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A physically-based model for retrieving foliar biochemistry and leaf orientation using close-range imaging spectroscopy

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Abstract

Radiative transfer models have long been used to characterize the foliar content at the leaf and canopy levels. However, they still do not apply well to close-range imaging spectroscopy, especially because directional effects are usually not taken into account. For this purpose, we introduce a physical approach to describe and simulate the variation in leaf reflectance observed at this scale. Two parameters are thus introduced to represent (1) specular reflection at the leaf surface and (2) local leaf orientation. The model, called COSINE (CLOse-range Spectral ImagiNg of lEaves), can be coupled with a directional-hemispherical reflectance model of leaf optical properties to relate

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the measured reflectance to the foliar content. In this study, we show that, when combining COSINE with the PROSPECT model, the overall PROCOSINE model allows for a robust sub-millimeter retrieval of foliar content based on numerical inversion and pseudo bidirectional reflectance factor hyperspectral measurements.

The relevance of the added parameters is first shown through a sensitivity analysis performed in the visible and near-infrared (VNIR) and shortwave infrared (SWIR) ranges. PROCOSINE is then validated based on VNIR and SWIR hyperspectral images of various leaf species exhibiting different surface properties. Introducing these two parameters within the inversion allows us to obtain accurate maps of PROSPECT parameters, e.g., the chlorophyll content in the VNIR range, and the equivalent water thickness and leaf mass per area in the SWIR range. Through the estimation of light incident angle, the PROCOSINE inversion also provides information on leaf orientation, which is a critical parameter in vegetation remote sensing.

Keywords: close-range, COSINE, hyperspectral, imaging spectroscopy, leaf optical properties, pigment retrieval, PROCOSINE, PROSPECT, radiative transfer, vegetation

1. Introduction

Due to the strong interactions occurring between vegetation and the incoming optical radiation through absorption and scattering processes, hyperspectral remote sensing from satellites and aircrafts provides critical information to assess the spatial and temporal variabilities of vegetation status from local to global scales. This has led to a number of agricultural, envi-

7 ronmental and ecological applications such as the retrieval of leaf pigments
8 (Zarco-Tejada et al., 2004; Ustin et al., 2009), the early detection of leaf
9 diseases (Mahlein et al., 2013) or the mapping of forest biodiversity (Féret
10 & Asner, 2014). As hyperspectral cameras are now becoming more afford-
11 able, close-range remote sensing data are also increasingly available to the
12 scientific community. Compared with air- and satellite-borne data, they gen-
13 erally offer a sub-milliter or millimeter spatial resolution, and they can be
14 acquired at a higher temporal frequency, which is particularly interesting for
15 precision agriculture. For example, these data can be used to identify plant
16 pigments (Blackburn, 2007), freezing stress (Nicotra et al., 2003) or leaf dis-
17 eases (Mahlein et al., 2013), each of which is of tremendous importance to
18 follow up the plant physiological status. These images are generally processed
19 by applying statistically-based methods to estimate various leaf biochemical
20 properties (Nicotra et al., 2003; Vigneau et al., 2011; Ji-Yong et al., 2012; Jay
21 et al., 2014). However, at this scale, a proper physical interpretation based
22 on radiative transfer modeling is needed to describe the interactions between
23 light and vegetation, especially for a spatially- and temporally-resolved quan-
24 tification of pigments (Blackburn, 2007).

25

26 Vegetation radiative transfer models are physically-based and simulate
27 light propagation within leaves and/or canopies, e.g., as a function of leaf
28 biochemical constituents, leaf anatomy or canopy structure. Whenever pos-
29 sible, model inversion allows for the retrieval of the variables of interest,
30 generally using iterative optimization, look-up tables, statistical methods or
31 machine learning algorithms.

32 At the leaf level, these models range from simple plate models, to ray-tracing,
33 radiosity and stochastic models that are computationally more difficult to in-
34 vert (Dorigo et al., 2007). For instance, PROSPECT (Jacquemoud & Baret,
35 1990) is based on the generalized plate model, and is particularly well suited
36 to estimate leaf biochemical constituents (e.g., chlorophyll content, water
37 content and leaf mass per area) based on spectral measurements in the op-
38 tical domain. The main reasons for the popularity of PROSPECT are its
39 accuracy, its computational efficiency (resulting in fast iterative model inver-
40 sion) and free distribution.

41 At the canopy level, various approaches of different complexities have been
42 developed for radiative transfer modeling, e.g., turbid medium approaches
43 (Verhoef, 1984), geometrical approaches (Chen & Leblanc, 1997) or the com-
44 bination of both (Gastellu-Etchegorry et al., 1996). Most of these models al-
45 low the canopy reflectance to be modeled as a function of parameters related
46 to canopy structure (such as leaf area index or leaf inclination distribution
47 function), leaf optical properties and sun-sensor geometry.

48

49 However, leaf and canopy radiative transfer models do not apply well
50 to close-range imaging spectroscopy. For example, at the leaf level, the
51 directional-hemispherical reflectance and transmittance simulated by PROSPECT
52 (Jacquemoud & Baret, 1990) are usually measured with an integrating sphere,
53 whose implementation is difficult (if not impossible) for every single pixel of
54 hyperspectral images. As a result, PROSPECT cannot be inverted based on
55 directional reflectance data as retrieved by a close-range hyperspectral cam-
56 era, unless it is assumed that leaves are Lambertian (Buddenbaum & Hill,

2015) and in fully horizontal position, which is an unrealistic hypothesis. Indeed, in most cases, leaf reflectance exhibits some anisotropy (Bousquet et al., 2005; Comar et al., 2012) and thus varies with respect to illumination and viewing angles. Furthermore, variation in leaf orientation prevent from achieving a proper reflectance correction for every pixel, because the reference surface used for reflectance correction is generally not submitted to the same local illumination conditions than leaf material.

At the canopy level, most radiative transfer models have to be applied to mixed pixels (containing both soil and leaf materials), for which effects of leaf composition, canopy structure, soil properties and viewing/illumination angles are integrated into a single spectrum. Canopy models are thus well suited for ground-based spectroradiometric measurements, as well as for air- and satellite-borne hyperspectral measurements, all of them being usually characterized by a spatial resolution coarser than one meter (Zarco-Tejada et al., 2003; Colombo et al., 2008; Schlemmer et al., 2013). However, most canopy models are not suitable for simulating hyperspectral data characterized by a higher spatial resolution (up to sub-millimeter level) for which the assumption of mixed pixel does not hold.

In this study, we propose a physically-based model, called COSINE (CLOse-range Spectral ImagiNg of lEaves), that describes the additional spectral variability induced by directional effects and variation in leaf orientation. Combining COSINE with a leaf directional-hemispherical reflectance model such as PROSPECT allows the simulation of leaf reflectance according to our experimental conditions: submillimetric spatial resolution and a single

light source assumed to be directional. When applied in inverse mode to close-range hyperspectral images, the overall PROCOSINE model enables the simultaneous retrieval of PROSPECT parameters (e.g., chlorophyll and water contents), bidirectional effects and leaf angle with respect to the light source.

The COSINE theory is described in Section 2. After recalling the necessary radiometric definitions, we develop a physically-based analytic expression of the reflectance quantity retrieved using close-range imaging spectroscopy. This expression is then related to PROSPECT to explain variations in leaf biochemistry and leaf anatomy. In Section 3, we present the data sets used in this article as well as details about model validation and sensitivity analysis. Results are presented and discussed in Section 4, and we finally draw some conclusions and perspectives in Section 5.

2. Theory

2.1. Radiometric considerations

2.1.1. Definitions

The definitions and notations of the main physical quantities used in this article and summarized in Table 1, are based on the initial terminology of Nicodemus et al. (1977), which has later been reviewed by Schaepman-Strub et al. (2006).

The spectral radiance L is the radiant flux in a beam per unit wavelength, per unit area and per unit solid angle, and is expressed in the SI unit $[\text{W} \cdot \text{sr}^{-1} \cdot \text{m}^{-2} \cdot \text{nm}^{-1}]$. This is the physical quantity measured by a hyper-

Table 1: Main parameters and acronyms.

Parameter	Definition [unit]
b_{spec}	Specular term [unitless]
C_{ab}	Chlorophyll a+b content [$\mu\text{g.cm}^{-2}$]
C_{bp}	Brown pigment content [unitless]
C_{cx}	Carotenoid content [$\mu\text{g.cm}^{-2}$]
C_m	Leaf mass per area [g.cm^{-2}]
C_w	Equivalent water thickness [cm]
E	Spectral irradiance [$\text{W.m}^{-2}.\text{nm}^{-1}$]
f_r	Bidirectional reflectance distribution function (BRDF) [sr^{-1}]
L	Spectral radiance [$\text{W.sr}^{-1}.\text{m}^{-2}.\text{nm}^{-1}$]
λ	Wavelength [nm]
N	Leaf structure parameter [unitless]
φ_l	Difference between illumination and leaf normal azimuth angles [$^\circ$]
φ_v	Difference between illumination and viewing azimuth angles [$^\circ$]
R	Bidirectional reflectance factor (BRF) [unitless]
R_{hsi}	Pseudo bidirectional reflectance factor [unitless]
ρ	Directional-hemispherical reflectance (DHR) [unitless]
θ_i	Light incident angle (angle between the light source and the normal to the leaf) [$^\circ$]
$\theta_l, \theta_v, \theta_s$	Leaf normal, viewing and illumination zenith angles [$^\circ$]
ϑ	PROCOSINE parameters
ϑ_{dhr}	Parameters of the leaf DHR model

106 spectral imaging sensor after spectral calibration. The spectral irradiance E
107 is the radiant flux in a beam per unit wavelength and per unit area and is
108 expressed in $[\text{W.m}^{-2}.\text{nm}^{-1}]$.

