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Evaluating the capabilities of Sentinel-2 for quantitative estimation of biophysical variables in vegetation

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ABSTRACT

The red edge position (REP) in the vegetation spectral reflectance is a surrogate measure of vegetation chlorophyll content, and hence can be used to monitor the health and function of vegetation. The Multi-Spectral Instrument (MSI) aboard the future ESA Sentinel-2 (S-2) satellite will provide the opportunity for estimation of the REP at much higher spatial resolution (20 m) than has been previously possible with spaceborne sensors such as Medium Resolution Imaging Spectrometer (MERIS) aboard ENVISAT. This study aims to evaluate the potential of S-2 MSI sensor for estimation of canopy chlorophyll content, leaf area index (LAI) and leaf chlorophyll concentration (LCC) using data from multiple field campaigns. Included in the assessed field campaigns are results from SEN3Exp in Barrax, Spain composed of 35 elementary sampling units (ESUs) of LCC and LAI which have been assessed for correlation with simulated MSI data using a CASI airborne imaging spectrometer. Analysis also presents results from SicilyS2EVAL, a campaign consisting of 25 ESUs in Sicily, Italy supported by a simultaneous Specim Aisa-Eagle data acquisition. In addition, these results were compared to outputs from the PROSAIL model for similar values of biophysical variables in the ESUs. The paper in turn assessed the scope of S-2 for retrieval of biophysical variables using these combined datasets through investigating the performance of the relevant Vegetation Indices (VIs) as well as presenting the novel Inverted Red-Edge Chlorophyll Index (IRECI) and Sentinel-2 Red-Edge Position (S2REP). Results indicated significant relationships between both canopy chlorophyll content and LAI for simulated MSI data using IRECI or the Normalised Difference Vegetation Index (NDVI) while S2REP and the MERIS Terrestrial Chlorophyll Index (MTCI) were found to have the strongest correlation for retrieval of LCC.

1. Introduction

Europe's Global Monitoring for Environment and Security (GMES) programme (ESA, 2011a) includes two Sentinel 2 (S-2) satellites designed to provide systematic global acquisitions of high resolution multispectral imagery. The Multi-Spectral Instrument (MSI) aboard S-2 has been designed to enable the continuity of Satellite Pour l'Observation de la Terre (SPOT) and Landsat type data into the future. MSI also builds upon the heritage of the ESA MEdium Resolution Imaging Spectrometer (MERIS) and experience with the NASA MODerate-resolution Imaging Spectroradiometer (MODIS) instruments in providing more spectral bands than Landsat or SPOT. Bands known to be important in sensing vegetation will have a spatial resolution of 10 m or 20 m, others will have 60 m resolution. S-2 will have a radiometric accuracy of <5% and operate at 12 bit radiometric resolution (ESA, 2010) which is suitable for vegetation (Tucker, 1980). The mission envisions a pair of satellites simultaneously circulating the Earth in a sun-synchronous 180° phase orbit with a 290 km swath (ESA, 2010). The first satellite, S-2A, is planned for launch in 2014 followed by S-2B currently planned for a tentative launch date in 2015 (ESA, 2011b). Tandem operation of S-2A and B will deliver a revisit period of up to five days under cloud free conditions.

Knowledge of canopy chlorophyll content and leaf chlorophyll concentration (LCC) can indicate plant health and potential gross primary productivity (Gitelson et al., 2006), while leaf area index (LAI) can provide an insight into the function and structure of the canopy (Wilhelm et al., 2000). Land cover (including vegetation type), LAI and the fraction of absorbed photosynthetically active radiation (FAPAR) are all Global Climate Observing System (GCOS) Essential Climate Variables (ECVs) required by the United Nations Framework Convention on Climate Change (UNFCCC) and the Intergovernmental Panel on Climate Change (IPCC) (GCOS, 2010). Satellite derived estimations of LAI and canopy chlorophyll content are key inputs into climate models as they provide estimates of carbon sequestration (Ciais et al., 1997). Consequently they have been used in services such as the Farmstar programme by EADS

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Infoterra to provide information supporting precision agriculture through timely and efficient use of fertilisers (Farmstar, 2011). A number of techniques have evolved in the past to derive the biophysical variables of vegetation using remote sensing data; these can be grouped into three broad categories: the inversion of radiative transfer models (Shultis and Myneni, 1988), machine learning (for example neural networks) (Carpenter et al., 1999) and the use of Vegetation Indices (VIs). Methods based on VIs have the benefit of being computationally simple while they are generally less site specific and more universally applicable than the other methods. Consequently VIs are a widely used method to provide quantitative ground measurements of the biophysical parameters of vegetation by contrasting specific spectral reflectance characteristics of vegetation and are frequently implemented operationally using remotely sensed data. Satellite derived VIs provide one of the best possible ways to obtain the biophysical parameters of vegetation over large areas (regional or global) while retaining the high temporal coverage required for many applications and consequently their development and validation is of great importance.

The first VIs contrasted the strong reflectance in the near-infrared (NIR) by plant matter with strong absorption by chlorophyll in the red part of the electromagnetic spectrum to quantify vegetation greenness parameters. Jordan (1969) made references to the retrieval of canopy chlorophyll content and LAI using the ratio of NIR/R which became known as the Simple Ratio (SR). The SR is the basis of the Normalised Difference Vegetation Index (NDVI) (Rouse et al., 1973) which is currently the most widely used VI as a measure for many variables. Much work has been done investigating the optimal reflectance wavelengths for use in the SR and the NDVI algorithms (for example, the Pigment Specific Simple Ratio ($PSSR_a$), Blackburn, 1998). Although VIs such as the NDVI were primarily developed for the purpose of LAI retrieval they have also been argued to be capable of canopy chlorophyll content estimations (Myneni et al., 1995; Huete et al., 2002). Refinements of the NDVI and SR such as the Perpendicular Vegetation Index (PVI) (Richardson and Wiegand, 1977) and the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988) aimed to account for uncertainty due to variation in background condition. The PVI achieved this through implementing NIR and red reflectance measurements of soil pixels into the equation while SAVI incorporated the correction factor L into the NDVI formula. L accounts for soil variation by varying the factor between 1, for low vegetation, and 0, for dense vegetation. This effectively retains original NDVI output at higher values of vegetation density. Qi et al. (1994) subsequently presented a modified version of the SAVI (MSAVI) which utilised a self-adjusting L factor as the product of NDVI and the Weighted Difference Vegetation Index (WDVI) (Clevers, 1988) which incorporates the slope of the soil line. It should be noted that the self-adjusting L means MSAVI adjusts SAVI, an index based around the NDVI, by NDVI and WDVI and in the process results in a loss in the vegetation dynamic response (Qi et al., 1994). Other VIs have also been developed to account for aerosol variation such as the atmospherically resistant vegetation index (ARVI) which makes use of aerosol resistance coefficients to reduce atmospheric influences (Kaufman and Tanré, 1992). Sequentially a combination of SAVI and ARVI was presented by Huete et al. (2002) as the enhanced vegetation index (EVI). Although NDVI refinements have aimed to account for, or mitigate, many of the uncertainties in VIs through doing so they often require additional scene specific information. Acquiring and applying such scene specific information can adversely affect the universal application of VIs as well as their dynamic response.

