Sensitivity Analysis of Vegetation Reflectance to Biochemical and Biophysical Variables at Leaf, Canopy, and Regional Scales

Yanfang Xiao, Wenji Zhao, Demin Zhou, and Huili Gong

Abstract—The objective of this paper is to investigate the sensitivity of reflectance to the variation in biochemical and biophysical variables at leaf, canopy, and regional scales using a modeling approach. The results show that, at the leaf scale, the variations in chlorophyll a+b content, the leaf structure parameter, and the water content dominate the reflectance variance in the visible light (VIS), near infrared (NIR), and short-wave infrared (SWIR) regions, respectively. At the canopy scale, the sensitivity of reflectance to variation in the leaf structure parameter is very slight. For sparse foliage cover (leaf area index (LAI) < 3), LAI is the most important variable to the canopy reflectance. As LAI increases, the sensitivity of reflectance to variation in LAI is reduced to a very low value. Moreover, chlorophyll a+b, dry matter, and water content control the variation of canopy reflectance in the VIS, NIR, and SWIR regions, respectively. At the regional scale, the sensitivity of reflectance to variation in vegetation variables is highly influenced by the mixed pixels. Thirty-six vegetation indices (VIs) are chosen in this paper to illustrate the scale dependence of the estimation accuracy of vegetation variables. The results show that the relationships between the VIs and the variables highly depend on the observation scale. For chlorophyll a+b content estimation, transformed chlorophyll absorption in reflectance index (TCARI), Blue Green pigment Index, leaf chlorophyll index (LCI), modified Normalized Difference (mND705), and Plant Biochemical Index at the leaf scale and canopy scale of LAI > 3 and TCARI at the canopy scale of LAI < 3 are highly related. The correlation between the indices and chlorophyll content in the regional scale is, however, much lower. For water content estimation, disease water stress index (DSWI), leaf water vegetation index 2 (LWVI_2), moisture stress index (MSTI), normalized difference infrared index (NDII), normalized difference water index (NDWI), hyperspectral perpendicular vegetation index (RV1), SWIR water stress index (SIWSI), SR water index (SRWI), and water index (WI) are good choices at the leaf scale and canopy scale of LAI > 3, while at the canopy scale of LAI < 3 and the regional scale, the correlation between the indices and water content is very low. For LAI estimation, VIs, including the Greenness Index, simple ratio (SR), Normalized Difference VI, modified soil-adjusted vegetation index (MSAVI), modified triangular vegetation index 1 (MTVI1), modified triangular vegetation index 2 (MTVI2), optimized soil-adjusted vegetation index (OSAVI), modified chlorophyll absorption ratio index 1 (MCARI1), modified chlorophyll absorption ratio index 2 (MCARI2), Enhanced VI, LAI Determining Index, renormalized difference vegetation index (RDVI), Spectral Polygon VI, Wide Dynamic Range VI, and triangular vegetation index (TVI), have high correlation with LAI at the canopy scale of LAI < 3 while a low correlation at the canopy scale of LAI > 3 and the regional scale.

Index Terms—Extended Fourier amplitude sensitivity test (EFAST), PROSPECT + SAIL, radiative transfer, scale, sensitivity analysis (SA), vegetation index (VI).

I. INTRODUCTION

ESTIMATING the vegetation biochemical and biophysical variables has important potential implications for many ecological, agronomic, and meteorological applications. The key variables include leaf chlorophyll content which affects photosynthetic capacity and productivity [5], [37], water content which is one of the key parameters in fire behavior models for its control on the initial probability of ignition, burning efficiency and the rate of fire propagation [10], and the leaf area index (LAI) defined as the single-sided area of green leaf area per unit ground, which governs net radiation and its expenditure, net primary production, evapotranspiration, and canopy interception [65]. Many vegetation variables show the diagnostic absorption features. For instance, leaf chlorophyll strongly affects the visible region of the reflectance spectra while LAI has a large impact on the near infrared (NIR) region. As a unique cost-effective resource, remote sensing data have been proposed as a good solution for the measurement of vegetation parameters [8]. There are two main approaches for estimating vegetation variables: the empirical–statistical approach and physically based models. The empirical–statistical approach seeks the relationship between the vegetation variable and single spectral reflectance or spectral indices. Many vegetation indices (VIs) were designed for estimating vegetation variables. For example, Blue Green pigment Index (BGI), Modified Chlorophyll Absorption in Reflectance (MCARI), Plant Biochemical Index (PBI), and Chlorophyll Absorption Ratio Index (CARI) were developed for estimating plant pigments [18], [46], [55], [72]; Enhanced VI (EVI), modified Normalized Difference (mND705), Normalized Difference VI (NDVI), and Wide Dynamic Range VI (WDRVI) were very useful for assessing
constituents (see Fig. 1). Therefore, in many cases, the pixel
the signal of remote sensing imagery is composed by multiple
neous characteristics, particularly for the open vegetation, and
However, it is hard for these data to obtain the absolute homoge-
cial role in estimating biochemical and biophysical variables.
medium resolution imaging spectrometer [2] still plays a cru-
mapper/enhanced thematic mapper [1], [71], moderate reso-
with moderate or low spatial resolution as Landsat thematic
The vegetation reflectance at different spatial resolution is controlled by diverse
variables simultaneously is critical to accurately estimate the
other variables which have more meanings in many ecological
The objective of this paper is then to investigate and quantify the sensitivity of reflectance to the variation in vegetation variables at leaf, canopy, and regional scales with a global sensitivity analysis (SA) method, the extended Fourier amplitude sensitivity test (EFAST). In this paper, leaf scale is defined as the data which can represent the leaf reflectance, canopy scale is defined as the data which can represent the canopy reflectance, and regional scale means that the obtained data are the mixed information of vegetation and other ground objects. There is no clear numerical definition for these scales because the scales are determined by both the spatial resolution of sensors and the research objects. A TM image with a 30-m resolution of a sparse forest may be dealt at the regional scale. However, this regional scale may be inaccurate for another TM image of a closed and continuous vegetation cover in which, in this case, the canopy scale would be more suitable.

This paper is organized in four sections. In Section II, the method and models are introduced, including EFAST global sensitivity, PROSPECT-5, and 4SAIL model. Section III shows the simulated database (including the value of vegetation variables and the simulated reflectance at leaf, canopy, and regional scales), and 36 published VIs. The results are presented in Section IV (the contribution of vegetation variables to the leaf, canopy, and regional reflectance and the relationship between VIs and chlorophyll a+b content, equivalent water thickness, and LAI). In Section V, a discussion addresses the main points of this study, including how the sensitivity of vegetation reflectance to vegetation variables changes, and what are the best VIs for estimating chlorophyll a+b content, equivalent water thickness, and LAI at leaf, canopy, and regional scales. A general conclusion summarizes the results and proposes the research prospect for future works.

II. METHODS AND MODELS

To quantify the contribution of vegetation variables to the variation in the reflectance data, a huge amount of ground data, including measured reflectance and vegetation variables at different scales, would be needed, which could be extremely expensive or even impossible. Consequently, in this paper, a

Fig. 1. Schematic drawing of vegetation reflectance at leaf, canopy, and regional scales.
database with a wide range of vegetation variables incorporating the vegetation reflectance at leaf, canopy, and regional scales is simulated from models. The well-known and modified PROSPECT-5 model is used to simulate the leaf reflectance. The link between the PROSPECT-5 and 4SAIL models which describes the canopy reflectance as a function of leaf biochemistry, canopy architecture, and illumination geometry, is used to simulate the canopy reflectance. EFASST is a global sensitivity method to calculate the sensitivity of reflectance to the variation in vegetation variables. A description of the main features of these models is given in the following sections. Refer to Jacquemoud and Baret [43], Verhoef [66], and Saltelli [59] for more details.

A. PROSPECT-5 and 4SAIL Models

1) PROSPECT-5 Model: Based on the assumption that a leaf is composed of a pile of N homogeneous layers separated by N – 1 air spaces, PROSPECT pioneered to simulate the directional–hemispherical reflectance and transmittance of various green monocotyledon and dicotyledon species, as well as senescent leaves over the solar spectrum of 400–2500 nm [43]. The PROSPECT-5 model is a robust version of PROSPECT, which is modified to include carotenoids and brown pigments.

The input parameters of the PROSPECT-5 model include leaf structure parameter N, chlorophyll a+b content C_{ab} (\mu g \cdot cm^{-2}), carotenoid content C_{ar} (\mu g \cdot cm^{-2}), brown pigment content C_{brown} (g \cdot cm^{-2}), equivalent water thickness C_{w} (g \cdot cm^{-2}), and dry matter content C_{m} (g \cdot cm^{-2}). The model simulates the leaf reflectance and transmittance spectra of 400–2500 nm with 1-nm resolution, using the specific absorption coefficient K which depends on wavelength but not botanical species. The total absorption coefficient k can be calculated as

\[ k(\lambda) = k_{c}(\lambda) + \frac{C_{ab}}{N} K_{ab}(\lambda) + \frac{C_{ar}}{N} K_{ar}(\lambda) + \frac{C_{brown}}{N} K_{brown}(\lambda) + \frac{C_{w}}{N} K_{w}(\lambda) + \frac{C_{m}}{N} K_{m}(\lambda) \]

where \( \lambda \) is the wavelength, \( k_{c}(\lambda) \) is the absorption of an albinos leaf, and \( K_{ab}, K_{ar}, K_{brown}, K_{w}, K_{m} \) are the absorption coefficients of chlorophyll a+b, carotenoid, brown pigment, water, and dry matter, respectively. They were determined by Feret et al. [25] using four data sets: leaf optical properties experiment (LOPEX) measured in 1993, center for advanced land management information technologies from 1995/1996, ANGERS measured in 2003, and HAWAII from 2007.