109 One of the main physical quantities used to describe angular patterns of
110 reflected light is the bidirectional reflectance distribution function (BRDF)
111 expressed in $[\text{sr}^{-1}]$. It describes how a parallel beam of incident light from
112 one direction in the hemisphere is reflected into another direction in the
113 hemisphere:

$$f_r(\theta_s; \theta_v, \varphi_v; \lambda) = \frac{dL_r(\theta_s; \theta_v, \varphi_v; \lambda)}{dE_i(\theta_s; \lambda)} \quad (1)$$

114 where subscripts i and r refer to incoming and reflected lights respectively,
115 θ_s and θ_v are respectively the illumination and viewing zenith angles, and
116 φ_v is the viewing azimuth angle relatively to the illumination azimuth an-
117 gle (see Fig. 1 for angle representation). The BRDF being the ratio of two
118 infinitesimal quantities, it cannot theoretically be measured. However, its
119 integration over the corresponding solid angles allows the derivation of many
120 other measurable physical quantities.

121 Usually, the reflectance correction process does not consist in retrieving di-
122 rectly the reflectance (defined as the ratio of the leaving radiant exitance
123 to the incident irradiance), but rather follows the definition of a reflectance
124 factor. In the specific case of single illumination and viewing directions, the
125 bidirectional reflectance factor (BRF, denoted by R) is given by the ratio of
126 the radiant flux dL_r reflected from the area element dA to the radiant flux
127 dL_r^{id} reflected from an ideal and diffuse surface of the same area dA under
128 identical illumination and viewing geometries. It is unitless and, as developed

Figure 1: Angle representation.

by Schaepman-Strub et al. (2006), it can be expressed as follows:

$$R(\theta_s; \theta_v, \varphi_v; \lambda) = \frac{dL_r(\theta_s; \theta_v, \varphi_v; \lambda)}{dL_r^{id}(\theta_s; \lambda)} \quad (2)$$

where dL_r^{id} does not depend on viewing angles because of the Lambertian nature of the reference surface.

The BRDF of an ideal and diffuse surface being $(1/\pi)$, the BRF of any surface is therefore related to its BRDF by:

$$R(\theta_s; \theta_v, \varphi_v; \lambda) = \pi f_r(\theta_s; \theta_v, \varphi_v; \lambda). \quad (3)$$

Let us finally define the directional-hemispherical reflectance (DHR) as the integration of BRDF over the whole viewing hemisphere. The DHR is unitless and is given by:

$$\rho(\theta_s; 2\pi; \lambda) = \int_0^{2\pi} \int_0^{\pi/2} f_r(\theta_s; \theta_v, \varphi_v; \lambda) \cos \theta_v \sin \theta_v d\theta_v d\varphi_v. \quad (4)$$

137 In the following, the spectral dependence will be omitted for more clarity in
138 notation. Similarly, spectral radiance and spectral irradiance will be simply
139 referred to as radiance and irradiance.

140 2.1.2. Radiometric expression of close-range hyperspectral measurement

141 The solid angles corresponding to incident and reflected light beams are
142 never purely directional, so rigorously, sensor measurements only allow the
143 retrieval of a biconical reflectance factor (Schaepman-Strub et al., 2006).
144 However, a close approximation of bidirectional reflectance can be obtained
145 under specific experimental and instrumental conditions, e.g., using a col-
146 limated light beam and a small sensor field of view (FOV) provided by a
147 push-broom hyperspectral camera. In this case, the leaf BRF R is approxi-
148 mated as follows:

$$R(\theta_s; \theta_v, \varphi_v) \approx \frac{L_r(\theta_s; \theta_v, \varphi_v)}{L_r^{id}(\theta_s)} \quad (5)$$

149 where L_r and L_r^{id} are the radiances respectively measured on the leaf and on
150 the reference surface with a hyperspectral camera.

151 Importantly, Eq. 5 requires the leaf and reference surface to be under identi-
152 cal illumination geometry (i.e., same θ_s values). However, at the pixel level,
153 the leaf position and leaf local orientation can make the irradiances received
154 by the leaf and reference surface strongly different. Indeed, considering a
155 directional light source, the irradiance received by an area element is propor-
156 tional to the cosine of the incident angle θ_i , i.e., the angle between the light
157 source and the normal to this element:

$$E_i(\theta_i) = E_0 \cos \theta_i \quad (6)$$

158 where E_0 is the irradiance received by an area element perpendicular to the
159 light source direction, and $\cos \theta_i = \cos \theta_s \cos \theta_l + \sin \theta_s \sin \theta_l \cos \varphi_l$ where θ_l
160 and φ_l characterize the normal to this area element (Bousquet et al., 2005;
161 Comar et al., 2014).

162 Therefore, we define two illumination geometries corresponding to either the
163 leaf or the reference surface. The irradiance received by the leaf is:

$$E_i^l(\theta_i^l) = E_0 \cos \theta_i^l \quad (7)$$

164 whereas the one received by the ideal and diffuse reference surface is:

$$E_i^{id}(\theta_i^{id}) = E_0 \cos \theta_i^{id}. \quad (8)$$

165 The reference surface is usually positioned horizontally so, in the following,
166 we note $\theta_i^{id} = \theta_s$ and $\theta_i^l = \theta_i$.

167 Similarly to Eq. 5, at each pixel, the physical quantity R_{hsi} retrieved using
168 a hyperspectral camera is given by:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx \frac{L_r(\theta_i; \theta_v, \varphi_v)}{L_r^{id}(\theta_s)}. \quad (9)$$

169 Assuming the light source is directional and the pixel FOV is small, combin-
170 ing Eq. 1 and Eq. 9 leads to the following equation:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx \frac{f_r(\theta_i; \theta_v, \varphi_v) E_i^l(\theta_i)}{(1/\pi) E_i^{id}(\theta_s)}. \quad (10)$$

171 Using Eq. 3, Eq. 7 and Eq. 8, R_{hsi} can finally be expressed as follows:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx R(\theta_i; \theta_v, \varphi_v) \frac{\cos \theta_i}{\cos \theta_s}. \quad (11)$$

172 Eq. 11 reveals that the physical reflectance quantity retrieved from a small
173 FOV sensor in presence of a directional light source does not correspond

174 to the leaf BRF if the leaf and reference surface are differently tilted with
175 respect to the light source. In the following, we call "leaf pseudo BRF" the
176 leaf BRF weighted by the ratio of the cosine of the angle between the light
177 source and the normal to the leaf, to the cosine of illumination zenith angle.
178 Therefore, Eq. 11 relates the measured leaf pseudo BRF to the illumination
179 zenith angle, the incident angle (related to local leaf angles and illumination
180 zenith angle) and the leaf BRF. To relate the latter to the foliar content, it
181 is then necessary to take into account leaf surface properties as described in
182 the next section.

183 2.2. COSINE: a model for ClOse-range Spectral ImagiNg of lEaves

184 In this study, we propose to adapt a leaf DHR model (such as PROSPECT
185 (Jacquemoud & Baret, 1990) or LIBERTY (Dawson et al., 1998)) to the close-
186 range case. Indeed, with the perspective of comparing leaf optical measure-
187 ments to DHR simulations, proper experimental acquisitions require using an
188 integrating sphere in order to match with the hemispherical simulations. As
189 a result, leaf DHR models cannot directly be applied to hyperspectral remote
190 sensing observations of vegetation that are affected by variable bidirectional
191 effects (or BRDF effects) depending on illumination and viewing geometries.
192 An important prerequisite before using these models for close-range imaging
193 spectroscopy, is therefore to relate the leaf DHR to the leaf BRDF.

194 2.2.1. Relationship between leaf BRDF and DHR

195 It is generally admitted that the leaf BRDF is the sum of a diffuse compo-
196 nent $f_{r,diff}$ and a directional component $f_{r,spec}$ (Bousquet et al., 2005; Comar

et al., 2014):

$$f_r(\theta_i; \theta_v, \varphi_v) = f_{r,spec}(\theta_i; \theta_v, \varphi_v) + f_{r,diff}(\theta_i; \theta_v, \varphi_v). \quad (12)$$

The diffuse component $f_{r,diff}$ characterizes absorption and scattering processes within the leaf volume and thus depends on optically-active biochemical and biophysical parameters. The directional component $f_{r,spec}$ characterizes leaf surface properties and describes how light is reflected at the surface. While $f_{r,diff}$ is strongly wavelength-dependent, $f_{r,spec}$ is assumed to be nearly wavelength-independent in the visible and near-infrared (VNIR) range (between 400 and 1000 nm) (Bousquet et al., 2005; Comar et al., 2014). In the shortwave infrared (SWIR) range (between 1000 and 2500 nm), this assumption does not hold because the leaf refractive index actually depends on wavelength (Féret et al., 2008; Vanderbilt & Grant, 1985), especially due to the non-negligible influence of water absorption.