A wealth of VIs have been developed to estimate canopy chlorophyll content with varying strengths and levels of robustness (e.g., Daughtry et al., 2000; Broge and Mortensen, 2002; Dash and Curran, 2004; Gitelson et al., 2005). Many such VIs presented band variations of the NDVI formula such as the Green Normalised Difference Vegetation Index (GNDVI) (Gitelson et al., 1996) which challenged the approach of using red reflectance and instead used the green reflectance in its place. It was argued to be at least five times more sensitive to chlorophyll-a concentration than the NDVI and specifically useful for differentiation in stressed and senescent vegetation. Daughtry et al. (2000) presented a modified chlorophyll absorption in reflectance index (MCARI) which was developed for minimising the effects of non-photosynthetic materials. Work reported strong response to LCC variation while noting that the index encounters issues at low LAI due to higher influence of background variation.

After the success of the NDVI and its specialised refinements subsequent work made use of developments in spectral capabilities to provide better characterisation of the red-edge (RE) which is the prominent spectral feature of vegetation located between the red absorption maximum and high reflectance in the NIR. Quantification of the RE is often achieved through calculation of the red-edge position (REP) which is recognised as the point of maximum slope along the RE and has been argued to provide enhanced estimates of LCC and canopy chlorophyll content (Horler et al., 1983; Curran et al., 1990). Evaluation of the REP at a global scale with high temporal resolution was first achieved using data from the MERIS sensor. MERIS had a spectral band located directly on the RE (band 9 708.75 ± 5 nm) which led to the development of

Table 1
Spectral bands of Sentinel-2 MSI.

S-2 band	1	2	3	4	5	6	7	8	8a	9	10	11	12
Central wavelength (nm)	443	490	560	665	705	740	783	842	865	945	1375	1610	2190
Bandwidth (nm)	20	65	35	30	15	15	20	115	20	20	30	90	180
Spatial resolution (m)	60	10	10	10	20	20	20	10	20	60	60	20	20

Table 2
A list of Vegetation Indices that have been analysed for use with Sentinel-2 using field data.

Vegetation index	Formulation	S-2 bands used	Original author
NDVI	(NIR − R)/(NIR + R)	(B7 − B4)/(B7 + B4)	Rouse et al. (1973)
NDI45	(NIR − R)/(NIR + R)	(B5 − B4)/(B5 + B4)	Delegido et al. (2011b)
MTCI	(NIR − RE)/(RE − R)	(B6 − B5)/(B5 − B4)	Dash and Curran (2004)
MCARI	[(RE − R) − 0.2(RE − G)] * (RE − R)	[(B5 − B4) − 0.2(B5 − B3)] * (B5 − B4)	Daughtry et al. (2000)
GNDVI	(NIR − G)/(NIR + G)	(B7 − B3)/(B7 + B3)	Gitelson et al. (1996)
$PSSR_a$	NIR/R	B7/B4	Blackburn (1998)
S2REP	705 + 35 * ((((NIR + R)/2) − RE1)/(RE2 − RE1))	705 + 35 * ((((B7 + B4)/2) − B5)/(B6 − B5))	
IRECI	(NIR − R)/(RE1/RE2)	(B7 − B4)/(B5/B6)	

Table 3
Biophysical parameters chosen for PROSAIL data set.

Model variables		Units	Range
PROSPECT			
N	Leaf structure index	Unitless	1.5
C_{ab}	Leaf chlorophyll content	($\mu g\ cm^{-2}$)	5–70
C_m	Leaf dry matter content	($g\ cm^{-2}$)	0.009
SAIL			
LAI	Leaf area index	($m^2\ m^{-2}$)	0–8
ALA	Average leaf angle	(°)	35
HotS	Hot spot parameter	($m\ m^{-1}$)	0.01
S	Sun zenith angle	(°)	30
V	View zenith angle	(°)	10

the MERIS Terrestrial Chlorophyll Index (MTCI) (Dash and Curran, 2004) a surrogate REP index which has been implemented operationally as a standard level 2 global product from the ENVISAT MERIS sensor. The MTCI has demonstrated that it is possible to use the REP parameter to estimate chlorophyll content over very extensive spatial areas at a high temporal resolution (Dash and Curran, 2006).

As S-2 will enable multiple operational reflectance measurements on and around the RE at a greatly enhanced spatial resolution of 20 m with a short revisit time it holds much appeal for vegetation monitoring. The combination of S-2 bands 5 and 6 (Table 1) provide the opportunity for improved characterisation of the RE than was previously possible operationally at a global scale. Consequently there is much scope for the development of algorithms to retrieve the biophysical parameters of vegetation using S-2. Some algorithms have already been presented in work by Delegido et al. (2011b) which specifically investigated the optimal bands to use in the NDVI formula with synthesised S-2 data. Research found that bands 4 and 5 were the optimal combination and the formula will be further investigated in this analysis and referred to as the NDI45. There are many different VIs each designed for a separate purpose and validated at varying levels using different datasets. Consequently each has its own strengths and weaknesses in application and some are more optimal at retrieving certain parameters of vegetation than others. With the caveat of saturation considered, this paper will investigate the strength of VIs presented in Table 2 for the SicilyS2EVAL and SEN3Exp field campaigns. VIs have been selected that do not self-normalise or linearise which forfeits sensitivity to vegetation variance. Also VIs that require the use of scene specific information that consequently affects their universal applicability and operational use with S-2 have also been excluded from analysis.

