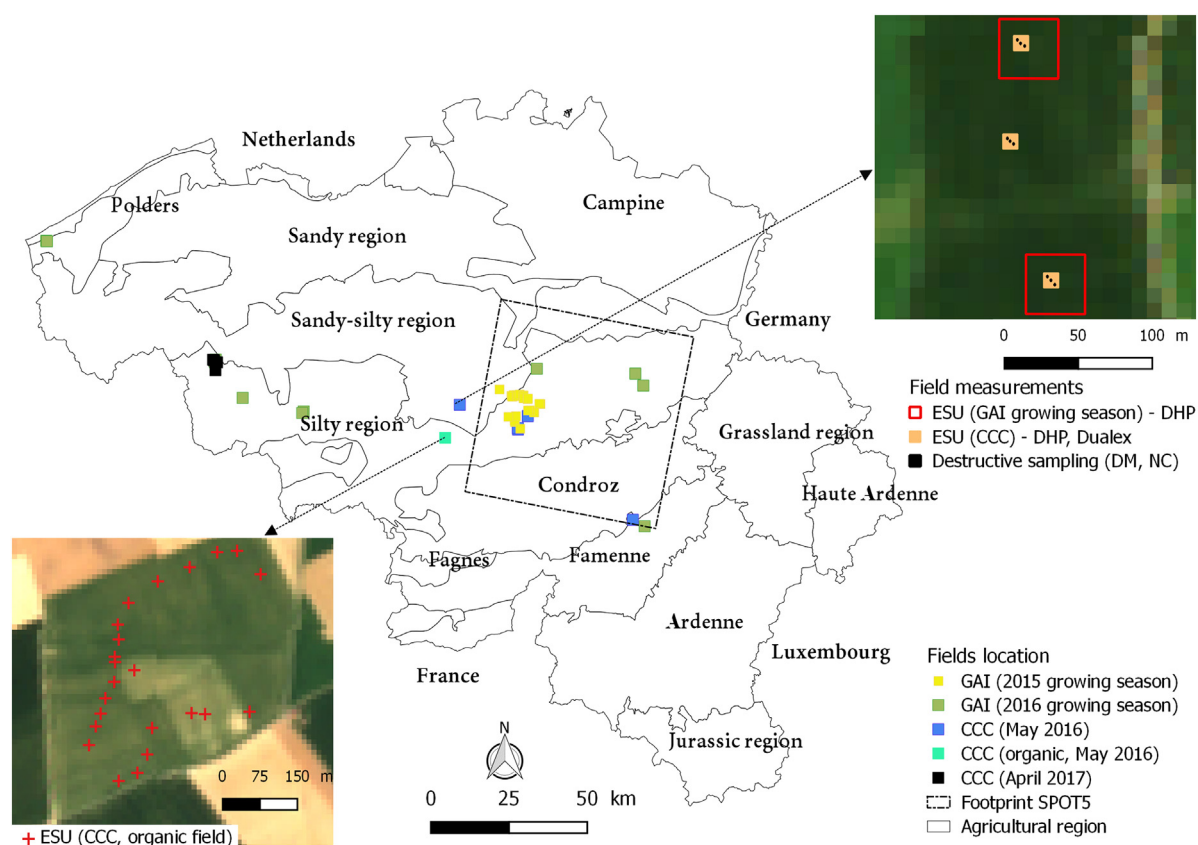


Fig. 2. Distribution of the fields monitored in four different agricultural regions in Belgium. *GAI* (yellow and green squares) stands for the 39 fields monitored with DHP in 2015 and 2016. *CCC* stands for the fields monitored for their N status during the periods of the 3rd and the 2nd N supply in May 2016 and April 2017, respectively (these were also monitored for the *GAI*). The upper right zoom presents one field monitored for both the *GAI* during the growing season (red ESU) and the N status (orange ESU), where the black squares represent the location of destructive sampling. The bottom left zoom illustrates the specific ESU distribution in the heterogeneous organic field. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2.2.2. *GAI* indirect measurements during the winter wheat growing season

The *GAI* was measured by acquiring Digital Hemispherical Photographs (DHP) in two Elementary Sampling Units (ESU) for each of the 39 sampled fields. In each ESU, the sampling was performed along 2 transects of 15 m with 5 DHPs by transect. The corresponding reflectances were then extracted by considering an area of 2 by 2 pixels (at 20 m spatial resolution) centred over the transects. DHPs were processed with the CAN-EYE version 6.4.1 software (Demarez et al., 2008). The *effective GAI* provided by CAN-EYE was considered for the comparison with the satellite estimates for the following reasons. First, the crop architecture can be approximated by a turbid medium since

rows are no longer apparent at this phenological stage of wheat (end of March), as demonstrated by Demarez et al. (2008) with very good agreement between CAN-EYE *effective GAI* estimates and destructive measurements for wheat ($GAI > 0.2$). Second, remote sensing data are better linked to the estimation of the *effective GAI* rather than the *true GAI*. Finally, the *true GAI* retrieval from DHP is more delicate since it requires the estimation of the clumping parameter to describe the canopy architecture.

2.2.3. *CCC* estimation and *CNC* during the key periods of N application

The *CCC* was estimated by the multiplication of the *GAI* and the *Cab*

Table 2

Agricultural practices and destructive measurements of the dry matter content (DM) and Nitrogen Content (NC) for the 10 fields studied for the *CCC* (6 in 2016 and 4 in 2017). The standard deviation is given in brackets.

Sampling date /type	Cultivar	TT ^a	UN ^b (kg/ha)	DM (t/ha)	BBCH stage	NC (%) ^c	Yield (t/ha) ^d
3rd N supply 06–09/05/2016, conventional	Atomic	1304	120	2.9 (0.9)	31–32	2.7 (0.2)	7
	Cellule (1)	1419	90	10.1 (1.8)	33	2.1 (0.2)	5.5
	Edgar	1467	121	7.6 (1.2)	32	2.3 (0.2)	7
	Cellule (2)	1338	145	4.3 (1.8)	33	2.9 (0.3)	6.5
	Anapolis	1431	130	11.2 (2.0)	32	2.1 (0.2)	7
19/05/2016, organic	Tybal	1120	90	7.3 (1.9)	37	1.7 (0.2)	3.6
2nd N supply 11/04/2017, conventional	Genius	896	65	1.4 (0.2)	30	3.0 (0.2)	–
	Cellule	994	78	2.2 (0.3)	31	3.3 (0.2)	–
	Gedser	967	78	2.5 (0.3)	30–31	3.0 (0.2)	–
	Bergamo	1172	78	2.1 (0.3)	30–31	3.3 (0.2)	–

^a Thermal time in degree days from the sowing date until the measurements day (Eq. (5)).

^b Synthetic/organic N fertilisation applied by the farmer during the period between the sowing and the measurements dates.

^c N content (%) of the dry aerial organs (leaf-stem), mean value based on 6 to 9 samples, the standard deviation is given in brackets.

^d Final yield estimated by the farmer at harvest.

Table 3

Distribution laws of input variables to generate the learning database in PROSAIL. Truncated Gaussian and uniform distribution laws are used, characterised by the mode, standard deviation (Std), minimum and maximum values. The co-distribution parameters between *Cab* and *GAI* are given in the last row (Weiss and Baret, 2016). ALA = Average Leaf Angle inclination; HsD = Hot-spot parameter; N = leaf structure parameter; Cdm = dry matter content; Cw = leaf water content; Cbp = brown pigment concentration.

	Variable	Min	Max	Mode	Std	Law
Canopy	GAI	0.0	15.0	2.0	3.0	Gauss
	ALA (°)	30	80	60	30	Gauss
	HsD	0.1	0.5	0.2	0.5	Gauss
Leaf	N	1.20	1.80	1.50	0.30	Gauss
	<i>Cab</i> ($\mu\text{g}\cdot\text{cm}^{-2}$)	20	90	45	30	Gauss
	Cdm ($\text{g}\cdot\text{m}^{-2}$)	0.0030	0.0110	0.0050	0.0050	Gauss
	Cw_Rel	0.60	0.85	0.75	0.08	Gauss
	Cbp	0.00	2.00	0.00	0.30	Gauss
	Bs	0.50	3.50	1.20	2.00	Uni
Co-distribution GAI-Cab						
Cabmin (0)		Cabmax (0)		Cabmin (GAI _{max})		Cabmax (GAI _{max})
20		90		45		90

that were indirectly measured, respectively, with DHPs and the Dualex 4 Scientific (Force A, Orsay, France). In parallel, the CNC was destructively measured by the multiplication of the aboveground DM and the N content (%) of the aerial part of the wheat. The sampling in the conventional fields consisted of three ESUs of 10 m × 10 m randomly selected in homogeneous areas. In each ESU corresponding to one 10 m S2 pixel, three rows of 1 m were geolocalised and delimited to perform 8 DHPs and 10 Dualex measurements per row. The plants in the row were then cut at ground level for DM and N content analyses in the laboratory. The Dualex measurements were systematically performed on the middle of the main shoot, i.e., the youngest upper fully developed leaf of the canopy, with the adaxial leaf side facing the light source (Cartelat et al., 2005; Cerovic et al., 2012). The N content (%) was determined with the NIR reflectance spectroscopy system (Foss NIRSystems 6500 spinning) operating between 1100 and 2500 nm. The values were then averaged by ESU and compared to the BV retrieved from S2 for the corresponding pixel. For the organic field, the sampling scheme was adapted to take into account its heterogeneity. Twenty-three ESUs of one row of 1 m were spread in the field (Fig. 2).

2.2.4. Calibration of the Dualex measurements

The Dualex 4 *Cab* estimates ($\mu\text{g}/\text{cm}^2$) are based on a generic equation established by the manufacturer. However, chlorophyll meters, such as SPAD and Dualex, are known to be instrument dependent and to saturate with high *Cab* (approximately 40–50 $\mu\text{g}/\text{cm}^2$) (Cartelat et al., 2005; Houborg and Boegh, 2008; Casa et al., 2015). To overcome this saturation problem and to obtain a specific relationship between the Dualex readings and the *Cab*, organic extraction is usually performed. As shown by Cartelat et al. (2005), the cultivar effect is not prominent, and the determination of the *Cab* with a same instrument should be cultivar independent. In this study, chlorophyll organic extraction was then completed on 18 winter wheat leaves of the most represented cultivar (Cellule) with 80% cold acetone. The absorbance of the supernatant was read using a spectrophotometer at 663.2 and 646.8 nm to calculate the *Cab* concentration according to Lichtenthaler (1987). The leaves were selected according to their colour from the lightest to the darkest to be representative of the chlorophyll range. A systematic bias was highlighted in the studied range, leading to the use of a linear relationship to convert the Dualex readings in *Cab* with a final RMSE of 2.6 $\mu\text{g}/\text{cm}^2$ on a range varying from 45 to 60 $\mu\text{g}/\text{cm}^2$:

$$C_{ab}(\mu\text{g}/\text{cm}^2) = \text{Dualex} + 12.24 \quad (1)$$

The linearity of the *Cab* - Dualex relationship confirms the results obtained by Cerovic et al. (2012). The *Cab* variability between actual

farmers' fields is relatively low because all of these fields correspond to high input-intensive cropping systems.