As a first approximation, $f_{r,diff}$ can be expressed as the ratio of leaf mesophyll Lambert coefficient k_l to π (Bousquet et al., 2005). To take into account the two-layer leaf structure (i.e. composed of an upper wax layer and a bottom leaf mesophyll layer), one should also consider the fraction of light that is reflected by the first wax layer and that does not reach the bottom layer (Stuckens et al., 2009; Ashikmin et al., 2000). The diffuse component is then expressed as a function of leaf mesophyll Lambert coefficient k_l and wax DHR ρ_{spec} (Stuckens et al., 2009):

$$f_{r,diff}(\theta_i) = \frac{k_l}{\pi}(1 - \rho_{spec}(\theta_i; 2\pi)) \quad (13)$$

where $f_{r,diff}$ does not depend on viewing angles and k_l only depends on

wavelength.

As defined by Eq. 4, the total DHR can then be obtained combining Eq. 12 and Eq. 13:

$$\begin{aligned} \rho(\theta_i; 2\pi) = & \int_0^{2\pi} \int_0^{\pi/2} f_{r,spec}(\theta_i; \theta_v, \varphi_v) \cos \theta_v \sin \theta_v d\theta_v d\varphi_v \\ & + \frac{k_l}{\pi} (1 - \rho_{spec}(\theta_i; 2\pi)) \int_0^{2\pi} \int_0^{\pi/2} \cos \theta_v \sin \theta_v d\theta_v d\varphi_v \end{aligned} \quad (14)$$

which can be rewritten as follows:

$$\rho(\theta_i; 2\pi) = \rho_{spec}(\theta_i; 2\pi) + k_l(1 - \rho_{spec}(\theta_i; 2\pi)). \quad (15)$$

This equation provides the necessary basis to relate a leaf DHR model to the leaf BRDF (through the Lambert coefficient).

2.2.2. The COSINE model

Assuming nadir illumination, a leaf DHR model expresses the DHR $\rho(0; 2\pi)$ as a function of leaf biochemical and biophysical contents characterized by the vector of input parameters $\boldsymbol{\vartheta}_{dhr}$. Following Eq. 15, the modeled Lambert coefficient can be expressed as a function of $\rho_{spec}(0; 2\pi)$ and DHR model $\tilde{\rho}(\boldsymbol{\vartheta}_{dhr})$ as:

$$\tilde{k}_l(\boldsymbol{\vartheta}_{dhr}) = \frac{\tilde{\rho}(\boldsymbol{\vartheta}_{dhr}) - \rho_{spec}(0; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \quad (16)$$

where $\sim$ refers to modeled quantities.

The leaf BRDF can then be modeled as a function of leaf parameters $\boldsymbol{\vartheta}_{dhr}$ by combining Eq. 12, Eq. 13 and Eq. 16:

$$\begin{aligned} \tilde{f}_r(\theta_i; \theta_v, \varphi_v; \boldsymbol{\vartheta}_{dhr}) = & f_{r,spec}(\theta_i; \theta_v, \varphi_v) \\ & + \frac{1}{\pi} \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right) (\tilde{\rho}(\boldsymbol{\vartheta}_{dhr}) - \rho_{spec}(0; 2\pi)). \end{aligned} \quad (17)$$

In order to estimate $\boldsymbol{\vartheta}_{dhr}$ from the pseudo BRF R_{hsi} retrieved using a hyperspectral camera, Eq. 3, Eq. 11 and Eq. 17 are combined to obtain the pseudo-BRF based COSINE model:

$$\begin{aligned} \widetilde{R_{hsi}}(\theta_s, \theta_i; \theta_v, \varphi_v; \boldsymbol{\vartheta}_{dhr}) = & \left(\frac{\cos \theta_i}{\cos \theta_s} \right) \left[\left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right) \tilde{\rho}(\boldsymbol{\vartheta}_{dhr}) \right. \\ & \left. + \pi f_{r,spec}(\theta_i; \theta_v, \varphi_v) - \rho_{spec}(0; 2\pi) \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right) \right] \quad (18) \end{aligned}$$

where only the first term of the sum is related to the leaf DHR model.
Note that $f_{r,spec}$ and ρ_{spec} could potentially be modeled using the leaf BRDF model developed by Bousquet et al. (2005) that expresses the directional component as a function of illumination and viewing geometries as well as on the wax refractive index and a surface roughness parameter. Unfortunately, the resulting model becomes over-parameterized so its inversion is an ill-posed problem and leads to poor estimation results (not shown).

2.2.3. A simplified COSINE model for the VNIR range

In the VNIR range, the second term in Eq. 18 is assumed to be wavelength-independent. Omitting its dependence in viewing angles, Eq. 18 can then be simplified as:

$$\widetilde{R_{hsi}}(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s} \right) \left[\left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right) \tilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec} \right] \quad (19)$$

where $b_{spec} = b_{spec}(\theta_i; \theta_v, \varphi_v) = \pi f_{r,spec}(\theta_i; \theta_v, \varphi_v) - \rho_{spec}(0; 2\pi) \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right)$.
Assuming that the fraction $\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}$ is nearly one (especially true for low incident angles), Eq. 19 can be approximated by:

$$\widetilde{R_{hsi}}(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s} \right) \left[\tilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec} \right]. \quad (20)$$

241 COSINE therefore simulates the pseudo-BRF as a function of incident an-
242 gle θ_i , illumination zenith angle θ_s , foliar content through the DHR model
243 parameters $\boldsymbol{\vartheta}_{dhr}$ and BRDF effect b_{spec} . Importantly, this model is presum-
244 ably only well suited for low incident angles. In high incidence, the fraction
245 $\frac{1-\rho_{spec}(\theta_i;2\pi)}{1-\rho_{spec}(0;2\pi)}$ may differ from one, which could lead to an incorrect estimation
246 of θ_i when inverting the model.
247 Finally, in order to model directly radiance measurements, a radiance-based
248 COSINE model can be derived from Eq. 9 as:

$$\widetilde{L}_r(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s} \right) \left[\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec} \right] L_r^{id}(\theta_s) \quad (21)$$

249 where $L_r^{id}(\theta_s)$ is the radiance measured on the reference surface.

250 3. Material and methods

251 3.1. Data acquisition

252 3.1.1. Spectral measurements

253 The COSINE model was tested using close-range hyperspectral images
254 acquired under laboratory conditions. Two push-broom hyperspectral cam-
255 eras were used, i.e., a HySpex VNIR-1600 camera (Norsk Elektro Optikk,
256 Norway) and a HySpex SWIR-320m-e camera (Norsk Elektro Optikk, Nor-
257 way). The HySpex VNIR-1600 camera acquired successive lines of 1600 pixels
258 and 160 spectral bands ranging from 415 to 994 nm with a 3.7 nm spectral
259 sampling interval. The pixel FOV was 0.18 and 0.36 mrad across- and along-
260 track respectively.

261 Even if COSINE is theoretically only well suited for the VNIR range for which
262 the directional BRDF component is assumed to be wavelength-independent,

Figure 2: Experimental setup for the horizontal (a) and tilted (b-c) configurations. For the VNIR camera, the corresponding average incident angles $\bar{\theta}_i$ are 20° (a), 40° (b) and 0° (c). For the SWIR camera, the corresponding average incident angles $\bar{\theta}_i$ are 30° (a), 10° (b) and 50° (c).

we also tested this model on SWIR images in order to see how this assumption was affecting the estimation results. The HySpex SWIR-320m-e camera acquired successive lines of 320 pixels and 256 spectral bands ranging from 960 to 2490 nm with a 6 nm spectral sampling interval. The pixel FOV was 0.75 mrad across- and along-track.

As shown in Fig. 2, in both cases, the camera was facing towards nadir at thirty centimeters above the imaged leaf, thus leading to across-track pixel FOV of 0.23 mm for the SWIR camera, and 0.11 mm for the VNIR camera (after an appropriate subsampling in the across-track direction so as to obtain square pixels). Both cameras were positioned thirty centimeters apart. The lighting was provided by two halogen sources (one for each camera) positioned close to the cameras. These light sources were collimated and

275 positioned so that each source was illuminating the same line than the line
276 imaged by the corresponding camera. The illumination zenith angles were
277 set to $\theta_s = 20^\circ$ and $\theta_s = 30^\circ$ for the VNIR camera and the SWIR camera
278 respectively. The incoming halogen irradiance was estimated on a line-by-
279 line basis by using a reference surface (Spectralon[®], Labsphere) horizontally
280 placed next to the imaged leaf. In order to limit saturation on the reference
281 surface while obtaining a low noise level in the strong absorption regions,
282 we chose a Spectralon[®] whose diffuse reflectance was approximately 40%
283 between 400 and 2500 nm. After acquisition, VNIR and SWIR images were
284 finally calibrated to spectral radiance.