2. Data and methods

The approach adopted in this paper compared simulated S-2 data with field measurements and the output of an established vegetation canopy model (PROSAIL) (Baret et al., 1992; Jacquemoud et al., 2009). The simulated data were derived from two airborne hyperspectral sensors, an Itres Instruments Compact Airborne Spectrographic Imager (CASI-1500) and a Specim AISA Eagle instrument collected during two field campaigns: SEN3Exp (SEN3Exp, 2011), and SicilyS2EVAL. SEN3Exp was conducted in June and July 2009 to prepare for the Sentinel 3 mission and to aid the development of scientific algorithms; however, ground data is highly suitible for S-2 investigations. SicilyS2EVAL was a campaign conducted in Sicily 2010 which was funded by ESA specifically to support validation of vegetation products for S-2. The combination of these two field campaign datasets provided 60 elementary sampling units (ESUs), from which ground canopy chlorophyll content measurements were obtained from sample areas of 10 × 10 m and 20 × 20 m to represent the spatial resolution of S-2.

2.1. PROSAIL model data

PROSAIL is the combination of the PROSPECT-5 leaf optical properties model (Jacquemoud and Baret, 1990) and the 4SAIL canopy bidirectional reflectance model (Verhoef, 1984, 1985). The model was used to simulate canopy reflectance for a range of leaf biochemistry and canopy parameters (Table 3). During the model simulation both LAI and LCC were varied to provide a good range (LAI was varied from 0 to 8, whereas LCC was varied from 5 to 70 $\mu g\ cm^{-2}$). Other parameters were taken as an average value from the literature; this was to ensure that the changes in the modelled spectral reflectance are only due to changes in LAI and leaf chlorophyll content. Two datasets were generated; All PROSAIL Data and SEN3Exp PROSAIL. The "All PROSAIL Data" was the correlation between reflectance and canopy chlorophyll content for a wide range of biophysical variables between the wavelengths of 500–800 nm. Alternatively, the SEN3Exp PROSAIL dataset represented reflectances generated from the PROSAIL model while using the same ESU biophysical variables of the SEN3Exp campaign. SicilyS2EVAL was not considered due to the low range of LAI and LCC compared to SEN3Exp.

2.1.1. In situ data collection: SicilyS2EVAL

SicilyS2EVAL targeted a single crop type, grillo (grapevine) during May 2010. Each of the 25 ESUs was a composition of multiple LAI and LCC measurements representing a 10 × 10 m sample area. LAI was systematically sampled 18 times at different locations within each ESU using the Li-Cor LAI-2000 near dusk and dawn under diffuse radiation conditions. A total of 81 Relative LCC measurements were taken using a SPAD, these measurements were spread evenly across the canopy of 9 separate plants at each ESU. In addition to the SPAD measurements leaf cuttings (5 mm diameter) were removed from 30 separate plants selected using a systematic sampling strategy. The leaf cuttings were taken at a consistent position of each leaf and stored in dimethylformamide for later analysis. Absorption in 647 nm and 664 nm were measured using a Rayleigh UV-1800™ spectrophotometer and used to estimate chlorophyll a and chlorophyll b of the sample using Eqs. (1) and (2) (Moran and Porath, 1980; Moran, 1982). Total chlorophyll concentration estimated from this analysis was correlated with the SPAD-502 measurements to provide an absolute LCC value using Eq. (3).

$$\text{Chlorophyll } a = 11.65 * A_{664} - 2.69 * A_{647} \tag{1}$$

$$\text{Chlorophyll } b = 20.81 * A_{647} - 4.53 * A_{664} \tag{2}$$

where A_{647} and A_{664} are sample absorptions at wavelengths of 647 nm and 664 nm.

$$\text{Total Chlorophyll} = 3.79 * S + 79.79 \tag{3}$$

where S is the representative SPAD value.

2.1.2. In situ data collection: SEN3Exp

Data from the SEN3Exp campaign, which took place in June and July 2009, included 35 canopy chlorophyll content measurements from agricultural sites in the Barrax region of Spain (SEN3Exp, 2011). The crop dataset composition consisted of: corn, garlic, oat, onion, potato, sunflower, alfalfa and grapevine. Within each of the 20 × 20 m ESUs, 24 LAI field measurements were taken using a Li-Cor LAI-2000™ (SEN3Exp, 2011) and relative LCC measurements were made using a Minolta SPAD-502™ (Delegido et al., 2011a). Relative LCC measurements were converted to absolute LCC using destructive leaf sampling of a subset of five samples

Table 4
Summary of field campaign data used in analysis.

Campaign	Location	Number of ESUs	ESU size	Date
SicilyS2EVAL	Castelvetrano – Sicily	25	10 × 10 m	May 2010
SEN3Exp	Barrax – Spain	35	20 × 20 m	June/July 2009

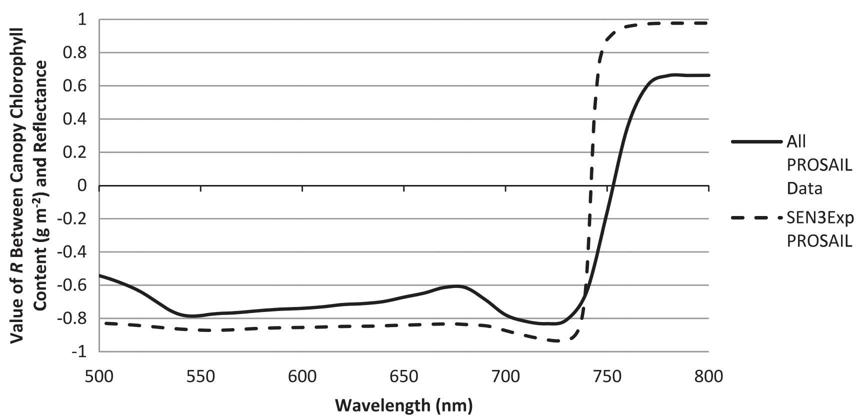

Fig. 1. Comparing the correlation coefficient (*R*) between spectral reflectance and canopy chlorophyll content with changing wavelength for both PROSAIL datasets.