2.3. Implementation of the BV-NET algorithm

The BV-NET algorithm developed by Weiss and Baret (1999) estimates BV from multi-spectral reflectance by inverting a RTM with a back-propagation ANN; its current implementation is described by Li et al. (2015). The architecture of the ANN is made up of two layers. The first layer is composed of 5 neurons with tangent sigmoid transfer functions, and the second layer contains 1 neuron with a linear transfer function allowing a larger dynamic in the output variables (Claverie, 2012). The training database is simulated by means of PROSAIL RTM (Jacquemoud et al., 2009) that couples PROSPECT-3 to simulate the leaf optical properties and SAIL-4 (Verhoef, 1984; Verhoef, 1985; Jacquemoud and Baret, 1990) to generate TOC reflectances. The generation of the learning database is the most critical step, since it should be composed of a representative set of TOC reflectances and incorporate prior information on the distribution of the input variables. Therefore, the distribution laws and associated parameters used in this study are those most recently defined by Weiss and Baret (2016), who consider the co-distribution between variables to reinforce the representativeness of the learning database. The BV-NET algorithm uses co-distribution for some variables, such as *Cab*, as a function of the *GAI*. Indeed, dense green wheat canopies are never associated with low *Cab*. Consequently, we assumed that the *Cab* variation range changes linearly with the *GAI* between *Cab*_{min}(0) and *Cab*_{min}(*GAI*_{max}). The distribution laws of the input variables used for this study are presented in Table 3 and justified in the Algorithm Theoretical Basis document (Weiss and Baret, 2016). The maximum *GAI* was artificially set to 15 to overcome the saturation problem currently observed for high *GAI* values.

To assess the impact of the spatial and spectral resolution of the new S2 bands on the retrieval performances of the three BVs (*GAI*, *Cab* and CCC), four band sets are investigated (Table 4). Note that band 2 and the 60 m bands designed for atmospheric correction are never included because of the possible residual atmospheric perturbation. To compare the different band combinations and ensure the comparability of the results, the ANNs were calibrated using the same learning database of PROSAIL input parameters. In this way, the tuned coefficients (synaptic weights and bias) are recomputed for each band set based on the same learning database. Together with the reflectances, the configuration of the image acquisition is used as inputs, i.e., the view and sun zenith angles, as well as the relative azimuth angle. The ANN performance for retrieving the BV with the different band sets is graphically and

Table 4

Selection of S2 band sets to assess the performance of the BV-NET algorithm. The “Code name” refers to the labelling in this paper and “#B” to the number of used bands in each tested set. The bands added in each band set are highlighted in bold.

Bands choice	Band sets	Code name	#B
All 10 m bands	B3, B4, B8	10 m bands	3
Equivalent SPOT5 bands	B3, B4, B8, B11	SPOT5 bands	4
Including red-edge bands	B3, B4, B8, B11, B5, B6, B7	Red-edge	7
All bands	B3, B4, B8, B5, B6, B7, B8a, B11, B12	All bands	9

statistically evaluated with the indicators described in Section 2.5. The simulated performances are assessed using the validation database corresponding to a random selection of 30% of the cases within the learning database, and the actual performances are then computed using in situ measurements (Fig. 3).

2.4. Sensitivity of the BV retrieval to the within-pixel heterogeneity

We study the impact of heterogeneity on the accuracy of the retrieved BV with the BV-NET algorithm in two ways. First, the pixel heterogeneity was simulated using a linear combination of the BV and associated reflectances from the synthetic dataset generated via PROSAIL. Heterogeneous pixels were made of 2 canopy cases randomly selected from the learning database, each canopy case including the BV and associated reflectances. The values of these pixels were computed via the relationship proposed by Weiss et al. (2000), which was slightly modified to address 2 canopy cases instead of 1 canopy and 1 soil case, and the value of each mixed pixel created synthetically corresponds to the mean value of the two randomly selected pixels:

$$X_w = w \cdot X_i + w \cdot X_j; w = 0.5 \quad (2)$$

where w corresponds to the fraction of the mixed pixel composed of the

canopy type i and the canopy type j , and X corresponds to the value of the BV or the associated reflectance. For each mixed pixel, a heterogeneity index (H) ranging from 0 to 1 was computed as follows (Weiss et al., 2000):

$$H = \frac{|X_i - X_j|}{\max_x} \quad (3)$$

where $\max_x$ corresponds to the maximum value of the considered X variable in the synthetic dataset. This new set of synthetic reflectances for all S2 bands was submitted to the calibrated ANN to retrieve the corresponding BV.

Second, the organic heterogeneous field was used to assess the impact of heterogeneity from actual reflectances. The S2 10 m reflectances were aggregated at 20 m resolution, and both sets of reflectances were applied in the trained ANN. The retrieval difference between the reflectance at 10 m and the reflectances aggregated at 20 m was assessed with the metrics described in Section 2.5.

2.5. Validation and evaluation of the ANN uncertainty

For validation purposes, it is necessary to have synchronous in situ measurements and satellite observations. Two strategies were adapted depending on the considered variable: for Cab , we used the closest satellite acquisition date to the measurement campaign, while for the GAI, the satellite estimates were interpolated using a crop functioning model. Indeed, the Cab of a crop varies in time according to the genotype and the environment (climatic, soil, nitrogen conditions, etc.) (Hamblin et al., 2014). Then, the interpolation of Cab in time is challenging and may lead to significant error. Therefore, Cab was validated with the closest S2 image, which involved a time lapse of 1 or 2 days and up to 11 days for the organic field. In contrast, the evolution of the GAI during the growing season presents a smooth temporal profile and can be interpolated over time with a crop-functioning model. The Canopy Structural Dynamic Model (CSDM) was chosen since it represents a good compromise between complexity (only 6 parameters) and

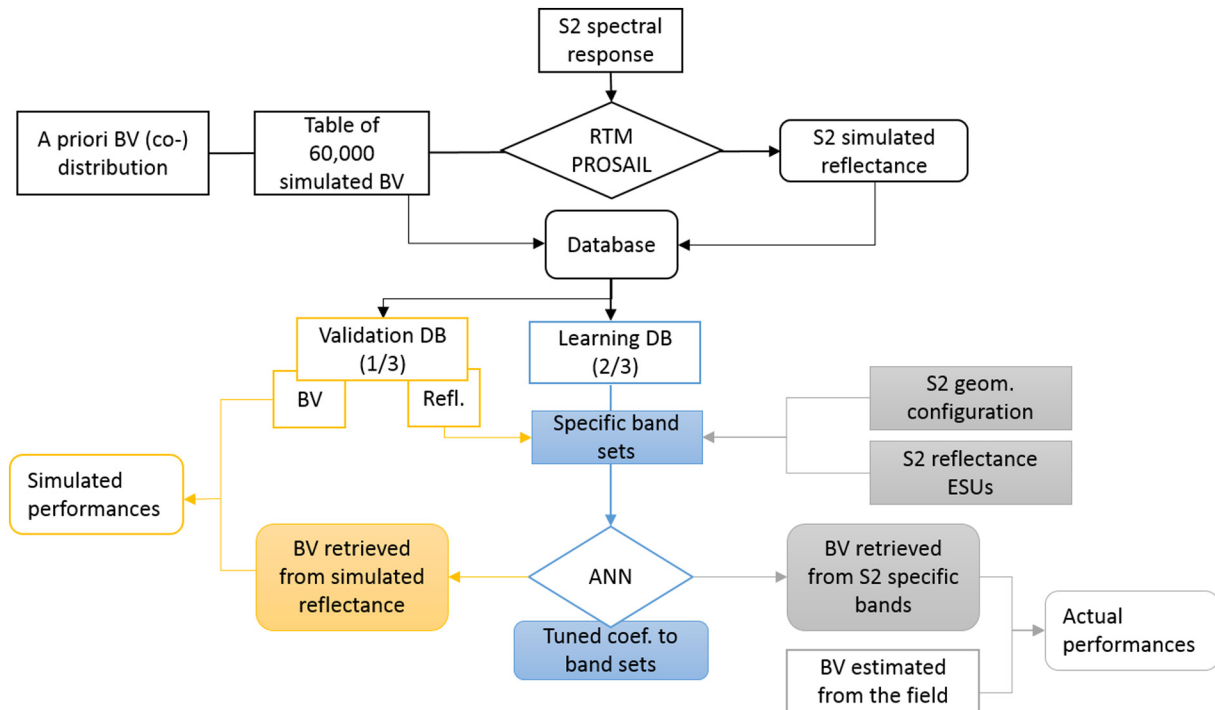


Fig. 3. Flowchart of the BV-NET algorithm and the methodology used to retrieve the BV (GAI , Cab and CCC) for the 4 band sets (Table 4). The implementation is divided into four steps: (i) creation of the learning database with PROSAIL for all S2 bands based on the distribution laws and associated parameters (Table 3), (ii) ANN calibration for each set of S2 bands by recomputing the synaptic weights and bias, (iii) ANN application on the reflectances of the validation DB to estimate the simulated performances and (iv) ANN application on S2 reflectances corresponding to the in situ validation dataset.

realism compared to a standard statistical smoothing algorithm. The CSDM partially takes climatic conditions into account in a simple way using the thermal time. The CSDM both smooths the residual errors associated with the individual *GAI* estimates and continuously describes the seasonal evolution of the BV from a limited number of observations during the growing cycle (Koetz et al., 2005). We used the CSDM improved by Lauvernet (2005):

$$GAI(tt) = k \left[\frac{1}{(1 + e^{-a(tt-T_0-T_a)})^c} - e^{b(tt-T_0-T_b)} \right] \quad (4)$$

where *a* and *b* define the rates of growth and senescence, respectively, *c* is a parameter conferring some plasticity to the shape of the curve, *k* is a scaling coefficient and *T₀*, *T_a* and *T_b* are, respectively, the thermal time of plant emergence, mid growth and senescence. *tt* is the cumulated thermal time corresponding to the sum of the thermal time between the sowing and the considered date (*t*):

$$tt = \sum_{day=sowing}^t \left[\frac{(T_{max}^{day} + T_{min}^{day})}{2} - T_{base} \right] \quad (5)$$

where the daily minimum (T_{min}^{day}) and maximum (T_{max}^{day}) air temperatures are recorded at the Pameseb local meteo station spread on a $10 \times 10 \text{ km}^2$ grid. *T_{base}* is the temperature below which the crop stops growing, corresponding to 0 °C for the winter wheat cultivated in this area.