285

286 The main data set contains leaves from five species commonly found in
287 the French Mediterranean region, namely bamboo (*Phyllostachys aurea*), ivy
288 (*Hedera helix*), laurestine (*Viburnum tinus*), bay laurel (*Laurus nobilis*) and
289 holly (*Ilex aquifolium*). Some of these leaves exhibited strong (resp. weak)
290 non-Lambertian behavior, e.g., bay laurel and holly (resp. bamboo). Also,
291 some of them had regular (resp. non-regular) surfaces, e.g., bay laurel (resp.
292 ivy and holly). All of these leaves were harvested in March, 2015 and selected
293 on a color basis, ranging from dark green for leaves with a high chlorophyll
294 content, to yellow for senescent leaves. As illustrated in Fig. 2, each leaf was
295 placed on a translation stage and was imaged in three positions using a 20°
296 tilted stand. As a result, the average incident angles $\bar{\theta}_i$ were 0° , 20° and
297 40° for VNIR camera, and 10° , 30° and 50° for SWIR camera. Note that
298 the translation stage had low reflectivity so we assumed that, after being
299 transmitted through the leaf, the light reflected from the translation stage

300 and re-transmitted through the leaf was negligible.
301 In addition, a SWIR image of a sugar beet leaf (*Beta vulgaris*) was ac-
302 quired, especially because this species shows interesting features in this spec-
303 tral range, i.e., very high equivalent water thickness ($C_w > 0.02$ cm) and low
304 leaf mass per area ($C_m < 0.005$ g.cm⁻²), as well as a strongly non-Lambertian
305 and non-regular surface, thereby illustrating well the relevance of our model.
306 This leaf was only imaged in horizontal position, its surface being already
307 highly non-regular.

308 3.1.2. Reference measurements

309 For each leaf, after spectral measurements, several leaf disks (from two to
310 seven disks depending on leaf size) of known area were sampled using a cork
311 borer. Each disk position was then recorded for further reference. A Dualex
312 scientific+TM (Force-A, Orsay, France), hereafter called Dualex, was used to
313 measure the chlorophyll a+b content C_{ab} in every disk. This leafclip allows
314 non-destructive transmittance-based C_{ab} measurements characterized by an
315 accuracy of around 5 μ g.cm⁻² (Cerovic et al., 2012). Compared with the well
316 known SPAD-502TM (Minolta, Japan), the Dualex uses a higher C_{ab} -sensitive
317 wavelength (710 nm) that allows it to have a nearly linear response to vari-
318 ation in C_{ab} for $C_{ab} < 40$ μ g.cm⁻². However, for dicotyledons, saturation
319 occurring beyond 40 μ g.cm⁻² leads the Dualex to underestimate such C_{ab}
320 values (Cerovic et al., 2012). The higher C_{ab} , the greater the underestima-
321 tion.

322 Leaf disks were then weighted and placed in a drying oven at 75°C for 48 h.
323 Subsequently, their dry mass was measured to obtain the equivalent water

Table 2: Characteristics of reference measurements for the main data set.

Parameter	Number of samples	Mean	Min/Max	Standard deviation
C_{ab} [$\mu\text{g.cm}^{-2}$]	93	29.4	5.2/54.6	11.1
C_w [cm]	22	0.0104	0.0049/0.0164	0.0040
C_m [g.cm^{-2}]	22	0.0091	0.0052/0.0129	0.0023

324 thickness C_w (in [cm]) and leaf mass per area C_m (in [g.cm^{-2}]) as follows:

$$C_w = \frac{FW - DW}{A} \times d_w \quad (22)$$

$$C_m = \frac{DW}{A} \quad (23)$$

325 where FW and DW are the fresh and dry weights of leaf disks respectively,
326 A is the total disk area, and $d_w = 1 \text{ g.cm}^{-3}$ is the water density.

327 Therefore, for each leaf, several measurements of C_{ab} and one measurement of
328 C_w and C_m were available. The ranges of C_{ab} , C_w and C_m for the main data
329 set are reported in Table 2 and were similar to those found in the literature
330 (Féret et al., 2008; Danson & Bowyer, 2004).

3.2. Retrieval of leaf parameters from model inversion

332 In this study, we used the PROSPECT (Leaf Optical Properties Spectra)
333 model to simulate the leaf DHR from 400 to 2500 nm as a function of the leaf
334 biochemistry and structure. The original version developed by Jacquemoud
335 & Baret (1990) has been successively improved over the years to take into
336 account other biochemical components and a broader spectral range (Jacque-
337 moud et al., 1996; Baret & Fourty, 1997a; Jacquemoud et al., 2000; Féret
338 et al., 2008; Gerber et al., 2011). The considered PROSPECT 5b version was
339 developed by Féret et al. (2008) (available at <http://teledetection.ipgp>.

jussieu.fr/prosail/) and simulates the leaf DHR as a function of the leaf structure parameter N , chlorophyll a+b content C_{ab} , carotenoid content C_{cx} , brown pigment content C_{bp} , equivalent water thickness C_w and leaf mass per area C_m .

In the following, leaf parameters were retrieved based on model inversion. The parameters that were only affecting the reflected radiation in the VNIR range (resp. the SWIR range), were kept constant when considering the SWIR range (resp. the VNIR range) so as to reduce the estimation uncertainty. Therefore, because water absorption is weak in the VNIR range and only occurs around 970 nm (Curran, 1989), the VNIR range was reduced to 410-900 nm (i.e., 135 bands) and C_w was fixed to the default value 0.01 cm. The vector of input PROSPECT parameters was thus $\boldsymbol{\vartheta}_{dhr} = [N, C_{ab}, C_{cx}, C_{bp}, C_m]^t$. Similarly, foliar pigments do not affect the SWIR reflectance so C_{ab} , C_{cx} and C_{bp} were fixed to the default values $30 \mu\text{g.cm}^{-2}$, $10 \mu\text{g.cm}^{-2}$ and 0 respectively. In the SWIR range, the vector of input PROSPECT parameters was $\boldsymbol{\vartheta}_{dhr} = [N, C_w, C_m]^t$. For each pixel, the combined pseudo-BRF based PROSPECT+COSINE model (named PROCOSINE hereafter) was numerically inverted by optimizing the following least square merit function:

$$\hat{\boldsymbol{\vartheta}}_{pseudo-brf} = \underset{\boldsymbol{\vartheta}}{\operatorname{argmin}} \sum_{\lambda_i} \left[R_{hsi}(\lambda_i) - \widetilde{R}_{hsi}(\lambda_i; \boldsymbol{\vartheta}) \right]^2 \quad (24)$$

where $\boldsymbol{\vartheta} = [\boldsymbol{\vartheta}_{dhr}, \theta_i, b_{spec}]^t$, R_{hsi} is the measured pseudo-BRF retrieved using Eq. 9 and $\widetilde{R}_{hsi}$ is the pseudo-BRF based PROCOSINE model given by Eq. 20. Similarly, the radiance-based PROCOSINE model was inverted by solving

Table 3: Lower bounds, upper bounds and initial values of the optimization problem.

Parameter	Lower bound	Upper bound	Initial value
N	1	3.5	1.5
C_{ab} [$\mu\text{g.cm}^{-2}$]	0	100	50
C_{cx} [$\mu\text{g.cm}^{-2}$]	0	30	10
C_{bp}	0	5	0
C_w [cm]	0.00005	0.1	0.01
C_m [g.cm $^{-2}$]	0.001	0.03	0.01
θ_i [$^\circ$]	0	90	20
b_{spec}	-0.2	0.6	0

the following optimization problem:

$$\hat{\boldsymbol{\vartheta}}_{radiance} = \underset{\boldsymbol{\vartheta}}{\operatorname{argmin}} \sum_{\lambda_i} \left[L_r(\lambda_i) - \widetilde{L}_r(\lambda_i; \boldsymbol{\vartheta}) \right]^2 \quad (25)$$

where L_r is the measured spectral radiance and $\widetilde{L}_r$ is the radiance-based PROCOSINE model given by Eq. 21.

To reduce the number of solutions to the inverse problem, the estimation range was restricted using lower and upper bounds. These bounds as well as initial values are provided in Table 3. Note that C_{bp} and C_w upper bounds are higher than those found in the literature because, at the sub-millimeter level, C_{bp} and C_w can be very high in necrotic regions and veins respectively. Optimization of Eq. 24 and Eq. 25 was performed using the trust-region reflective algorithm implemented in MATLAB[®] (version 8.0.0, The MathWorks Inc., Natick, MA, 2012) within the "lsqcurvefit" function.

3.3. PROCOSINE sensitivity analysis

Before assessing PROCOSINE in terms of estimation results, we performed a global sensitivity analysis in order to study the relative contribution of each parameter to the modeled pseudo-BRF as a function of wavelength. Global sensitivity analysis informs us on which variation in the model output is produced by variation in the model input parameters, both individually and collectively through their interactions with each other. When studied as a function of wavelength, it provides interesting insights regarding the optimal spectral bands that can be used to retrieve model parameters.

In this paper, we implemented the EFAST (Extended Fourier Amplitude Sensitivity Transform) method (Saltelli et al., 1999) that was already applied to PROSAIL and PROGEOSAIL models by Bowyer & Danson (2004). EFAST is a quantitative variance-based method, i.e., it allows the derivation of sensitivity indices from the decomposition of the total variance of the model output into variance terms induced by every input parameter. In this paper, we only used the first-order index S_i that represents the percentage of output variance explained by the i^{th} parameter alone. The remaining percentage of variance is explained by interactions between parameters and is given by $S_{int} = 1 - \sum_i S_i$. S_i (and S_{int}) ranges from 0 to 1, and the higher S_i , the more sensitive the model output is to the i^{th} parameter.