2) 4SAIL Model: The 4SAIL canopy reflectance model used in this paper is a numerically robust and speed-optimized version of SAIL. In the SAIL model, the canopy layer is assumed to be homogeneous, horizontal, and infinitely extend with small and flat leaves as the only canopy components. Essentially, the SAIL model is a four-flux theory, with four differential equations and nine coefficients which are given by

\[ dE_s/dz = k(\theta_t)E_s \]
\[ dE_- / dz = -\sigma(\theta_t)E_+ + \alpha(\theta_t)E_- - s(\theta_t)E_s \]
\[ dE_+ / dz = -\alpha(\theta_t)E_+ + \alpha(\theta_t)E_- + s(\theta_t)E_s \]
\[ dE_o / dz = w(\theta_t)E_s + v(\theta_t)E_- + u(\theta_t)E_+ - K(\theta_t)E_o \]

where \( E_s \) is a direct solar flux, \( E_+ \) is a diffuse upward flux, \( E_- \) is a diffuse downward flux, and \( E_o \) is a radiance flux in the direction of observation. \( \theta_t \) stands for the leaf inclination angle, \( k \) and \( K \) for the extinction coefficient for \( E_s \) and \( E_o \), respectively, and \( \alpha \) for the attenuation coefficient for diffuse fluxes \( E_+ \) and \( E_- \). \( \sigma \) respectively describes the backscatter and forward scattering of the \( E_+ \) and \( E_- \), \( s \) and \( s' \) describe the scattering from \( E_s \) to \( E_+ \) and \( E_- \), and \( w, v, \) and \( u \) describe the scattering from \( E_s, E_+, \) and \( E_- \) to \( E_o \), respectively.

To simulate canopy reflectance spectra in the optical domain of 400–2500 nm with 1-nm resolution, the 4SAIL model requires the leaf area index (LAI), mean leaf inclination angle (\( \alpha \)), hot spot parameter (\( s_1 \)), soil reflectance assumed Lambertian (\( \rho_s \)), ratio of diffuse to total incident radiation (\( \sigma_{SKYL} \)), zenith angle of solar (\( \theta_s \)) and viewing (\( \theta_v \)), relative azimuth angle (\( \phi_{az} \)), and leaf reflectance (\( \rho_l \)) and transmittance (\( \tau_l \)) which can be obtained from the PROSPECT-5 leaf reflectance model. The canopy reflectance \( \rho(\lambda) \) can be expressed as

\[ \rho(\lambda) = SAIL(LAI,a,p_l(\lambda),\tau_l(\lambda),\rho_l(\lambda),\theta_s,\theta_v,\phi_{az},s_1,\sigma_{SKYL}) \]

B. EFAST Method

Two different schools of SA have been implemented, local SA and global SA. The difference between these two SA schools is that the local SA provides information on how variation in each parameter individually accounts for variation in the model output and ignores any interaction among model parameters, while the global SA provides information on how the variation of model output is produced by the variation of model input parameters individually and globally through the interactions with each other [6], [26], [59].

Due to the intrinsic difficulty of local SA in analyzing the variation of model output induced by the interactions among model input parameters, global SA has been widely adopted in recent research works. The Fourier amplitude sensitivity test (FAST) introduced in the 1970s [13]–[15], [61] was, at the time, one of the most elegant methods of global SA, with the core feature of exploring the input parameters in a multidimensional space by a suitably defined search curve. The FAST method efficiently computes the “main effect,” which stands for the contribution of each input parameter to the variation in the output. In 1993, Sobol [64] published a sensitivity measure, which was superior to FAST in computing the higher interaction terms [9], [11], [20]. The superior feature of FAST compared to Sobol’s method is that FAST is computationally more efficient [60]. In 1999, Saltelli [59] developed a method called EFAST, which combined the better efficiency of FAST with the capacity of Sobol’s method to compute the total effects. EFAST can qualitatively rank the importance of each input parameter by calculating the contribution of each parameter to the model output variation. The model sensitivity is decomposed into the first-order index, which represents the individual effect of each model parameter in accounting for model output variation, and the total-order index, which represents the overall effect of each parameter in accounting for model output variation, including the interactions between this parameter and all the
other parameters. The results presented in this paper were obtained using the EFAST method.

The EFAST method first defines a search curve to scan the multidimensional space of model input parameters and then generates the samples of model input parameters by searching each axis of the multidimensional space at different frequencies. These samples are entered into the models to obtain the model output value. Fourier decomposition is used to compute the first-order and the total-order index. For example, supposing a model with only three input parameters, the total variance \( V \) of the model output is given by

\[
V = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}
\]

where \( V_1, V_2, \) and \( V_3 \) are the variances of model input parameters 1, 2, and 3; \( V_{12}, V_{13}, \) and \( V_{23} \) are the variances of interactions between model parameters 1 and 2, 1 and 3, and 2 and 3, respectively; and \( V_{123} \) is the variance of interactions between model parameters 1, 2, and 3. The first-order sensitivity index of the model input parameters, \( S_1, S_2, \) and \( S_3 \), can be calculated as

\[
S_1 = V_1/V \quad S_2 = V_2/V \quad S_3 = V_3/V.
\]

The second-order sensitivity indices \( S_{12}, S_{13}, \) and \( S_{23} \) are defined as

\[
S_{12} = V_{12}/V \quad S_{13} = V_{13}/V \quad S_{23} = V_{23}/V.
\]

Moreover, the total sensitivity index of each parameter, parameter 1 for example, \( ST_1 \) is obtained from

\[
ST_1 = S_1 + S_{12} + S_{13} + S_{123} = (V_1 + V_{12} + V_{13} + V_{123})/V.
\]

The variance caused by the interactions among these parameters may be calculated as

\[
I = 1 - (S_1 + S_2 + S_3).
\]

### III. SIMULATED REFLECTANCE DATA AND VEGETATION INDICES

#### A. Leaf Scale Simulation

The SA at the leaf scale is processed using the PROSPECT-5 model, with the chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, and leaf structure parameter varied, while the brown pigment content is fixed as zero for the low content of brown pigment in healthy leaves.

The value range of model input parameters was referred to the \textit{a priori} information from the LOPEX’93 database [35] and the related literature [7], [36], [50] (see Table I). A total of 2000 sets of model input parameters were generated in SimLab 3.2 (a professional tool interacted with Matlab environment to perform SA with several methods, including EFAST). The model input parameters were entered into the PROSPECT-5 model to simulate leaf reflectance and transmittance at the 400–2500-nm domain with a 1-nm interval.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorophyll a+b content (C\text{ch}) (µg cm(^{-2}))</td>
<td>10-120</td>
</tr>
<tr>
<td>Carotenoid content (C\text{cr}) (µg cm(^{-2}))</td>
<td>5-30</td>
</tr>
<tr>
<td>Brown pigment content (C\text{brn}) (µg cm(^{-2}))</td>
<td>0</td>
</tr>
<tr>
<td>Equivalent water thickness (C\text{w}) (g cm(^{-2}))</td>
<td>0.005-0.04</td>
</tr>
<tr>
<td>Dry matter content (C\text{dm}) (g cm(^{-3}))</td>
<td>0.002-0.014</td>
</tr>
<tr>
<td>Leaf structure parameter (N)</td>
<td>1-2</td>
</tr>
</tbody>
</table>

#### B. Canopy Scale Simulation

At the canopy scale, the combination of PROSPECT-5 and the canopy model 4SAIL was adopted to simulate the canopy reflectance. The value range of the main input parameters of the integrated model showed in Table II were generated based on the LOPEX’93 database [35] and some related literatures [36], [50]. The range of these parameters describing leaf properties was the same as that at the leaf scale in order to analyze the sensitivity change only caused by the difference in spatial scale. LAI, leaf angle \( \alpha \), and soil coefficient \( p_{\text{soil}} \) were allowed to vary, and \( s_t, SKYL, \) and illumination geometry (including \( \theta_s, \theta_v, \) and \( \phi_{sv} \)) were fixed, without taking account of directional variation.

A total of 5000 sets of model parameters were produced using SimLab 3.2 and Matlab. The samples were entered into the PROSPECT-5 + 4SAIL model and generated 5000 simulated canopy reflectances over the range of 400–2500 nm at a 1-nm interval.
C. Regional Scale Simulation

At the regional scale, particularly for the sparse vegetation areas, the remote sensing image has difficulty obtaining the information of pure canopy. The retrieval functions calibrated at the leaf or canopy scale may induce scaling biases in vegetation variable estimation, when they were used at the regional scale. To analyze the impact of the mixed pixel on the spectral response to vegetation variables, suppose that the pixel was composed of only two compositions, vegetation and soil with various proportions (see Fig. 1), and the pixel reflectance was the linear combination of canopy reflectance and soil reflectance through the following formula:

\[ R = \frac{a_1}{A} R_v + \frac{a_2}{A} R_s \]

where \( R \), \( R_v \), and \( R_s \) are the pixel reflectance, canopy reflectance, and soil reflectance, respectively. \( A \) is the pixel area, \( a_1 \) is the area of vegetation in the pixel, and \( a_2 \) is the area of soil in the pixel. The value range of \( a_1/A \) and \( a_2/A \) is 0–1.

To guarantee that the new variation of reflectance at the regional scale was only caused by the mixed pixel, the simulated canopy reflectances in Section III-B were used here to simulate 5000 reflectance spectra of the mixed pixel with the standard soil reflectance and the randomly obtained vegetation fraction values.

D. Various Vegetation Indices

Thirty-six VIs, traditionally used to detect vegetation characteristics, were chosen to illustrate the impact of the observation scale on estimation accuracy and find the best indices of estimating vegetation variables at different scales (see Table III). These VIs were classified into three categories according to their characteristics and functions: 16 VIs, including GI, TCARI, SR, BGI, blue red pigment index (BRI), CARI, LCI, mND705, modified SR index with index wavelength of 705nm (mND705), and Plant biochemical Index (PBI), for chlorophyll estimation, 15 VIs, including GI, SR, NDVI, MSAVI, MTVI-1, MTVI-2, OSAVI, MCARI1, MCARI2, EVI, LAIDI, RDVI, SPVI, WDRVI, and TVI, for estimating LAI estimation, and ten VIs, including DSWI, LWVI-1, LWVI-2, MSI, NDII, NDWI, RVI, SIWSI, SRWI, and WI, for water content estimation.