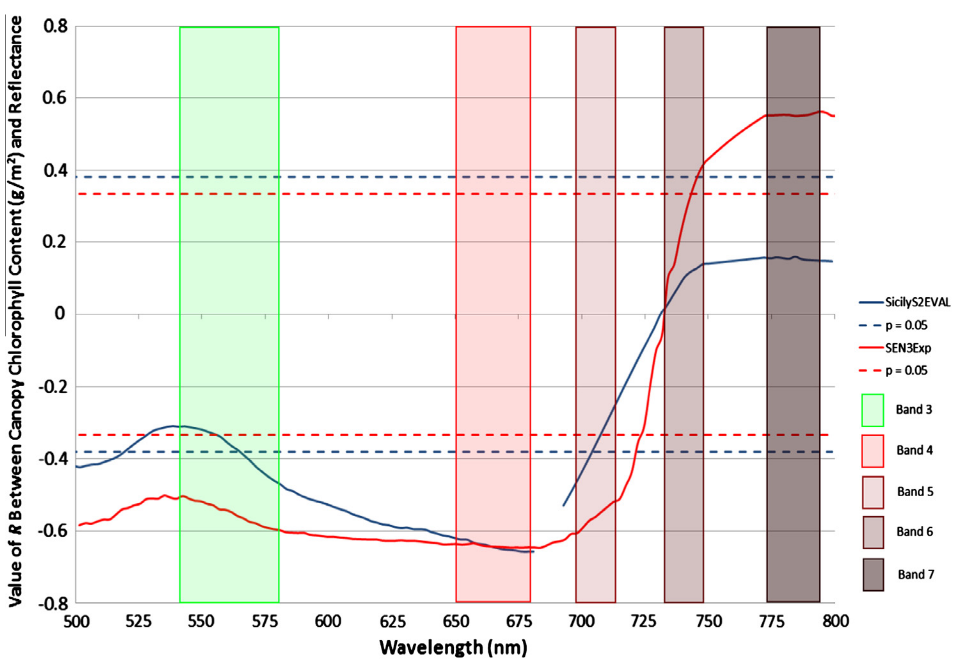

Fig. 2. Comparing the correlation coefficient (*R*) between spectral reflectance and canopy chlorophyll content with changing wavelength for the SicilyS2EVAL and SEN3Exp field campaigns with indications of S-2 band positions and dashed lines to show where $p = 0.05$.

per ESU in a Varian spectrophotometer after extraction of chlorophyll with dimethylformamide (SEN3Exp, 2011).

Table 4 provides a summary of the field campaign data used in this analysis.

2.2. Airborne acquisitions

SEN3Exp hyperspectral data was collected using a CASI-1500 sensor operating at 2.4 nm spectral and 1.5 m spatial resolution. Five flight lines were acquired with an overlap of 50% at an altitude of 2743 m. Atmospheric conditions were good with some reported high cloud appearing during the survey (SEN3Exp, 2011). For the SicilyS2EVAL campaign hyperspectral airborne data was collected and processed to level 1B by the natural environment research council (NERC) airborne research and survey facility (ARSF) using a Specim EAGLE sensor. The sensor operated at a spectral resolution of 2.2 nm between the range of 400 and 1000 nm with a spatial resolution of less than 1.5 m flying at an altitude of 5000 m under clear sky conditions with a solar zenith angle of 70°. All ESUs were contained within two flight lines with an overlap of 50%.

2.3. Band weighting and data processing

Prior to simulating S-2 bands, the Eagle data from SicilyS2EVAL were geometrically corrected using a parametric method, AZGCORR (Azimuth Systems, 2005) based on in-flight altitude and

Table 5
Outcomes of correlation signal investigation.

Part of spectrum	Central wavelength			Range of correlation		
	SicilyS2EVAL (nm)	SEN3Exp (nm)	PROSAIL SEN3Exp (nm)	SicilyS2EVAL (nm)	SEN3Exp (nm)	PROSAIL SEN3Exp (nm)
NIR	750	770	770	750+	750+	760+
RE 0	730	730	742	n/a	n/a	n/a
Red	678	677	725	660–685	600–690	705–735
Green	543	540	555	528–558	525–555	545–565

heading data. Geometrically corrected images were atmospherically corrected using ATCOR-4 (ReSe Applications 2011) which is based around an atmospheric look-up table (Richter, 2008) that contains the results of radiative transfer calculations from the MODTRAN-4 model. After atmospheric correction the available S-2 bands were synthesised from CASI and Eagle data using a weighting function based on the S-2 spectral response files.

3. Designing optimal indices for biophysical variable retrieval from Sentinel 2 data

Direct assessments have been made between canopy chlorophyll content measurements and spectral reflectances for available wavelengths. Canopy chlorophyll content ($g\,m^{-2}$), the product of LCC and LAI, is the total amount of chlorophyll in a given area. The following results show how reflectance is affected for a range of canopy chlorophyll contents over a large part of the visible and NIR spectrum. The method aimed to highlight the strongest vegetative absorption and reflectance signatures and subsequent analysis explored how well they could be harnessed using the available S-2 bands.

3.1. Relationship between spectral reflectance generated from PROSAIL and canopy chlorophyll content

Analysis of the PROSAIL results provided insight into; (i) how reflectance related to the biophysical variables of interest, and; (ii) how these correlations compared to ground data from the field campaigns presented in this paper. This method of investigation highlighted the most highly correlated vegetative features with respect to wavelength for the two PROSAIL datasets and is presented in Fig. 1.