In this study, 5000 combinations of model parameters were randomly generated using appropriate probability distributions because the latter strongly affects the results of sensitivity analysis (Bowyer & Danson, 2004; Wallach

Table 4: Estimated parameter distributions (μ : mean; σ : standard deviation; α : shape parameter; β : scale parameter).

Parameter	Distribution	μ	σ	α	β
N	Gamma	1.52	0.23	47.50	0.032
C_{ab} [$\mu\text{g.cm}^{-2}$]	Gamma	32.8	18.87	1.99	16.45
C_{cx} [$\mu\text{g.cm}^{-2}$]	Gamma	8.51	3.92	3.83	2.22
C_w [cm]	Gamma	0.0122	0.0061	6.45	0.0019
C_m [g.cm^{-2}]	Gamma	0.0078	0.0036	4.20	0.0018
θ_i [$^\circ$]	Gamma	25	10	6.25	4
b_{spec} (VNIR)	Normal	-0.009	0.0375	-	-
b_{spec} (SWIR)	Normal	0.0346	0.0403	-	-

et al., 2014). The distributions of PROSPECT parameters were estimated from seventeen independent data sets made available by Féret et al. (2011); Féret, personal communication. They include a wide range of leaf spectral, chemical, and structural properties, i.e., 1417 leaves corresponding to about 120 different species from various growing conditions and developmental stages. Note that C_{ab} , C_{cx} , C_w and C_m data were obtained in a destructive way, whereas N data were obtained from PROSPECT inversion on DHR data. It can be shown that these data are well described by Gamma distributions ($p < 0.001$). Using such distributions (instead of normal ones) prevented us from generating samples with negative content values. Regarding brown pigments, we assumed that leaves under study were green so C_{bp} was set to zero. Finally, θ_i and b_{spec} distributions were retrieved from the estimation results presented in Section 4 using a Gamma distribution for θ_i and a normal distribution for b_{spec} (not shown). The characteristics of all of these distributions are presented in Table 4, where the shape parameter α

and the scale parameter β of the Gamma distribution were given by their maximum likelihood estimates. Note that two b_{spec} distributions were used for the two spectral domains. Importantly, the covariance between parameters could not be considered when generating the samples. Consequently, the actual influences of C_{ab} and C_{cx} are likely to be slightly different, both parameters being highly correlated (Féret et al., 2008). For each EFAST run, 5000 leaf reflectance spectra were therefore simulated using PROSPECT and PROCOSINE (Eq. 20) so as to compute first-order indices and interactions. Average indices were finally computed over 15 runs.

4. Results and discussion

4.1. Sensitivity analysis

In Figure 3, we compare the first-order indices and interactions obtained with PROSPECT and PROCOSINE over the VNIR and SWIR ranges. Fig. 3.a and Fig. 3.b reveal the same features already observed in previous studies using other methods and/or models (Jacquemoud & Baret, 1990; Jacquemoud et al., 2009; Bacour et al., 2001, 2002; Bowyer & Danson, 2004). In the visible range (400-730 nm), photosynthetic pigments (i.e., chlorophyll and carotenoids) drive most of the reflectance variability. Between 400 and 525 nm where the carotenoid absorption is the strongest (Féret et al., 2008), the contributions of C_{ab} and C_{cx} are similar in magnitude and range from 20 to 40%. Between 525 and 730 nm, reflectance mainly depends on C_{ab} , its contribution ranging from 40 to 90%. The influence of interactions is higher in strong absorption regions, which means that the effects of other parameters depend on C_{ab} and C_{cx} values. For example, the relative increase in

Figure 3: First-order sensitivity indices and interactions for (a) PROSPECT in the VNIR range, (b) PROSPECT in the SWIR range, (c) PROCOSINE in the VNIR range, and (d) PROCOSINE in the SWIR range ($\theta_s = 26^\circ$).

reflectance due an increase in N (reflecting higher scattering within the leaf internal structure) will be high in case of low absorption and low in case of strong absorption.

In the NIR plateau, variation in reflectance is mainly produced by variation in leaf structure (80%) and leaf mass per area (14%) through scattering processes (Knyazikhin et al., 2013). In the SWIR range, only leaf structure, equivalent water thickness and leaf mass per area have significant contributions. In particular, C_w strongly influences reflectance in the water absorption peaks located around 1450 and 1950 nm (about 75%), whereas variation in C_m has a significant contribution around 1720 and 2250 nm (resp. 24% and 30%).

Taking into account BRDF effects and leaf orientation through the b_{spec} and θ_i parameters within the PROCOSINE model modifies the reflectance sensitivity as shown in Figure 3.c and Figure 3.d. Compared with PROSPECT sensitivity analysis, the overall contributions of PROSPECT parameters are mostly similar in shape but still, they decrease to account for variance in b_{spec} and θ_i . For example, the C_{ab} contribution at around 550 nm decreases from 90 to 70%.

The contributions of b_{spec} and θ_i are quite different. Overall, variance in b_{spec} highly influences reflectance in strong absorption regions (both due to C_{ab} and C_w), accounting for up to 90% near 400 nm and 75% near 1930 and 2500 nm. In these regions, the diffuse part of reflectance is very low so the influence of the surface-reflected flux (that does not interact with the leaf volume) dominates. Interestingly, an analogy can be made with high-

463 resolution water remote sensing, in that the sun glint (i.e., the amount of
464 flux directly reflected at the water surface) is usually estimated in the NIR
465 region, where the water-leaving signal is negligible because of strong water
466 absorption (Hochberg et al., 2003). Overall, the b_{spec} contribution is always
467 greater than 15% between 400 and 2500 nm, thereby indicating that this pa-
468 rameter should not be neglected when dealing with close-range hyperspectral
469 images.

470

471 The contribution of the incident angle θ_i significantly varies over the whole
472 spectral domain. It mostly affects reflectance in the NIR plateau, accounting
473 for about 30% of the variance of the PROCOSINE output. Conversely, its
474 influence is much weaker in the visible range, where its contribution does
475 not exceed 5%, as well as in water absorption regions. Generally, because
476 it affects the model through a multiplicative term (see Eq. 20 and Eq. 21),
477 the spectral profile of its contribution is similar to a common leaf spectral
478 signature: the higher the reflectance, the higher its contribution. Interest-
479 ingly, this profile is also similar to the contribution of the average leaf angle
480 (ALA) to the PROSAIL model (Jacquemoud et al., 2009). In the latter case,
481 ALA has more influence at weakly absorbing wavelengths because the effect
482 of multiple scattering within the canopy is stronger (Knyazikhin et al., 2013).

483

484 To summarize, this sensitivity analysis shows that both b_{spec} and θ_i sig-
485 nificantly affect the measured signal and definitively have to be taken into
486 account in the case of close-range imaging spectroscopy.

487 4.2. Quantitative assessment of model inversion

488 The performances of model inversion were quantitatively assessed both
489 in terms of spectral fitting and parameter retrieval. Note that we had only
490 reference measurements integrated over one (for C_{ab}) or several (for C_w and
491 C_m) leaf disk(s) of a few square centimeters. As a result, in this section,
492 the means and standard deviations of C_{ab} , C_w and C_m estimated values were
493 computed from the values estimated within the corresponding leaf disk(s).

494 4.2.1. PROCOSINE spectral accuracy

495 We first quantified how accurate was PROCOSINE in fitting the pseudo-
496 BRF and radiance measurements retrieved at the pixel level. In Fig. 4, we
497 show some fitting results obtained with an ivy leaf both for the VNIR and
498 SWIR ranges, this leaf surface being non-Lambertian and non-regular.
499 Overall, strong agreements were obtained between measured and simulated
500 spectra in the two ranges (RMSE < 4%). As expected, high b_{spec} values were
501 retrieved in areas affected by specular reflection, and high θ_i values were
502 retrieved where the light incident angle was high. Compared with the VNIR
503 range, the obtained RMSE were about twice higher for the SWIR range.
504 This is in agreement with the mismodeling of specular reflection in the SWIR
505 range mentioned in Section 2.2.1 and discussed further in Section 4.2.4. These
506 results thus demonstrate the accuracy of PROCOSINE in accounting for the
507 spectral variability induced by BRDF effects and leaf orientation, especially
508 in the VNIR range.

Figure 4: Fitting results obtained for the VNIR range (a-c) and the SWIR range (d-f) using the pseudo-BRF model (b,e) and the radiance model (c,f). Solid (resp. dashed) lines correspond to measurements (resp. simulations). Blue curves correspond to areas strongly affected by specular reflection, while red curves correspond to areas characterized by a high incident angle.

Figure 5: C_{ab} estimation results (mean $\pm$ standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PROCOSINE model (green) and with $\bar{\theta}_i = 20^\circ$ (a-c), $\bar{\theta}_i = 0^\circ$ (d-f) and $\bar{\theta}_i = 40^\circ$ (g-i). The R² and RMSE values are computed for actual C_{ab} values lower than $40 \mu\text{g.cm}^{-2}$ and are given in parentheses.