The accuracy of the tested models was compared with the statistics given in Table 5 and the adjusted coefficient of determination. The mean absolute error (MAE) is the most representative of the average model error in comparison with the RMSE (Willmott and Matsuura, 2005). The RMSE and RRMSE are used for comparison purposes with other papers, as they are still widely published. The RMSE was decomposed in proportions of systematic and unsystematic errors for an in-depth model analysis (Willmott, 1984). The proportion of systematic error quantifies the model-induced errors that are linked to the bias and reflects improvement possibilities, while the unsystematic error is linked to the data variability and noise. Finally, the index of agreement was computed instead of the usual relative MAE, as it has the advantage of being bounded between 0 and 1 (Willmott, 1984). An index of agreement of 1 indicates perfect agreement between the observed and predicted values, while 0 stands for complete disagreement. These three last metrics facilitate comparisons between the different band sets and BVs studied, regardless of their associated units.

In parallel to the accuracy estimation based on statistical metrics, the ANN uncertainties were evaluated. The performance of BV retrieval is influenced by several sources of error, including external sources,

such as the noise in the input field data set, the sensors, the spatial resampling linked to the Point Spread Function (PSF), atmospheric correction and so on, as well as errors arising from the retrieval method itself, e.g., the ANN. The uncertainties associated with the ANN involve several levels of the retrieval chain, i.e., the simulated database, the training of the ANN, the model developed and the sensitivity of the model to noise.

We theoretically evaluated part of the estimation errors by considering two levels: (i) errors due to the training process by itself, e.g., the theoretical performances of the ANN, and (ii) the cumulated error associated with both the training process and the noise in the input dataset, e.g., the theoretical uncertainty. For the theoretical performances, we fitted a polynomial function using the actual BV value as the input and the RMSE between the estimated and the actual value of the BV. Then, to assess the theoretical uncertainties, we considered the sensitivity of the ANN to the noise associated with the data. We first defined confidence intervals around each input reflectance, which were taken as equivalent to the noise that was added to the data when simulating the learning database. For each input case in the validation database, all the cases within the vicinity defined by the confidence intervals were selected, and the RMSE between the estimated BV value for this case and the observed BV values of all the cases in the vicinity was computed. Then, a second ANN (UANN) was trained for each BV to estimate the computed RMSE from the input reflectance values corresponding to each case.

3. Results and discussion

3.1. Evaluation of the uncertainties

As expected and partly shown in Fig. 4, the median of the residuals between the estimated and actual variable is centred at approximately 0 for the three BVs, showing no bias in the estimation. Some deviation is observed for the highest values due to the combined effect of reflectance saturation and the limited number of cases observed within this range in the validation database (*GAI* > 6.5, *Cab* > 80, *CCC* > 600). For the three variables, the RMSE increases with the estimated value of the BV, the relationship between the estimated BV and corresponding RMSE being almost linear for the *GAI* (with a saturation for values higher than 6) and *CCC*. The RMSE increases from 0.32 to 1.3 for *GAI* values of 1 and 6, respectively. The RMSE increases from 0.18 to 0.75 for *CCC* values of 0.5 and 3 g/m², respectively. While for *Cab*, the slope is almost equal to zero, meaning a low sensitivity of the ANN to this BV and a relatively constant high RMSE level (7 to 11 µg/cm² for *Cab* values ranging between 30 and 65 µg/cm²).

The theoretical uncertainties (Fig. 5) are quite well estimated by the UANN using reflectances and angles as inputs for the *GAI* and *CCC*; higher scattering is observed for higher values, which may be mainly due to the number of cases used in the training process (only 7% of the *GAI* training data have a RMSE higher than 2.5). Furthermore, high RMSE values are associated with high *GAI* values for which saturation is observed (especially in the NIR), making the ANN more sensitive and less accurate to small reflectance variations in that domain. Concerning the *Cab* variable, the uncertainties in modelling give very poor results, including at a low RMSE level, which was expected due to the poor capability of the ANN to estimate the chlorophyll content at the leaf level. It should be noted that the shape of the relationship obtained for the theoretical uncertainties is very similar to the one modelled for the simulated performances (Fig. 7) since we used the same dataset and same level of noise for the training of the ANN and the training of the UANN.

Overall, this analysis remains incomplete since the uncertainties are estimated by assuming a perfect radiative transfer model and a given noise estimation, but that does not take into account the noise co-distributions between bands. Furthermore, although the noise applied on TOC reflectance is realistic, according to our knowledge, there are no

Table 5

Statistics computed to compare the results of the different band sets used for the three BVs. *P* stands for the predicted value from the ANN and *O* is the observed value, measured from the field. $\hat{P}_i = a + b O_i$, where *a* and *b* are the parameters associated with a simple linear regression between *O* and *P*. $\bar{O}$ is the mean value of *O* based on *N* observations.

Statistics	Formula
Mean absolute error	$MAE = \frac{\sum_{i=1}^N P_i - O_i }{N}$
Root mean square error	$RMSE = \sqrt{\frac{\sum_{i=1}^N (P_i - O_i)^2}{N}}$
Relative RMSE	$RRMSE = RMSE / \bar{O}$
Bias	$Bias = \frac{\sum_{i=1}^N (P_i - O_i)}{N}$
Systematic error	$RMSE_s = \sqrt{\frac{\sum_{i=1}^N (\hat{P}_i - O_i)^2}{N}}$
Proportion of systematic error	$s = \left(\frac{RMSE_s}{RMSE} \right)^2$
Proportion of unsystematic error	$u = 1 - s$
Index of agreement	$d = 1 - \frac{N \times MAE}{\sum_{i=1}^N (P_i - \bar{O} + O_i - \bar{O})}$

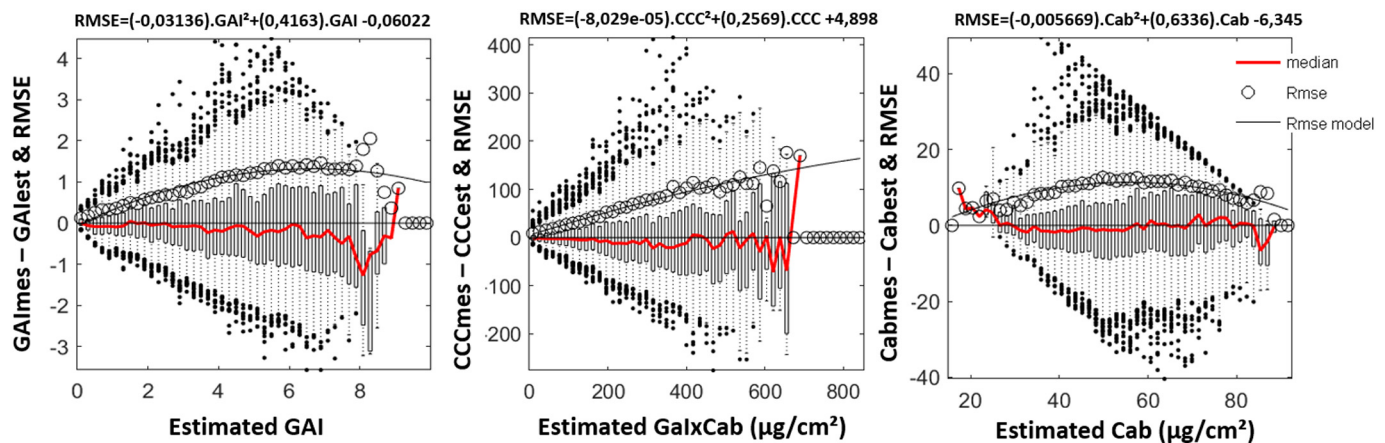


Fig. 4. Theoretical evaluation of the errors due to the training process. The RMSE between the estimated and the actual value of the considered BV was computed as a second order polynomial function. The variation of the RMSE is presented according to the level of the BV.

quantitative results providing the propagated uncertainties for the level 2A surface reflectances taking into account radiometric calibration, the PSF effect, geometric resampling and residual atmospheric noise.

3.2. Impact of S2 bands on GAI retrieval

The GAI was successfully retrieved with the ANN, and the accuracy presents a good consistency between the theoretical analysis and the analysis based on field data (Fig. 6). The overall results show an increase of performances with the addition of the S2 spectral bands. From 3 to 9 bands, the MAE decreases from 0.75 to 0.56 (RMSE from 1.12 to 0.88 using the simulated dataset), and the coefficient of determination increases from 0.57 to 0.85.

The estimation of the GAI using only the 3 S2 bands at 10 m presents the highest MAE and an obvious saturation at approximately 4, leading to a relatively low coefficient of determination ($R^2 = 0.57$) (Fig. 6b). This error is of the same magnitude as the one obtained for the 2015 SPOT5 Take5 dataset (MAE = 0.81, Fig. 6a). The replication of SPOT5 bands by including the S2 SWIR band (B11) in the ANN increases the coefficient of determination to 0.69. This increase is due to (i) the limitation of the points spreading around the 1:1 axis, especially for the GAI value below 2, and (ii) the saturation threshold at 5 instead of 4. The sensitivity of the SWIR to the soil spectral signature and its better resistance to atmospheric perturbation than the visible bands explain the increased performance for low GAI values, where small variations in reflectance are critical.