LAI and LCC were varied between 0–8 using increments of 0.2 and 5–70 $\mu g\,cm^{-2}$ using increments of 5 $\mu g\,cm^{-2}$ respectively for the All PROSAIL Data while SEN3Exp PROSAIL represented reflectances generated from the PROSAIL model by inputting biophysical variables attributes as the SEN3Exp campaign. There were issues with using the all PROSAIL dataset in this correlation analysis as the difference between the lower and higher step values of LCC cause the red edge to be more drawn out, as can be seen in Fig. 1, in comparison to the smaller SEN3Exp PROSAIL dataset. PROSAIL was found to highlight the correlation between reflectance and canopy chlorophyll content in the red to peak between 705 and 735 nm and after a very steep and narrow RE it can be seen that spectral reflectance is positively correlated to canopy chlorophyll content above 750 nm.

3.2. Relationship between spectral reflectance and canopy chlorophyll content for SicilyS2EVAL

Fig. 2 illustrates the relationship between canopy chlorophyll content and spectral reflectance for 25 ESU locations in SicilyS2EVAL. Firstly, assessing the NIR correlation showed that the relationship was consistently positive above 745 nm. Increased reflectance in the NIR due to vegetation is a well documented feature of vegetation density due to internal leaf scattering (Gausman, 1974; Knipling, 1970). The correlation coefficient (R value) of the relationship between the canopy chlorophyll content and wavelength in the NIR was low partly due to the vegetative sample having a relatively low LAI range (0.16–1.05) but also due to the influence of soil background reflectance at low LAI. Although the resulting correlation strength was low (Fig. 2) and the *p value of* >0.05 indicated that the result was not significant, the change in correlation with respect to the transition of the red edge is noteworthy when compared to results from SEN3Exp highlighted in Section 3.3. During atmospheric correction several bands in the red (680–690 nm) had to be removed due to sensor saturation issues. Noting this caveat, the red part of the spectrum was found to have a strong and statistically significant ($p < 0.05$) negative relationship between spectral reflectance and canopy chlorophyll content with maximum correlation at 678 nm. This was primarily due to absorption by canopy chlorophyll content. The strength of the red correlation decayed either side of this narrow peak, especially above 690 nm. Correlation between visible light reflectance and canopy chlorophyll content can be seen to decay to a minimum strength in the green (543 ± 15 nm) where chlorophyll absorption reached a minimum. The green relationship had a negative correlation with canopy chlorophyll content due to the sparse ESU locations of bright soil having higher reflectance than the vegetated pixels. Nevertheless, the trend specifically showed the strongest green signal according to this dataset (528–558 nm).

3.3. Relationship between spectral reflectance and canopy chlorophyll content for SEN3Exp

Fig. 2 displays the correlation between the spectral reflectance and canopy chlorophyll content at specific wavelengths for the 35 ESU SEN3Exp dataset. The NIR correlation can be seen to be stronger and statistically significant ($p < 0.05$) compared to the SicilyS2EVAL data above 750 nm reaching maximum strength above 770 nm. The correlation between red reflectance and canopy chlorophyll content reached a maximum at 680 nm and, as with the SicilyS2EVAL dataset, quickly decayed above 690 nm. Similar to the SicilyS2EVAL results the SEN3Exp results show visible absorption correlation decayed to a minimum in the green at 540 nm (± 15 nm).

3.4. Comparison between field campaign data and PROSAIL

Table 5 summarises the outcomes of the correlation coefficient analysis for both SEN3Exp, SicilyS2EVAL and the PROSAIL SEN3Exp data. The "central wavelength" is the point at which the correlation reaches a maximum strength of R in the NIR, red and green. However, in the case of "RE 0" it was where the correlation in the RE = 0. It should be noted that "RE 0" was not a REP measurement but used as a statistical measure to compare between datasets. In Table 5 the "range of correlation" is the extent of the strongest correlation with regards to wavelength for each dataset that can be used to characterise the three key spectral reflectance features in the green, red and NIR.

Table 5 highlights close similarities between the two field campaigns in most parts of the visible and NIR spectrum with the only noticeable differences being; (i) the width of the red correlation feature which is narrower in SicilyS2EVAL towards the green than SEN3Exp, and; (ii) the strength, but not position, of the NIR reflectance feature. However there are significant differences between the field and PROSAIL datasets.

The PROSAIL model data was compared with SEN3Exp data in which is displayed in Fig. 3. It is interesting to note that the PROSAIL data had a strong negative correlation with canopy chlorophyll content until 735 nm. This was not the same for the SEN3Exp and SicilyS2EVAL field data where the correlation between spectral reflectance and canopy chlorophyll content in the red part of the spectrum rapidly decreased above 690 nm (see Fig. 2) and is positive above 730 nm.

In light of the differences in correlation between the field and PROSAIL data in the RE reflectance was compared at 680 nm and 730 nm (Fig. 4). It can be seen that at 680 nm the field data (Fig. 4a) and the PROSAIL data (Fig. 4b) shows a decline in reflectance with an increase in chlorophyll content. However, at 730 nm no relationship was present for the field data (Fig. 4c) while the PROSAIL data (Fig. 4d) remained negative with an R^2 of 0.87 where $p < 0.001$. Although the slope between reflectance and canopy chlorophyll content at this wavelength was 0.05 for the RTM this still results in a 23% reduction in absolute reflectance over the range of 0.05–1.84 g m^{-2} canopy chlorophyll content. In the NIR part of the spectrum, PROSAIL data results are similar to the field campaign data becoming strongly positive at 750 nm and reaching maximum strength at 770 nm (Fig. 4). There was also a difference between the datasets in the green. The field data showed a weakening of the negative relationship while the PROSAIL data showed the negative relationship becoming slightly stronger. Upon further investigation the cause of this difference with the PROSAIL data was an issue of saturation of canopy chlorophyll content with change in green reflectance. When ESUs with high canopy chlorophyll content values were removed the R^2 between canopy chlorophyll content and spectral reflectance in the green was weaker than in blue and red for the SEN3Exp PROSAIL dataset correlating with the SEN3Exp field data trend.