509 4.2.2. Results of parameter retrievals in the VNIR range

510 As recalled by the sensitivity analysis, the VNIR reflectance is mainly
511 driven by the chlorophyll a+b content. In Fig. 5, we show the means and
512 standard deviations of C_{ab} estimation obtained for each leaf disk with leaves
513 in horizontal position (Figure 5.a-c) and tilted position (Figure 5.d-i). We
514 compare the results obtained with PROSPECT (in blue), the pseudo-BRF
515 based PROCOSINE model (in orange) and the radiance-based PROCOSINE
516 model (in green). Because of the saturation in the reference measurement
517 (see Section 3.1.2), the RMSE and R^2 values were computed from samples
518 for which the measured C_{ab} values were lower than $40 \mu\text{g.cm}^{-2}$.

519
520 On average, when tested with horizontal leaves, the radiance-based PRO-
521 COSINE model led to a higher accuracy ($R^2 = 0.92$; $\text{RMSE} = 3.23 \mu\text{g.cm}^{-2}$)
522 than the pseudo-BRF PROCOSINE model ($R^2 = 0.89$; $\text{RMSE} = 3.73 \mu\text{g.cm}^{-2}$)
523 and PROSPECT ($R^2 = 0.81$; $\text{RMSE} = 4.88 \mu\text{g.cm}^{-2}$). Applying the same
524 models to leaves in tilted position decreased the estimation accuracy, how-
525 ever to a variable extent. For $\bar{\theta}_i = 0^\circ$, the radiance-based PROCOSINE
526 model ($R^2 = 0.93$; $\text{RMSE} = 4.44 \mu\text{g.cm}^{-2}$) still performed better than the
527 pseudo-BRF based PROCOSINE model ($R^2 = 0.92$; $\text{RMSE} = 4.71 \mu\text{g.cm}^{-2}$)
528 and PROSPECT ($R^2 = 0.81$; $\text{RMSE} = 6.45 \mu\text{g.cm}^{-2}$). The same trend was
529 also observed for $\bar{\theta}_i = 40^\circ$, the radiance-based PROCOSINE model leading
530 to a better accuracy ($R^2 = 0.91$; $\text{RMSE} = 3.65 \mu\text{g.cm}^{-2}$) than the pseudo-
531 BRF based PROCOSINE model ($R^2 = 0.86$; $\text{RMSE} = 4.63 \mu\text{g.cm}^{-2}$) and
532 PROSPECT ($R^2 = 0.87$; $\text{RMSE} = 5.87 \mu\text{g.cm}^{-2}$).
533 Overall, both PROCOSINE implementations obtained significantly lower

Figure 6: Histograms of estimated θ_i values for every pixel for the VNIR range and the three acquisition configurations ($\bar{\theta}_i = 0^\circ$, $\bar{\theta}_i = 20^\circ$, and $\bar{\theta}_i = 40^\circ$): (a) pseudo-BRF based PROCOSINE model, and (b) radiance-based PROCOSINE model.

standard deviations of C_{ab} estimation than PROSPECT.

Lastly, for $C_{ab} > 40 \mu\text{g.cm}^{-2}$, model inversion always provided higher C_{ab} values than those measured with the Dualex.

The incident angle estimation within the whole leaves is evaluated in Fig. 6. The results are presented using histograms to account for within-leaf variability of leaf orientation. For both model implementations, we represent the distributions of θ_i values estimated for every pixel for the three acquisition configurations (i.e., average incident angles $\bar{\theta}_i$ of 0° , 20° , and 40°).

Surprisingly, strong differences were observed between both model inversions. On the one hand, the pseudo-BRF based model gave poor estimation results with estimated $\bar{\theta}_i$ of 3.3° , 5.1° and 11.7° (and the same estimated distribution mode, i.e., 2.4°) for $\bar{\theta}_i = 0^\circ$, $\bar{\theta}_i = 20^\circ$, and $\bar{\theta}_i = 40^\circ$ respectively. On the other hand, the radiance-based model gave better estimation results with estimated $\bar{\theta}_i$ of 9.7° , 16.9° and 19.6° (and estimated distribution modes of 6.3° , 14.8°

549 and 14.8°) for $\bar{\theta}_i = 0^\circ$, $\bar{\theta}_i = 20^\circ$, and $\bar{\theta}_i = 40^\circ$ respectively.

550 It is worth noting that poorer angle estimation results were generally obtained
551 for bamboo leaves (results not shown) with estimated distribution modes of
552 15.4° , 28.6° and 28.6°) for $\bar{\theta}_i = 0^\circ$, $\bar{\theta}_i = 20^\circ$, and $\bar{\theta}_i = 40^\circ$ respectively.

553 4.2.3. Results of parameter retrievals in the SWIR range

554 Regarding PROSPECT original parameters, variation in SWIR reflectance
555 is mainly produced by variation in equivalent water thickness, leaf mass per
556 area and leaf structure.

557 In Fig. 7, we show the means and standard deviations of C_w estimation
558 obtained with leaves in horizontal position (Fig. 7.a-c) and in tilted posi-
559 tion (Fig. 7.d-i). For horizontal leaves, PROCOSINE performed better than
560 PROSPECT in terms of R^2 ($R^2 = 0.91$ for PROSPECT, $R^2 = 0.93$ for
561 the pseudo-BRF based PROCOSINE model and $R^2 = 0.94$ for the radiance-
562 based PROCOSINE model), but worse in terms of RMSE (RMSE = 0.0016 cm,
563 RMSE = 0.0083 cm and RMSE = 0.0025 cm resp.). However, the PRO-
564 COSINE performances remained mostly unchanged when applied to tilted
565 leaves, while PROSPECT obtained poorer performances, either for $\bar{\theta}_i = 10^\circ$
566 (a 125% increase in RMSE) or $\bar{\theta}_i = 50^\circ$ (a 15% decrease in R^2).

567 The RMSE values obtained with PROCOSINE were primarily due to a sys-
568 tematic bias, the R^2 values being higher than 0.91 for the three acquisition
569 configurations. This bias was more pronounced for the pseudo-BRF based
570 model, and led to a systematic overestimation of C_w .

571 Lastly, similarly to C_{ab} estimation, PROCOSINE obtained lower standard
572 deviations of C_w estimation than PROSPECT, especially for tilted leaves.

573

Figure 7: C_w estimation results (mean $\pm$ standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PROCOSINE model (green) and with $\bar{\theta}_i = 30^\circ$ (a-c), $\bar{\theta}_i = 10^\circ$ (d-f) and $\bar{\theta}_i = 50^\circ$ (g-i). R^2 and RMSE values are given in parentheses.

Figure 8: C_m estimation results (mean $\pm$ standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PRO-COSINE model (green) and with $\bar{\theta}_i = 30^\circ$ (a-c), $\bar{\theta}_i = 10^\circ$ (d-f) and $\bar{\theta}_i = 50^\circ$ (g-i). R^2 and RMSE values are given in parentheses.

Figure 9: Histograms of estimated θ_i values in every pixel for the SWIR range and the three acquisition configurations ($\bar{\theta}_i = 10^\circ$, $\bar{\theta}_i = 30^\circ$, and $\bar{\theta}_i = 50^\circ$): (a) pseudo-BRF based PROCOSINE model, and (b) radiance-based PROCOSINE model.

574 The C_m retrieval results are presented in Fig. 8 in a similar fashion to C_w .
575 The radiance-based PROCOSINE model gave significantly lower RMSE than
576 the pseudo-BRF based PROCOSINE model and PROSPECT, i.e., $\text{RMSE} =$
577 0.0013 g.cm^{-2} , $\text{RMSE} = 0.0032 \text{ g.cm}^{-2}$, and $\text{RMSE} = 0.0024 \text{ g.cm}^{-2}$ respec-
578 tively on average for the three acquisition configurations. The PROCOSINE
579 performances weakly depended on leaf position, whereas the R^2 dropped
580 from 0.89 for $\bar{\theta}_i = 10^\circ$ and $\bar{\theta}_i = 30^\circ$, to 0.30 for $\bar{\theta}_i = 50^\circ$ when inverting only
581 PROSPECT. For such high incident angles, the uncertainty of C_m estimation
582 was much higher with PROSPECT than with PROCOSINE.
583 Lastly, C_m was generally underestimated by PROSPECT and overestimated
584 by the pseudo-BRF based PROCOSINE model.

585

586 The two PROCOSINE inversions were also compared based on θ_i esti-
587 mation results in Fig. 9, in which we represent the histograms of estimated
588 θ_i distributions. As expected, in both cases, the highest (resp. the lowest)

angles were mostly retrieved from the $\bar{\theta}_i = 50^\circ$ (resp. $\bar{\theta}_i = 10^\circ$) configuration, the dispersions around the mean values being due to the variation in leaf orientation. θ_i was more accurately predicted using the radiance-based model since the estimated $\bar{\theta}_i$ were 19.7° , 27.7° and 36.4° for $\bar{\theta}_i = 10^\circ$, $\bar{\theta}_i = 30^\circ$, and $\bar{\theta}_i = 50^\circ$ respectively. The pseudo-BRF based model globally overestimated θ_i since the estimated $\bar{\theta}_i$ were 38.0° , 47.2° and 53.0° for $\bar{\theta}_i = 10^\circ$, $\bar{\theta}_i = 30^\circ$, and $\bar{\theta}_i = 50^\circ$ respectively.