IV. RESULTS

A. Leaf Level SA

Fig. 2 shows the first-order sensitivity indices of chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, and leaf structure parameter and the impact of the interactions among these parameters on leaf reflectance variability. It can be seen that the variation in \( C_{ab} \) strongly affects the leaf reflectance in the visible light (VIS) region. The great contribution of \( C_{ab} \) exceeding 70% is at 540–720 nm, which includes the absorption features of chlorophyll a+b at wavelengths near 550 and 660 nm, and the red edge of vegetation near 700 nm. In the same region, the first-order sensitivity indices of \( C_{ab} \) near 660 nm are relatively low compared to the sensitivity indices at other bands, and it may be because the reflectance around 660 nm is easy to approach to saturation with the increase of chlorophyll content.

\( C_{nr} \) is another parameter influencing the reflectance in VIS, but the contribution of \( C_{nr} \) is much less than that of \( C_{ab} \). The variation in \( C_{nr} \) dominates the reflectance variability in

<table>
<thead>
<tr>
<th>Vegetation index</th>
<th>Definition</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Greenness Index (GI)</td>
<td>( R_R/S_{R=0.1} )</td>
<td>Zarco-Tejada et al. 2005</td>
</tr>
<tr>
<td>Transformed Chlorophyll Absorption in Reflectance Index (TCARI)</td>
<td>( \frac{R_{705}+R_{865}+R_{865}+R_{705}}{R_{865}+R_{705}} )</td>
<td>Ibobiande et al. 2002</td>
</tr>
<tr>
<td>Simple Ratio (SR)</td>
<td>( R_{550}/R_{810} )</td>
<td>Jordan, 1969</td>
</tr>
<tr>
<td>Blue Green Pigment Index (BGI)</td>
<td>( R_{550}/R_{705} )</td>
<td>Zarco-Tejada et al. 2005</td>
</tr>
<tr>
<td>Blue Red Pigment Index (BRI)</td>
<td>( R_{660}/R_{705} )</td>
<td>Zarco-Tejada et al. 2005</td>
</tr>
<tr>
<td>Chlorophyll Absorption Ratio Index (CARI)</td>
<td>( \left( \frac{R_{550}+R_{800}+R_{865}}{R_{550}+R_{800}+R_{865}} \right) )</td>
<td>Kim et al. 1994</td>
</tr>
<tr>
<td>Leaf Chlorophyll Index (LCI)</td>
<td>( R_{550}/R_{705} )</td>
<td>Sims and Gamoer 2002</td>
</tr>
<tr>
<td>Modified Normalized Difference Index with Index Wavelength of 705nm (mND705)</td>
<td>( R_{550}/R_{705} )</td>
<td>Sims and Gamoer 2002</td>
</tr>
<tr>
<td>Modified SR Index with Index Wavelength of 705nm (mSR705)</td>
<td>( R_{550}/R_{705} )</td>
<td>Peltohées et al. 1994</td>
</tr>
<tr>
<td>Normalized Total Pigment to Chlorophyll Index (NPCI)</td>
<td>( (R_{865}/R_{550}) )</td>
<td>Rumah Rauo et al. 2008</td>
</tr>
<tr>
<td>Plant biochemical Index (PBI)</td>
<td>( R_{550}/R_{705} )</td>
<td>Gamoer et al. 1992</td>
</tr>
<tr>
<td>Photochemical Reflectance Index (PRI)</td>
<td>( R_{550}/R_{705} )</td>
<td>Roque et al. 1973</td>
</tr>
<tr>
<td>Normalized Difference Vegetation Index (NDVI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Duangtrag et al. 1999</td>
</tr>
<tr>
<td>Modified Normalized Difference Vegetation Index (MSAVI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Gri et al. 1994</td>
</tr>
<tr>
<td>Modified Triangular Vegetation Index (MTVI-1)</td>
<td>( R_{550}/R_{705}/R_{660} )</td>
<td>Haboudane et al. 2004</td>
</tr>
<tr>
<td>Modified Triangular Vegetation Index (MTVI-2)</td>
<td>( R_{550}/R_{705}/R_{660} )</td>
<td>Haboudane et al. 2004</td>
</tr>
<tr>
<td>Optimized Soil-adjusted Vegetation Index (OSAVI)</td>
<td>( 1.5(R_{550}/R_{660}) )</td>
<td>Rondeaux et al. 1996</td>
</tr>
<tr>
<td>Modified Chlorophyll Absorption Ratio Index (MCARI)</td>
<td>( (R_{670}/R_{660}) )</td>
<td>Druey et al. 1999</td>
</tr>
<tr>
<td>Triangular Vegetation Index (TVI)</td>
<td>( (R_{705}/R_{810}) )</td>
<td>Broge and LeBlanc 2000</td>
</tr>
<tr>
<td>Modified Chlorophyll Absorption Ratio Index (MCARI1)</td>
<td>( (R_{705}/R_{810}) )</td>
<td>Haboudane et al. 2004</td>
</tr>
<tr>
<td>Modified Chlorophyll Absorption Ratio Index (MCARI2)</td>
<td>( (R_{705}/R_{810}) )</td>
<td>Haboudane et al. 2004</td>
</tr>
<tr>
<td>Enhanced vegetation Index (EVI)</td>
<td>( 2.5(R_{670}/R_{810}) )</td>
<td>Huete et al. 2002</td>
</tr>
<tr>
<td>LAI Determining Index (LADI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Deleuze et al. 2008</td>
</tr>
<tr>
<td>Renormalized Difference Vegetation Index (NDVI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Roujean et al. 1995</td>
</tr>
<tr>
<td>Spectral Polynome Vegetation Index (SPVI)</td>
<td>( (3.7R_{660}/R_{660}) )</td>
<td>Vinci et al. 2006</td>
</tr>
<tr>
<td>Wide Dynamic Range Vegetation Index (WDRVI)</td>
<td>( (R_{550}/R_{660}) )</td>
<td>Griepen 2004</td>
</tr>
<tr>
<td>Leaf Water Vegetation Index 1 (LWVI-1)</td>
<td>( (R_{550}/R_{660}) )</td>
<td>Galvao et al. 2005</td>
</tr>
<tr>
<td>Leaf Water Vegetation Index 2 (LWVI-2)</td>
<td>( (R_{550}/R_{660}) )</td>
<td>Galvao et al. 2005</td>
</tr>
<tr>
<td>Moisture Stress Index (MSI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Hunt and Rock 1989</td>
</tr>
<tr>
<td>Normalized Difference Infrared Index (NDII)</td>
<td>( R_{660}/R_{705} )</td>
<td>Lundqvist et al. 1983</td>
</tr>
<tr>
<td>Normalized Difference Water Index (NDWI)</td>
<td>( R_{550}/R_{705} )</td>
<td>Drat et al. 2003</td>
</tr>
<tr>
<td>Hyperspectral Perpendicular Vegetation Index (RPVI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Schlief et al. 2006</td>
</tr>
<tr>
<td>SWIR Water Stress Index (SWISI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Fensholt and Sandholt 2003</td>
</tr>
<tr>
<td>SR Water Index (SRWI)</td>
<td>( R_{550}/R_{660} )</td>
<td>Zarco-Tejada et al. 2003</td>
</tr>
<tr>
<td>Water Index (WI)</td>
<td>( R_{660}/R_{705} )</td>
<td>Peltohées et al. 1997</td>
</tr>
</tbody>
</table>
the spectral range of 400–550 nm, accounting for 0%–40% of the variation. The greatest contribution is exhibited in the absorption feature of carotenoid around 500 nm, and only in about 500–530 nm does the importance of $C_{w}$ in explaining the leaf reflectance variation exceed that of $C_{ab}$. In the 400–530-nm region, the interactions between these leaf variables have the greatest contribution to leaf reflectance, accounting for 3%–71% of the variation.

The variation of $C_{w}$ is expressed in the short-wave infrared (SWIR) region and NIR region, accounting for 45%–83% of the variability in leaf reflectance. At the wavelengths around 1430, 1950, and 2440 nm, which are the main water absorption features, the sensitivity indices reach the maximum value. In the VIS region, $C_{w}$ has no significant contribution to the variation of leaf reflectance.

The variation in $C_{m}$ affects the leaf reflectance in the NIR and SWIR regions, accounting for only 0%–12% of the variation. The contribution of $C_{m}$ is much less than that of $C_{w}$, which would lead to more obvious error in the inverting process.

It can be seen that the variation in $N$ impacts the leaf reflectance in the whole optical domain of 400–2500 nm. In the VIS region, the contribution of $N$ expresses 2%–27% of the variation in reflectance. In the NIR region, $N$ has the most significant influence on leaf reflectance, accounting for 30%–90% of the variation, and in 750–1300 nm, up to 80% of the variation in leaf reflectance is expressed by the variation in $N$. In the SWIR region, the contribution of $N$ accounts for 5%–44% of the variation in leaf reflectance, with the contribution trend consistent with $C_{m}$ and contrary to $C_{w}$.

**B. Canopy Level SA**

As shown in Fig. 3, $C_{ab}$ drives about 70% of the canopy reflectance variation in 540–720 nm of the VIS region, with two contribution peaks near 560 and 720 nm. The contribution valley of $C_{ab}$ around 680 nm is more apparent than that shown at the leaf scale. It is illustrated that, at the canopy scale, the reflectance around 680 nm is much easier to approach saturation at high chlorophyll content. In 400–540 nm, the importance of $C_{ab}$ is reduced, and $C_{w}$ accounts for 1%–42% of the variation in canopy reflectance. The additional parameters LAI and $\alpha$ affect the canopy reflectance in 400–540 nm, accounting for 1%–32% and 0%–24% of the variation, respectively.