3.5. Suitability of S-2 bands for retrieval of biophysical variables

SicilyS2EVAL and SEN3Exp field campaigns correlation results at specific wavelengths are combined in Fig. 2 which also highlights the available bands for S-2 near the red edge (Table 2). Firstly, according to the two field campaign datasets, S-2 band 3 (542.5–577.5 nm, green band) does not cover the optimal wavelengths where, due to increased canopy chlorophyll content, the green reflectance is less strongly correlated to canopy chlorophyll content than in the red and blue parts of the visible spectrum. Using a band width of 525–555 nm would be theoretically optimal for the datasets presented. Secondly S-2 band 4 (red band) captures absorption due to chlorophyll as its bandwidth extends until just before the RE where spectral reflectance beings to shift from a negative to positive relationship with canopy chlorophyll content. Furthermore, the bandwidth of S-2 band 4 is not adversely wide whereas, according to the two datasets and especially SicilyS2EVAL, if the lower band limit extended below 650 nm the bands strength of characterising the chlorophyll absorption feature would be weakened. The MERIS continuation RE band (S-2 band 5: 705 ± 7.5 nm) has increased spectral bandwidth compared to MERIS band 9 (708.75 ± 5 nm). However, with the central band position only slightly changed this should not make significant impact for RE characterisation considering it is situated over a linear part of the RE. S-2 band 6 is a new RE/NIR band with respect to previous satellite sensors such as RapidEye and MERIS. Considering vegetative monitoring and capturing the NIR feature S-2 band 6 will, as a replacement for MERIS band 10 (753.75 ± 3.75 nm), receive increased mixed signal from the RE as it is situated at the peak of the RE rather than slightly beyond it. However the position of the band and its combination with S-2 band 5 will, consequently, provide the opportunity for enhanced estimation of the REP compared to MERIS or RapidEye. Finally S-2 band 7, which is similar to MERIS band 12 (775 ± 7.5 nm), is the optimal band in the NIR for capturing the vegetative signal in the NIR based on SicilyS2EVAL and SEN3Exp data sets.

It should be highlighted that, with reference to Table 5, the correlation in vegetation spectral reflectance and canopy chlorophyll content shown between these two separate field campaigns is consistent considering their differences with respect to airborne sensor, location, operating team, time of year and field campaign procedures. Taking this into account gives confidence in using this presented dataset to compare methods for canopy chlorophyll content, LAI and LCC retrieval from S-2 data.

3.6. New vegetation indices for S-2

Based on the relationship between spectral reflectance in individual S-2 MSI bands and canopy chlorophyll content, LAI and LCC, this paper proposes two new methods to estimate biophysical

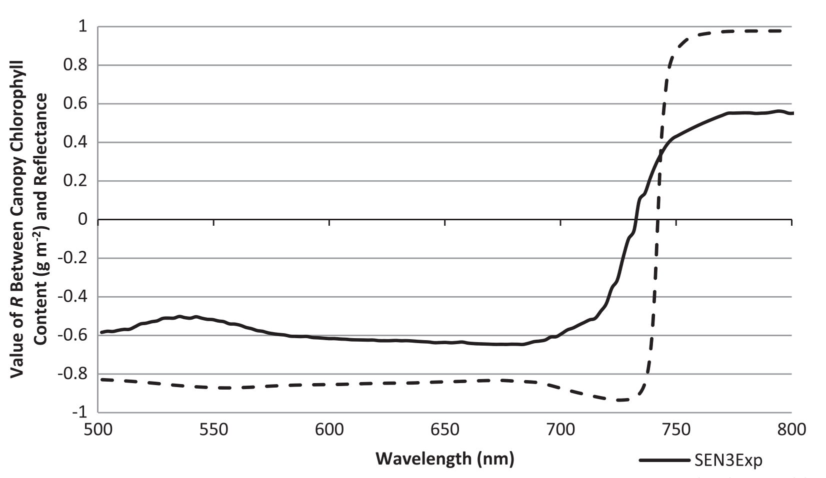

Fig. 3. Comparing the correlation coefficient (R) between canopy chlorophyll content and spectral reflectance for the SEN3Exp field campaign and SEN3Exp PROSAIL with changing wavelength.

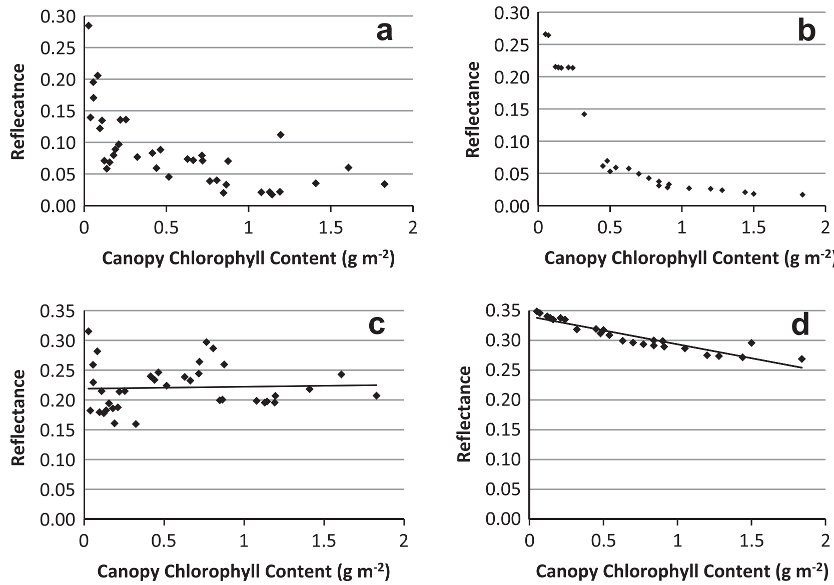

Fig. 4. Comparison of PROSAIL SEN3Exp (b and d) and SEN3Exp field data (a and c) at 680 nm (a and b) and 730 nm (c and d).

variables for use with S-2 MSI data. First, the inverted red-edge chlorophyll index (IRECI, Eq. (4)) which incorporates the reflectance in four S-2 bands to estimate canopy chlorophyll content, and second, the Sentinel-2 red-edge position (S2REP, Eq. (5)); a version of REP estimation for S-2 using linear interpolation (Guyot and Baret, 1988; Clevers et al., 2000).

$$\mathrm{IRECI} = \frac{\rho\mathrm{NIR} - \rho R}{\rho\mathrm{RE2}/\rho\mathrm{RE1}} = \frac{\rho 783 - \rho 665}{\rho 705/\rho 740} \tag{4}$$