Similarly to the VNIR range, poorer estimation results were generally obtained for bamboo leaves (results not shown). For example, the radiance-based model led to estimated $\bar{\theta}_i$ of 38.0° , 43.4° and 47.0° for $\bar{\theta}_i = 10^\circ$, $\bar{\theta}_i = 30^\circ$, and $\bar{\theta}_i = 50^\circ$ respectively.

4.2.4. Discussion about parameter retrievals

Estimation of chlorophyll content. In the VNIR range, both PROCOSINE implementations performed better than PROSPECT in retrieving C_{ab} . For leaves in horizontal position, the 34% improvement in RMSE when using the radiance-based PROCOSINE model instead of PROSPECT is likely to be due mainly to the modeling of BRDF effects. Not taking them into account leads to a greater uncertainty as shown through the estimation standard deviations computed within each leaf disk. For example, as illustrated in Fig. 5.a with the sample corresponding to an actual mean value of $53 \mu\text{g}\cdot\text{cm}^{-2}$, a local BRDF effect induces an overall increase in reflectance, which is misinterpreted by PROSPECT as a decrease in C_{ab} . This result confirms one of the conclusions drawn from the sensitivity analysis, which has already showed that b_{spec} significantly affects leaf close-range hyperspectral measurements. The difference between PROCOSINE and PROSPECT was even greater

when considering leaves in tilted position, for which the modeling of leaf inclination was more important. In particular, for the highest incident angle ($\bar{\theta}_i = 40^\circ$), both the modeling of BRDF effects and leaf orientation within the radiance-based PROCOSINE model led to an actual 38% improvement over PROSPECT. It is worth noting that taking θ_i into account improves the C_{ab} estimation results even if C_{ab} is mainly retrieved between 400 and 750 nm, in which the effect of θ_i is lower (see Fig. 3.c). In fact, the difference in retrieval performance in VNIR between PROSPECT and PROCOSINE is even greater for N leaf structure parameter that mainly affects reflectance in the NIR plateau, where both θ_i and b_{spec} have a strong influence on reflectance (N maps are only shown for the SWIR range, see Fig. 12).

The PROCOSINE inversion performed well compared with the accuracy provided by the Dualex manufacturer, i.e., $RMSE = 5 \mu g.cm^{-2}$ (Cerovic et al., 2012), especially considering that spectral measurements are affected by extra variability and that the method is based on reflectance, which is known to be less sensitive to C_{ab} than transmittance (Baret & Fourty, 1997b). Importantly, the apparent C_{ab} overestimation for $C_{ab} > 40 \mu g.cm^{-2}$ was rather due to the saturation in the reference measurement (see Section 3.1.2), as also suggested by the similar trend observed for both PROSPECT and PROCOSINE. Further experiments conducted on hyperspectral data associated with laboratory extraction based measurements of pigment contents (including C_{cx}) would, however, be interesting to fully characterize the pigment retrieval.

The main difference between both PROCOSINE inversions arose for high incident angles, since the RMSE decreased by 21% when using the radiance-

639 based model. This result confirms that this implementation better handles
640 variation in leaf orientation as displayed in Fig. 6.

641 *Estimation of equivalent water thickness and leaf mass per area.* Somewhat
642 different observations could be made from the SWIR range. In most cases,
643 the retrievals of C_w and C_m resulted in lower RMSE when using the radiance-
644 based PROCOSINE model. In particular, the C_m estimation was very accu-
645 rate even if C_m is not the most influential parameter in this spectral domain
646 (see Fig. 3.d). The poor R^2 value and very high standard deviations obtained
647 with PROSPECT and $\bar{\theta}_i = 50^\circ$ again demonstrate the need for accounting
648 for BRDF effects and leaf orientation, especially when the targeted parame-
649 ter does not have a strong influence on reflectance.

650

651 However, as recalled in Section 2.2.1, BRDF effects are not properly taken
652 into account for the SWIR range because, unlike the VNIR range, b_{spec} de-
653 pends on wavelength. Indeed, the BRDF directional component depends on
654 the leaf refractive index (Bousquet et al., 2005), whose imaginary part is
655 proportional to absorption (Born & Wolf, 1980). Especially at the far end
656 of the SWIR range, water absorption is so strong (Hale & Querry, 1973)
657 that the imaginary part of the leaf refractive index is no longer negligible
658 compared with the real part (Gerber et al., 2011). This may explain why
659 PROSPECT is more accurate than PROCOSINE in retrieving C_w on leaves
660 in horizontal position. Presumably, PROCOSINE systematically overesti-
661 mates C_w to mimic the decrease of the leaf refractive index (Féret et al.,
662 2008). The compensation between C_w and b_{spec} allows the proposed models
663 to be adjusted to the SWIR range and to obtain better estimation results

664 for other PROSPECT parameters such as C_m . For leaves in tilted position,
665 the influence of leaf orientation, whose modeling does not depend on wave-
666 length, again makes the radiance-based PROCOSINE model more accurate
667 than PROSPECT.

668

669 Importantly, the high R^2 values obtained with PROCOSINE for C_w and
670 C_m retrievals make it possible to calibrate strong linear relationships between
671 the actual values and the estimated values. Indeed, in every case, the ob-
672 tained RMSE is driven more by the estimation bias than by the variance. As
673 carried out by Cheng et al. (2011), applying such an indirect retrieval could
674 correct this bias and significantly enhance the estimation results obtained
675 with a given experimental setup.

676 *Angle estimation.* Both in the VNIR and SWIR ranges, the performances of
677 PROCOSINE weakly depended on leaf position. This tends to prove that
678 non-regular surfaces can be handled properly by introducing the θ_i parame-
679 ter. However, some clear differences arose between pseudo-BRF and radiance
680 inversions. Overall, inverting the radiance-based model provided the best re-
681 sults, the strongest difference between both ranges lying in θ_i estimation,
682 especially in the VNIR range. θ_i was indeed better retrieved using radiance-
683 based inversion, the θ_i underestimation for high incident angles and both
684 ranges being presumably due to the assumption $\frac{1-\rho_{spec}(\theta_i;2\pi)}{1-\rho_{spec}(0;2\pi)} \approx 1$ in Eq. 20.
685 It could be shown that confounding effects between θ_i and N (as well as C_m
686 in the VNIR range) were responsible for poor θ_i estimation results obtained
687 through pseudo-BRF inversion. For example, as observed in Fig. 3, both θ_i
688 and N have similar contributions to the model output. However, they also

689 have opposite effects, which may lead the inversion process to misinterpret
690 an increase in θ_i as a decrease in leaf structure N . Therefore, in the VNIR
691 (resp. SWIR) range, this model compensates θ_i underestimation (overesti-
692 mation) by N underestimation (overestimation).

693 On the other hand, several assumptions can be made regarding the good
694 performances obtained by radiance-based inversion. First, this may be due
695 to the noise level in the spectral measurements: as the ratio of two radi-
696 ance spectra is noisier than both radiance spectra independently, retrieved
697 pseudo-BRF spectra thus have a lower signal-to-noise ratio than originally
698 measured radiance spectra. This problem is critical near 400 nm and in the
699 NIR plateau where the sensitivity of the VNIR camera is lower compared
700 with most of the visible range (see Fig. 4). This emphasizes the necessity
701 of acquiring spectral measurements as clean as possible. Alternatively, such
702 differences in the inversion performances may be due to the numerical imple-
703 mentation of the inversion process (e.g., through the considered cost function,
704 optimization algorithm or initialization). Further investigation is therefore
705 needed to fully optimize the PROCOSINE inversion.

706

707 Finally, the poorer angle estimation results obtained with bamboo leaves
708 were likely to be due to the azimuthally anisotropic roughness properties of
709 monocotyledon leaves, that mainly originate from the longitudinal orienta-
710 tion of veins (Comar et al., 2012, 2014). Unlike regular surfaces for which
711 the BRF is azimuthally symmetric, such an organized arrangement of the
712 leaf surface leads the specular lobe not to be in the principal plane (Miesch
713 et al., 2002). In this case, it may seem inappropriate to represent the local

714 leaf inclination at the pixel level using only a single mean angle, especially
715 because the image spatial resolution is comparable to the inter-vein distance
716 for monocotyledons, i.e., a few hundred micrometers (Comar et al., 2014).
717 However, other estimation results presented in this paper strongly suggest
718 that this does not affect the retrievals of leaf biochemical properties.

719 4.3. Leaf parameter mapping

720 Hyperspectral imaging allowed us to obtain high-resolution maps of model
721 parameters by inverting the model for each pixel. Compared with the results
722 obtained from estimated values averaged within one or several leaf disk(s)
723 (each of which contains several hundreds of pixels), such maps provide a
724 deeper insight in how these effects actually affect the estimation process.
725 In Fig. 10 and Fig. 11, we show some estimated maps obtained using PROSPECT
726 and the radiance-based PROCOSINE model respectively, the radiance-based
727 inversion performing better than the pseudo-BRF inversion as seen in Sec-
728 tion 4.2. The considered bay laurel leaf was chosen due to its strong non
729 Lambertian behavior and to the presence of a large range of C_{ab} and C_{bp}
730 values. The actual chlorophyll content in the greenest area was close to
731 $40 \mu\text{g}.\text{cm}^{-2}$, while the equivalent water thickness and leaf mass per area were
732 0.0088 cm and $0.0099 \text{ g}.\text{cm}^{-2}$ respectively.