In the 720–1150 nm of NIR, the canopy reflectance variability is dominated by $C_{m}$, LAI, and $\alpha$, which account for 1%–45%, 1%–36%, and 1%–15% of the variation, respectively. Compared to the leaf scale, the importance of $C_{m}$ is significantly higher, while the contribution of leaf structure parameter $N$ is much lower, with explaining only 1%–2.5% of the variation in canopy reflectance. The results prove the finding of Jacquemoud [42] that $N$ only slightly changed the canopy reflectance over the whole solar domain. At the 1150–1500-nm wavelength region of NIR, the importance of $C_{w}$ to canopy reflectance exceeds that of $C_{m}$, and it becomes the most important parameter. Moreover, the contribution of LAI is reduced to 0%–5%.

Variation in $C_{w}$ is expressed strongly in the SWIR region, with about 20%–89% of the variation in canopy reflectance explained. Compared to the leaf scale, the contribution peaks are less visible, and at around 2440 nm, the contribution peak at the leaf scale became a valley at the canopy scale. The importance of $C_{w}$ at around 1920 nm is significantly reduced from 75% to 20%. The sensitivity change of reflectance variability to $C_{w}$ at 2440 and 1920 nm is contrary to LAI. The results show that the addition of the canopy structure properties varies the contribution of leaf biochemical and biophysical parameters to the reflectance variation, and some VIs that worked well at the leaf scale would not be suitable or should be improved as they are used at the canopy scale. Compared with the results at the leaf scale, the interactions among the canopy parameters have less contribution to the canopy reflectance variation of VIS accounting for 7%–52% and larger contribution to the canopy reflectance variation of NIR and SWIR accounting for 3%–28%.

LAI is an important variable to canopy reflectance, and many researchers have proved that vegetation reflectance is strongly affected by LAI. In this paper, three scenarios were built: $0 < \text{LAI} < 3$ for sparse foliage cover, $3 < \text{LAI} < 6$ for middense foliage cover, and $6 < \text{LAI} < 9$ for dense foliage cover. Fig. 4 shows the sensitivity of canopy reflectance to the variation in biochemical and biophysical parameters in these three scenarios. It can be seen that, at sparse foliage cover, LAI is the most important parameter to the variation in the reflectance of 400–2500 nm. The dominance of LAI in...
the NIR and SWIR regions exceeds the contribution of $C_w$ and $C_m$ to the variation of canopy reflectance and makes it extremely difficult to estimate the two vegetation parameters. In the 400–530-nm region of VIS, the reflectance variance is also mainly controlled by LAI, accounting for 40%–70% of the variation, and the result makes it almost impossible to estimate $C_{ab}$ at sparse foliage cover. Due to the high sensitivity at around 560 and 710 nm, LAI might not strongly affect the estimation accuracy of chlorophyll content if these two narrow bands were used. Another phenomenon observed at sparse foliage cover is the increase of the importance of soil coefficient $p_{soil}$, accounting for 4%–34% of the variation in reflectance.

At middense and dense foliage cover, the influence of LAI on the canopy reflectance variation is reduced to 0%–14%, and the contribution of $p_{soil}$ to canopy reflectance can be neglected. $C_{ab}$, $C_m$, and $C_w$ explain the most of canopy reflectance variability in the VIS, NIR, and SWIR regions, respectively. At the 400–480-nm region of VIS, average leaf angle $a$ explains up to 90% of the variation in reflectance. Canopy reflectance variability is dominated by the interactions among vegetation parameters, accounting for 1%–55%.

C. Regional Scale SA

At the regional scale, vegetation fraction $frac$ in a pixel is the additional factor which affects the signals obtained by the remote sensor. In this condition, the vegetation parameters impacting leaf and canopy reflectance would not have the same contribution to the pixel reflectance. Fig. 5 shows the results of the first-order sensitivity indices and interactions among the vegetation parameters for two scenarios. In the first scenario, the LAI of the vegetation in the pixel is set 0–3, and in the second scenario, LAI is set 3–9. As shown in Fig. 5(a), when the LAI of the vegetation cover in the pixel is low, the reflectance variability in the VIS and SWIR regions is dominated by the variation in $frac$, accounting for about 65%. In the NIR region, the reflectance variability is dominated by vegetation fraction $frac$, leaf angle $a$, and LAI accounting for 0%–20%, 4%–14%, and 25% of the variation in pixel reflectance. At 730 and 1325 nm, the contribution of LAI is very low, while $p_{soil}$ can explain about 40% of the variation. The interactions have the greatest impact on the pixel reflectance in the NIR region. As
Fig. 6. Correlations between VIs and vegetation variables. (a) Correlations between VIs and chlorophyll a+b content. (b) Correlations between VIs and equivalent water thickness. (c) Correlations between VIs and LAI.

shown in Fig. 5(b), when the LAI of vegetation cover in the pixel is high, the variability of pixel reflectance is strongly controlled by the vegetation fraction $frac$. In these two scenarios, the results show that very little variation in pixel reflectance is caused by chlorophyll a+b content $C_{ab}$, carotenoid content $C_{ar}$, equivalent water thickness $C_{eq}$, dry matter content $C_{dm}$, and leaf structure parameter $N$.

D. Correlations Between VIs and Vegetation Variables

In order to illustrate the change of estimation accuracy at the leaf, canopy, and regional scales, we calculated 36 hyperspectral VIs from the simulated reflectance. The correlations between VIs and chlorophyll a+b content, equivalent water thickness, and LAI were calculated at different scales (see Fig. 6). It should be noted that, at the regional scale, the correlations are between VIs and the parameters averaged in a pixel.

The results show that the relationships between VIs and the focal variables heavily depend on the observation scale. VIs have lower correlations with the variables as the spatial resolution reduced. For chlorophyll content estimation [see Fig. 6(a)], at the leaf scale, TCARI, BGI, LCI, mND705, and PBI are highly correlated to chlorophyll content with the correlation coefficient ($R^2$) approaching 0.8. At the canopy scale, when LAI is less than 3, TCARI has the highest correlation with chlorophyll content, while there are high correlations between TCARI, BGI, BRI, mND705, PBI, and chlorophyll content when LAI is greater than 3. At the regional scale, the relativity between these VIs and chlorophyll content is lower than that at the leaf and canopy scales, with the maximum correlation coefficient of about 0.5. For water content estimation, all the VIs except LWVI_1 are highly correlated with equivalent water thickness at the leaf scale and canopy scale of LAI greater than 3, while at the canopy scale of LAI less than 3 and the regional scale, all the selected indices have very low correlations with the equivalent water thickness. For LAI estimation, the correlations between VIs and LAI show significant variance as the observation scale changed. Most of the VIs have high correlations with LAI when LAI is low, while at the canopy scale of LAI $>3$ and the regional scale, the correlations between all the VIs and LAI are low.

V. DISCUSSION AND CONCLUSION

The sensitivity of reflectance in the 400–2500-nm range to the variation in vegetation biochemical and biophysical parameters at the leaf, canopy, and regional scales were explored in this paper using the global SA method EFAST with the simulated database from PROSPECT-5 and 4SAIL models. The vegetation parameters include chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, leaf structure parameter, LAI, soil moisture, average leaf angle, and vegetation fraction in a pixel. The variation in view and solar geometry are not considered in this paper.

At the leaf scale, the most influential parameters are chlorophyll a+b content, leaf structure parameter, and equivalent water thickness, which dominate the most variability of reflectance in VIS, NIR, and SWIR, respectively. The sensitive wavelength region of carotenoid content is narrow, and the sensitivity is also easily disturbed by the variation in chlorophyll a+b content. Dry matter content affects the leaf reflectance variability in the NIR and SWIR regions with a little contribution. In the SWIR region, the variation in reflectance is also affected by the leaf structure parameter, and the contribution tendency of the leaf structure parameter is opposite to the equivalent water thickness, which supports the conclusion of Jacquemoud and Baret [43] that the leaf structure parameter was well correlated with leaf biomass. The results indicate that chlorophyll a+b content has no effect on the reflectance variation in the SWIR region, carotenoid content has no effect on the reflectance variation in NIR and SWIR regions, and dry matter content and equivalent water thickness have no contribution to the variation of leaf reflectance in the VIS region. The results also show that at the leaf scale, chlorophyll a+b content and equivalent water thickness can be estimated with high accuracy. However, it is
extremely difficult to inverse carotenoid content and dry matter content.

Compared to the leaf scale, the importance of the leaf structure parameter is reduced to a very low value at the canopy scale, which indicates that the leaf structure parameter is insensitive to canopy reflectance. The result is consistent with Jacquemoud and Bacour’s conclusion. The importance of chlorophyll a+b content, equivalent water thickness, dry matter content, and average leaf angle to the canopy reflectance variation is strongly correlated to LAI (see Fig. 4). For sparse foliage cover (LAI < 3), the variation in LAI is the dominant factor to reflectance variability in NIR and SWIR regions, and the sensitivity of reflectance to variation in equivalent water thickness and dry matter content is covered. The results presented here show that it is difficult to estimate equivalent water thickness and dry matter content when LAI is low. In addition, soil moisture is a relatively important factor to the canopy reflectance variability. In the VIS region, chlorophyll a+b content still has two contribution peaks to reflectance variation at around 560 and 715 nm. The result indicates that estimating chlorophyll a+b content should focus on using the data near these two bands when LAI is low. For middense and dense foliage cover (LAI > 3), the canopy reflectance is less responsive to the variation in LAI and soil moisture, and the reflectance variation is explained by one specific parameter at different wavelength regions, with chlorophyll a+b content, dry matter content, and equivalent water thickness respectively dominating the variation of reflectance in the VIS, NIR, and SWIR regions. The results indicate that the requirement for the accurate estimation of LAI is most pressing for very thick vegetation. Higher estimation accuracy of chlorophyll a+b content, water content, and dry matter content is to be expected for vegetation with medium and high LAIs than that with low LAI.