The integration of the new S2 red-edge bands enhances the accuracy

by decreasing the MAE to 0.55 and increasing the coefficient of determination to 0.84 (Fig. 6d). The improvement is linked to two positive impacts on the GAI retrieval already slightly present with the SWIR band. First, it removes the saturation effect, leading to a slight over-estimation of the GAI value, and second, it reduces the GAI dispersion for values below 3. The added value of using all S2 bands, including the additional band in the SWIR (B12) and a redundancy in the NIR (B8a), is not significant (Fig. 6e). The improved performance using the 3 red-edge bands is due to the combination of two effects: (i) the known sensitivity of the red-edge position and shape to the vegetation biomass and the GAI (Segl et al., 2012), and (ii) the inclusion of a more informative dataset in the ANN. The inclusion of the SWIR and red-edge bands that are less sensitive to the atmosphere while being sensitive to the vegetation (Li et al., 2014b) increases the GAI estimation accuracy.

These first results highlight the added value of S2 20 m bands in estimating the GAI with good accuracy that is slightly better than several studies relying on RTM inversion. Duveiller et al. (2012) obtained a RRMSE of 31% for wheat after linearisation due to a high saturation effect with the combination of SPOT 1, 2 and 4 at 20 m resolution. Additionally, for wheat, Li et al. (2015) reached a RMSE of 0.74 with the combination of SPOT4 Take5 and Landsat at 30 m resolution. Claverie (2012) achieved a lower RRMSE (21%) with Forisat-2 (8 m resolution) and showed that the results are species-dependent, with a higher RRMSE for sunflowers (40%) than for maize and soybean (10% and 14%, respectively). Houborg et al. (2015) estimated the GAI for maize and soybean with a RRMSE of 33% from Landsat 7. The results from Li et al. (2015) and Claverie (2012) dealing with a GAI

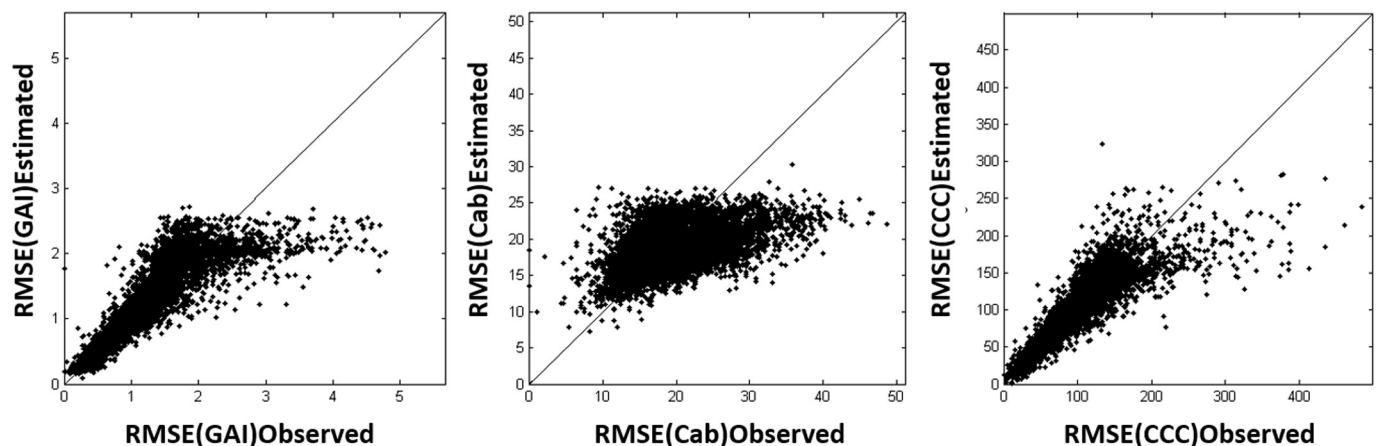


Fig. 5. Theoretical uncertainties results. Scatterplot between the observed RMSE computed from the learning database between each selected BV and the BVs in the confidence interval, and the retrieved RMSE with the UANN.

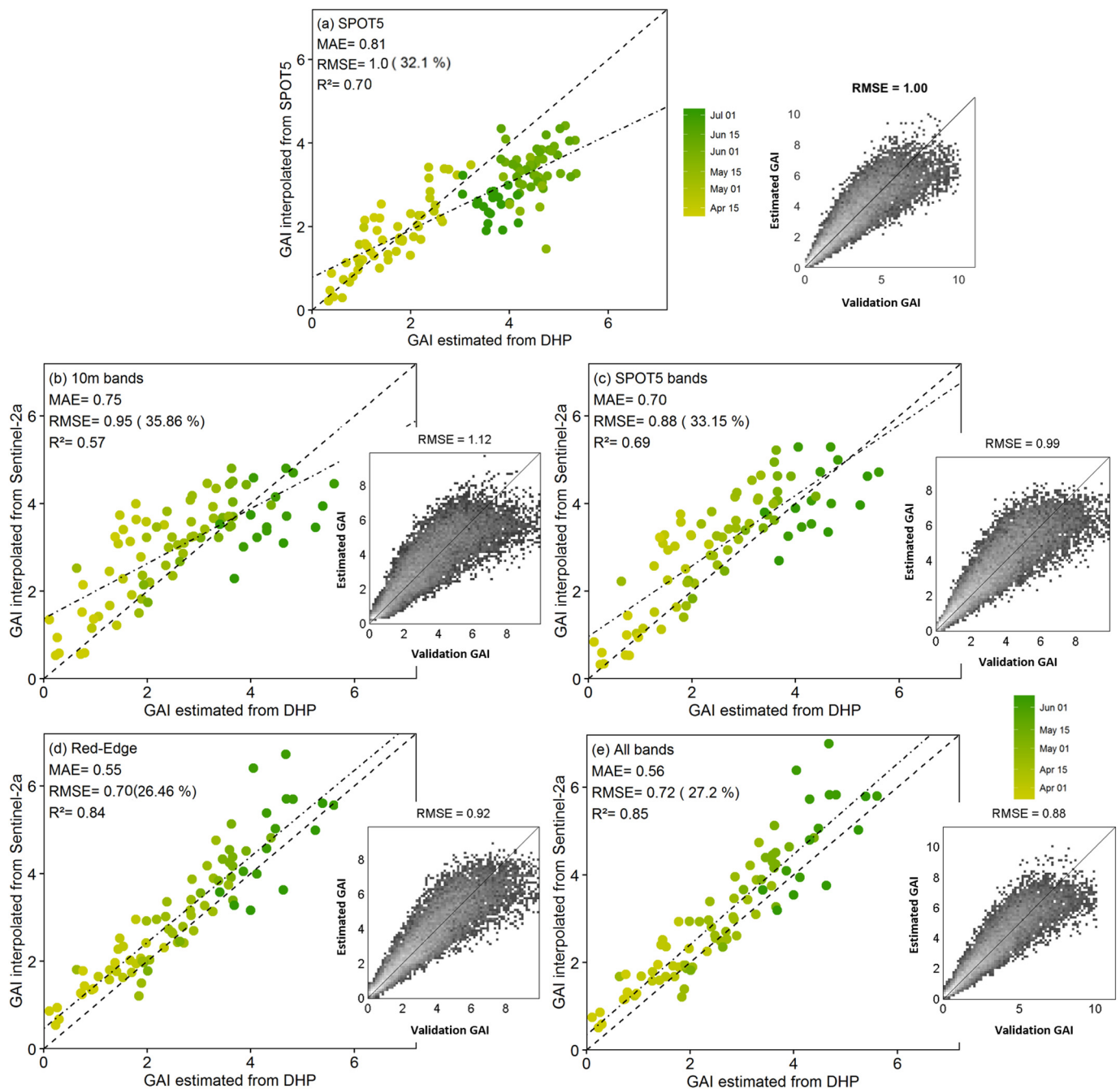


Fig. 6. (a; colour) Scatterplot and statistics computed for the GAI retrieved from SPOT5 Take5 images through the growing season and validated with 2015 field data ($N = 125$). (b–e; colour) Actual accuracy of the GAI retrieved from S2 2016 images for the 4 different band sets described in Table 4 ($N = 83$). (a–e; grey levels) Simulated performances of the S2 algorithm over the simulated validation dataset. For comparison with field data, the satellite estimate was interpolated at the date of field data acquisition by fitting the CSDM over the GAI values retrieved from all the available images during the growing season. The RRMSE is given in brackets.

up to 5 presented a slight or no saturation effect. In contrast, Duveiller et al. (2011) and Houborg et al. (2015) worked with the highest GAI values (up to 7) and demonstrated a clear saturation effect from a GAI of 3, as observed in the present study with the SPOT5 satellite and S2 band set equivalent to SPOT5 bands.

3.3. Impact of the growing season on the GAI retrieval with S2

While the above results are quite interesting for monitoring crop development, an operational diagnostic for the 2nd or 3rd N supply addresses a much smaller range of GAI values. The challenge is then to retrieve accurately the field GAI with values of approximately 3. The

performance metrics of the GAI estimated before the key period of the 2nd and 3rd N applications are given in Table 6. The 3rd N supply coinciding with the end of the stem elongation stage (May 2016 conventional dataset) corresponds to the most accurate estimation of the GAI. The validation is quite promising, with a constant MAE of approximately 0.30 for all the band sets. The results obtained for the 2nd N supply, corresponding to the end of tillering-beginning of stem elongation stage (early April 2017) highlight the importance of the red-edge bands in the accurate estimation of the GAI at that period. As demonstrated previously, the 20 m bands gather the points together around the 1:1 axis, decreasing the MAE from 1.03 to 0.42. Nonetheless, the organic field studied for its high heterogeneity presents a

Table 6

Assessment of the *GAI* retrieved with 4 different band sets of S2 with regards to the validation dataset acquired during the key periods for the 3rd (2016) and the 2nd (2017) N application. The MAE is given and the RRMSE is in brackets.

Stat.\band sets	10 m bands	SPOT5 bands	Red-edge	All bands
3rd N supply (May 2016, conventional)				
MAE (RRMSE)	0.28 (11.9%)	0.29 (12.7%)	0.27 (11.4%)	0.27 (12%)
Bias	−0.19	−0.09	−0.11	−0.13
R ²	0.85	0.78	0.82	0.80
3rd N supply (May 2016, organic)				
MAE (RRMSE)	0.53 (23.6%)	0.57 (25.6%)	0.71 (31.8%)	0.84 (35.4%)
Bias	−0.44	−0.52	−0.71	−0.84
R ²	0.58	0.58	0.48	0.65
2nd N supply (April 2017)				
MAE (RRMSE)	1.03 (40%)	0.88 (39.2%)	0.43 (18.5%)	0.42 (16.6%)
Bias	1.03	0.88	0.32	−0.36
R ²	0.71	0.71	0.71	0.69

reduction of accuracy with the inclusion of the 20 m bands (MAE from 0.53 to 0.84) due to a systematic underestimation of the *GAI* (bias of −0.84). This issue is further investigated in Section 3.7.

