International Journal of Applied Earth Observation and Geoinformation 57 (2017) 24–35

Contents lists available at ScienceDirect

International Journal of Applied Earth Observation and Geoinformation

journal homepage: www.elsevier.com/locate/jag

Assessment of leaf carotenoids content with a new carotenoid index: Development and validation on experimental and model data

Xianfeng Zhou[a,b], Wenjiang Huang[a,*], Weiping Kong[a], Huichun Ye[a], Yingying Dong[a], Raffaele Casa[c]

[a] Key Laboratory of Digital Earth Science, Institute of Remote Sensing and Digital Earth, Chinese Academy of Science, Beijing 100094, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China
[c] Department of Agricultural and Forestry scieNcEs (DAFNE), Universita' della Tuscia, via San Camillo de Lellis, 01100 Viterbo, Italy

ARTICLE INFO

Article history:
Received 18 July 2016
Received in revised form 9 December 2016
Accepted 14 December 2016

Keywords:
Leaf carotenoids content
Hyperspectral
Spectral index
Radiative transfer model

ABSTRACT

Leaf carotenoids content (LCar) is an important indicator of plant physiological status. Accurate estimation of LCar provides valuable insight into early detection of stress in vegetation. With spectroscopy techniques, a semi-empirical approach based on spectral indices was extensively used for carotenoids content estimation. However, established spectral indices for carotenoids that generally rely on limited measured data, might lack predictive accuracy for carotenoids estimation in various species and at different growth stages. In this study, we propose a new carotenoid index (CARI) for LCar assessment based on a large synthetic dataset simulated from the leaf radiative transfer model PROSPECT-5, and evaluate its capability with both simulated data from PROSPECT-5 and 4SAIL and extensive experimental datasets: the ANGERS dataset and experimental data acquired in field experiments in China in 2004. Results show that CARI was the index most linearly correlated with carotenoids content at the leaf level using a synthetic dataset ($R^2 = 0.943$, RMSE = 1.196 μg/cm^2), compared with published spectral indices. Cross-validation results with CARI using ANGERS data achieved quite an accurate estimation ($R^2 = 0.545$, RMSE = 3.413 μg/cm^2), though the RBRI performed as the best index ($R^2 = 0.727$, RMSE = 2.640 μg/cm^2). CARI also showed good accuracy ($R^2 = 0.639$, RMSE = 1.520 μg/cm^2) for LCar assessment with leaf level field survey data, though PRI performed better ($R^2 = 0.710$, RMSE = 1.369 μg/cm^2). Whereas RBRI, PRI and other assessed spectral indices showed a good performance for a given dataset, overall their estimation accuracy was not consistent across all datasets used in this study. Conversely CARI was more robust showing good results in all datasets. Further assessment of LCar with simulated and measured canopy reflectance data indicated that CARI might not be very sensitive to LCar changes at low leaf area index (LAI) value, and in these conditions soil moisture influenced the LCar retrieval accuracy.

1. Introduction

Photosynthetic pigments that mainly include chlorophylls and carotenoids are of great importance in the biosphere. Their photosynthetic function is essential for plant and mammal survival (Blackburn, 2007). Within leaf chloroplasts, chlorophylls (Chl), composed of chlorophyll *a* (Chl *a*) and chlorophyll *b* (Chl *b*), represent the principal class of pigments responsible for light absorption in photosynthesis (Nobel, 1999). Carotenoids (Car), that include carotenes and xanthophylls, are the second major group of plant pigments (Blackburn, 2007). They are part of the essential structures of the photosynthetic antenna and reaction center, and help stabilize chlorophyll–protein complexes (Frank and Cogdell, 1996; Strzałka et al., 2003). Besides their function in photosynthesis, previous studies suggest that the assessment of the variation of Car and of their ratio to Chl could shed light on the understanding of photoprotection, photosynthetic acclimation, and photosynthetic efficiency in plants (Demmig-Adams and Adams, 1996; Fang et al., 1998; Gamon and Surfus, 1999; Merzlyak et al., 1999; Richardson et al., 2002; Young and Britton, 1990). Within the plant growth cycle, Chl decrease normally indicates that plants are affected by environmental stresses, while the variation of Car reflects the physiological status of vegetation (Young and Britton, 1990). For instance, it has been observed that Car content would change

* Corresponding author.
E-mail address: huangwj@radi.ac.cn (W. Huang).

http://dx.doi.org/10.1016/j.jag.2016.12.005
0303-2434/

when plants are in sun-intense and high temperature conditions, or when nitrogen availability is low, or at the onset of leaf senescence (Demmig-Adams and Adams, 1996; Kirchgeßner et al., 2003; Munné-Bosch and Peñuelas, 2003). Therefore, quantitative estimation of Car content is extremely useful, in order to clarify the mechanisms of photoprotection and light-adaption, and for early diagnosis of stress in vegetation.