At the regional scale, it shows that the sensitivity of pixel reflectance to the variation in vegetation biochemical and biophysical parameters is very different from the sensitivity at the canopy scale because of the additional factor of vegetation fraction. The vegetation fraction in a pixel is the dominant factor. Chlorophyll a+b content, carotenoid content, equivalent water thickness, and dry matter content have no significant contribution to the variation of pixel reflectance. The sensitivity of pixel reflectance to LAI is much less when compared to that at the canopy scale. The results show that it is a great challenge to accurately estimate these biochemical and biophysical variables without any a priori knowledge.

The relationships between VIs and chlorophyll a+b content, equivalent water thickness, and LAI illustrate the change of reflectance sensitivity to vegetation biochemical and biophysical parameters at different scales. The results show that the VIs which are highly correlated with these parameters at a certain scale may have a very low correlation at another scale. For example, LCI and PBI have high correlations with chlorophyll content at the leaf scale while low correlations at the canopy scale of LAI < 3. TVI has a very low correlation with chlorophyll content, but the correlation is much higher at the canopy scale of LAI > 3.

To accurately estimate a certain vegetation variable, it is important to use the wavelength regions which are sensitive to the variable and insensitive to the other variables. The research demonstrates that, at different scale, the sensitivity of reflectance to the variation in vegetation variables and the sensitive wavelength regions are significantly different, which means that various inversion strategies should be adopted for improving the estimating precision. Inversion strategies should be chosen according to both the condition of the study area and the spatial resolution of the sensor. For the very thick forests, Landsat TM with 30-m spatial resolution could provide “canopy” scale data. In this condition, chlorophyll content maybe can be accurately estimated using VIs like TCARI, BGI, and BRI calculated from TM data. For the sparse forest, it is likely that a TM image could only provide “regional” scale data, and the estimation of chlorophyll content becomes more challenging. Information from the SA of vegetation biochemical and biophysical parameters would also help to develop new methods to estimate various vegetation parameters with higher accuracy. Furthermore, the results also highlight the importance of using a priori knowledge which is a key issue in inversion work. For example, at sparse foliage cover, LAI must be a prerequisite as a priori knowledge to accurately estimate leaf biochemical parameters. To get the variation and distribution of vegetation variables at the regional scale, acquiring vegetation fraction of each pixel is very critical.

The remote sensing data from satellites usually do not have the ability to capture the information on leaf or canopy. The methods used to estimate vegetation biochemical and biophysical variables from the satellite remote sensing data should be improved. According to the study area and the available data, multiple step inversion strategy with the help of a priori knowledge may be one way to estimate vegetation biochemical and biophysical parameters more accurately.

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Sensitivity Analysis of Vegetation Reflectance to Biochemical and Biophysical Variables at Leaf, Canopy, and Regional Scales

Yanfang Xiao, Wenji Zhao, Demin Zhou, and Huili Gong

Abstract—The objective of this paper is to investigate the sensitivity of reflectance to the variation in biochemical and biophysical variables at leaf, canopy, and regional scales using a modeling approach. The results show that, at the leaf scale, the variations in chlorophyll a+b content, the leaf structure parameter, and the water content dominate the reflectance variance in the visible light (VIS), near infrared (NIR), and short-wave infrared (SWIR) regions, respectively. At the canopy scale, the sensitivity of reflectance to variation in the leaf structure parameter is very slight. For sparse foliage cover (leaf area index (LAI) < 3), LAI is the most important variable to the canopy reflectance. As LAI increases, the sensitivity of reflectance to variation in LAI is reduced to a very low value. Moreover, chlorophyll a+b, dry matter, and water content control the variation of canopy reflectance in the VIS, NIR, and SWIR regions, respectively. At the regional scale, the sensitivity of reflectance to variation in vegetation variables is highly influenced by the mixed pixels. Thirty-six vegetation indices (VIs) are chosen in this paper to illustrate the scale dependence of the estimation accuracy of vegetation variables. The results show that the relationships between the VIs and the variables highly depend on the observation scale. For chlorophyll a+b content estimation, transformed chlorophyll absorption in reflectance index (TCARI), Blue Green pigment Index, leaf chlorophyll index (LCI), modified Normalized Difference (mND705), and Plant Biochemical Index at the leaf scale and canopy scale of LAI > 3 and TCARI at the canopy scale of LAI < 3 are highly related. The correlation between the indices and chlorophyll content in the regional scale is, however, much lower. For water content estimation, disease water stress index (DSWI), leaf water vegetation index 2 (LWVI_2), moisture stress index (MSI), normalized difference infrared index (NDII), normalized difference water index (NDWI), hyperspectral perpendicular vegetation index (RV1), SWIR water stress index (SIWSI), SR water index (SRWI), and water index (WI) are good choices at the leaf scale and canopy scale of LAI > 3, while at the canopy scale of LAI < 3 and the regional scale, the correlation between the indices and water content is very low. For LAI estimation, VIs, including the Greenness Index, simple ratio (SR), Normalized Difference VI, modified soil-adjusted vegetation index (MSAVI), modified triangular vegetation index 1 (MTVI1), modified triangular vegetation index 2 (MTVI2), optimized soil-adjusted vegetation index (OSAVI), modified chlorophyll absorption ratio index 1 (MCARI1), modified chlorophyll absorption ratio index 2 (MCARI2), Enhanced VI, LAI Determining Index, renormalized difference vegetation index (RDVI), Spectral Polygon VI, Wide Dynamic Range VI, and triangular vegetation index (TVI), have high correlation with LAI at the canopy scale of LAI < 3 while a low correlation at the canopy scale of LAI > 3 and the regional scale.

Index Terms—Extended Fourier amplitude sensitivity test (EFAST), PROSPECT + SAIL, radiative transfer, scale, sensitivity analysis (SA), vegetation index (VI).

I. INTRODUCTION

Estimating the vegetation biochemical and biophysical variables has important potential implications for many ecological, agronomic, and meteorological applications. The key variables include leaf chlorophyll content which affects photosynthetic capacity and productivity [5], [37], water content which is one of the key parameters in fire behavior models for its control on the initial probability of ignition, burning efficiency and the rate of fire propagation [10], and the leaf area index (LAI) defined as the single-sided area of green leaf area per unit ground, which governs net radiation and its expenditure, net primary production, evapotranspiration, and canopy interception [65].

Many vegetation variables show the diagnostic absorption features. For instance, leaf chlorophyll strongly affects the visible region of the reflectance spectra while LAI has a large impact on the near infrared (NIR) region. As a unique cost-effective resource, remote sensing data have been proposed as a good solution for the measurement of vegetation parameters [8]. There are two main approaches for estimating vegetation variables: the empirical–statistical approach and physically based models. The empirical–statistical approach seeks the relationship between the vegetation variable and single spectral reflectance or spectral indices. Many vegetation indices (VIs) were designed for estimating vegetation variables. For example, Blue Green pigment Index (BGI), Modified Chlorophyll Absorption in Reflectance (MCARI), Plant Biochemical Index (PBI), and Chlorophyll Absorption Ratio Index (CARI) were developed for estimating plant pigments [18], [46], [55], [72]; Enhanced VI (EVI), modified Normalized Difference (mND705), Normalized Difference VI (NDVI), and Wide Dynamic Range VI (WDRVI) were very useful for assessing
constituents (see Fig. 1). Therefore, in many cases, the pixel of remote sensing imagery is composed by multiple consequent characteristics, particularly for the open vegetation, and however, it is hard for these data to obtain the absolute homogeneity in estimating biochemical and biophysical variables. Medium resolution imaging spectrometer [2] still plays a crucial role in estimating biochemical and biophysical variables. For example, the impact of chlorophyll content on the estimation accuracy. As shown in Fig. 1, the vegetation reflectance at different scales, would be needed, which could be extremely expensive or even impossible. Consequently, in this paper, a research prospect for future works. A general conclusion summarizes the results and proposes the implications. The objective of this paper is then to investigate and quantify the sensitivity of reflectance to the variation in vegetation variables at leaf, canopy, and regional scales with a global sensitivity analysis (SA) method, the extended Fourier amplitude sensitivity test (EFAST). In this paper, leaf scale is defined as the data which can represent the leaf reflectance, canopy scale is defined as the data which can represent the canopy reflectance, and regional scale means that the obtained data are the mixed information of vegetation and other ground objects. There is no clear numerical definition for these scales because the scales are determined by both the spatial resolution of sensors and the research objects. A TM image with a 30-m resolution of a sparse forest may be dealt at the regional scale. However, this regional scale may be inaccurate for another TM image of a closed and continuous vegetation cover in which, in this case, the canopy scale would be more suitable.

This paper is organized in four sections. In Section II, the method and models are introduced, including EFAST global sensitivity, PROSPECT-5, and 4SAIL model. Section III shows the simulated database (including the value of vegetation variables and the simulated reflectance at leaf, canopy, and regional scales), and 36 published VIs. The results are presented in Section IV (the contribution of vegetation variables to the leaf, canopy, and regional reflectance and the relationship between VIs and chlorophyll a+b content, equivalent water thickness, and LAI). In Section V, a discussion addresses the main points of this study, including how the sensitivity of vegetation reflectance to vegetation variables changes, and what are the best VIs for estimating chlorophyll a+b content, equivalent water thickness, and LAI at leaf, canopy, and regional scales. A general conclusion summarizes the results and proposes the research prospect for future works.