The influence of the development stage on the accuracy of the *GAI* retrieval is illustrated in the literature. Duveiller et al. (2011) showed the influence of winter wheat growing stages on the performance of the ANN for retrieving the *GAI*. The RRMSE decreases from the leaf development stages (87%) until heading (17%), and then increases with flowering (27%) until senescence (483%). Delloye et al. (2016) noted the same decrease of the RRMSE relative to the period of N application with SPOT5 Take5 images, the lowest RRMSE (10%) corresponding to the stem elongation stage (~BBCH stage 33–37), i.e., the third N application, which explains the great potential of remote sensing in adjusting N splitting for the 3rd and even 2nd fraction.

3.4. *Cab* retrieval and S2 bands contribution

Cab retrieval using BV-NET is characterised by a significant scattering and a systematic overestimation with regards to the Dualex measurements despite the correction applied in Eq. (1) (Fig. 7). However, the *Cab* retrieved from the 10 m and SPOT5 band sets is in the same range of variation as the one measured with the Dualex ($Cab_{max} - Cab_{min} \sim 20 \mu\text{g}/\text{cm}^2$). The red-edge band set integration reduces the bias from 11.8 to 7.26 $\mu\text{g}/\text{cm}^2$ and the MAE from 11.8 to 9.14 $\mu\text{g}/\text{cm}^2$, providing the best performance metrics. The simulated performances confirm this analysis, with a systematic overestimation of low *Cab* (< 50 $\mu\text{g}/\text{cm}^2$) while high *Cab* values tend to be underestimated, especially from 70 $\mu\text{g}/\text{cm}^2$. This behaviour is clearly mitigated by the use of the new S2 bands, but still exists specifically for the extreme values approximately 30 and 80 $\mu\text{g}/\text{cm}^2$, typically outside the range measured with the Dualex.

Further, the red-edge bands provide good differentiation between the fields selected in this study, i.e., organic versus conventional and 2nd versus 3rd N supply, which is promising to distinguish different growing stages and farming practices. Migdall et al. (2012) confirmed this difference in *Cab* between conventional and organic fields with hyperspectral data, where organic fields are associated with lower *Cab* values. Indeed, *Cab* differences induce large variation in canopy reflectance in the visible domain, with the sharpest variation of reflectance located in the red-edge, while saturation occurs for high *Cab* values in the red (680 nm), corresponding to strong chlorophyll absorption (Baret and Fourty, 1997).

The RMSE obtained in this study is lower than the one reported by Sehgal et al. (2016) (23 $\mu\text{g}/\text{cm}^2$), who worked on a wider range of *Cab* (25–65 $\mu\text{g}/\text{cm}^2$) with an ANN applied to IRS-P6 images for winter wheat in an experimental field. Using a physically based model, Houborg et al. (2009) obtained a better RRMSE for a maize field (17%)

based on SPOT5 imagery. Based on S2 simulation data, Verrelst et al. (2012) reported a RRMSE of approximately 20% for 9 crops, including winter wheat, and showed the importance of adding the red-edge in the configuration to improve performances. Finally, relying on a fully theoretical study, Segl et al. (2012) showed a RMSE between 17 and 19 $\mu\text{g}/\text{cm}^2$ by means of an inverted-Gaussian Reflectance Model applied on 4 S2 bands systematically, including B4 to 6, and alternatively, B7, 8 and 8a.

It is important to mention that the *Cab* estimation at the field scale is particularly complex due to the vertical gradient of *Cab*, which increases from the stem to the upper leaves and may explain the poor performances of the ANN. In addition, these results (errors) must also be discussed in light of the accuracy of Dualex field measurements. Beyond the usual large *Cab* variation of experimental plots, the Dualex seems to show sensitivity limitations in the range of *Cab* considered in this study. Indeed, in spite of the correction applied in Eq. (1), the measured Dualex *Cab* values remain relatively low (below 60 $\mu\text{g}/\text{cm}^2$) compared to the spectrophotometry analysis (up to 74 $\mu\text{g}/\text{cm}^2$). Irrespective of S2 potential in estimating crop *Cab*, this raises the question of the ability of the Dualex to capture the slight heterogeneity of winter wheat *Cab* at these development stages in input-intensive cropping systems. Hence, the low coefficient of determination ($R^2 = 0.26$) between the *Cab* measured with the Dualex and that retrieved from S2 should be considered cautiously, mainly in light of the high coefficient of determination obtained between the CNC and the CCC ($R^2 = 0.90$) (Section 3.6). The development of alternative methods, such as those based on spectrometers or multispectral devices combined with a leaf optical properties model, could be considered to acquire an accurate field validation dataset. Spectrometers that acquire data in the hyperspectral domain are useful in precisely characterising the inflexion point in the red-edge, which is strongly correlated to *Cab*. Indeed, Liu et al. (2010) reported a very low error (2.6 $\mu\text{g}/\text{cm}^2$) with hyperspectral images. In addition, the development of crop specific algorithms that combine 3D models with machine learning techniques could constitute a way of increasing the performance of the retrieval process. Indeed, a main restriction of the BV-NET algorithm considers a turbid medium in the inversion model and therefore does not take into account the different optical properties of the plant organs.

3.5. CCC retrieval using S2 data and performance comparison

Directly estimating the CCC with the ANN avoids ambiguities between the *GAI* and *Cab* during the inversion process. Indeed, the combined retrieval of the one variable with the ANN offers the advantage that the reflectance, especially in the red-edge, provides composite information on both canopy structure and *Cab*, making it difficult to decouple individual effects from the *Cab*. The simultaneous retrieval of both BVs makes it possible to overcome the confounding factors by compensation effects (Baret and Fourty, 1997; Weiss et al., 2000).

The coefficient of determination increases to 0.62 when considering the red-edge bands (Fig. 8c). The effects due to the increasing number of bands in the ANN are similar to those observed for both individual variables: a decrease of the saturation behaviour at high CCC values and of the data scattering around the 1:1 axis, leading to a significant lower MAE (from 0.34 to 0.26). The range value of the studied fields is below 3 g/m², which is out of the CCC saturation zone, as shown by the simulated performances, which systematically provides a better MAE value when compared to field data.

However, slight scattering occurs with the red-edge band set at approximately 2 g/m², which corresponds to the combination of 2 results highlighted previously, namely, the heterogeneity effect at 20 m for the organic field (green dots; Fig. 8c–d) and the dispersion of the *Cab* value related to the red-edge bands but combined with a possible saturation of the DUALEX instrument. Indeed these CCC results also include some uncertainty in the field data that is difficult to assess directly, since in situ CCC values combine the inaccuracies of 2 devices

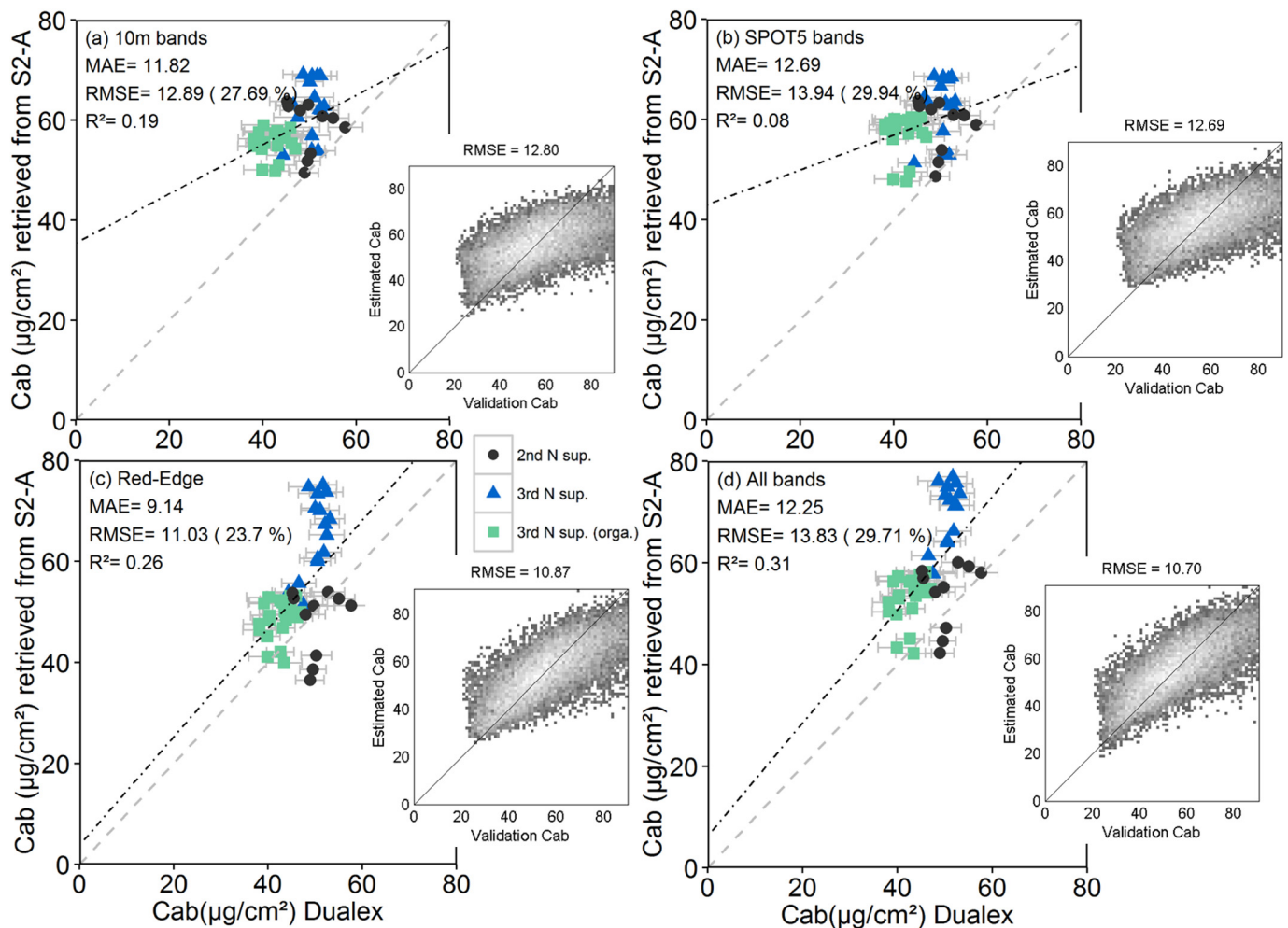


Fig. 7. (a–d, colour) Scatterplots of *Cab* measured with the Dualex Scientific Force A during the 3rd (2016) and the 2nd (2017) N supply and *Cab* retrieved from the different S2 band sets using the BV-NET algorithm ($N = 48$). The blue triangles and the green squares represent the sampling before the 3rd N supply in the conventional and the organic fields, respectively (May 2016). The black circles stands for the measurements before the 2nd N supply (April 2017). (a–d, grey levels) Simulated performances of the S2 algorithm over the simulated validation dataset. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

with different footprints and instrument errors (DHP and Dualex), making difficult to estimate the retrieval accuracy exactly.