During the last decade, a series of attempts have been undertaken to use spectroscopy techniques to estimate Car content at both the leaf and canopy level, exploiting its absorption features in the visible range (Gitelson et al., 2002). Based on ratio analysis of reflectance spectra (RARS) method, Chappelle et al. (1992) suggested that the absorption band at 500 nm had the highest correlation with Car and was least affected by confounding effects from other pigments, thus they proposed a ratio index (RARS*c*, R_{760}/R_{500}) for Car estimation. Research conducted by Datt (1998) indicated that the maximum sensitivity of reflectance to variation in pigment content was in the green band region at 550 nm and at 708 nm in the red edge region, thus they put forward a reflectance band ratio index (RBRI, $R_{672}/(R_{550} \times R_{708})$), which had a good correlation with Car. In an attempt to evaluate spectral indices for estimating pigment concentrations at the leaf scale, Blackburn (1998) developed two new indices (PSSR*c* and PSND*c*) with the optimal wavebands 470 nm and 800 nm for Car retrieval. Having found that the spectral band around 510 nm was sensitive to Car content, Gitelson et al. (2002) developed two carotenoid reflectance indices (CRI_{550} and CRI_{700}), with the reciprocal reflectance at 510, 550 and 700 nm and found that these two indices were accurate indicator of leaf carotenoids content (LCar). Furthermore, Gitelson et al. (2006) investigated the applicability of a conceptual three-band model to estimate the content of various pigments and they established two carotenoid indices ($CAR_{rededge}$ and CAR_{green}) with three bands located at 510–520 nm, 690–710 nm (560–570 nm for CAR_{green}) and a NIR band, which showed accurate estimation of Car. Hernández-Clemente et al. (2012) found that vegetation canopy structure severely affected the performance of spectral index for Car assessment at crown level. A simple ration index (SR_{car}, R_{515}/R_{570}) was then proposed and it showed good correlation with Car content at both leaf and canopy levels.

For the development of robust indices for plant biochemical content assessment with spectroscopic techniques, the quality of the training dataset, the selection of the wavelengths and the availability of an independent dataset for the validation are essential (Féret et al., 2011). The above mentioned studies have indeed made much progress in Car content estimation in different vegetation species at the leaf or canopy scales. Nevertheless, most of the research focused on establishing spectral indices or models for Car retrieval, with calibration and validation datasets that were generally limited. These limited data might not be generic enough in order to provide a robust method of assessing Car composition and distribution, at a range of phenological stages and leaf structures. Spectral indices or models based on these datasets might be site- or species-specific, their robustness and capability deserves further investigation when applied to a wide variety of plant leaves and conditions.

Radiative transfer models (RTMs) are effective tools to clarify the mechanism describing the relationships between spectral reflectance and plant parameters. They provide an analysis of the remote sensing signal based on a robust understanding of the physical, chemical, and biological processes, allowing to assemble rapidly abundant simulation datasets (Féret et al., 2008). In recent years, the RTMs have been used extensively for various applications on the vegetation studies (Jacquemoud et al., 2009). Based on spectral data sets simulated from leaf scale RTMs, Blackburn and Ferwerda (2008) proposed a method to estimate leaf chlorophylls content (LChl) from reflectance using wavelet analysis. By coupling the leaf model PROSPECT (Jacquemoud and Baret, 1990) with the multi-layer canopy model Scattering by Arbitrary Inclined Leaves (SAIL) (Verhoef, 1984) into the PROSAIL model, le Maire et al. (2008) conducted a research to select optimal narrow-band vegetation indices for the retrieval of LChl and leaf mass per area (LMA). Féret et al. (2008) successfully estimated the concentrations of carotenoids and total chlorophyll by inverting the PROSPECT model from tree leaf reflectance and transmittance measurements. Di Vittorio (2009) focused on the incorporation of three pigments, including chlorophyll *a*, chlorophyll *b*, and total carotenoids, into the Leaf Incorporating Biochemistry Exhibiting Reflectance and Transmittance Yields (LIBERTY) model (Dawson et al., 1998), obtaining good estimates of the concentrations of these pigments. Vincini et al. (2016), used PROSAIL simulations to explore the sensitivity of canopy scale estimators of leaf chlorophylls, obtainable with Sentinel-2 satellite spectral resolution, to soil, canopy and leaf mesophyll factors.

Nevertheless, attention on Car assessment using RTMs has been smaller than that for Chl estimation. For LCar retrieval with leaf spectra, the proper combination of various plant parameters in leaf model PROSPECT, could generate a series of simulated datasets useful for an investigation of the spectral interactions among Car and other leaf characteristics, also providing a database for evaluating the performance of spectral indices for LCar assessment. Different from LCar retrieval with leaf level reflectance, LCar assessment with canopy spectra is much more complex, since spectra acquired at the canopy could be affected by complicating factors other than biochemical content, such as canopy structure, illumination and viewing geometry, as well as the optical properties of the soil (Lemaire, 2012). These effects can induce ambiguities in LCar assessment from canopy reflectance. Among these factors, leaf area index (LAI), one of the key parameters describing the canopy structure, and the soil background, has a large effect on canopy reflectance signals (Yu et al., 2014; Zou et al., 2015). The utilization of the PROSAIL model could generate an extensive canopy level dataset useful for better understanding the relationship between canopy geometry, background environment and canopy reflectance, thus it could shed light on the effect of LAI and soil background on LCar assessment and provide the basis for an accurate and robust LCar estimation with spectral index methods.

Therefore, the aim of the present study was to develop an accurate and robust LCar estimation index, using simulated and measured datasets based on their absorption features in the visible spectrum. The specific objectives were to: i) establish a new carotenoid index (CARI) for LCar estimation, assess and compare its performance with published carotenoid indices using leaf level simulated data obtained from PROSPECT-5; ii) evaluate the capability and robustness of the newly CARI and published carotenoid indices with various leaf level measured data including the widely used ANGERS dataset (Féret et al., 2008) and field survey data; iii) clarify the effect of LAI and soil background on LCar assessment with the CARI using an extensive synthetic dataset obtained from 4SAIL and measured data at the canopy scale.

2. Material and methods

2.1. Study site

The study site was located at the National Experimental Station for Precision Agriculture (40°10.6′ N, 116°26.3′ E), Beijing, China. The field site has a warm temperate climate, with a mean annual rainfall of 507.7 mm, a mean annual temperate of 13.8 °C and the soil is classified as silt-clay loam. Winter wheat (*Triticum aestivum* L.), one of the major crops in China, was used in this study. In 2004, twenty-one cultivars of winter wheat were grown in plots of 30 m × 5.4 m size. Fertilization and irrigation were applied accord-