II. METHODS AND MODELS
To quantify the contribution of vegetation variables to the variation in the reflectance data, a huge amount of ground data, including measured reflectance and vegetation variables at different scales, would be needed, which could be extremely expensive or even impossible. Consequently, in this paper, a
database with a wide range of vegetation variables incorporating the vegetation reflectance at leaf, canopy, and regional scales is simulated from models. The well-known and modified PROSPECT-5 model is used to simulate the leaf reflectance. The link between the PROSPECT-5 and 4SAIL models which describes the canopy reflectance as a function of leaf biochemistry, canopy architecture, and illumination geometry, is used to simulate the canopy reflectance. EFAST is a global sensitivity method to calculate the sensitivity of reflectance to the variation in vegetation variables. A description of the main features of these models is given in the following sections. Refer to Jacquemoud and Baret [43], Verhoef [66], and Saltelli [59] for more details.

A. PROSPECT-5 and 4SAIL Models

1) PROSPECT-5 Model: Based on the assumption that a leaf is composed of a pile of N homogeneous layers separated by N − 1 air spaces, PROSPECT pioneered to simulate the directional–hemispherical reflectance and transmittance of various green monocotyledon and dicotyledon species, as well as senescent leaves over the solar spectrum of 400–2500 nm [43]. The PROSPECT-5 model is a robust version of PROSPECT, which is modified to include carotenoids and brown pigments.

The input parameters of the PROSPECT-5 model include leaf structure parameter N, chlorophyll a+b content $C_{ab}$ (μg·cm$^{-2}$), carotenoid content $C_{ar}$ (μg·cm$^{-2}$), brown pigment content $C_{brown}$ (g·cm$^{-2}$), equivalent water thickness $C_{w}$ (g·cm$^{-2}$), and dry matter content $C_{m}$ (g·cm$^{-2}$). The model simulates the leaf reflectance and transmittance spectra of 400–2500 nm with 1-nm resolution, using the specific absorption coefficient $K$ which depends on wavelength but not botanical species. The total absorption coefficient k can be calculated as

$$k(\lambda) = k_{e}(\lambda) + \frac{C_{ab}}{N} K_{ab}(\lambda) + \frac{C_{ar}}{N} K_{ar}(\lambda) + \frac{C_{brown}}{N} K_{brown}(\lambda) + \frac{C_{w}}{N} K_{w}(\lambda) + \frac{C_{m}}{N} K_{m}(\lambda)$$

where $\lambda$ is the wavelength, $k_{e}(\lambda)$ is the absorption of an albinos leaf, and $K_{ab}, K_{ar}, K_{brown}, K_{w}, K_{m}$ are the absorption coefficients of chlorophyll a+b, carotenoid, brown pigment, water, and dry matter, respectively. They were determined by Feret et al. [25] using four data sets: leaf optical properties experiment (LOPEX) measured in 1993, center for advanced land management information technologies from 1995/1996, ANGERS measured in 2003, and HAWAII from 2007.

2) 4SAIL Model: The 4SAIL canopy reflectance model used in this paper is a numerically robust and speed-optimized version of SAIL. In the SAIL model, the canopy layer is assumed to be homogeneous, horizontal, and infinitely extend with small and flat leaves as the only canopy components. Essentially, the SAIL model is a four-flux theory, with four differential equations and nine coefficients which are given by

$$\frac{dE_s}{dz} = k(\theta_t)E_s$$
$$\frac{dE_-}{dz} = -\alpha(\theta_t)E_+ + \alpha(\theta_t)E_+ - s(\theta_t)E_s$$
$$\frac{dE_+}{dz} = -\alpha(\theta_t)E_- + \alpha(\theta_t)E_- + s(\theta_t)E_s$$
$$\frac{dE_o}{dz} = w(\theta_t)E_s + v(\theta_t)E_- + u(\theta_t)E_+ - K(\theta_t)E_o$$

where $E_s$ is a direct solar flux, $E_+$ is a diffuse upward flux, $E_-$ is a diffuse downward flux, and $E_o$ is a radiance flux in the direction of observation. $\theta_t$ stands for the leaf inclination angle, $k$ and $K$ for the extinction coefficient for $E_s$ and $E_o$, respectively, and $\alpha$ for the attenuation coefficient for diffuse fluxes $E_+$ and $E_-$. $\sigma$ respectively describes the backscatter and forward scattering of the $E_+$ and $E_-$. $s$ and $s'$ describe the scattering from $E_s$, $E_+$, and $E_-$. $w$, $v$, and $u$ describe the scattering from $E_s$, $E_+$, and $E_-$. $o$, and $E_-$.

To simulate canopy reflectance spectra in the optical domain of 400–2500 nm with 1-nm resolution, the 4SAIL model requires the leaf area index (LAI), mean leaf inclination angle ($\alpha$), hot spot parameter ($s_l$), soil reflectance assumed Lamber-Donor ($\rho_s$), ratio of diffuse to total incident radiation (SKYL), zenith angle of solar ($\theta_s$) and viewing ($\theta_v$), relative azimuth angle ($\phi_\infty$), and leaf reflectance ($\rho_l$) and transmittance ($\tau_l$) which can be obtained from the PROSPECT-5 leaf reflectance model. The canopy reflectance $\rho(\lambda)$ can be expressed as

$$\rho(\lambda) = SAIL[LAI, \alpha, \rho_l(\lambda), \tau_l(\lambda), \rho_s(\lambda), \theta_s, \theta_v, \phi_\infty, s_l, SKYL]$$.  

B. EFAST Method

Two different schools of SA have been implemented, local SA and global SA. The difference between these two SA schools is that the local SA provides information on how variation in each individual parameter accounts for variation in the model output and ignores any interaction among model parameters, while the global SA provides information on how the variation of model output is produced by the variation of model input parameters individually and globally through the interactions with each other [6], [26], [59].

Due to the intrinsic difficulty of local SA in analyzing the variation of model output induced by the interactions among model input parameters, global SA has been widely adopted in recent research works. The Fourier amplitude sensitivity test (FAST) introduced in the 1970s [13]–[15], [61] was, at the time, one of the most elegant methods of global SA, with the core feature of exploring the input parameters in a multidimensional space by a suitably defined search curve. The FAST method efficiently computes the “main effect,” which stands for the contribution of each input parameter to the variation in the output. In 1993, Sobol [64] published a sensitivity measure, which was superior to FAST in computing the higher interaction terms [9], [11], [20]. The superior feature of FAST compared to Sobol’s method is that FAST is computationally more efficient [60]. In 1999, Saltelli [59] developed a method called EFAST, which combined the better efficiency of FAST with the capacity of Sobol’s method to compute the total effects. EFAST can qualitatively rank the importance of each input parameter by calculating the contribution of each parameter to the model output variation. The model sensitivity is decomposed into the first-order index, which represents the individual effect of each model parameter in accounting for model output variation, and the total-order index, which represents the overall effect of each parameter in accounting for model output variation, including the interactions between this parameter and all the
other parameters. The results presented in this paper were obtained using the EFAST method.

The EFAST method first defines a search curve to scan the multidimensional space of model input parameters and then generates the samples of model input parameters by searching each axis of the multidimensional space at different frequencies. These samples are entered into the models to obtain the model output value. Fourier decomposition is used to compute the first-order and the total-order index. For example, supposing a model with only three input parameters, the total variance $V$ of the model output is given by

$$V = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}$$

where $V_1$, $V_2$, and $V_3$ are the variances of model input parameters 1, 2, and 3; $V_{12}$, $V_{13}$, and $V_{23}$ are the variances of interactions between model parameters 1 and 2, 1 and 3, and 2 and 3, respectively; and $V_{123}$ is the variance of interactions between model parameters 1, 2, and 3. The first-order sensitivity index of the model input parameters, $S_1$, $S_2$, and $S_3$, can be calculated from

$$S_1 = V_1 / V \quad S_2 = V_2 / V \quad S_3 = V_3 / V.$$ 

The second-order sensitivity indices $S_{12}$, $S_{13}$, and $S_{23}$ are defined as

$$S_{12} = V_{12} / V \quad S_{13} = V_{13} / V \quad S_{23} = V_{23} / V.$$ 

Moreover, the total sensitivity index of each parameter, parameter 1 for example, $ST_1$ is obtained from

$$ST_1 = S_1 + S_{12} + S_{13} + S_{123} = (V_1 + V_{12} + V_{13} + V_{123}) / V.$$ 

The variance caused by the interactions among these parameters may be calculated as

$$I = 1 - (S_1 + S_2 + S_3).$$

### III. SIMULATED REFLECTANCE DATA AND VEGETATION INDICES

#### A. Leaf Scale Simulation

The SA at the leaf scale is processed using the PROSPECT-5 model, with the chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, and leaf structure parameter varied, while the brown pigment content is fixed as zero for the low content of brown pigment in healthy leaves.

The value range of model input parameters was referred to the *a priori* information from the LOPEX’93 database [35] and the related literature [7], [36], [50] (see Table I). A total of 2000 sets of model input parameters were generated in SimLab 3.2 (a professional tool interacted with Matlab environment to perform SA with several methods, including EFAST). The model input parameters were entered into the PROSPECT-5 model to simulate leaf reflectance and transmittance at the 400–2500-nm domain with a 1-nm interval.

#### B. Canopy Scale Simulation

At the canopy scale, the combination of PROSPECT-5 and the canopy model 4SAIL was adopted to simulate the canopy reflectance. The value range of the main input parameters of the integrated model showed in Table II were generated based on the LOPEX’93 database [35] and some related literatures [36], [50]. The range of these parameters describing leaf properties was the same as that at the leaf scale in order to analyze the sensitivity change only caused by the difference in spatial scale. LAI, leaf angle $\alpha$, and soil coefficient $p_{soil}$ were allowed to vary, and $s_l$, $SKYL$, and illumination geometry (including $\theta_s$, $\theta_v$, and $\phi_{sv}$) were fixed, without taking account of directional variation.

A total of 5000 sets of model parameters were produced using SimLab 3.2 and Matlab. The samples were entered into the PROSPECT-5 + 4SAIL model and generated 5000 simulated canopy reflectances over the range of 400–2500 nm at a 1-nm interval.