Sehgal et al. (2016), working on a trial field with different N treatments, reached a larger RMSE (0.54) but a higher coefficient of determination ($R^2 = 0.92$) because of the range of CCC considered. Houles et al. (2007), who studied the elaboration of a nitrogen nutrition index (NNI) for winter wheat based on the same two BVs (*GAI* and *Cab*), drew the conclusion that the most useful variable in studying the CNC is the CCC in place of the *Cab* alone. Given the sound rationale of directly retrieve the CCC and the results highlighted in the literature and demonstrated in this study, we now focus on the CCC to estimate the N absorbed by the canopy (Section 3.6).

To further analyse and compare the performances of the ANN to retrieve the three BVs, the statistics that allow the comparison of errors regardless of their units were used (Table 7: Statistics to compare the accuracy of the 3 BVs retrieved with the ANN. d = index of agreement, s and u = proportion of systematic (s) and unsystematic (u) error computed from the RMSE. The band sets are abbreviated to 10 m, R-E = red-edge, All = all bands.). The configurations, including the 20 m bands, perform best for all BVs. The *GAI* retrieval gives the highest performances ($d = 0.77$), and there are possibilities for improvement ($s = 0.37$) suggesting possible modifications of the ANN through the training database or the network architecture to increase the accuracy of the retrieved *GAI*. The retrieval of the CCC is also associated with a

high index of agreement ($0.63 < d < 0.71$). The integration of the 20 m bands in the ANN reduces the systematic error to almost zero ($s = 0.03$); supposing that there is no possibility to improve the estimation of the CCC with the ANN, the remaining error is associated with the variability and noise in the field dataset. The performances of the model to retrieve the *Cab* remain low with all the tested configurations. The red-edge band set decreases the part of the error due to the model from 88% to 43%, which remains larger than the error for the *GAI* and the CCC (37% and 5%, respectively). This result confirms the theoretical analyses, i.e., the largest part of the error is due to the poor sensitivity of the ANN to the *Cab*, and a large potential for improvement remains.

3.6. CNC estimated from S2 data and potential for N recommendation

The N absorbed by the wheat in conventional fields is estimated with a high coefficient of determination via a linear relationship based on the CCC retrieved from the red-edge configuration. This correlation is as high during the period of the 2nd N supply as during the 3rd N supply, at 0.90 and 0.87, respectively (Fig. 9). The model error during the 2nd N supply, corresponding to the end of tillering-beginning of stem elongation, is very low with the red-edge band set (approximately 4 kg/ha), providing excellent accuracy for developing the N recommendation. This model error increases with the growing stage (3rd

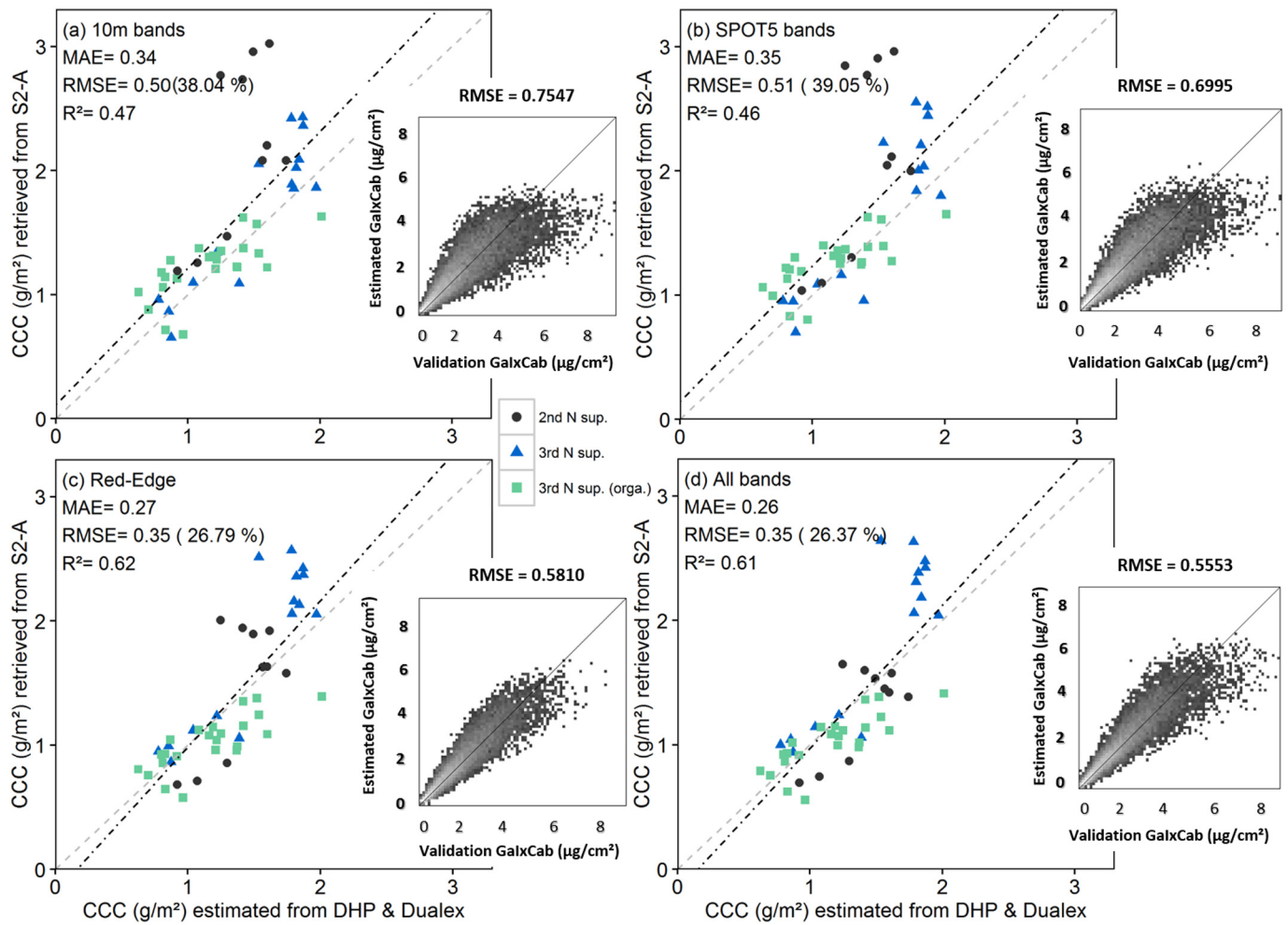


Fig. 8. (a–d, colour) Scatterplots of the CCC measured with DHP and the Dualex Scientific Force A and estimated from the different S2 band sets using the BV-NET algorithm ($N = 48$). The blue triangles and the green squares represent the sampling before the 3rd N supply in the conventional and the organic fields, respectively (May 2016). The black circles stands for the measurements before the 2nd N supply (April 2017). The RRMSE is given in brackets. (a–d, grey levels) Simulated performances of the S2 algorithm over the simulated validation dataset. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 7

Statistics to compare the accuracy of the 3 BVs retrieved with the ANN. d = index of agreement, s and u = proportion of systematic (s) and unsystematic (u) error computed from the RMSE. The band sets are abbreviated to 10 m, R-E = red-edge, All = all bands.

Band set/BV	d			s			u		
	10 m	R-E	All	10 m	R-E	All	10 m	R-E	All
GAI	0.63	0.77	0.77	0.44	0.37	0.37	0.56	0.63	0.63
Cab	0.50	0.49	0.50	0.88	0.43	0.70	0.12	0.57	0.30
CCC	0.63	0.71	0.70	0.25	0.05	0.03	0.75	0.95	0.97

N supply) to 21 kg/ha using the best band set (red-edge).

Bao et al. (2013) obtained the same level of accuracy ($RMSE = 24$ kg/ha, $R^2 \sim 0.9$) based on hyperspectral data acquired on the ground using a spectrometer with a linear model multiplying the first derivative of the red-edge reflectance spectra by a ratio of NIR/red-edge. They worked on 27 experimental winter wheat fields in China sown with the same cultivar and under the same farming practices. A strong linear relationship (very close to 1) between the CCC and the CNC was also demonstrated by Houles et al. (2007), who worked only on destructive data in 2 experimental plots with three winter wheat cultivars in the north of France. Like the present study, they outlined

two groups of points: one before stage 32 (two-node) and one from then onwards. They predicted the nitrogen absorption deficit, which is computed based on the critical nitrogen absorption curve, with an error of approximately 20 kg/ha, which is considered to be fairly acceptable for the range of nitrogen absorption deficit that varies from -120 to 20 kg/ha.