IRECI makes use of both RE bands, that S-2 will provide, to characterise the RE slope by using the reflectance at 740 nm and 705 nm (Table 1) while also making use of the maximum and minimum vegetation reflectances found in the NIR and red at 783 nm and 665 nm respectively. By using the LCC indicative RE reflectance IRECI does not put heavy emphasis on the red, which will help to avoid saturation, while still utilising the strong contrast of the SR sensitive to LAI. Based on field dataset from SEN3Exp and SicilyS2EVAL campaigns, IRECI is a near direct calculation of field measured canopy chlorophyll content (g m^{-2}) with a slope of 0.9004 and intercept of 0.1795 with a coefficient of determination of 0.87 (see Section 4.3., Table 6). However, further validation will be required with other datasets and specifically a larger range of canopy chlorophyll content.

$$\begin{aligned}\mathrm{S2REP} &= 705 + 35 * \frac{\left(\frac{\rho\mathrm{NIR}+\rho R}{2}\right) - \rho\mathrm{RE1}}{\rho\mathrm{RE2} - \rho\mathrm{RE1}}\\ &= 705 + 35 * \frac{\left(\frac{\rho 783+\rho 665}{2}\right) - \rho 705}{\rho 740 - \rho 705}\end{aligned} \tag{5}$$

S2REP (Eq. (5)) is based on linear interpolation as presented by Guyot and Baret (1988) where the reflectance at the inflexion point is estimated and in turn the REP is retrieved through interpolation of S-2 band 5 and 6 which are positioned on the RE slope. This linear interpolation method has been previously applied to MERIS data by Clevers et al. (2000) and was found to be more robust than the Lagrangian method (Dawson and Curran, 1998) with the benefit of requiring a limited number of spectral bands making it suitable for spaceborne sensors (Clevers et al., 2002). S-2 has a key benefit compared to MERIS for the application of the linear interpolation method. S-2 band 6 (740 nm) measures the reflectance situated at the top of the linear part of the RE slope whereas MERIS band 10 (753.75 nm) measures reflectance slightly above the linear part of the RE where the gradient in decreasing as it reaches the NIR plateau. In theory this means that S2REP should provide better characterisation of the RE slope compared to application of the method using the MERIS or the future Sentinel-3 sensors.

Table 6
Coefficient of determination results of each Vegetation Index for varying field data sets and biophysical variables.

Variable	Data Set	NDVI	NDI45	MTCI	MCARI	GNDVI	PSSR	S2REP	IRECI
Canopy Chlorophyll Content	Combined	0.70*	0.78*	0.51*	0.42*	0.66*	0.72*	0.47*	0.87*
	SicilyS2EVAL	0.83*	0.78*	0.65*	0.66*	0.45*	0.84*	0.35	0.64*
	SEN3Exp	0.62*	0.70*	0.24	0.75*	0.58*	0.59*	0.23	0.84*
LAI	Combined	0.63*	0.76*	0.39	0.55*	0.58*	0.61*	0.36	0.88*
	SicilyS2EVAL	0.86*	0.84*	0.55*	0.72*	0.42*	0.83*	0.19	0.74*
	SEN3Exp	0.57*	0.68*	0.15	0.88*	0.49*	0.51*	0.12	0.84*
LCC	Combined	0.56*	0.30*	0.77*	0	0.58*	0.36	0.91*	0.24
	SicilyS2EVAL	0.62*	0.63*	0.39	0.35	0.54*	0.62*	0.24	0.35
	SEN3Exp	0	0	0.25	0	0.02	0.03	0.51*	0

*Have p values of <0.001.

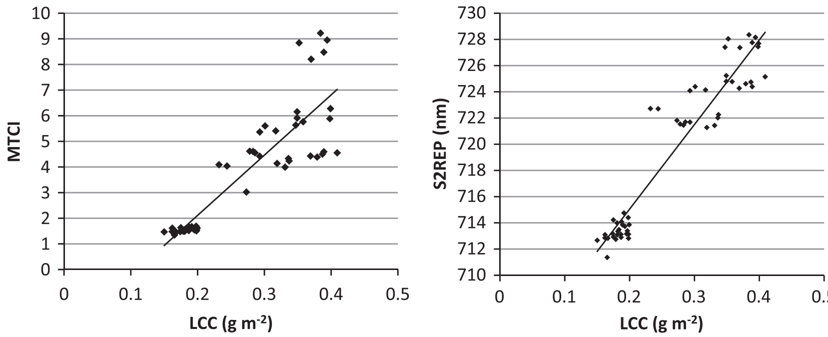

Fig. 5. Coefficient of determination comparisons between MTCI, an estimate of the REP and LCC.

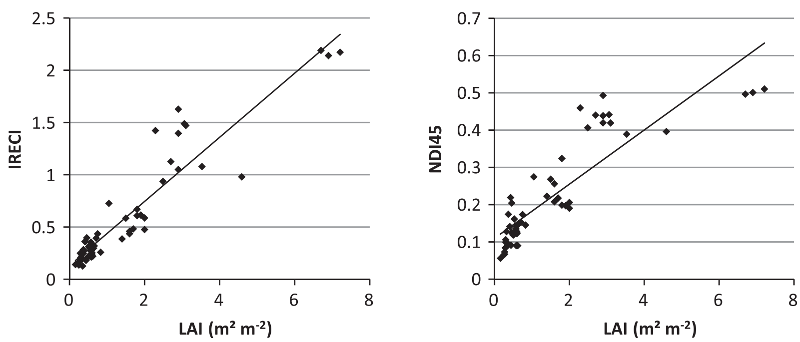

Fig. 6. IRECI and NDI45 compared for LAI from SEN3Exp and SicilyS2EVAL field campaigns.