<table>
<thead>
<tr>
<th>TABLE I</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>VALUE RANGE OF PROSPECT-5 INPUT PARAMETERS FOR THE SA AT LEAF SCALE</strong></td>
</tr>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>Chlorophyll a+b content ($C_{ab}$) (µg. cm$^{-2}$)</td>
</tr>
<tr>
<td>Carotenoid content ($C_c$) (µg. cm$^{-2}$)</td>
</tr>
<tr>
<td>Brown pigment content ($C_{brown}$) (µg. cm$^{-2}$)</td>
</tr>
<tr>
<td>Equivalent water thickness ($C_w$) (g. cm$^{-2}$)</td>
</tr>
<tr>
<td>Dry matter content ($C_m$) (g. cm$^{-2}$)</td>
</tr>
<tr>
<td>Leaf structure parameter ($N$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TABLE II</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>VALUE RANGE OF PROSPECT-5 + 4SAIL MODEL INPUT PARAMETERS FOR THE SA AT CANOPY SCALE</strong></td>
</tr>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>Leaf area index (LAI)</td>
</tr>
<tr>
<td>Average leaf angle ($\alpha$) (°)</td>
</tr>
<tr>
<td>Soil coefficient ($p_{soil}$)</td>
</tr>
<tr>
<td>Hot spot parameter ($s_l$)</td>
</tr>
<tr>
<td>Ratio of diffuse to total incident radiation ($SKYL$)</td>
</tr>
<tr>
<td>illumination geometry</td>
</tr>
<tr>
<td>solar zenith angle ($\theta_s$) (°)</td>
</tr>
<tr>
<td>viewing zenith angle ($\theta_v$) (°)</td>
</tr>
<tr>
<td>relative azimuth angle ($\phi_{sv}$) (°)</td>
</tr>
</tbody>
</table>
C. Regional Scale Simulation

At the regional scale, particularly for the sparse vegetation areas, the remote sensing image has difficulty obtaining the information of pure canopy. The retrieval functions calibrated at the leaf or canopy scale may induce scaling biases in vegetation variable estimation, when they were used at the regional scale. To analyze the impact of the mixed pixel on the spectral response to vegetation variables, suppose that the pixel was composed of only two compositions, vegetation and soil with various proportions (see Fig. 1), and the pixel reflectance was the linear combination of canopy reflectance and soil reflectance through the following formula:

\[ R = \frac{a_1}{A} R_v + \frac{a_2}{A} R_s \]

where \( R, R_v, \) and \( R_s \) are the pixel reflectance, canopy reflectance, and soil reflectance, respectively. \( A \) is the pixel area, \( a_1 \) is the area of vegetation in the pixel, and \( a_2 \) is the area of soil in the pixel. The value range of \( a_1 / A \) and \( a_2 / A \) is 0–1.

To guarantee that the new variation of reflectance at the regional scale was only caused by the mixed pixel, the simulated canopy reflectances in Section III-B were used here to simulate 5000 reflectance spectra of the mixed pixel with the standard soil reflectance and the randomly obtained vegetation fraction values.

D. Various Vegetation Indices

Thirty-six VIs, traditionally used to detect vegetation characteristics, were chosen to illustrate the impact of the observation scale on estimation accuracy and find the best indices of estimating vegetation variables at different scales (see Table III). These VIs were classified into three categories according to their characteristics and functions: 16 VIs, including GI, TCARI, SR, BGI, blue red pigment index (BRI), CARI, LCI, mND705, modified SR index with index wavelength of 705 nm (mSR705), Normalized Total Pigment to Chlorophyll Index (NPCI), Plant biochemical Index (PBI), Photochemical Reflectance Index (PRI), Normalized Difference Vegetation Index (NDVI), Modified Normalized Difference Vegetation Index with Index Wavelength of 705 nm (mND705), Modified SR Index with Index Wavelength of 705 nm (mSR705), and the randomly obtained vegetation fraction values.

IV. Results

A. Leaf Level SA

Fig. 2 shows the first-order sensitivity indices of chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, and leaf structure parameter and the impact of the interactions among these parameters on leaf reflectance variability. It can be seen that the variation in \( C_{ab} \) strongly affects the leaf reflectance in the visible light (VIS) region. The great contribution of \( C_{ab} \) exceeding 70% is at 540–720 nm, which includes the absorption features of chlorophyll a+b at wavelengths near 550 and 660 nm, and the red edge of vegetation near 700 nm. In the same region, the first-order sensitivity indices of \( C_{ab} \) near 660 nm are relatively low compared to the sensitivity indices at other bands, and it may be because the reflectance around 660 nm is easy to approach to saturation with the increase of chlorophyll content.

\( C_{at} \) is another parameter influencing the reflectance in VIS, but the contribution of \( C_{at} \) is much less than that of \( C_{ab} \). The variation in \( C_{at} \) dominates the reflectance variability in
the spectral range of 400–550 nm, accounting for 0%–40% of the variation. The greatest contribution is exhibited in the absorption feature of carotenoid around 500 nm, and only in about 500–530 nm does the importance of $C_{aw}$ in explaining the leaf reflectance variation exceed that of $C_{ab}$. In the 400–540 nm region, the interactions between these leaf variables have the greatest contribution to leaf reflectance, accounting for 3%–71% of the variation.

The variation of $C_{aw}$ is expressed in the short-wave infrared (SWIR) region and NIR region, accounting for 45%–83% of the variability in leaf reflectance. At the wavelengths around 1430, 1950, and 2440 nm, which are the main water absorption features, the sensitivity indices reach the maximum value. In the VIS region, $C_{aw}$ has no significant contribution to the variation of leaf reflectance.

The variation in $C_{m}$ affects the leaf reflectance in the NIR and SWIR regions, accounting for only 0%–12% of the variation. The contribution of $C_{m}$ is much less than that of $C_{aw}$, which would lead to more obvious error in the inverting process.

It can be seen that the variation in $N$ impacts the leaf reflectance in the whole optical domain of 400–2500 nm. In the VIS region, the contribution of $N$ expresses 2%–27% of the variation in reflectance. In the NIR region, $N$ has the most significant influence on leaf reflectance, accounting for 30%–90% of the variation, and in 750–1300 nm, up to 80% of the variation in leaf reflectance is expressed by the variation in $N$. In the SWIR region, the contribution of $N$ accounts for 5%–44% of the variation in leaf reflectance, with the contribution trend consistent with $C_{m}$ and contrary to $C_{aw}$.

### B. Canopy Level SA

As shown in Fig. 3, $C_{ab}$ drives about 70% of the canopy reflectance variation in 540–720 nm of the VIS region, with two contribution peaks near 560 and 720 nm. The contribution valley of $C_{ab}$ around 680 nm is more apparent than that shown at the leaf scale. It is illustrated that, at the canopy scale, the reflectance around 680 nm is much easier to approach saturation at high chlorophyll content. In 400–540 nm, the importance of $C_{ab}$ is reduced, and $C_{aw}$ accounts for 1%–42% of the variation in canopy reflectance. The additional parameters LAI and $a$ affect the canopy reflectance in 400–540 nm, accounting for 1%–32% and 0%–24% of the variation, respectively.

In the 720–1150 nm of NIR, the canopy reflectance variability is dominated by $C_{m}$, LAI, and $a$, which account for 1%–45%, 1%–36%, and 1%–15% of the variation, respectively. Compared to the leaf scale, the importance of $C_{m}$ is significantly higher, while the contribution of leaf structure parameter $N$ is much lower, with explaining only 1%–2.5% of the variation in canopy reflectance. The results prove the finding of Jacquemoud [42] that $N$ only slightly changed the canopy reflectance over the whole solar domain. At the 1150–1500-nm wavelength region of NIR, the importance of $C_{aw}$ to canopy reflectance exceeds that of $C_{m}$, and it becomes the most important parameter. Moreover, the contribution of LAI is reduced to 0%–5%.

Variation in $C_{aw}$ is expressed strongly in the SWIR region, with about 20%–89% of the variation in canopy reflectance explained. Compared to the leaf scale, the contribution peaks are less visible, and at around 2440 nm, the contribution peak at the leaf scale became a valley at the canopy scale. The importance of $C_{aw}$ at around 1920 nm is significantly reduced from 75% to 20%. The sensitivity change of reflectance variability to $C_{aw}$ at 2440 and 1920 nm is contrary to LAI. The results show that the addition of the canopy structure properties varies the contribution of leaf biochemical and biophysical parameters to the reflectance variation, and some VIs that worked well at the leaf scale would not be suitable or should be improved as they are used at the canopy scale. Compared with the results at the leaf scale, the interactions among the canopy parameters have less contribution to the canopy reflectance variation of VIS accounting for 7%–52% and larger contribution to the canopy reflectance variation of NIR and SWIR accounting for 3%–28%.

LAI is an important variable to canopy reflectance, and many researchers have proved that vegetation reflectance is strongly affected by LAI. In this paper, three scenarios were built: 0 < LAI < 3 for sparse foliage cover, 3 < LAI < 6 for middense foliage cover, and 6 < LAI < 9 for dense foliage cover. Fig. 4 shows the sensitivity of canopy reflectance to the variation in biochemical and biophysical parameters in these three scenarios. It can be seen that, at sparse foliage cover, LAI is the most important parameter to the variation in the reflectance of 400–2500 nm. The dominance of LAI in
the NIR and SWIR regions exceeds the contribution of $C_{w}$ and $C_{m}$ to the variation of canopy reflectance and makes it extremely difficult to estimate the two vegetation parameters. In the 400–530-nm region of VIS, the reflectance variance is also mainly controlled by LAI, accounting for 40%–70% of the variation, and the result makes it almost impossible to estimate $C_{ar}$ at sparse foliage cover. Due to the high sensitivity at around 560 and 710 nm, LAI might not strongly affect the estimation accuracy of chlorophyll content if these two narrow bands were used. Another phenomenon observed at sparse foliage cover is the increase of the importance of soil coefficient $p_{soil}$, accounting for 4%–34% of the variation in reflectance.