The critical nitrogen absorption curve derived from the dilution curve developed by Justes et al. (1994) and calculated based on Eq. (6) is a common method in deciding whether the crops require additional N fertilisation (Zhao et al., 2016; Chen, 2015; Chen et al., 2010; Lemaire, 2008; Baret et al., 2007a; Blondlot et al., 2005; Cartelat et al., 2005).

$$N_C = 53.5DM^{0.558} \quad (6)$$

where N_C is the critical nitrogen absorbed by the canopy (kg/ha) under optimal conditions, and DM is the dry matter of the shoot (t/ha). This equation was recently adapted by Zhao et al. (2014) to directly derive the critical N absorbed in the canopy (N_C) from the GAI instead of the DM and opens up new perspectives for remote sensing applications. Based on Eq. (6), the NNI is computed as the ratio between the CNC and the N_C . A NNI smaller than 1 indicates that the crop could absorb additional N to reach the potential maximal yield. The required N quantity can just be computed as the difference between N_C and CNC. Considering Eq. (6) and the DM measured in the laboratory (1.4 to 2.5 t/ha and 2.9 to 11.2 t/ha for the 2nd and 3rd N supply, respectively,

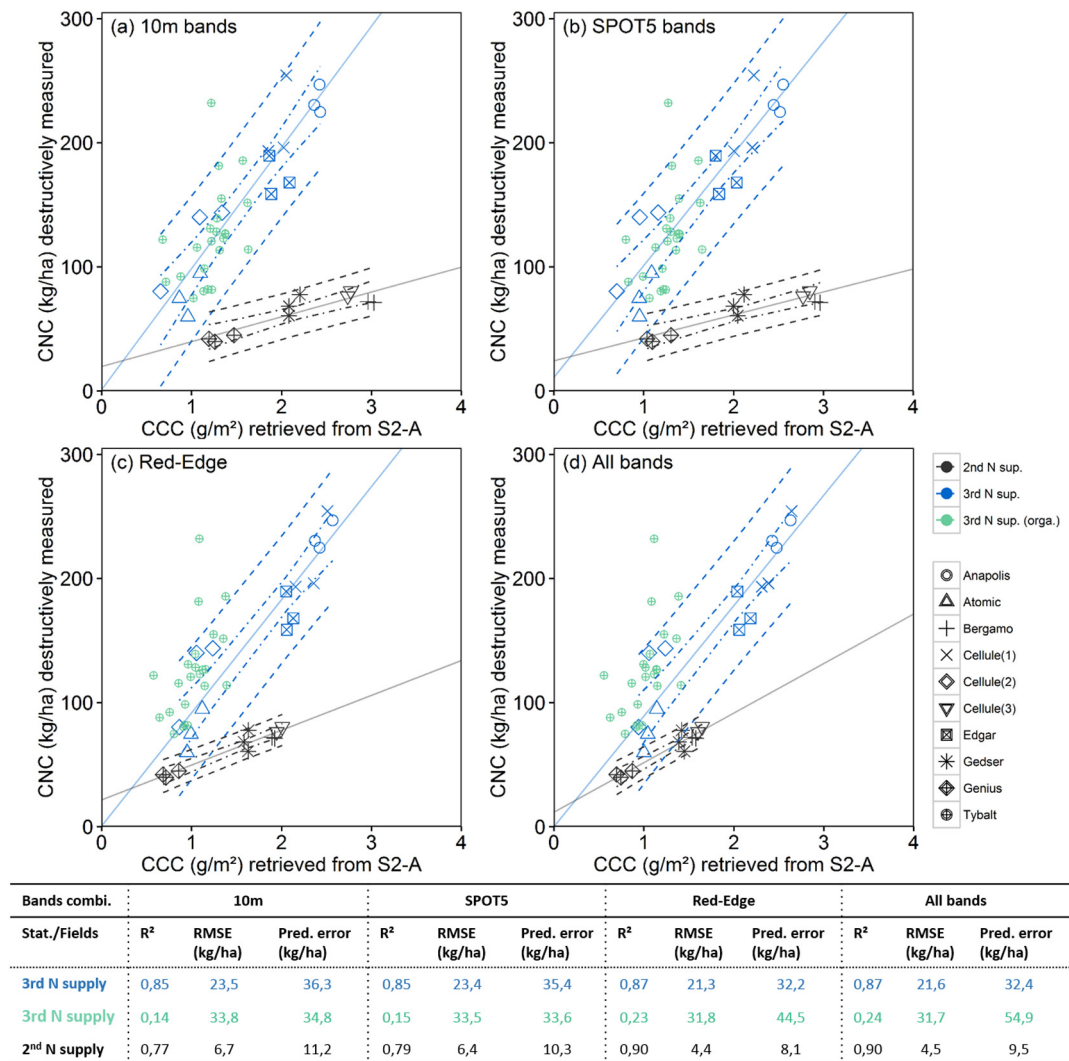


Fig. 9. Linear relationships between the CCC (g/m²) retrieved from S2 images and the CNC (kg/ha) destructively measured in the conventional fields for the 2nd (black) and the 3rd N supply, respectively, in the conventional and the organic fields (blue and green, respectively). The cultivars are distinguished by symbols. The confidence (dotdash) and prediction (dashed) intervals at 95% are drawn. The associated table includes the performance metrics: the coefficient of determination (R²); the RMSE and the standard deviation of the prediction (Pred. error) computed as the sum of the square roots of residual and model variances for conventional fields. For the organic field, the prediction error corresponds to the RMSE between the CNC measured and predicted based on the linear model obtained for the conventional fields in the same period (3rd N). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

see Table 2), the N_C varies in an interval of 25 kg/ha for the 2nd N supply and 110 kg/ha for the 3rd N supply. The model errors of 4 and 21 kg/ha, respectively, achieved in this study are compatible with the detection of fields that present an obvious N shortage or excess.

Despite this accuracy reached for conventional fields, there is no significant relationship between the CCC and the CNC for the organic heterogeneous field selected for this study. Migdall et al. (2012) demonstrated that the variation coefficient of the chlorophyll inside a field is higher for organic (approximately 0.23) than for conventional (approximately 0.12) fields. This variability of the chlorophyll added to the existing heterogeneity in the organic field studied may be a factor explaining the weakness of the CCC-CNC relationship. Apart from its organic management, 3 characteristics distinguish this field from the conventional fields and are potential sources of the discrepancy: (i) the lowest percentage of N measured in the plants (1.7% against 2.1% and up to 3.3% for the 2nd N supply; Table 2); (ii) the advanced BBCH stage (37 against 30–33); and (iii) the interval between field measurements and the acquisition of the S2 image (11 days against 1 and 2 days).

Since the literature have regularly reported a relationship between

Cab and the crop N content (%), the potential to estimate the N content from the Cab retrieved from S2 was investigated. The results show lower correlation between these two variables. The coefficient of determination is acceptable only for the 3rd N supply for the conventional fields (R² = 0.64), while the field N variability appears not to be related to the Cab estimated at leaf level during the 2nd N supply and for the organic field (R² of 0.08 and 0, respectively).

Whereas Hamblin et al. (2014) highlighted the dependency of Cab on the cultivar and the environment, the resulting relationships of this study seem to be cultivar independent. The set of 7 cultivars included in this analysis may belong to cultivars adapted to high N supply, which decreases the difference between cultivars (Hamblin et al., 2014). Moreover, given the importance of the environment, another important concern to address is the operational scale of the relationships. The relationships derived in this study are expected to be different for more contrasted cultivars and agroecological zones. Moreover, the operational aspect of applying such relationships is still a key issue since they are sensitive to both environmental conditions and differences between cultivars. High-throughput phenotyping techniques indeed appear very

promising to conduct such investigations.

A last important point to address is the difference in the CNC-CCC relationships between the 2nd and 3rd N application periods, which may be explained by both the impact of wheat physiology and weather conditions. Justes et al. (1994) have shown that plant physiology notably influences the dilution curve, especially before and after the reproductive period, which was also demonstrated by Houllès et al. (2007), who outlined a different CNC-CCC relationship before and after the two-node stage, and Peng et al. (2017), who showed differences in reflectances for vegetative and reproductive stages. Indeed, in this study, the 3rd N supply was achieved just before the reproductive phase. Furthermore, Houllès et al. (2007) also showed that the CNC-CCC relationship is affected by water stress. In this study, the two field campaigns correspond to two highly contrasting situations: the 2017 early growing season was particularly dry (rainfall deficit of 230.7 mm between autumn 2016 and spring 2017), while the 2016 early growing season was marked by a rainfall excess of 104 mm compared to an average amount of 628.2 mm during this season. This result highlights the importance of acquiring additional field data under contrasting weather conditions to draw a conclusion on the possibility of using these relationships independently of field calibration data.

3.7. Sensitivity of the BV retrieval to the within-pixel heterogeneity

Increasing the heterogeneity simulated by linear combination of two different BV values impacts the GAI and *Cab* retrieval differently (Fig. 10). A substantial underestimation of the retrieved GAI is linked to the increasing degree of heterogeneity (*H*), while there is no effect of the simulated heterogeneity on the *Cab* retrieval. The mixed pixels associated with a high degree of heterogeneity are underestimated by 50% and more when considering the GAI, while the *Cab* is over- and underestimated independently of *H* (Fig. 10a–b). The GAI is not an additive variable, and its relationship with the reflectance is not linear, which explains its sensitivity to scaling issue (Weiss et al., 2000). Garrigues et al. (2006) also highlighted the negative scaling bias on the GAI estimation when combining heterogeneous pixels and a non-linear transfer function.

The analysis of the *Cab* synthetic dataset (Fig. 7) highlighted the same behaviour as observed in Fig. 10b, i.e., a systematic over- and underestimation of the low and high *Cab* values, respectively. This very poor performance of the ANN in estimating *Cab* may explain the insensitivity of the retrieved *Cab* to the simulated heterogeneity, even though it is a non-additive variable.

These synthetic results are confirmed when aggregating actual S2 reflectances from 10 to 20 m for the heterogeneous organic field (Fig. 10d–f). Indeed, a systematic underestimation of the GAI is observed for the aggregated reflectances (bias = −0.34, MAE = 0.38). This error corresponds to the increase in MAE (+0.31) observed with the inclusion of the 20 m bands for the heterogeneous field (Table 6). As postulated from the theoretical analysis, the aggregation of the reflectances confirms the insensitivity of the retrieved *Cab* to the down-scaling issue (Fig. 10e).

The conclusions on the CCC integrative variable are driven by the influence of the GAI leading to the same observations, i.e., an underestimation of heterogeneous pixels (Fig. 10c). The analysis of S2 10 m reflectance spatially degraded to 20 m shows the same underestimation, but it is associated with a high decrease in the accuracy of the retrieved CCC ($R^2 = 0$ versus 0.80 Fig. 10c–f). This lack of consistency between the retrieved CCC at 10 and 20 m of the organic field combined with the insensitivity of the retrieved *Cab* to variation in reflectances may partly explain the absence of correlation between the N and the chlorophyll for this heterogeneous organic field (Section 3.6). These preliminary analyses seem to demonstrate a greater impact of the spatial variations at the field scale on the accuracy of the BV estimation compared to the spectral component (red-edge contribution). Nonetheless, a larger field dataset would be required to draw further conclusions on the weak

correlation between the retrieved CCC at 10 and 20 m. Therefore, based on the theoretical results (Fig. 10a–c) and the high correlation found between CCC and CNC, we would advise estimating the CNC at the spatial resolution of 10 m based on the integrative variable CCC rather than on *Cab*. The use of the 10 m bands only, offers the advantages of obtaining more information at the field scale and taking into account the spatial field heterogeneity without a significant increase of the prediction error on the CNC for the conventional field (the prediction error increases by 4 and 2 kg/ha for the 3rd and 2nd N supply, respectively). In addition, instead of applying a specific model for the organic/heterogeneous fields, one can use the same model for the organic and the conventional fields. The RMSE of the prediction increases by only 1 kg/ha with the 10 m bands configuration in comparison to the use of the red-edge configuration, which increases the RMSE of prediction by 12.7 kg/ha.