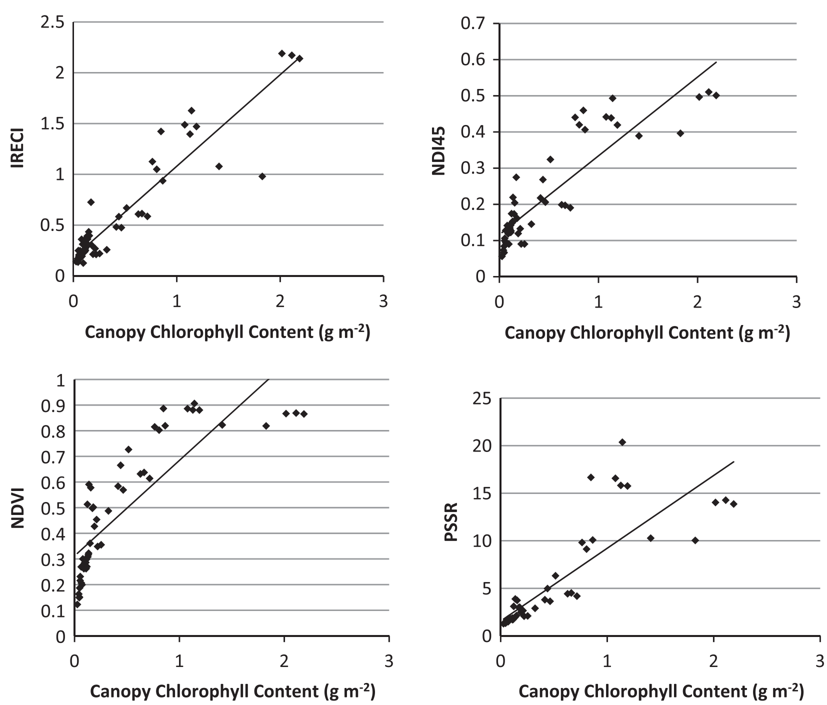

Fig. 7. IRECI, NDI45, NDVI and PSSR compared to canopy chlorophyll content for field data from SicilyS2EVAL and SEN3Exp field campaigns.

4. Evaluation of the spectral indices

Each VI output was derived from the synthesised S-2 data for the field campaigns presented in Table 3. The correlation with LAI, LCC and canopy chlorophyll content for each assessed VI is presented in Table 6.

4.1. Leaf chlorophyll concentration

Although majority of VIs had poor correlation with LCC (Table 6) the MTCI and S2REP achieved strong correlation with leaf chlorophyll concentration with R^2 of 0.77 and 0.91 respectively (Fig. 5).

The MTCI and S2REP are the only two VIs in the analysis that solely characterise the RE which has been shown to be sensitive to variation in LCC (Horler et al., 1983; Curran et al., 1990; Dash and Curran, 2004). Increases in LCC result in a broadening of the major red absorption feature which causes a shift in the REP towards longer wavelengths (Boochs et al., 1990). Previous experimental studies have shown low LCC to be associated with REP values near 700 nm and high LCC to attain REP results closer to 725 nm (Boochs et al., 1990; Horler et al., 1980; Lamb et al., 2002). S2REP performed with similar results for the combined SicilyS2EVAL and SEN3Exp datasets producing REP results of 711–728 nm for LCC values of 0.16–0.41 g/m^2.

4.2. Leaf area index

The IRECI and the NDI45 were the best performing VIs with respect to LAI with R^2 values of 0.88 and 0.76 respectively. Although developed for correlation with canopy chlorophyll content IRECI is shown in Fig. 6 to be linear with LAI. When compared for lower values of LAI below 2 the IRECI and the NDI45 have an R^2 of 0.77 and 0.62 ($p < 0.001$) respectively.

4.3. Canopy chlorophyll content

The four best performing VIs (NDVI, PSSR, NDI45 and IRECI) (Table 6) in terms of correlation coefficient with respect to canopy chlorophyll content are compared in Fig. 7. Saturation is noticeably present above a canopy chlorophyll content value of 1 g/m^2 for the NDVI ($R^2 = 0.70$) due to saturation of red reflectance (Kanemasu, 1974; Tucker, 1979; Horler et al., 1983; Buschmann and Nagel, 1993.) The PSSR ($R^2 = 0.72$) functions linearly with canopy chlorophyll content although its spread increases significantly at higher values. When comparing the NDVI and the NDI45 this dataset suggests the change from using reflectance measurements in the NIR (band 7) to RE1 (band 5) has increased spread at lower canopy chlorophyll content values but made NDI45 more linear with less saturation at higher values than the NDVI. The IRECI was the best performing measure of canopy chlorophyll content using synthesised S-2 field data for the two presented campaigns. The index can be seen to have a strong linear relationship with canopy chlorophyll content without saturation at higher values. As highlighted earlier in Section 5, the IRECI also has the useful trait of being a near direct calculation of canopy chlorophyll content in g/m^2 for this dataset. The inclusion of RE bands improved correlation over the entire data set while mitigating the saturation effect at higher canopy chlorophyll content. However, the inclusion of these bands also increased the spread of the IRECI at very low canopy chlorophyll content (<0.13 g/m^2) compared to the NDVI and PSSR$_a$.

5. Conclusions

S-2 provides a great opportunity for global vegetation monitoring due to its enhanced spatial, spectral and temporal characteristics compared with Landsat and SPOT. Simulated S-2 data has been compared to a combined field dataset of 60 + ESUs across two field campaigns covering eight separate crops. Although the field campaigns varied with respect to year, location, airborne sensors and field teams, similar relationships between spectral reflectance and canopy chlorophyll content were obtained. All bands around the RE have been shown to be useful in assessing vegetation condition, specifically canopy chlorophyll content. However, there is a need for further investigation of the green reflectance region 525–555 nm and its potential role in estimating canopy chlorophyll content. The results suggest that the wavelengths covered by the S-2 green band may not be optimal to capture the changes in reflectance due to canopy chlorophyll content.

It has been highlighted that many VIs attempt to correct for uncertainties or inaccuracies through incorporation of scene specific parameters or normalisation functions. Application of such methods affects the universal applicability and ease of operational use. S2REP has been presented and shown as the most suitable method for quantifying LCC using these datasets; nevertheless the MTCI also had noteworthy results. A novel index the IRECI has been shown to be linearly related to canopy chlorophyll content at a near 1:1 ratio in g m^{-2} while still performing well for LAI up to and beyond the common saturation point. It achieves this as it utilises the opportunities S-2 bands 5 and 6 present for RE characterisation while still incorporating the robustness of the SR. Further validation is required with other field campaigns and synthetic S-2 data to reinforce findings.

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