At middense and dense foliage cover, the influence of LAI on the canopy reflectance variation is reduced to 0%–14%, and

the contribution of $p_{soil}$ to canopy reflectance can be neglected. $C_{ab}$, $C_{m}$, and $C_{w}$ explain the most of canopy reflectance variability in the VIS, NIR, and SWIR regions, respectively. At the 400–480-nm region of VIS, average leaf angle $a$ explains up to 90% of the variation in reflectance. Canopy reflectance variability is dominated by the interactions among vegetation parameters, accounting for 1%–55%.

### C. Regional Scale SA

At the regional scale, vegetation fraction $frac$ in a pixel is the additional factor which affects the signals obtained by the remote sensor. In this condition, the vegetation parameters impacting leaf and canopy reflectance would not have the same contribution to the pixel reflectance. Fig. 5 shows the results of the first-order sensitivity indices and interactions among the vegetation parameters for two scenarios. In the first scenario, the LAI of the vegetation in the pixel is set 0–3, and in the second scenario, LAI is set 3–9. As shown in Fig. 5(a), when the LAI of the vegetation cover in the pixel is low, the reflectance variability in the VIS and SWIR regions is dominated by the variation in $frac$, accounting for about 65%. In the NIR region, the reflectance variability is dominated by vegetation fraction $frac$, leaf angle $a$, and LAI accounting for 0%–20%, 4%–14%, and 25% of the variation in pixel reflectance. At 730 and 1325 nm, the contribution of LAI is very low, while $p_{soil}$ can explain about 40% of the variation. The interactions have the greatest impact on the pixel reflectance in the NIR region. As
Fig. 6. Correlations between VIs and vegetation variables. (a) Correlations between VIs and chlorophyll a+b content. (b) Correlations between VIs and equivalent water thickness. (c) Correlations between VIs and LAI.

shown in Fig. 5(b), when the LAI of vegetation cover in the pixel is high, the variability of pixel reflectance is strongly controlled by the vegetation fraction $\text{frac}$. In these two scenarios, the results show that very little variation in pixel reflectance is caused by chlorophyll a+b content $C_{\text{ab}}$, carotenoid content $C_{\text{ar}}$, equivalent water thickness $C_{\text{w}}$, dry matter content $C_{\text{m}}$, and leaf structure parameter $N$.

D. Correlations Between VIs and Vegetation Variables

In order to illustrate the change of estimation accuracy at the leaf, canopy, and regional scales, we calculated 36 hyperspectral VIs from the simulated reflectance. The correlations between VIs and chlorophyll a+b content, equivalent water thickness, and LAI were calculated at different scales (see Fig. 6). It should be noted that, at the regional scale, the correlations are between VIs and the parameters averaged in a pixel. The results show that the relationships between VIs and the focal variables heavily depend on the observation scale. VIs have lower correlations with the variables as the spatial resolution reduced. For chlorophyll content estimation [see Fig. 6(a)], at the leaf scale, TCARI, BGI, LCI, mND705, and PBI are highly correlated to chlorophyll content with the correlation coefficient ($R^2$) approaching 0.8. At the canopy scale, when LAI is less than 3, TCARI has the highest correlation with chlorophyll content, while there are high correlations between TCARI, BGI, BRI, mND705, PBI, and chlorophyll content when LAI is greater than 3. At the regional scale, the relativity between these VIs and chlorophyll content is lower than that at the leaf and canopy scales, with the maximum correlation coefficient of about 0.5. For water content estimation, all the VIs except LWVI_1 are highly correlated with equivalent water thickness at the leaf scale and canopy scale of LAI greater than 3, while at the canopy scale of LAI less than 3 and the regional scale, all the selected indices have very low correlations with the equivalent water thickness. For LAI estimation, the correlations between VIs and LAI show significant variance as the observation scale changed. Most of the VIs have high correlations with LAI when LAI is low, while at the canopy scale of LAI $> 3$ and the regional scale, the correlations between all the VIs and LAI are low.

V. DISCUSSION AND CONCLUSION

The sensitivity of reflectance in the 400–2500-nm range to the variation in vegetation biochemical and biophysical parameters at the leaf, canopy, and regional scales were explored in this paper using the global SA method EFAST with the simulated database from PROSPECT-5 and 4SAIL models. The vegetation parameters include chlorophyll a+b content, carotenoid content, equivalent water thickness, dry matter content, leaf structure parameter, LAI, soil moisture, average leaf angle, and vegetation fraction in a pixel. The variation in view and solar geometry are not considered in this paper.

At the leaf scale, the most influential parameters are chlorophyll a+b content, leaf structure parameter, and equivalent water thickness, which dominate the most variability of reflectance in VIS, NIR, and SWIR, respectively. The sensitive wavelength region of carotenoid content is narrow, and the sensitivity is also easily disturbed by the variation in chlorophyll a+b content. Dry matter content affects the leaf reflectance variability in the NIR and SWIR regions with a little contribution. In the SWIR region, the variation in reflectance is also affected by the leaf structure parameter, and the contribution tendency of the leaf structure parameter is opposite to the equivalent water thickness, which supports the conclusion of Jacquemoud and Baret [43] that the leaf structure parameter was well correlated with leaf biomass. The results indicate that chlorophyll a+b content has no effect on the reflectance variation in the SWIR region, carotenoid content has no effect on the reflectance variation in NIR and SWIR regions, and dry matter content and equivalent water thickness have no contribution to the variation of leaf reflectance in the VIS region. The results also show that at the leaf scale, chlorophyll a+b content and equivalent water thickness can be estimated with high accuracy. However, it is
extremely difficult to inverse carotenoid content and dry matter content. Compared to the leaf scale, the importance of the leaf structure parameter is reduced to a very low value at the canopy scale, which indicates that the leaf structure parameter is insensitive to canopy reflectance. The result is consistent with Jacquemoud and Bacour’s conclusion. The importance of chlorophyll a+b content, equivalent water thickness, dry matter content, and average leaf angle to the canopy reflectance variation is strongly correlated to LAI (see Fig. 4). For sparse foliage cover (LAI < 3), the variation in LAI is the dominant factor to reflectance variability in NIR and SWIR regions, and the sensitivity of reflectance to variation in equivalent water thickness and dry matter content is covered. The results presented here show that it is difficult to estimate equivalent water thickness and dry matter content when LAI is low. In addition, soil moisture is a relatively important factor to the canopy reflectance variability. In the VIS region, chlorophyll a+b content still has two contribution peaks to reflectance variation at around 560 and 715 nm. The result indicates that estimating chlorophyll a+b content should focus on using the data near these two bands when LAI is low. For middense and dense foliage cover (LAI > 3), the canopy reflectance is less responsive to the variation in LAI and soil moisture, and the reflectance variation is explained by one specific parameter at different wavelength regions, with chlorophyll a+b content, dry matter content, and equivalent water thickness respectively dominating the variation of reflectance in the VIS, NIR, and SWIR regions. The results indicate that the requirement for the accurate estimation of LAI is most pressing for very thick vegetation. Higher estimation accuracy of chlorophyll a+b content, water content, and dry matter content is to be expected for vegetation with medium and high LAIs than that with low LAI.

At the regional scale, it shows that the sensitivity of pixel reflectance to the variation in vegetation biochemical and biophysical parameters is very different from the sensitivity at the canopy scale because of the additional factor of vegetation fraction. The vegetation fraction in a pixel is the dominant factor. Chlorophyll a+b content, carotenoid content, equivalent water thickness, and dry matter content have no significant contribution to the variation of pixel reflectance. The sensitivity of pixel reflectance to LAI is much less when compared to that at the canopy scale. The results show that it is a great challenge to accurately estimate these biochemical and biophysical variables without any a priori knowledge.

The relationships between VIs and chlorophyll a+b content, equivalent water thickness, and LAI illustrate the change of reflectance sensitivity to vegetation biochemical and biophysical parameters at different scales. The results show that the VIs which are highly correlated with these parameters at a certain scale may have a very low correlation at another scale. For example, LCI and PBI have high correlations with chlorophyll content at the leaf scale while low correlations at the canopy scale of LAI < 3. TVI has a very low correlation with chlorophyll content, but the correlation is much higher at the canopy scale of LAI > 3.

To accurately estimate a certain vegetation variable, it is important to use the wavelength regions which are sensitive to the variable and insensitive to the other variables. The research demonstrates that, at different scale, the sensitivity of reflectance to the variation in vegetation variables and the sensitive wavelength regions are significantly different, which means that various inversion strategies should be adopted for improving the estimating precision. Inversion strategies should be chosen according to both the condition of the study area and the spatial resolution of the sensor. For the very thick forests, Landsat TM with 30-m spatial resolution could provide “canopy” scale data. In this condition, chlorophyll content maybe can be accurately estimated using VIs like TCARI, BGI, and BRI calculated from TM data. For the sparse forest, it is likely that a TM image could only provide “regional” scale data, and the estimation of chlorophyll content becomes more challenging. Information from the SA of vegetation biochemical and biophysical parameters would also help to develop new methods to estimate various vegetation parameters with higher accuracy. Furthermore, the results also highlight the importance of using a priori knowledge which is a key issue in inversion work. For example, at sparse foliage cover, LAI must be a prerequisite as a priori knowledge to accurately estimate leaf biochemical parameters. To get the variation and distribution of vegetation variables at the regional scale, acquiring vegetation fraction of each pixel is very critical.

The remote sensing data from satellites usually do not have the ability to capture the information on leaf or canopy. The methods used to estimate vegetation biochemical and biophysical variables from the satellite remote sensing data should be improved. According to the study area and the available data, multiple step inversion strategy with the help of a priori knowledge may be one way to estimate vegetation biochemical and biophysical parameters more accurately.

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