733 On the one hand, as observed in Fig. 10, PROSPECT estimation was strongly
734 affected by BRDF effects both in the VNIR and SWIR ranges. This increase
735 in reflectance is not taken into account by PROSPECT, which resulted in
736 some compensations during the inversion, here corresponding to an increase
737 in C_{bp} and decreases in C_{ab} (as already mentioned in Section 4.2.2), C_w and
738 C_m . On the other hand, in Fig. 11, we show that these BRDF effects were

Figure 10: Estimated maps obtained using PROSPECT in the VNIR (a-c) and SWIR (d-f) ranges: (a) true color composite image, (b) C_{ab} , (c) C_{bp} , (d) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (e) C_w , (f) C_m .

739 correctly interpreted as local increases in b_{spec} within the PROCOSINE in-
740 version. Accurate descriptions of the actual regular leaf orientation were also
741 obtained through homogeneous θ_i maps and average θ_i of 15° and 30° for the
742 VNIR and SWIR ranges respectively.

743 Modeling such extra variability therefore allowed us to obtain consistent maps
744 of foliar content. In the VNIR range, the highest C_{ab} values were obtained
745 in the greenest parts with values close to $40 \mu\text{g}.\text{cm}^{-2}$, while very low chloro-
746 phyll contents were retrieved in senescent parts, especially in the necrotic
747 area on the top (Fig. 11.b). This latter area was also exhibiting a high con-
748 tent in brown pigments as shown in Fig. 11.c, thereby proving the reliability

Figure 11: Estimated maps obtained using the radiance-based PROCOSINE model in the VNIR (a-e) and SWIR (f-j) ranges: (a) true color composite image, (b) C_{ab} , (c) C_{bp} , (d) b_{spec} , (e) θ_i , (f) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (g) C_w , (h) C_m , (i) b_{spec} , (j) θ_i .

749 of PROSPECT for retrieving pigments.

750 Consistent maps were obtained in the SWIR range as well. As expected,
751 veins were found to contain a lot of water, unlike the upper part where
752 necrosis was causing a strong water loss (Fig. 11.g). Although being a bit
753 more affected than C_w by mismodeled BRDF effects, C_m was estimated more
754 accurately than C_w since both C_w and C_m average estimated values were close
755 to 0.011 g.cm^{-2} .

756 In particular, these maps are very appealing for identifying plant diseases at
757 leaf scale. As described by Mahlein et al. (2013), different diseases may lead
758 to different symptoms that can be characterized by local changes in optical
759 properties, e.g., a higher chlorophyll/carotenoid ratio for sugar beet rust, or
760 necrosis for *Cercospora* leaf spot. Therefore, inverting PROCOSINE based
761 on VNIR and SWIR hyperspectral images of the same leaf offers very inter-
762 esting perspectives for early detection of many plant diseases.

763

764 Finally, in Fig. 12, we provide a last example that again demonstrates the
765 potential of PROCOSINE in the SWIR range when tested with a sugar beet
766 leaf characterized by high C_w ($C_w = 0.0355 \text{ cm}$) and low C_m ($C_m = 0.0040 \text{ g.cm}^{-2}$)
767 values, and by a strongly non-regular and non-Lambertian leaf surface. Even
768 if PROSPECT obtained better results when considering estimated values av-
769 eraged over the five sampled leaf disks ($\hat{C}_w = 0.0370 \text{ cm}$; $\hat{C}_m = 0.0032 \text{ g.cm}^{-2}$),
770 it also led to highly heterogeneous and inconsistent maps, whose variances
771 obviously did not reflect the actual ones but rather expressed unmodelled
772 variability. Conversely, the PROCOSINE inversion led to homogeneous and
773 consistent maps, either for leaf structure ($\hat{N} = 1.30$; to compare with

Figure 12: Estimated maps obtained in the SWIR range using the radiance-based PRO-COSINE model (b-f) and PROSPECT (g-i): (a) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (b) b_{spec} , (c) θ_i , (d) N , (e) C_w , (f) C_m , (g) N , (h) C_w , (i) C_m .

the mean value of 1.225 provided by Jacquemoud et al. (1996) for the same species), equivalent water thickness ($\hat{C}_w = 0.042$ cm) and leaf mass per area ($\hat{C}_m = 0.0052$ g.cm⁻²). In particular, the strongly non regular leaf orientation was greatly retrieved through the estimated θ_i map (Fig. 12.c): regions with low estimated θ_i were indeed facing the light source while regions with high estimated θ_i were facing the opposite side (note that shadows were interpreted as high θ_i values). Interestingly, most imaging techniques allowing the retrieval of leaf (or even plant) orientation are either based on depth imaging systems (Chn et al., 2012) or on 3D models built from multi-angular observations using stereovision (Lati et al., 2013) or photogrammetry (Jay et al., 2015). In comparison, it is worth noting that in this study, the retrieval of leaf orientation only necessitates a single-angular observation and is based on spectral information only.

5. Conclusions and perspectives

In this study, we propose a physically-based model that allows for applying rigorously a DHR model of leaf optical properties to pseudo-BRF hyperspectral (or multispectral) images acquired with close-range imaging spectroscopy. The proposed COSINE model describes the spectral variability caused by variable BRDF effects and leaf orientation, that, depending on leaf surface, can make the acquired pseudo-BRF measurements very different from DHR measurements. In this paper, COSINE is coupled with PROSPECT and the numerical inversion of the resulting PROCOSINE model led to accurate leaf-level mappings of foliar content and above leaf surface properties, both in the VNIR and SWIR ranges.

Figure 13: Use of the PROCOSINE model for image pretreatment in the VNIR (a-c) range: (a) DHR image reconstructed with PROSPECT and estimated parameters, (b) *SBRI* map (Mahlein et al., 2013) obtained with the original image, and (c) *SBRI* map (Mahlein et al., 2013) obtained with the reconstructed image.

798 Besides avoiding the need for hemispherical measurements, the proposed ap-
799 proach allows the non-destructive biochemical characterization of small leaves
800 thanks to the sub-millimeter resolution of hyperspectral images. Potentially,
801 it could represent a practical solution for optical characterization of needles,
802 whose optical properties were found to be well described by PROSPECT
803 (Moorthy et al., 2008) (usual needle optical measurements involving using
804 complex experimental setups to handle irregularities in size, shape and cur-
805 vature). As previously mentioned, it can also be combined with other leaf
806 DHR models such as LIBERTY (Dawson et al., 1998).

807 The accurate retrieval of C_m makes it possible to derive mass-based quantities
808 from surface-based quantities. In particular, strong correlations ($R^2 > 0.85$)
809 were obtained for the estimation of Gravimetric Water Content (being ex-
810 pressed as C_w/C_m), which is an important indicator for fire risk modeling
811 (Chuvieco et al., 2004).

812 Potential applications also include the use of PROCOSINE as a pretreat-
813 ment for further processing. To illustrate, in Fig. 13.a, we show a DHR
814 image reconstructed by running PROSPECT in a forward mode with pa-
815 rameters previously estimated with the radiance-based PROCOSINE model

(the original image is presented in Fig. 10). For example, computing spectral indices designed for plant disease identification based on this cleaned image is much more reliable to detect these diseases at early infection stages, especially when these indices are based on wavelengths strongly affected by BRDF effects, e.g., the SBRI (Mahlein et al., 2013). Alternatively, PROCOSINE could allow the design of spectral indices adapted to close-range imaging spectroscopy, similarly to Féret et al. (2011).

Further investigation is however needed to properly model the specular component in the SWIR range. In this case, the effect of water absorption on leaf refractive index should be considered to reliably model the wavelength-dependency of b_{spec} parameter. Also, confounding effects between PROCOSINE parameters (e.g., N , θ_i and C_m in the VNIR range) should be studied more deeply by optimizing the numerical implementation of the iterative optimization or by considering regularization strategies as reviewed by Baret & Buis (2008) and Verrelst et al. (2015), e.g., by using prior knowledge to constrain some model variables, or by generating a look-up table and averaging the N best solutions. As noted in the discussion, a more exhaustive assessment of PROCOSINE should also be performed over a larger data set encompassing a wider range of pigment, water and dry matter contents properly measured using laboratory extraction methods. This would allow us to fully validate the proposed model. Lastly, it is worth mentioning that the use of COSINE based on images acquired under outdoor conditions requires assuming that diffuse illumination (coming from either the sky and/or the surrounding terrain) is negligible compared with direct sunlight. We are currently working towards an improvement of COSINE to account for these

841 influences within the modeling, thus transforming the BRDF-based model into
842 a hemispherical-directional reflectance factor based model. This would allow
843 processing spatially-resolved data acquired from near-ground remote sensing,
844 e.g., from a tower or low flying unmanned aerial vehicle.

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