4. Conclusions

We highlighted the strong linear correlation between the integrative variable CCC (g/m^2) and the CNC (kg/ha) for all the tested S2 band sets (R^2 from 0.77 to 0.90). The accuracy reached in this study (RMSE = 4 and 21 kg/ha for the 2nd and the 3rd N supply, respectively, with the prediction errors of 8 and 32 kg/ha) is promising in the detection of a field's N shortage or excess in an operational way through using BV-NET, which does not require a field training dataset. Unlike most of the research on the subject, these results were obtained for regular farmers' fields in intensive cropping systems, meaning that they correspond precisely to the conditions and N level to be assessed by an operational service. While this experiment relies on a large multi-year and multi-cultivar dataset, the relationships have to be confirmed with a larger number of fields. Indeed, we showed that a different CNC-CCC relationship has to be defined for different stages and years. Such information is crucial in a pre-operational context, such as for the BELCAM collaborative platform. This platform aims to set up a constructive exchange between farmers and scientists to build consistent and useful products for precision farming applications. It may help to obtain reference field data over several years under contrasting weather conditions to determine definition domains associated with specific relationships that can be used afterwards without any field data. Then, some remaining questions have to be fine-tuned, mainly concerning (i) the validity intervals of the relationships according to the N supply in terms of development stages or thermal time and input reflectances, (ii) the dependency of the relationships on the years, (iii) the dependency of the relationships on other cultivars and (iv) agricultural management impact (mainly organic versus conventional). If this validity interval can be defined in terms of the thermal time associated with reflectances, only the sowing date would be required from the farmers to provide them with an operational service advising them of the opportunity to reduce the standard N recommendation or the relevance of applying additional N based, for example, on the critical N absorption curve. Another option is to integrate the CCC in crop-functioning models taking into account weather conditions and growing stages. In this case, the models, currently integrating *true* BV values, have to be fine-tuned to integrate satellite inputs which include *effective* BV values, as the GAI studied in this paper.

The added value in estimating the CNC at the canopy level with the integrative variable CCC at 10 m resolution was demonstrated by the highest sensitivity of this variable to the N content. Working at 10 m resolution with this variable allows the use of a single relationship for the conventional and organic fields and the inclusion of heterogeneous fields in terms of biomass, thus opening the way to precision agriculture using S2 satellite data. The retrieval of *Cab* with an ANN showed poor performances from the theoretical as well as from the field data analyses, and low or no correlation was highlighted with the N content (%). Nonetheless, the red-edge bands enable the differentiation between conventional and organic fields, which are associated with lower *Cab*

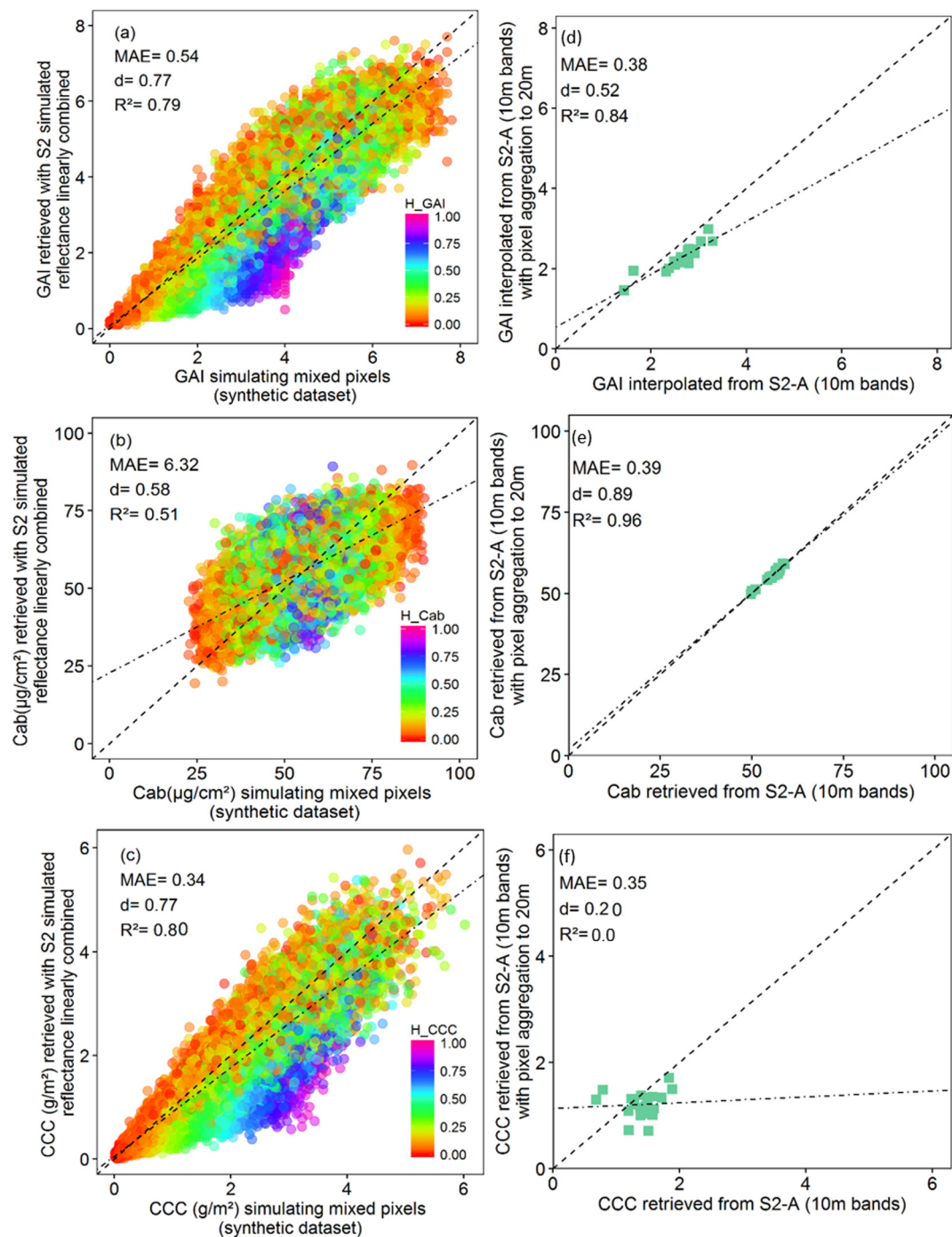


Fig. 10. (a–c) Scatterplots of the synthetic dataset created to simulate pixel heterogeneity for (a) the *GAI*, (b) *Cab* and (c) the *CCC*. The different colours represent the degree of heterogeneity: 0 stands for no heterogeneity (reflectance combination of 2 BVs of the same value) and 1 for the maximum heterogeneity (reflectance combination of 2 BVs with the maximum difference) ($N = 40,277$). (d–f) Scatterplots of the retrieved BV from the actual S2 10 m reflectances of the organic heterogeneous field and the same reflectances aggregated to 20 m ($N = 23$).

values, as confirmed by Migdall et al. (2012).

The contribution of the red-edge bands at a 20 m resolution is significant when considering only the BVs. This contribution increased the accuracy of the 3 studied BVs, i.e., the *GAI*, *Cab* and *CCC*, with the exception of the *GAI* during the 3rd period of N application, which presented the highest accuracy with the 10 m bands. The red-edge bands show clear potential for quantitative crop growth monitoring using the *GAI*. The growing season analysis showed a decrease of the MAE from 0.75 to 0.55 and an increase of the coefficient of determination from 0.57 to 0.84. While during the period of the 2nd N

application, the MAE also decreased significantly due to the red-edge bands (from 1.11 to 0.46), it did not impact accuracy during the 3rd N supply, which was constantly high (MAE approximately 0.35). However, this BV is very sensitive to the scaling effect, and only the 10 m bands should be used to retrieve the *GAI* before the 3rd N supply in fields with high spatial heterogeneity. On the other hand, the *Cab* retrieval was insensitive to the downscaling issue, but the differentiation of the low *Cab* range was increased with the red-edge band set, allowing better discrimination of the different growing stages and farming practices (organic versus conventional). Finally, the *CCC*,

mainly impacted by the *GAI*, presented the same accuracy improvement due to the inclusion of the red-edge bands in the ANN.

There was a very small gain in accuracy due to the inclusion of the 2 remaining S2 bands, i.e., the SWIR band (B12), and a redundancy in the NIR wavelengths (B8a). Among the tested band sets, the use of 7 bands, including the 3 red-edge bands, was optimal for retrieving the 3 considered BVs. Weiss et al. (2000) reached similar conclusions working with 9 bands between 500 and 882 nm; they demonstrated that a combination of 6 bands is optimal for estimating the *GAI* and *Cab*, while implementation of 9 bands in the Look-up table decreased the performances. Verger et al. (2011) found that 7 bands was the optimal number for retrieving the *LAI* with an ANN based on a 62-band initial dataset. Verrelst et al. (2012) accurately retrieved the *LAI* using the 4 simulated S2 10 m bands, while the retrieval of *Cab* required the use of the red-edge bands and 60 m bands, which was not appropriate in the context of our study.

Acknowledgements

This research was completed in the framework of the BELCAM project funded by the Belgian Science Policy Office (BELSPO) in the STEREO II program (contract SR/00/300). Many thanks to the CRAW-w team who helped to collect and process the field data, specifically J.P. Goffart, A. Leclef and W. Philippe, as well as F. Baret from INRA, who contributed to the analyses of uncertainties and interpretation of results. The authors would like to thank the Sentinel-2 for Agriculture system, who provided NRT L2A S2 images as well as the Theia land data services centre for SPOT5 Take 5 images distribution.

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